Solids

Rose-Hulman Institute of Technology (1972)
Texas Tech University (1975)
R.J. Marks II Class Notes
(1975)
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Note: The image contains hand-drawn elements and a small head illustration.
3-14-72 (TUES)

ABRAHAMS: "ELECTRONIC PROCESSES" CHAPT. 3
TIPLER: "MODERN PHYSICS" SEC. 3-4, 5-1, 5-2, 5-5, 5-6, 5-7, 5-8, 5-9, 122-1

COURSE OUTLINE

CRYSTAL STRUCTURE

LATTICE VIBRATIONS, THERMAL PROPERTIES

DIELECTRICS

MAGNETIC PROPERTIES

ELECTRICAL CONDUCTION

FREE ELECTRON THEORY METALS

BAND THEORY - METALS, SEMICONDUCTORS, INSULATORS

LIGHT-WAVE (SO THOUGHT)

PHOTOELECTRIC EFFECT

LIGHT showed PARTIAL PROPERTY OF LIGHT

PARTICLE (PHOTON)

WAVE (ELECTROMAGNETIC) DUAL NATURE OF LIGHT

\[ E = hf \]

E = ENERGY

h = PLANCK'S CONSTANT

f = FREQUENCY

p = \( \frac{h}{\lambda} = \frac{m}{k} \)

p = MOMENTUM

m = \( \frac{h}{2\pi} \)

k = \( \frac{2\pi}{\lambda} \)

\( \lambda \) = WAVELENGTH

k is IN DIRECTION OF MOTION OF WAVE

HIGH FREQ \( \rightarrow \) HIGH ENERGY
Increasing $V$ lifts energy of electrons on the right (lifting entire right picture). When $\bar{I}$ is opposite $\bar{I}^2$, increase $V$ further. Tunneling increases.

(Data by Skeeter)
SEMICONDUCTORS

CONDUCTION

$E_c$  
$E_v$

VALANCE BAND

$T > T_D$, ALL VALANCE BAND STATES OCCUPIED BY $e^-$
$T < T_D$, $n = 0$, FOR DISCRETE $e^-$'S (METALS)

FOR SEMICONDUCTORS

$\psi = \frac{1}{V \text{ Volume}} \int \psi^* \psi \text{ dV}$

$\psi = \text{ Electrons near the bottom of the conduction band}$

$\psi (E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} (E-E_v)^{1/2}$

FOR HOLES NEAR THE TOP OF VALENCE BAND

$\psi (E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} (E-E_v)^{-1/2}$

FOR $T < T_D$

$E_F = \text{Fermi energy}$

$n_e < \psi_c$

$n = \int_{E_F}^{\infty} \psi (E) \text{ dE}$

$= \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \int_{E_F}^{\infty} (E-E_v)^{1/2} \text{ dE}$

$\approx \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \left[ \frac{2}{3} (E-E_v) \right]_{E_F}^{\infty}$

$= \frac{2}{3} \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \frac{E_v-E_c}{kT}$

$= N_e e^{-(E_v-E_c)/kT}$
\[
\rho = \frac{N_e^2}{\pi^2} \delta(E) \left[ 1 - f(E) \right] dE
\]

**Bottom Value**

\[
= \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \int_{-\infty}^{E_F} (E - E_F)^{3/2} \left[ 1 - \frac{e^{(E - E_F)/kT}}{e^{(E - E_F)/kT} + 1} \right] dE
\]

\[
= \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \int_{E_F}^{E} \frac{1}{e^{(E - E_F)/kT} + 1} dE
\]

**Assume** \( E_F - E \gg kT \)

**Yielding**

\[
\rho = \left( \frac{2\pi m^* kT}{\hbar^2} \right)^{3/2} \frac{e^{-(E_F - E)/kT}}{1 + e^{(E_F - E)/kT}}
\]

\[
= N_e e^{-(E_F - E)/kT}
\]

**Intrinsic (Pure) Semiconductor**

Set \( T = 0 \)

\[
\Rightarrow E_F = \frac{E_F^0}{3} + \frac{3}{4} \frac{kT}{\ln \left( \frac{m^*}{m_e} \right)}
\]

\( T = 0 \) \( \Rightarrow E_F^0 \) is halfway 'twixt bands

\[
E^0 = \frac{h^2}{8\pi^2 e^2 m^*}
\]

\[
np = N_e N_v e^{-(E_F - E)/kT}
\]

\[
n = N_e e^{-(E_F - E)/kT}
\]

\[
\rho = \sqrt{np} = \sqrt{2N_e N_v \frac{1}{2} e^{-(E_F - E)/kT}}
\]

\[
(N_e N_v)^{1/2} = 2 \left( \frac{2\pi m^*}{\hbar^2} \right)^{3/2} \left( \frac{m^*}{m_e} \right)^{3/4}
\]

Now

\[
\sigma = \frac{e^2}{2\hbar^2} \ln \left[ (N_e N_v)^{1/2} e^{-(E_F - E)/kT} \right] \frac{e^{-(E_F - E)/kT}}{e^{-(E_F - E)/kT} + 1}
\]

**Find \( E_F \)**
DETERMINATION OF $E_g$ BY INFRARED ABSORPTION

$$h \nu \rightarrow h \nu$$

TRANSMISSION

VALENCE

TRANSITION

PHOTONS HAVE ENOUGH ENERGY TO GIVE TO $\downarrow \downarrow \to$ TO MOVE TO COND. BAND

ABSORPTION EDGE

$T_c$

AND $E_g = \frac{h \nu}{2}$

$\rightarrow \downarrow \downarrow \rightarrow 1.5 \text{ eV}$

$E_g \approx 2.75$ (DUE)

$E_g \approx 3.72$ (WED)

FREE ELECTRON

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

BOUNDARY CONDITIONS TELL US

2N STATES PER BAND, WHERE N IS NUMBER OF CELLS TWIXT ATOMS

VELOCITY OF ELECTRONS IN PERIODIC LATTICE

$V = \frac{qU}{mk}$

$E = h \nu = \frac{p^2}{m}$ $\Rightarrow$ $V = \frac{1}{m} \frac{dE}{dk}$

APPLY $E$ FIELD

$E = \frac{qE}{mk}$

$\frac{dE}{dx} = \frac{E}{m} \frac{dE}{dk}$

$E = \frac{dE}{dk}$

$\frac{dE}{dt} = \frac{dE}{dk} \frac{dk}{dt}$

$\Rightarrow \frac{dE}{dt} = \frac{1}{m} \left( \frac{dE}{dk} \right) \frac{dk}{dt}$

$\Rightarrow \frac{dE}{dt} = \frac{E}{m} \frac{dE}{dk}$

$\Rightarrow \frac{dE}{dt} = \frac{1}{m} \frac{dE}{dk}$

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$\Rightarrow \frac{dE}{dt} = \frac{1}{m} \frac{E}{E} \frac{dE}{dk}$
EFFECTIVE MASS

\[ m^* = \frac{m}{1 - \frac{e^2}{\hbar^2}} \]

When \( m^* \) and \( m \) are in opposite directions, \( m^* \ll m \)

\[ \frac{E}{\hbar^2} \frac{2k^2}{m^*} = \frac{E}{\hbar^2} \frac{2k^2}{m} \implies m^* = \frac{m}{(2\hbar^2/E)^{1/2}} \]

FOR FREE ELECTRONS

\[ E = \hbar^2 k^2/2m \]

\[ v = \frac{\hbar k}{m} \]

\[ \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} \]

\[ m^* = \frac{1}{\frac{m}{\hbar^2}} = m \]

CONDUCTION DUE TO FULL BAND \( \Rightarrow 0 \)

APPLY \( E \) TO FULL BAND

YOU CAN'T ACCELERATE THE ELECTRON AS A GROUP

(NO CONDUCTION)

GOOD CONDUCTOR

GOOD INSULATOR

METAL

ALKALI-METAL HAVE

HALF FULL CONDUCTION BAND

FULL HALF FULL

3 DIMENSIONAL CASE

IF OVERLAPPING, OCCURS A METAL

GO TO \( E \implies E^2 \) (FBI)
5-16-72  (Tues)

INTRINSIC SEMICONDUCTOR

\[ N = D \Rightarrow \delta = \frac{E_F}{E_C + E_V} \]

\[ n = p = \left( N_c N_v \right)^{1/2} \exp\left( -\frac{E_F}{kT} \right) \]

FERMI ENERGY IS HALFWAY TWIXT HIGHEST VALENCE E AND LOWEST CONDUCTION E

EXTRINSIC (IMPURITY) SEMICONDUCTOR

SILICON

PENTAVALENT IMPURITY

\[ \text{Pb, As} \]

EXTRA-LOOSELY BOUND ELECTRON IN BORA, ORBIT OF BIG RADIUS

\[ \text{Linear states may move to conduction band at high } T \]

AND IONIZING IMPURITY FOR \( n > p \), \( n \)-TYPE SEMICONDUCTOR

TRI-VALENT IMPURITY WITH \( S_i \); ONE EXTRA PLACE FOR \( \Theta^- \) IN A BOND

\[ E_C \quad E_V \quad \text{ACCEPTOR LEVELS} \]

\[ \text{(IT)} \]

As \( T \) \( \uparrow \) A BIT, SOME \( \Theta^- \) WILL JUMP TO ACCEPTOR LEVELS, CREATING HOLES IN THE VALENCE BAND.
\[ P > N \Rightarrow p \text{ type} \]

\[
N_0 = \# \text{ DONOR LEVELS/VOL}
\]

\[
N_0^+ = \# \text{ IONIZED LEVELS/VOL (LOST E-')}
\]

\[
N = N_0^+ - N_0 e^{-(E_c - E_F)/kT} = N_0 \left[ 1 - f(E) \right]
\]

\[
N_c e^{-(E_c - E_F)/kT} = N_0 e^{(E_2 - E_F)/kT}
\]

\[
\ln N_c + \frac{(E_F - E_0)/kT}{kT} = \ln N_0 + \frac{(E_2 - E_0)/kT}{kT}
\]

\[
E_F = E_2 + E_0 + kT \ln \left( \frac{N_0^+}{N_0} \right)
\]

\[
\text{at } T = 0^\circ K
\]

\[
N = N_c e^{-(E_c - E_F)/kT}
\]

\[
\ln N = \ln N_c + \frac{E_F - E_0}{kT}
\]

\[
= \ln N_0 + \frac{1}{kT} \left( \frac{E_2 - E_0 + kT \ln(N_0^+)}{kT} \right)
\]

\[
= \ln N_0 + \frac{1}{2} \ln \left( \frac{N_0^+}{N_0} \right) - \frac{E_0}{2kT}
\]

\[
n = (N_c N_0)^{1/2} e^{-E_0/2kT}
\]
\[ \sigma = \frac{n e \mu_e}{\mu} \]

**Hall Effect**

\[ R_H = \frac{E_y}{j B} = \frac{n e E}{j B} = \frac{\eta e E}{j B} \]

\[ \eta = \frac{e^2 \tau}{m_e^*} = \frac{n e \mu_e}{j B} \]

\[ E_y = \frac{e \tau}{m_e^*} \]

\[ E_y = \frac{e \tau}{m_e^*} \]

**Measure** \[ E_y, \eta \] (Hall Mobility)

\[ \ln \eta \]

Increasing impurity

- Slope \(-3/2\)
- \(\mu \sim T^{-3/2}\)

\[ \ln \eta \]

- Minimum

- Maximum

\[ \frac{1}{T} \]
5-17-72 (Wed)

N-TYPE

P-TYPE

N-TYPE

P-TYPE

DONOR LEVELS

ACCEPTOR LEVELS

P-N JUNCTION

\[ P \quad N \]

\[ P \quad + \quad N \]

BARRIER FOR DIFFUSION TO LEFT

\[ P \quad N \]

\[ e^- \quad n \rightarrow p \]

REVERSE V POLARITY TOO

BREAKDOWN DUE TO IONIZATION OF ATOMS (AVALANCHE EFFECT)
ELECTRON AND HOLE CONDUCTION

\[ \sigma = n e \mu + p \mu \nu \]
\[ \eta = \mu = \text{MOBILITY} \]

HALL EFFECT

\[ E = q \nabla \times B = q \nabla B \]

For holes
\[ \mathbf{F} = \mathbf{E} + \mathbf{v} \times \mathbf{B} \]
For electrons

\[ \mathbf{F} = q \mathbf{E} \]

(CAPACITOR ANALOGY)

May thus determine majority carriers
Suppose \( p = 0, n \neq 0 \)
\[ E = q \nabla \times B = q \nabla B = E_y, E_y = VB \]
\[ E_x = VB, E_y = V \]

Hall Coefficient:
\[ R_h = E_y / J B \]
\[ J = \frac{E_y}{A} \]
\[ \Rightarrow R_h = \frac{V B}{J B} = \frac{ne v B}{ne v B} = \frac{1}{e} \] (ne v B)

Thus measuring \( R_h \) yields \( n \)

For \( p \) material \( R_h = \frac{1}{e} \)

When both types of carriers are important
\[ R_h = \frac{\mu_p^2 n - \mu_n^2 p}{\mu_p^2 n + \mu_n^2 p} \]
BANDS IN THREE DIMENSIONS

CUBIC

\[ \theta = \frac{\pi}{2\sin \frac{k}{q}} = \frac{\pi}{\frac{k}{q}} = \frac{\pi}{k} \]

BRAGG'S LAW: FOR FIRST ZONE:

FREE ELECTRON

CONSTANT E SURFACE \( E = \frac{1}{2} k \cdot k \)

FOR NON-FREE E...
Metal - no E gaps \((E_A > E_B)\)
Semiconductor \(E_B < E_A\)

5-8-72 (Mon)

One Dimension

\[
\sigma = \frac{n e^2 v}{m^*}
\]

In Three Dimensions

Cubic Lattice

Sharing -> Occupied Space
In 3 dimensions:

\[ \psi = \frac{1}{L} \left( e^{i \mathbf{k} \cdot \mathbf{r}} - e^{i \mathbf{k} \cdot \mathbf{r}} \right) \]

\[ \nabla \psi = \frac{-i \mathbf{E}}{m} \]

\[ Q_x = e \frac{F_x}{m}, \quad F_x = -\frac{dE}{dy} \]

\[ Q_y = e \frac{F_y}{m}, \quad F_y = -\frac{dE}{dx} \]

\[ Q_z = e \frac{F_z}{m}, \quad F_z = -\frac{dE}{dz} \]

\[ \omega = \frac{e E_z}{m} \]

**Free Electrons**

\[ E = \frac{p^2}{2m} = \frac{\mathbf{k} \cdot \mathbf{k}}{2m} \]

\[ \frac{\hbar^2}{m} \frac{\partial^2 \psi}{\partial \mathbf{r}^2} = \frac{-\hbar^2}{m} \nabla^2 \psi + \frac{1}{\hbar^2} (\mathbf{E} \cdot \mathbf{r}) \psi \]

\[ \mathbf{E} = \frac{\mathbf{E} \cdot \mathbf{r}}{m} \]

\[ \frac{1}{m} \mathbf{k} = \frac{\mathbf{E} \cdot \mathbf{r}}{m} \]

Then:

\[ Q_x = \frac{e}{m} F_x, \quad Q_y = \frac{e}{m} F_y, \quad Q_z = \frac{e}{m} F_z \]

**Cyclotron Resonance Frequency**

Electron moving upward with energy near \( E_F \) (Fermi energy)

\( E_{\text{res}} = B \omega_c \)

\[ \omega_c = \frac{e B}{m} \]

If radio frequency matches \( \omega_c \), then one could get a large amount of absorption of energy from \( E_F \).
CHANGE P AND LOOK FOR LARGE

RESONANCE ABSORPTION OF E

AT NEAR BOTTOM OF CONDUCTION BAND

HOLE NEAR TOP OF VALENCE BAND

B IN SOME PARTICULAR DIRECTION

K = \frac{2\pi n}{a} = n = \pm 1, \pm 2, \ldots \text{ (one dimension)}

R states in first band

in three dimensions

L = \frac{2\pi n}{b}

\psi(x) \quad \psi(x+L)

k_x = \frac{2\pi n_x}{\frac{a}{N}} \quad n_x = 1, 2, \ldots

k_y = \frac{2\pi n_y}{\frac{b}{N}} \quad n_y = \ldots

k_z = \frac{2\pi n_z}{\frac{c}{N}} \quad n_z = \ldots

Number of states (in 2 states/point in spin)

N^3 = \text{no. of unit cells in lattice}
CYCLIC BOUNDARY CONDITION: \( \psi(x) \equiv \psi(x + L) \)

NEED TO KNOW HOW ENERGY IS DISTRIBUTED TO KNOW CONDUCTION

\( g(E) = \text{const. for free } E \)

HOW MANY STATES TWIXT \( E \) AND \( E + dE \) \( (g(E)\,dE) \)

VOLUME OF FIRST ZONE IN \( k \)-SPACE

\[ V = \left( \frac{2\pi}{a} \right)^3 \]

DENSIY OF STATES IN \( k \)-SPACf

\[ \frac{dN}{dE} = \frac{2Nk^3}{E^3} = \frac{2N^2\omega^3}{h^3} \Rightarrow (\text{vol. of crystal}) \]

\[ \Rightarrow \frac{dN}{dE} \cdot \frac{1}{V} = \frac{2N^2\omega^3}{h^3} \text{ states/unit volume in } k \text{-space} \]

\[ g(E)\,dE = \frac{dN}{dE} \times \text{volume twixt } E \text{ and } E + dE \]

\( \text{IN } k \text{-SPACE} \)

\( ds = \text{surface element} \)

CYLINDER \( dk_n \) IS THE CHANGE IN \( k \)

(VOLUME = \( dk_n \cdot ds \)) GOING FROM \( E \) TO \( E + dE \)

IN THE NORMAL DIRECTION

SECTION OF ENERGY SURFACE

\[ dE = |\nabla_E \cdot dk_n| = |\text{grad}_k E| \, dk_n \Rightarrow dk_n = \frac{dE}{|\text{grad}_k E|} \]

\[ \Rightarrow \frac{2N^2\omega^3}{h^3} \int dk_n \cdot ds \text{ (INTEGRATE OVER CONST. ENERGY SURFACE)} \]

\( \int dk_n \cdot ds = \text{TOTAL VOLUME TWIXT } E \text{ AND } E + dE \)
EXAMPLE - FREE ELECTRON

\[ E = \frac{\hbar^2}{2m} \left( k_x^2 + k_y^2 + k_z^2 \right) \]

\[ \nabla E = \nabla \left( \frac{\hbar^2}{2m} \right) \nabla k = \frac{\hbar^2}{2m} \left( 2k_x + 2k_y + 2k_z \right) \]

\[ = \frac{\hbar^2}{2m} \left( 2k_x^2 + 2k_y^2 + 2k_z^2 \right) \]

\[ = \frac{\hbar^2}{2m} k \Rightarrow |\nabla k| = \frac{\hbar^2}{2m} \Rightarrow k \text{ is not a vector.} \]

This is expression for constant \( E \) surface.

\[ \Rightarrow \int dS = 4\pi k^2 \Rightarrow \text{is over constant } E \text{ surface.} \]

\[ \Rightarrow \xi(E) dE = \frac{2}{\sqrt{2\pi \hbar^2/m}} \frac{dE}{E} \left( 2\pi \right) \]

\[ \Rightarrow \xi(E) = \frac{1}{\sqrt{2\pi \hbar^2/m}} \cdot \frac{1}{\sqrt{E}} \left( \frac{2\pi \hbar^2}{m} \right)^{3/2} E^{1/2} = C E^{-1/2} \]

Because \( k = \sqrt{\frac{E}{\hbar^2}} \) from \( E = \frac{\hbar^2 k^2}{2m} \)

The previously derived answer.

SOME OTHER RESULTS

ELECTRON IN A CRYSTAL (GENERALLY NOT FREE)

\[ \xi(E) \]

Number of states drop off since we run out of the cube.

Near the bottom of the Band:

\[ \xi(E) = \frac{1}{2\pi} \times \left( \frac{2\pi^2}{h^2} \right)^{3/2} (E - E_B)^{1/2} \]

Assuming we're not in the first band, \( E_B = 0 \) in first band.

Near the top of the Band:

\[ \xi(E) = \frac{1}{2\pi} \times \left( \frac{2\pi^2}{h^2} \right)^{3/2} (E - E_d) \]

Electrons near the top and bottom of the bands are the ones generally of interest.
ALKALI METALS HAVE FULL ALAS. MOLD STATES AS THEY HAVE ELECTRONS TO PUT IN THEM, YIELDING HALF FULL BANDS. THIS GUARANTEES IT IS A METAL GOOD CONDUCTOR CHANGES STATE EASILY

CALCIUM (DIVALENT METAL): 2 VALENE ELECTRONS AS MANY ELECTRONS AS STATES. SINCE IT IS METAL, IT MUST HAVE BAND OVERLAP.

TRANSITION METALS: OVERLAPPING BAND. LARGE $m^*$ NOT A GOOD CONDUCTOR. WIDE BAND

$$m^* = \frac{\hbar^2}{2\epsilon_{G}}$$ IF BAND IS NARROW, $m^*$ IS LARGE NARROW BAND IS POOR CONDUCTOR SINCE $m^*$ IS HARD TO ACCELERATE

DIAMOND: GAP OF ENERGY: $E_g = 7.4 \text{ eV} (8.6)$ HARD TO BRIDGE GAP. FULL AND EMPTY BAND SEPARATED BY $E_g$

GERMANIUM SIMILAR TO DIAMOND BUT $E_g = 7.4 \text{ eV}$ SO SOME ELECTRONS CAN JUMP GAP USING ABSORBING PHONON (IF $T > 0 K$) AND ENTER THE CONDUCTION BAND. NUMBER OF ELECTRONS BAND LIMIT (UNLIKE METALS) SEMICONDUCTOR
HOW TO INVESTIGATE BANDS (EXPERIMENT)

FAST ELECTRONS

EBand

KNOCK OUT ELECTRON FROM LOWER LEVEL, SO THE ELECTRON DROPS AND EMITS X-RAYS

NORMAL RESISTANCE

\( p \) is residual resistance, due to lattice defects & impurities

\( p @ \text{ room temperature} \) & above is dependent on lattice vibrations

For superconductivity, we must do away with the problem of defects and impurities
5-10-71 (W.E.O.)

\[ \rho \] = NORMAL RESISTIVITY (METALS)

\[ \rho(T) \]

\[ \rho(0) \]

DUE TO LATTICE VIBRATIONS

\[ \rho(T) \] VERSUS T

ONNES-1911-SUPERCONDUCTIVITY

\[ \rho \] (HE WIRE)

WITH IMPURITIES

\[ T_c \]

3.23. SUPERCONDUCTOR ELEMENTS, 2 HUNDREDS OF ALLOYS

\[ \rho (\text{lead}) \]

CRITICAL FIELD \[ H_c \]

NORMAL

SUPER CONDUCTORS

\[ T_c \] (0K)

BEST SUPERCONDUCTORS ARE POOREST

NORMAL CONDUCTORS

APPLY MAGNETIC FIELD AND TAKE DOWNWARD THRU \[ T_c \]

SURFACE CURRENT SET UP THAT CANCELS

FIELD INSIDE THE SUPERCONDUCTOR (MEISSNER EFFECT)

\[ T < T_c \]
For a doughnut:

Field off trap lines giving magnet with current

Isotope effect

$T_c \sim \frac{1}{\sqrt{M}}$

$M = \text{mass of the atom (for particular atom)}$

$\Rightarrow$ less inertia $\Rightarrow$ less moveable

$\Rightarrow$ higher $T_c$ $\Rightarrow$ better superconductivity

(effect causing superconductivity is stronger)

Theory developed in 1958

BCS theory (Bardeen, Cooper, Schrieffer)

Simplified BCS theory

Another $e^-$ might be attracted to region of high density charge. Pairs of attracting electrons (via lattice waves), electrons having lower energies than single electrons would have

$\uparrow^5 \quad \uparrow_5$

Cooper pairs, will react

$\uparrow \downarrow \rightarrow \uparrow \downarrow$ up to $10^{-4}$ cm
ELECTRON BEAM

\[ \text{MAY DETERMINE } A \text{ FROM ABOVE} \]
\[ \text{CAN ALSO DETERMINE } \mathbf{P} \text{ (MOMENTUM)} \]
\[ \text{AGAIN: } \mathbf{P} = \frac{\hbar}{\lambda}, \quad E = \frac{\mathbf{P}^2}{2m} \]
\[ \text{POTENTIAL ENERGY} \]

DUAL NATURE OF WAVE-PARTICLES:
1. LIGHT: \[ E = hf, \quad \mathbf{P} = \frac{\hbar}{\lambda}, \quad \mathbf{K} = \frac{2\pi}{\lambda} \]
2. MATTER: \[ \mathbf{P} = \frac{\hbar}{\lambda}, \quad E = \frac{\mathbf{P}^2}{2m} \]

HEISENBERG UNCERTAINTY PRINCIPLE:

IT IS IMPOSSIBLE TO SIMULTANEOUSLY DETERMINE A POSITION COORDINATE AND THE CORRESPONDING MOMENTUM COORDINATE TO ANY GREATER PRECISION THAN:
\[ \Delta x \Delta p \geq \hbar \]

INVENT "WAVE FUNCTION": \[ \psi \] (HAS VALUE AT ALL POINTS IN SPACE, CAN BE REAL OR COMPLEX)

THE PROBABILITY OF FINDING A PARTICLE IN VOLUME ELEMENT \( dV \) AT POSITION \( x, y, z \) IS:
\[ \text{PROB} = \frac{1}{V} \psi^*(x, y, z) \psi dydz \]

\[ \text{PROBABILITY OF BEING IN SOME FINITE VOLUME } V: \]
\[ \rho = \int \frac{1}{V} |\psi|^2 dydz \]
SCHROEDINGER EQUATION (CONSERVATION OF ENERGY AND WAVE)

For time independence: \( (\hat{V} + \hat{H}) \psi = \epsilon \psi \)

\[-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = \epsilon \psi \]

EX) VIBRATING ATOM (LINEAR HARMONIC OSCILLATOR)

\[ V = \frac{1}{2} k x^2 \]

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} x^2 + \frac{1}{2} k x^2 \psi = \epsilon \psi \]

Each solution, a set of \( \psi \)'s is obtained, for each \( \psi \), there is a distinct energy \( \epsilon \).

In order to satisfy differential equation

STATE 1: \( \psi_1 \quad \epsilon_1 \)

STATE 2: \( \psi_2 \quad \epsilon_2 \)

\( \epsilon \) is quantized

\[ \epsilon_n = \frac{(n+\frac{1}{2}) \hbar^2}{2m} \]

[NO SOLUTION FOR \( \epsilon = 0 \); \( \psi = 0 \); \( \text{ATOM IS NEVER AT REST} \)]

3-15-72 (WSD)
Levy: pg 22

Note:

a) WAVE-LIKE QUALITY
2) LIGHT \( \epsilon = h \nu \quad p = h/\lambda \quad \epsilon = h \nu \sim \frac{h}{\lambda} \)
3) MATTER \( \epsilon = m c^2 \quad p = m \nu \quad \epsilon = m c^2 \sim m \nu \)
4) UNCERTAINTY \( \Delta \epsilon \Delta p \sim \hbar \) \( \frac{\hbar}{m} \Delta \nu \Delta v = \hbar \)

\[ \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \psi = \epsilon \psi \] (SCHROEDINGER'S EQUATION)

b) ONE ELECTRON ATOM: \( V = \frac{1}{4 \pi \epsilon_0} \frac{e^2}{r} \)

Yielding the following results:

\[ \epsilon_n = \frac{\pi^2 \hbar^2}{2m a^2} \quad n = 1, 2, 3, \ldots \]

PRINCIPLE QUANTUM NUMBER

\[ n = 1, 2, 3, \ldots \]

\[ \epsilon_0 = \frac{\pi^2 \hbar^2}{a^2} \]

\[ \epsilon_1 = \frac{\pi^2 \hbar^2}{a^2} \]

\[ \epsilon_2 = \frac{4 \pi^2 \hbar^2}{a^2} \]

\[ E_f = 0 \]
\[ \ell = \ell \mathbf{p} \quad \text{(Angular Momentum)} \]

\[ \ell \text{- have same } \ell \text{, but have different } \ell \]

Allowed Angular Momenta (Orbital)

\[ \ell = \sqrt{\ell (\ell + 1)} \hbar \quad \ell = 0, 1, 2, 3, \ldots \]

\( \ell \) called Azimuthal Quantum Number

Suppose \( \ell = 2 \), then \( \ell = 1, 0 \)

\[ \ell = 1 \Rightarrow \text{p electron} \]
\[ \ell = 2 \Rightarrow \text{d electron} \]
\[ \ell = 3 \Rightarrow \text{f electron} \]

Electron Spin Angular Momentum

\[ \ell \left( \ell + 1 \right) \hbar \leq \frac{1}{2} \hbar \]

In presence of magnetic field, only certain directions allowed for \( \ell \) and \( \ell \) vector.

\[ \ell = 2 \Rightarrow \ell = \begin{cases} \sqrt{1} \hbar, \hbar & \ell = 2 \hbar \end{cases} \]

\[ \ell = 1 \Rightarrow \ell = \begin{cases} \sqrt{2} \hbar, 0, -\hbar, -2\hbar \end{cases} \]

\[ \ell = 2 \Rightarrow \ell = \begin{cases} \sqrt{3} \hbar, 0, -\hbar, -2\hbar \end{cases} \]
PAULI: EXCLUSION PRINCIPLE (APPLIES TO ODD-HALF INTEGRAL SPIN PARTICLES): NO TWO ELECTRONS (ODD-HALF INTEGRAL SPIN PARTICLES) IN THE SAME (QUANTUM MECHANICAL SYSTEM) ATOM MAY HAVE IDENTICAL SETS OF QUANTUM NUMBERS \((n, l, m, m_s)\)

<table>
<thead>
<tr>
<th>Atom</th>
<th>Quantum Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_2^+)</td>
<td>((1, 0, 0, +\frac{1}{2}))</td>
</tr>
<tr>
<td>He</td>
<td>((1, 0, 0, +\frac{1}{2}))</td>
</tr>
<tr>
<td>Li</td>
<td>((1, 0, 0, +\frac{1}{2}))</td>
</tr>
<tr>
<td>Be</td>
<td>(1s^22s^2)</td>
</tr>
<tr>
<td>B</td>
<td>(1s^22s^22p)</td>
</tr>
<tr>
<td>C</td>
<td>2(p^2): ((2, 1, 0, +\frac{1}{2}))</td>
</tr>
<tr>
<td>N</td>
<td>2(p^3): ((2, 1, -1, +\frac{1}{2}))</td>
</tr>
<tr>
<td>O</td>
<td>2(p^4): ((2, 1, 1, -\frac{1}{2}))</td>
</tr>
<tr>
<td>F</td>
<td>2(p^5): ((2, 1, 1, -\frac{1}{2}))</td>
</tr>
<tr>
<td>Ne</td>
<td>2(p^6): ((2, 1, 1, -\frac{1}{2}))</td>
</tr>
</tbody>
</table>

\(n\): ENERGY
\(l\): ORBITAL ANGULAR MOMENTUM
\(m\): Z DIRECTIONAL COMPONENT OF \(\ell\)
\(m_s\): Z COMPONENT OF \(m\)
\(s\): +\(\frac{1}{2}\)
CRYSTALLINE SOLIDS: REGULAR ATOM ARRANGEMENTS
AMORPHOUS SOLIDS: RANDOM (DIFFICULT TO ANALYZE)

FORCES TWIST ATOMS
A) IONIC FORCES (Na⁺ Cl⁻)
   - COULOMB ATTRACTION OF IONS
   - STRONG FORCE
   - HIGH MELTING POINT
   - LOW ELECTRICAL THERMAL CONDUCTION
B) COVALENT FORCE (SHARED ELECTRONS)
   2 CL SHARES 7 3P ELECTRONS
   14! FROM 16 FIND NO. 6 5 4 3 2 1 ATOMS
   EXCESS NEGATIVE CHARGE
   "Fandscape"

GO TO FRIDAY, 4/9
3/28 (THU) 100 NEXT WEEK TUES, 4/13
1+1 = 2
0 = B = Z = 90°

FRONT FACE
\[ \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \]
TAKE REC. C 0 1 0 (MILLER INDICES)

\[ \begin{bmatrix} 1 \ 0 \ 0 \end{bmatrix} \begin{bmatrix} 100 \end{bmatrix} \]

DESIGNATION OF POINTS IN UNIT CELL
BODY-CENTERED POSITION IS \( \left( \frac{1}{2} \frac{1}{2} \frac{1}{2} \right) \)
FOR BODY-CENTERED POSITION:
\( \left( \frac{1}{2} \frac{1}{2} \frac{1}{2} \right) \rightarrow \left( 1, 1, \frac{1}{2} \right) \)
SPACING BETWEEN PLAINS CONTAINING LATTICE POINTS (PRIMITIVE CELL)

\[
\begin{align*}
(100^2) & \quad d = \frac{a}{2} \\
(110) & \quad d = \frac{a}{\sqrt{2}} \\
(111) & \quad d = \frac{a}{\sqrt{3}} \\
\end{align*}
\]

\[d = \frac{a}{\sqrt{n^2 + k^2 + l^2}}\]

X-RAY DIFFRACTION DETERMINATION OF UNIT CELLS

IF \(2d \sin \theta = n \lambda \) : CONSTRUCTIVE INTERFERENCE (Bragg's Law)

MONOCRHHOMATIC DEUTER (GRAY'S LAW)

INTENSITY (FOR PRIMITIVE CUBE)

\[
\begin{align*}
(100) & \quad n = 1 \\
(110) & \quad n = 1 \\
(111) & \quad n = 1 \\
(002) & \quad n = 2 \\
(210) & \quad n = 2 \\
\end{align*}
\]

PRIMITIVE CUBE: \( d = \frac{a}{\sqrt{n^2 + k^2 + l^2}} \)

\[2d \sin \theta = n \lambda \]

\[\Rightarrow \quad \sin \theta = \frac{n \lambda}{2d}\]

SOLVE FOR \(d\) (LATTICE CONSTANT)
(1) Assume first peak is $(100) \Rightarrow$ calculate $q$
- See if other peaks fit with this value of $q$ and some $h k l$
(2) Assume BCC, first peak $(h k l) = (110)$
- Calculate $q$, see if other peaks fit
(3) Assume FCC, first peak $(h k l) = (111)$
- Calculate $q$, see if other peaks fit
FORCES 'TWIXT ATOMS

1. IONIC (STRONG ATTRACTION)
2. COVALENT (FAIRLY STRONG)
3. METALLIC BOND (SHARED ELECTRONS 'TWIXT ALL ATOMS OF THE MATERIAL)
4. VAN DER WAALS FORCE (MOLECULAR CRYSTALS)
   - VERY WEAK DIPOLE ATTRACTIVE FORCE
   - THESE MATERIALS ARE SOLIDS ONLY AT TEMPS NEAR 0°K
5. REPULSIVE FORCES (DUE TO EXCLUSION PRINCIPLE)

CRYSTAL STRUCTURE

SPACE LATTICE: REGULAR (REPEATING)
- ARRANGEMENT OF POINTS SUCH THAT THE ARRANGEMENT OF ATOMS ABOUT EACH POINT IS IDENTICAL

TO GET FROM ONE LATTICE POINT TO ANY OTHER LATTICE POINT
\[ \mathbf{r} = \mathbf{m}_1 \mathbf{a} + \mathbf{m}_2 \mathbf{b} + \mathbf{m}_3 \mathbf{c} \]
THE VOLUME FOR WHICH \( a, b, \) AND \( c \) INSCRIBE THE EDGES IS CALLED A "UNIT CELL"

PRIMITIVE UNIT CELL - THAT CELL HAVING SMALLEST POSSIBLE VOLUME (LATTICE POINTS ONLY @ CORNERS).

SINGLE CRYSTAL LATTICE CONTINUES FROM ONE EDGE OF CRYSTAL TO THE OTHER WITH NO BREAKS.

POLYCRYSTALLINE BREAKS IN THE LATTICE - GRAIN BOUNDARY

SPACE LATTICE SYMMETRY

1) MIRROR PLANE
2) ROTATION SYMMETRY (n-fold)
   n- THE NUMBER OF EQUAL ANGLES OF ROTATION TO GET BACK TO ORIGINAL CONFIGURATION (EACH OF THE EQUAL ROTATIONS MUST YIELD THE SAME CONFIGURATION AS ORIGINAL)

CUBIC CRYSTALS: 4-3 FOLD ROTATION AXES

MILLER INDICES

1) INTERCEPTS
2) RECIPROCAL
3) CLEAR FRACTIONS

GO TO MONDAY, P3 6
IONIC CRYSTALS

RESTORING FORCE: $F = kx$

$F_n = \beta (\mu_{nn} - \mu_{nn}) = \beta (\mu_{nn} + 2\mu_{nn})$

$M_{nn} = \beta (\mu_{nn} + 2\mu_{nn})$ - wave equation

$\omega^2 M_0 = \beta \left( e^{i(k_0 - k_0)} - e^{-i(k_0 + k_0)} \right)$

$\omega^2 M_0 = -\frac{4\pi e^2 \kappa_0^2}{\epsilon_0 m^2 k_0^2}$

$\Rightarrow \omega^2 = \frac{-4\pi e^2 \kappa_0^2}{\epsilon_0 m^2 k_0^2}$

$\Rightarrow \omega = \sqrt{\frac{-4\pi e^2 \kappa_0^2}{\epsilon_0 m^2 k_0^2}}$

RELATION $\omega = \frac{1}{\lambda}$
\[ \mathbf{w} = \mathbf{A} \mathbf{v} \]

\[ \mathbf{v} \equiv \frac{\mathbf{w}}{k} \]

\[ v_p = \frac{\lambda}{k} \]

SPEED DECREASES FOR HIGHER FREQUENCIES

TRANSMISSION OF ENERGY FROM ONE POINT TO ANOTHER: GROUP VELOCITY

\[ v_g = \frac{\lambda}{k} \]

DIATOMIC LATTICE

\[ \begin{array}{c|c|c|c|c} \hline 1 & 2 & 3 & 4 \hline \end{array} \]

\[ \begin{array}{c|c|c|c} \hline a & b & c & d \hline \end{array} \]

\[ \mathbf{M} \mathbf{v}_m = \mathbf{E} \mathbf{E} \mathbf{v}_m = \beta \left( \mathbf{H}_2 \mathbf{v}_m - 2 \mathbf{H}_2 \mathbf{v}_m \right) \]

\[ \mathbf{M} \mathbf{v}_m = \beta \left( \mathbf{H}_2 \mathbf{v}_m + 2 \mathbf{H}_2 \mathbf{v}_m \right) \]

\[ \mathbf{v}_m = \mathbf{M}^{-1} \mathbf{E} \mathbf{E} \mathbf{v}_m = \mathbf{M}^{-1} \mathbf{E} \mathbf{E} \left( \mathbf{w} + 2 \pi n \mathbf{v} \right) \]

\[ \omega^2 = \beta \left( \frac{1}{m} + \frac{1}{M} \right) \pm \beta \left[ \left( \frac{1}{m} + \frac{1}{M} \right)^2 - \frac{4 \pi^2 \mathbf{v} \mathbf{v}}{MM} \right] \]

OPTICAL BAND

ACOUSTIC BAND

\[ \begin{array}{c|c|c|c} \hline -\pi/2 & \pi/2 \hline \end{array} \]

\[ \mathbf{v} \]

\[ \mathbf{F} \]

\[ \mathbf{M} \]

\[ \mathbf{E} \]

\[ \mathbf{H}_2 \]

\[ \mathbf{w} \]

\[ \mathbf{v}_m \]

THE SPLINE OF ATOMS BEHAVES LIKE A SPRING WHEN ONE IS PULLED
IONIC CRYSTALS

A: LATTICE POTENTIAL ENERGY (E)

\[ E = \frac{91.98}{4.13 \times 10^{-8}} + \frac{91.98}{4.13 \times 10^{-8}} + \frac{91.98}{4.13 \times 10^{-8}} + \ldots \]

\[ E_{\text{excl}} = \frac{-9.198}{4.13 \times 10^{-8} \left( \frac{3}{2} + \frac{1}{2} + \frac{3}{2} - \frac{1}{2} \right)} \]

INCLUDING ONLY THAT PART OF THE ATOM INSIDE CUBE:

\[ E_{\text{incl}} = \frac{-9.198}{4.13 \times 10^{-8} \left( \frac{3}{2} + \frac{1}{2} + \frac{3}{2} - \frac{1}{2} \right)} \]

CALLED EDEN METHOD OF CUTTING OFF THE SERIES
\[ E_0 = \frac{-\alpha e^2}{4\pi \varepsilon_0 R} \]

\[ \alpha = \text{Modeling constant} = 1.747 \text{ for NaCl} \]

**Ion #1: Exclusion Principle Repulsion**

We worry about nearest neighbor only.

\[ E_{1} = \frac{-\alpha e^2}{4\pi \varepsilon_0 R} - \frac{A}{R^6} \]

**Total P.E.:**

\[ E_{T} = -\frac{-\alpha e^2}{4\pi \varepsilon_0 R} - \frac{A}{R^6} \]

Recall ion pairs in whole crystal (2N ions)

Total Energy:

\[ E = N \left[ -\frac{-\alpha e^2}{4\pi \varepsilon_0 R} + \frac{A}{R^6} \right] \]

\[ E_T \quad R \quad R \quad T = 0 \quad K, \quad R = R_0 \]

\[ \frac{6 N e^2}{4 \pi \varepsilon_0 R^2} \]

\[ A = \frac{e^2}{4 \pi \varepsilon_0 R^6} \]

\[ E_T = \frac{-N e^2}{4 \pi \varepsilon_0 R^2} \left[ 1 - \frac{1}{R_0^6} \right] \]

\[ \alpha N \text{ is related to compressibility } k \]

\[ k = -\frac{1}{V} \frac{\partial p}{\partial V} \]

\[ \frac{dW = p \, dV = \Delta E}{dV} \]

\[ \frac{1}{k} = -V \frac{dp}{dV} = V \frac{d^2 E}{dV^2} \]

\[ \frac{dE}{dV} = \frac{dE}{dR} \frac{dR}{dV} \text{ and } \frac{d^2 E}{dV^2} = \frac{dE}{dR} \frac{d^2 R}{dV^2} + \frac{d^2 E}{dR^2} \frac{dR}{dV} \frac{dR}{dV} \]

From (1) and (2):

\[ R_0 = V \left[ \frac{dE}{dR} \frac{d^2 R}{dV^2} + \frac{d^2 E}{dR^2} (dR)^2 \right] \]

\[ = V \left[ \frac{dE}{dR} \right]^2 \]
\[ \frac{dV}{dt} = 3CNR^2 \]
\[ \frac{d}{dR} \left[ \frac{1}{k}R \right] = \frac{qCNRe^2}{4\pi \varepsilon_0} \left[ \frac{n-1}{R_e^3} \right] \]
\[ \frac{d^2E}{dR^2} \bigg|_{R=R_e} = \frac{Na^2}{4\pi \varepsilon_0} \left[ \frac{1}{R_e^2} \right] \]

\[ \frac{1}{k}R_e = \frac{qCNRe^2}{4\pi \varepsilon_0} \left[ \frac{n-1}{R_e^3} \right] \]

\[ = \frac{36\pi \varepsilon_0 R_e^5}{4\pi \varepsilon_0} \]

0 is what we'll solve for; all other constants we'll know.

Go to Wednesday, 3/11

3-24-72 (Fri) test on Monday (Sec 3.4, 7)

Diatomic lattice

\[ \omega = 2\pi \sqrt{\frac{k}{m}} \]

\[ \omega = 2\pi \sqrt{\frac{k}{m}} \]

\[ \omega = 2\pi \sqrt{\frac{m + M}{2m + M}} \]

Optical (out of phase) \quad m > M

Acoustic (in phase)
MONOTONIC LATTICE

\[ \omega = \sqrt{ \frac{4M}{M} \omega \cdot \frac{K}{2} } \]

\[ -\frac{T}{2}, \quad \frac{T}{2} \quad \quad k = \frac{2\pi}{L} \]

\[ \text{TRANSMISSION OF } E \quad 100\% \]

\[ \text{ABSORPTION RESONANCE} \]

\[ \omega = 2\pi f \]

3 VIBRATING DIRECTIONS IN 3-D

\[ \nu_p = \frac{\omega}{k} \]

\[ "\text{TRANSVERSE WAVES}" \]

\[ \text{REAL PART} \]

\[ \alpha \quad \text{AND} \quad \beta \quad \text{FREQUENCIES} \]

\[ \text{STANDING WAVES} \]

\[ \text{DISCRETE } k \text{ AND } \omega! \]
REVIEW FOR TEST:

1) FORCES BETWEEN IONS

2) CRYSTAL STRUCTURE
   (i) LATTICE, UNIT CELLS, CUBIC LATTICES, LATTICE CONSTANTS
   (ii) MILLER INDICES
   (iii) SPACING BETWEEN PLANES
   (iv) X-RAY DIFFRACTION DETERMINATION OF UNIT CELL, LATTICE CONSTANTS

3) IONIC CRYSTALS
   (i) POTENTIAL ENERGY
   (ii) COMPRESSIBILITY AND DENSITY
   (iii) ELASTIC WAVES
      (a) FREQUENCY, WAVELENGTH, WAVE SPEEDS
      (b) INFRARED ABSORPTION
      (c) STANDING WAVE NODES
GO TO TUES. (PG. 21)

SUN 5-29-72 (TUE) 10 3-11 12-34

SPECIFIC HEAT OF SOLID

$C_v = \frac{3}{2}R$ (PER MOLE)

$C_v = \frac{3}{2} R \frac{1}{v}$

FROM CLASSICAL CALCULATION: $U = \beta \cdot RT$ (ANY ENERGY ALLOWED)

$C_v = \beta \cdot R$

FROM QUANTUM MECHANICAL OSCILLATORS

$E_n = (n - \frac{1}{2}) \hbar \omega$; $n = 0, 1, 2, ...$

EINSTEIN MODEL OF SOLID

1) ALL ATOMS VIBRATE WITH SINGLE FREQUENCY $\omega$

2) EACH OSCILLATOR IS A LINEAR HARMONIC OSCILLATOR (NATURALLY 1 VIBRATIONS)

3) $N$ ATOMS $\Rightarrow$ $3N$ LINEAR OSCILLATORS

4) GIBBS DISTRIBUTION: $U = 3N \frac{E}{kT}$ (E-AKIN)

$N \frac{E}{kT} = \sum_{n=0}^{\infty} e^{-E_n/kT}$

$E = \frac{3}{2} \hbar \omega$ (SIMPLIFIED)

$E = \frac{3}{2} \hbar \omega e^{-\hbar \omega / kT}$

$= \frac{3}{2} \hbar \omega$ (APPROXIMATION)

$= \frac{3}{2} \hbar \omega e^{-\hbar \omega / kT}$

$= \frac{3}{2} \hbar \omega e^{-\hbar \omega / kT}$

$+ \frac{3}{2} \hbar \omega e^{-2\hbar \omega / kT}$

$+ \frac{3}{2} \hbar \omega e^{-3\hbar \omega / kT}$ + ...

$\Rightarrow E = \frac{3}{2} \hbar \omega + \hbar \omega (1 + e^{-\hbar \omega / kT} + e^{-2\hbar \omega / kT} + ...)$

LET $u = 1 + e^x + e^{2x} + e^{3x} + ... = \frac{e^{nx} - 1}{n(-e^{nx})}$

$\Rightarrow E = \frac{3}{2} \hbar \omega + \hbar \omega (1 + u)$
\[ \frac{dy}{dx} = e^x + 2e^{2x} + 3e^{3x} = \text{NUMERATOR} = \frac{d}{dx} \left( \frac{1}{1-e^{-x}} \right) = e^x (1-e^{-x})^2 \]

\[ \bar{E} = \frac{1}{2} \hbar f + \hbar f \left( \frac{1-e^{-x}}{1-e^{-x}} \right) \]

\[ = \frac{1}{2} \hbar f + \hbar f \left( \frac{1}{1-e^{-x}} \right) \]

\[ \therefore \quad \bar{E} = \frac{1}{2} \hbar f + \hbar f \left( \frac{e^{-x}}{2} \right) = \frac{1}{2} \hbar f + \hbar f \left( e^{\frac{\hbar f}{kT}} - 1 \right) \]

**TOTAL ENERGY**

\[ U = 3N \times \bar{E} = 2N \hbar f + 3N \hbar f \left( e^{\frac{\hbar f}{kT}} - 1 \right) \]

\[ C_V = \frac{\partial U}{\partial T} = 3N \hbar f \left( e^{\frac{\hbar f}{kT}} - 1 \right) \cdot \frac{1}{kT} \]

\[ = 3N \hbar f \left( \frac{1}{kT} \right) \left( e^{\frac{\hbar f}{kT}} - 1 \right) \cdot e^{\hbar f/kT} \left( - \frac{\hbar f}{kT} \right) \]

\[ = 3N \left[ (\frac{\hbar f}{kT})^2 e^{\hbar f/kT} / (e^{\hbar f/kT} - 1)^2 \right] \]

**FOR 1 MOLE** \( N = N_0 \):

\[ \Rightarrow C_V = 3R \left[ (\frac{\hbar f}{kT})^2 e^{\hbar f/kT} / (e^{\hbar f/kT} - 1)^2 \right] \]

As \( T \to \infty \):

\[ e^{\hbar f/kT} \to 1 \quad \hbar f \quad \therefore \quad \lim_{T \to \infty} C_V = 3R \]

As \( T \to 0 \):

\[ C_V \to 3R \left( \frac{\hbar f}{kT} \right)^2 e^{\hbar f/kT} \]

\[ \lim_{T \to 0} C_V = 3R \quad (\text{USING HOSPITALS}) \]

\[ T \quad \text{EINSTEIN MODEL} \]
DEBYE MODEL

1) 3N LINEAR HARMONIC OSCILLATORS

2) MAXWELL DISTRIBUTION

3) INSTEAD OF SINGLE VIBRATION FREQUENCY
   4) ASSUMED FREQUENCIES PRESENT ARE
      STANDING WAVE FREQUENCIES OF
      CONTINUOUS MEDIUM

\[ f = \frac{v}{\lambda} \]

5) ASSUMPTION: ALL WAVES TRAVEL AT SAME
       SPEED (NON-DISPERSIVE)

\[ \frac{\varepsilon_0 \varepsilon''}{\varepsilon''} + \frac{\varepsilon_0 \varepsilon''}{\varepsilon''} + \frac{\varepsilon_0 \varepsilon''}{\varepsilon''} \frac{v^2}{c^2} = \frac{1}{2} \frac{\varepsilon_0 \varepsilon''}{\varepsilon''} \]

FOR 1-DIMENSIONAL (STANDING WAVE)

\[ u = u_0 \sin \left( \frac{n \pi x}{L} \right) \cos \omega t \]

FOR 3D

\[ u = u_0 \sin \left( \frac{n \pi x}{L} \right) \sin \left( \frac{n \pi y}{L} \right) \sin \left( \frac{n \pi z}{L} \right) \cos \omega t \]
TUES (2-28-72) PR. 13:12

SPECIFIC HTS.

(1) CLASSICAL STATISTICAL MECHANICS

TO DETERMINE EQUILIBRIUM ENERGY DISTRIBUTION

MOMENTUM SPACE

FREE PARTICLES

ENERGY DEPENDS ONLY ON Mom

IF PARTICLE IS NOT FREE:

\[ E(p_x, p_y, p_z, x, y, z) \] : CONSERVATIVE SYSTEM

6-DIMENSIONAL GRAPH: PHASE SPACE, WITH

BOXES OF \( dp_x dp_y dp_z dx dy dz \)

DISTRIBUTION OF PARTICLES AMONG CELLS

IN PHASE SPACE WILL GIVE ENERGY DISTRIBUTION

\[ n_1, n_2, n_3, n_4, n_5 \]

\( N = \text{TOTAL PARTICLES} \)

EQUILIBRIUM DISTRIBUTION = MOST PROBABLE

DISTRIBUTION OF PTS. AMONG CELLS

EXAMPLE: 2 BOXES: 4 PARTICLES

a) ALL 4 IN A CELL (ONE WAY)

b) 2 IN A, 1 IN B (4 WAYS)

c) 2 IN A, 2 IN B (6 WAYS)

\[ \text{WAYS} = \frac{n!}{n_1! n_2! n_3!} \ldots \]

PROBABILITY OF A DISTRIBUTION OF PTS

AMONG CELLS IS: \( \text{WAYS} \)

WHICH DISTRIBUTION HAS MAXIMUM

PROBABILITY WITH RESTRICTIONS:

\[ H = n_1 + n_2 + \ldots = \text{CONSTANT} \]

\[ E = n_1 E_1 + n_2 E_2 + \ldots = \text{CONSTANT} \]
LE GRANGER: MULTIPLIERS:

\[ N = e^{-\frac{E}{kT}} \] \( \text{MAXWELL-BOLTZMANN DISTRIBUTION} \)

\( E_1, E_2, E_3, \ldots \Rightarrow \text{DISCRETE ENERGIES (QUANTUM)} \)

\( N \) = \# PARTICLES WITH ENERGY \( E \)

CONTINUOUS ENERGY DISTRIBUTION

BOXES HAVE "VOLUME" IN PHASE SPACE:

\[ dN = dp_x dp_y dp_z dx dy dz \]

\[ \Rightarrow dN = e^{-\frac{E}{kT}} d\frac{E}{kT} d\Omega \] \( \text{(MAXWELL-BOLTZMANN)} \)

EXAMPLE: CLASSICAL VIBRATING ATOM \( \Rightarrow \) NO \( E \) RESTRICTIONS

FRACTION OF THE PARTICLES \( \propto \rho (p_x p_y p_z) \)

AND POSITION \( x, y, z \) IN PHASE SPACE IN \( d\Omega \)

\[ \frac{dN}{N} = e^{-\frac{E}{kT}} d\frac{E}{kT} d\Omega / \int_{-\infty}^{\infty} e^{-\frac{E}{kT}} d\frac{E}{kT} d\Omega \]

\[ \frac{E}{N} = \frac{\int E d\Omega}{\int e^{-\frac{E}{kT}} d\Omega} = 3kT \]

TOTAL \( E \) ON \( N \) VIBRATING ATOMS:

\[ U = 3NkT \]

FOR 1 GRAMS MOLE

\[ U = 3N_0 kT = 3RT \]

\( N_0 = \text{AVAGADRO'S NUMBER} \)

\( R = \text{IDEAL GAS CONSTANT} \)

SPECIFIC HEAT PER MOLE

\[ C_V = \frac{8T}{3} \left( \frac{\delta U}{\delta T} \right)_V = 3 \left( \frac{\delta U}{\delta T} \right)_V = 3.72 \text{ CALORIES/MOLE } \cdot \text{K} \]

\[ C_V \]

EXPERIMENTAL

VIBRATING PARTICLE CAN HAVE ENERGIES

\[ E = (n + \frac{1}{2}) \hbar \omega \quad ; n = 0, 1, 2, 3, \ldots \]

TO WED (P3, 19)
LATTICE VIBRATION SPECIFIC HEAT OF SOLID

(1) EINSTEIN MODEL

\[ \frac{\xi^2}{2} \left( \frac{\xi}{\xi + 2} \right) + \frac{\xi^2}{2} = \frac{\xi^2}{\xi + 2} \]

\[ \mu = \mu_0 \sin \left( \frac{n_\xi \pi x}{a} \right) \sin \left( \frac{n \pi y}{a} \right) \]

\[ \sin \left( \frac{n \pi z}{a} \right) \cos \left( \frac{2 \pi z}{a} \right) \]

FREQUENCIES ARE CONTINUOUS MEDIUM

STANDING WAVE FREQUENCIES

\[ f = \sqrt{2 \xi^2 + \xi_0^2 + \xi_z^2} \]

\[ n^2 \text{ IS STANDING WAVE MODE (YIELDS "CRYSTAL LATTICE")} \]

\[ n^2 = n_\xi^2 + n_0^2 + n_z^2 \]

Moving from origin f goes up

\[ \frac{\partial}{\partial \xi} \left( \frac{1}{2} \right) + \frac{\partial}{\partial \xi} \left( \frac{1}{2} \right) \]

\[ dR = \frac{2 \xi^2 f}{\xi_0^2} \]

TO GET # OF VIBRATION MODES 'TWIXT f AND \[ f + df = df \]

\[ N \] (COUNT # OF PTS 'TWIXT \( R \) & \( R + dR \))

VOLUME 'TWIXT \( R \) & \( R + dR \) (ELLIPSOID)
WILL GIVE A SPHERE SHELL

\[ dN = \frac{1}{\beta} (4\pi R^2) dR \]

\[ = \frac{1}{\beta} R^3 \frac{dR^2}{\sqrt{1 - \left( \frac{R}{V_0} \right)^2}} \]

\[ = \frac{4\pi V^3}{V_0^3} \int_0^V f^2 df \]

\[ = \frac{4\pi V}{V_0^3} \int_0^V f^2 df \quad \Rightarrow \ V^3 = \text{CUBE VOLUME} = \frac{4}{3} \pi r^3 \]

\[ \text{CUT-OFF (} f_0) \]

\[ dN \]

\[ f_0 = \sqrt{\frac{3}{4\pi V_0^3}} \left( \frac{\theta}{V_0^3} + \frac{1}{V_0^2} \right) \]

\[ N = \int_0^{f_0} dN \]

\[ = 4\pi \left( \frac{3}{V_0^3} + \frac{1}{V_0^2} \right) \int_0^{f_0} f^2 df \]

\[ \Rightarrow f_0 = \left[ \frac{3}{4\pi} \frac{N}{V_0^3} \left( \frac{3}{V_0^3} + \frac{1}{V_0^2} \right) \right]^{1/3} \]

LET EACH OSCILLATOR HAVE ENERGY EQUAL TO AVERAGE ENERGY OF EINSTEIN'S OSCILLATORS:

\[ E = \frac{h^2}{2m} - 1 \]

TOTAL ENERGY:

\[ U = \int_0^{f_0} E dN \]

\[ U = 4\pi \left( \frac{3}{V_0^3} + \frac{1}{V_0^2} \right) \int_0^{f_0} \left( \frac{h^2}{2m} - 1 \right) df \]

SUBSTITUTE \( \left( \frac{3}{V_0^3} + \frac{1}{V_0^2} \right) \) FROM EXPRESSION FOR \( f_0 \)

LET \( x = \frac{h^2}{2m} - 1 \) ANO \( x_0 = \frac{h^2}{kT} \)

\[ \Rightarrow 3N \left( \frac{kT}{h^2} \right)^3 \int_0^{x_0} e^{x^3} dx \]

\[ \Rightarrow U = 3N \left( \frac{kT}{h^2} \right)^3 \int_0^{x_0} e^{x^3} dx \]

\[ \Rightarrow \frac{3 \text{N} \text{K}T}{3 \text{R}} = 3 \text{R} \text{JOULES/MOLE} \]

\[ \Rightarrow c_v = \frac{3}{5} \cdot 3R = 3R \]
LOW TEMP

\[ U = qT \left( \frac{kT^2}{\hbar^2} \right) kT \int_0^{\infty} \frac{x^2 \, e^{-x}}{e^x - 1} \, dx \]

\[ \Rightarrow U = qT \left( \frac{kT^2}{\hbar^2} \right) kT \int_0^{\infty} \frac{x^2 \, e^{-x}}{e^x - 1} \, dx \]

\[ \frac{e^{-x} x^2}{e^x - 1} = \frac{\pi^4}{15} \]

\[ U = \frac{3}{5} \pi^4 N kT \left( \frac{T}{T_0} \right) \]

\[ \Theta_0 = \text{DEBYE TEMPERATURE} \]

\[ C_V = \frac{\pi^2}{5} \frac{U}{kT} \]

\[ C_V = \frac{8}{3} \pi^4 R \left( \frac{T}{T_0} \right) \]

\[ \Theta_0 \text{ TO MAKE CURVE FIT} \]

\[ \Theta_0 \text{ TO MAKE CURVE FIT} \]

\[ \text{THE EXPERIMENT} \]

\[ \Theta_0 \text{ TO MAKE CURVE FIT} \]

\[ \text{BEGIN ON THE SUBSTANCE} \]

4-4-72 (TUES) TEST NEXT WEDNESDAY 09 197-59

SPECIFIC HEAT \( C_V \)

1. INSULATORS: \( C_V = \left( \frac{\hbar \nu_{\text{lib}}}{kT} \right) \)

2. METALS: \[ C_V = \left[ \left( \frac{\hbar \nu_{\text{lib}}}{kT} \right) + \left( \frac{\hbar \nu_{\text{elec}}}{kT} \right) \right] \]

\[ C_V = C_V^{\text{lib}} + C_V^{\text{elec}} \]

\[ \uparrow \]

\[ \frac{\hbar \nu}{kT} \]

\[ \uparrow \]

\[ \nu \]

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DIELECTRICS

1. ELECTRONIC POLARIZATION (σ-electrons)
   - Relative to nucleus

2. IONIC POLARIZATION
   - \( \text{Na}^+ \text{Cl}^- \)

3. ORIENTATIONAL POLARIZATION (Reorientation of permanent dipole on \( E \))

Definitions:

1. Dipole moment: \( \vec{p} = q \vec{d} \)

2. Polarization: \( \vec{P} = \varepsilon \frac{\vec{P}}{V} = \text{dipole moment/unity volume} \)

3. Displacement: \( \vec{D} = \varepsilon_0 \varepsilon \vec{E} + \vec{P} \) (MKS)
   \( \vec{D} = \varepsilon \vec{E} + \varepsilon_0 \vec{P} \) (CGS)

\[ \varepsilon \text{electric decreases } \varepsilon \text{ if charge on plates is the same} \]

4. Dielectric constant: \( k \)
   \( \vec{D} = k \varepsilon_0 \varepsilon \vec{E} = \varepsilon_0 \varepsilon \vec{E} + \vec{P} \)
   \[ \Rightarrow k = 1 + \varepsilon_0 \varepsilon \]
$E_{100}$ = LOCAL FIELD @ POSITION OF ATOM DUE TO OTHER CHARGES

$E_{20}$ = FIELD OUT, DUE TO PLATES

$E_{30}$ = FIELD OUT, DUE TO OUTSIDE SURFACE

POLARIZATION CHARGE

$E_{3}$ = FIELD DUE TO CHARGE ON CAVITY SURFACE

$E_4$ = FIELD INSIDE THE CAVITY

$\Rightarrow E_{100} = E_1 + E_2 + E_3 + E_4 = E + E_3 + E_4$

Polarization in a Dielectric

$E_0$ DUE TO INDIVIDUAL CIRCLES

$E_{100} = E + E_3 + E_4$

$\Rightarrow E_3 = \int_{\Sigma} \frac{\partial \Phi}{\partial n} \cdot dS$

$\Theta$ = (FOR CLOSED) = $\int_{\Sigma} \sigma \cdot dS = -P \cdot \cos \Theta \cdot dS$

$\Rightarrow \sigma = -P \cdot \cos \Theta$

$\text{AREA} = \pi R \cdot d\Theta \cdot 2 \cdot R \cdot d\Theta$

$\Rightarrow \sigma = C \cdot R \cdot \sin \Theta \cdot d\Theta$

$dE = \frac{1}{2} \int_{\Sigma} \frac{\partial E}{\partial n} \cdot dS$

$\Rightarrow E_3 = \frac{1}{2} \iiint_{\Sigma} \frac{\partial E}{\partial n} \cdot dS$

$E_3 = \frac{P}{2 \epsilon_0}$

$\Rightarrow E_{100} = E + \frac{P}{2 \epsilon_0} + E_4$
For cubic lattice of same atom: $E_0 \Rightarrow E_{\text{tot}} = E_0 + \frac{p}{2E_0}$.

2) Some other lattice: $E_{\text{tot}} \Rightarrow E_{\text{tot}} = E + \frac{p}{2E_0}$.

Atomic polarization: $\alpha = \frac{p}{E_0}$. 

Cubic lattice of identical atoms:

$E_{\text{tot}} = E_0 + \frac{p}{2E_0}$

$\alpha = \frac{p}{E_0}$

$E_{\text{tot}} = E_0 + \frac{p}{2E_0}$

$P = (k-1)E_0 E$

$P = \frac{kE_0 E}{2}$

$N$ atoms per unit volume,

$\lambda = 10^{-10}$ m$^3$.

$\text{Na}^+ : 1.29 \times 10^{-6}$

$\text{Li}^+ : 3.94 \times 10^{-6}$

Ionic polarization:

Apply field $E$.

Shift of $E_0$ ions relative to negative ions.

Polar moment $\chi = 2E_0 \chi / \beta$

$\lambda = \frac{N_\text{x}}{\text{x}}$

$\lambda = \frac{N_\text{Na}^+ \text{e}^{+} + N_\text{Na}^+ \text{e}^{-} + N_\text{Na}^+ \text{e}^{-} / 3}$

$W = \sqrt{\lambda}$
ORIENTATIONAL POLARIZATION ALIGNMENT OF PERMANENT DIPOLES

WITH ELECTRIC FIELD PRESENT, FIELD TENDS TO
LINE UP DIPOLES, WHILE INTERACTIONS
'TWIST' THE DIPOLES THEMSELVES TEND TO
RANDOMIZE DIRECTION.

\[ U = \beta \cdot \mathbf{E} - \beta \mathbf{E} \cos \Theta \]
\[ U = \pi \mathbf{d} \mathbf{n} \cdot \mathbf{E} \cos \Theta \]
\[ -\int \mathbf{E} \cos \Theta \mathbf{E} \cdot \mathbf{E} \cos \Theta / kT \, d\Omega \]
\[ = \int \mathbf{E} \mathbf{E} \cdot \mathbf{E} \cos \Theta / kT \, d\Omega \]
\[ \mathbf{E} \cdot \mathbf{E} \mathbf{E} \cdot \mathbf{E} \cos \Theta / kT \]
\[ d\Omega \text{ IS THE SOLID ANGLE} \]
\[ 'TWIST' \Theta \text{ AND} \Theta + d\Theta \]

\[ \theta = \frac{\text{AREA SUBT. ON SPHERE}}{R^2} \]

\[ \Rightarrow \beta \mathbf{E} \mathbf{E} \cdot \mathbf{E} \cos \Theta = \int \beta \mathbf{E} \cos \Theta \mathbf{E} \cdot \mathbf{E} \cos \Theta / kT \, d\Omega \]
\[ \Rightarrow \mathbf{E} \cos \Theta = \int \beta \mathbf{E} \cos \Theta \mathbf{E} \cos \Theta / kT \, d\Omega \]
\[ \text{NOW} \ dx = \sin \Theta \, d\Theta; \ x = \cos \Theta; \ q = -\mathbf{E} / kT \]
\[ -\int x^2 e^q \, dx = \frac{e^q - e^{-q}}{2} \]
\[ \cos \Theta = \text{COTH} 0 - \frac{1}{a} = \text{LANGEVIN FUNCTION} \]
\[ \cos \Theta = \text{ORDINARY T} \& \mathbf{E} \]
\[ \frac{1}{a} \text{ LOW} T \text{ OR} \mathbf{E} \text{ OR BOTH} \]
\[ a = \beta \mathbf{E} / kT \]
For normal $T$ and $E \ll 1$

$$\theta = \theta_0^3 \quad \text{(exp in series)}$$

$$P = Np \frac{\theta}{3kT} \quad \text{where } N = \text{number of dipoles per unit volume}$$

$$p = Np \frac{E}{3kT} = Np^0 E / 3kT$$

$$k = 1 + \frac{p}{Np^0}$$

$$= 1 + \frac{E}{3kT}$$

If other polarization besides dipole orientation

$$s = k_0 + C/T \quad \text{(Curie Law)}$$

\[ K \]

\[ H \cdot S \]

\[ \text{Structure 2} \]

\[ \text{Structure 1} \]

\[ \text{Liquid} \]

4-10-72 (Monday)

**Alternating Electric Fields (D Electric)**

$$E = E_0 e^{i\omega t}$$
\[ \Sigma F = m \frac{d^2x}{dt^2} = q E_0 e^{i\omega t} - \beta x - \gamma x \frac{dx}{dt} \]

\[ \beta = \text{RESTORING COEFFICIENT} \]

\[ m = \text{MASS} \]

\[ \gamma = \text{RADIATION LOSS} \]

\[ \Rightarrow \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \omega_0^2 x = \frac{q E_0 e^{i\omega t}}{m} \]

\[ x = m \left[ \frac{E_0 e^{i\omega t}}{\omega_0^2 - \omega^2 + i\omega} \right] = \frac{q E_0 e^{i\omega t}}{m} \left[ \frac{\omega_0^2 - \omega^2 \pm i\omega}{(\omega_0^2 - \omega^2)^2 + \omega^2 \omega_0^2} \right] \]

\[ = \frac{q E_0}{m} e^{i\omega t} \left\{ \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \omega^2 \omega_0^2} \right\} - \frac{i\omega}{(\omega_0^2 - \omega^2)^2 + \omega^2 \omega_0^2} \]

\[ \rho = qx \Rightarrow P = Nq \rho = \frac{Nq^2 E_0}{m} e^{i\omega t} \]

**FOR A SLOWLY VARYING FIELD (\( \omega < \omega_0 \))**

\[ P_{in} = \frac{Nq^2 E_0}{m} e^{i\omega t} \left( \frac{\omega_0^2 \pm i\omega}{\omega_0^2} \right) ; \quad \text{\( \omega \) NUGLIGIBLE} \]

\[ P_{out} = 0 \]

**NEAR \( \omega = \omega_0 \)**

\[ P_{in} = 0 \Rightarrow P_{out} = \frac{Nq^2 E_0}{m} e^{i\omega t} \]

**RESULTS:**

\[ P_{in} \]

\[ \omega \rightarrow \omega_0 \rightarrow \text{RESONANCE} \]
\[ P_{in} = \frac{N_0^2 E_0}{m} \left( \frac{-\omega^2}{\omega^2 - 2 \omega \omega_0 + \omega_0^2} \right) \]

Heads toward zero, after hump after \( \omega_0 \).

\[ P_{out} \rightarrow \text{Heads toward zero} \]

Power: \( \frac{dW}{d\tau} = FV \)

Power input maximum \( @ \) resonance: \( \omega = \omega_0 \).

\( E_0 \) \( @ \) max when \( x = 0 \), since velocity \( V \) is max \( @ \) \( x = 0 \).

\[
K = 1 + \frac{P_{in}}{E_0 E} ; \quad K' = 1 + \frac{P_{in}}{E_0 E} ; \quad K'' = 1 + \frac{P_{out}}{E_0 E}
\]

\( K' \): Orientation

\( K'' \): Electronic

Absorption:

Microwave, infrared; Ultra, V. Violet.
FERRO-ELECTRICITY:

INVERSION CENTER OF SYMMETRY
- ALL POINTS INVERTED THRU
  INVERSION CENTER

FERRO-ELECTRICITY
1) UNIT CELLS HAVE NO INVERSION CENTER
   OF SYMMETRY
2) ALTERNATE POSITIONS FOR SOME ATOMS
   IN UNIT CELLS
3) DIPOLE IN ONE CELL HAS STRONG
   ENOUGH FIELD TO PRODUCE SIMILAR
   DIPOLE IN NEXT, ETC.
   (CO-OPERATIVE PHENOMENON)

EX) $\text{BaTi}_2\text{O}_3$

$\bullet \text{Ba}^{+2}$

$\bullet \text{Ti}^{4+}$

$\bullet \text{O}^{-2}$

$\bullet \text{O}^{-2}$

$\text{Ti}^{4+}$ OFF CENTER BY 0.66 Å
$\text{O}^{-2}$ 0.69 Å
TETRAGONAL 278-3930 K
(WILL CHANGE FROM CUBIC IN
ABOVE TEMPERATURE CHANGE)

→ POLARIZATION WITH ALL DIPOLE
MOMENTS IN A GIVEN REGION OF
CRYSTAL (DOMAIN) IN THE SAME
DIRECTION

FOR $\text{BaTi}_2\text{O}_3$ (SINGLE CRYSTAL)

NO APPLIED E FIELD
Applying electric field because regions don't line up the same as they were due to regular polarization due to regions lining up with each other.

Ferroelectric

Regular

\[ K = 1 + \frac{dP}{dE} \bigg|_{E=0} \]

Triglycine sulphate

\[ K = K_0 + \frac{C}{T - T_c} \]

\[ T_c = \text{Curie temp} \]
TEST 2

I) SPECIFIC HT. OF INSULATORS
   (NO SPECIFIC QUESTIONS ON STATISTICS)
   1) EINSTEIN MODEL
      MODEL, DERIVATION OF Cv, COMPARISON W/ EXPERIMENT
   2) DEBYE MODEL
   3) PHONON - PACKET OF VIBRATIONAL ENERGY

II) DI-ELECTRICS
   1) DEFINITIONS OF \( \tilde{p}, \tilde{P}, \tilde{D}, k, \alpha \)
   2) TYPES OF POLARIZATION
   3) LOCAL FIELD @ ATOMIC POSITION
      (DUE TO OTHER DIPOLES AND CHARGES)
   4) CLAUSIUS-MOSotti EQUATION
      (DERIVATION, USE IN FINDING \( \alpha \))
   5) IONIC POLARIZATION
   6) ORIENTATIONAL POLARIZATION
      (DERIVATION, DEPENDENCE OF \( P \) ON E & T)
   7) DIELECTRIC IN ALTERNATING FIELD
   8) FERRO-ELECTRICS
MAGNETIC PROCESSES

IF APPLY MAGNETIC FIELD OF INTENSITY $\vec{H}$ TO A MATERIAL $\rightarrow$ INDUCED MAGNETIZATION $\vec{M}$

$\vec{M} = \frac{\varepsilon \vec{P}}{\gamma}$

$\vec{B} = \mu_0 \vec{H} + \vec{M}$; $\vec{B}$ = MAGNETIC INDUCTION

$\vec{M} = (\mu_0 + \chi) \vec{H}$; $\chi = \frac{\vec{M}}{\vec{H}}$ = MAGNETIC SUSCEPTIBILITY

MAGNETIC MOMENTS

ORBITAL MAGNETIC MOMENT (CIRCLE)

$\vec{P}_m = IA \hat{\vec{n}}$

$\vec{P}_m = \frac{2\pi}{2m} (2\pi r^2) \hat{\vec{r}}$

$\vec{L} = \frac{2\pi}{2m} - \vec{mv} \hat{\vec{n}}$

$\vec{L} = \frac{2\pi}{2m} \vec{l}$ — ORBITAL ANGULAR MOMENTUM

2) SPIN MAGNETIC MOMENT

$\vec{P}_s = g \left( \frac{\hbar}{2m} \right) \hat{\vec{s}}$; $\vec{s}$ = SPIN ANGULAR MOMENTUM

APPLY MAGNETIC FIELD

$\vec{F} = \vec{P} \times \vec{B}$

$\dot{\vec{s}} = -\vec{P}_m \cdot \vec{B}$

DIAMAGNETISM DUE TO LARMOR PRECESSION OF ELECTRON ORBIT

TORQUE INTO PAPER

$F = \vec{P}_m \cdot \vec{B}$
\[ \mathbf{r} = \frac{\mathbf{I}}{\mathbf{r}} : \mathbf{I} = \mathbf{r} \times \mathbf{B} = \mathbf{r} \times \mathbf{B} \] 

\[ d\mathbf{\hat{r}} = \left( \frac{\mathbf{I}}{2m} \right) \mathbf{r} \times \mathbf{B} \] 

\[ \omega_L = \text{Larmor precessional frequency} \quad \text{(in Hz)} \] 

\[ \omega_L = \frac{d\theta}{dt} \] 

\[ d\theta = \omega_L dt \Rightarrow \theta = \omega_L t \] 

\[ d\phi = \omega_L \sin \phi \quad d\phi = |\omega_L| \sin \phi \, dt \] 

Solving for \( \omega_L \): 

\[ \omega_L = \left( \frac{e}{2m} \right) B \Rightarrow \text{Larmor precision error} \] 

Induced angular momentum \( \rightarrow \) Diamagnetic effect \( \text{(all in electrons orbit)} \) 

\[ L_{\text{ind}} = m \omega_L r^2 \] 

\[ W_0(x) = \frac{\hbar}{2m} \text{Ind} = \frac{e}{2m} m \omega_L r^2 \] 

- Spherical radius \( r = R \) 

\[ r^2 = x^2 + y^2 + z^2 = 3x^2 \] 

\[ \rho^2 = y^2 + z^2 = 2x^2 \] 

\[ \rho^2 = \frac{2}{3} r^2 \] 

\[ \rho \text{rno} = -\mathbf{e} \left( \frac{e}{2m} \right) m \omega_L \left( \frac{3}{2} r^2 \right) \] 

Assume molecules/volume 

\[ M = N \text{ atoms} \quad B = N \text{ atoms} \] 

\[ N = \frac{M}{14} = \frac{N \text{ atoms}}{14} \] 

\[ N_e = N \text{e} \left( \frac{3}{2} \right) m \omega_L \left( \frac{r^2}{2} \right) \]
TOTAL ORBITAL ANGULAR MOMENTUM
\( L = \sqrt{J(J+1)} \), \( K = \) ORBITAL ANGULAR MOM. - INTEGER
\( S = \sqrt{J(J+1)} \), \( \Lambda = \) TOTAL SPIN ANGULAR MOM. - INTEGER
\( J = L + S \), \( \Lambda = \) TOTAL TOTAL ANGULAR MOM. - INTEGER
\( \Lambda = \) NUMBER OF ELECTRONS IN ELLIPTICAL ORBITS

HAY CONTINUOUS INNER SHELL

TOTAL MAGNETIC MOMENT
\( m_u = m_s + m_l \)
\( J_z = \sqrt{J(J+1)} \)
\( q = 1 \)

APPLY MAGNETIC FIELD TO ATOM'S TOTAL MAGNETIC MOMENT

\( J_z \) COMPONENT OF \( \mathbf{J} \)

\( m \equiv J_z, J = 1, \ldots, \frac{J(J+1)}{2} \)

SET \( J = \frac{3}{2} \)

\( m_J = \pm \frac{3}{2}, \pm \frac{1}{2}, 0 \)

NOW \( U = -\mu m \cdot B = U \) ENERGY

\( B = \) \( \Rightarrow \) HIGH \( m_J \) \( \Rightarrow \) HIGHER \( U \)

AND \( (\mu m) = -q_f \left( \frac{2}{\hbar} \right) J_z \)

\( U = -\frac{1}{2} q_f (\frac{2m}{\hbar}) J_z \)

\( U = \frac{1}{2} q_f \left( \frac{2m}{\hbar} \right) B \)

\( U = \frac{1}{2} q_f \left( \frac{2m}{\hbar} \right) B \)

\( U = \frac{1}{2} q_f \left( \frac{2m}{\hbar} \right) B \)

ETC.
PARAMAGNETISM

\[ U = \frac{\Sigma q_i B_i e^{-m_i q_i B_i / kT}}{\Sigma e^{-m_i q_i B_i / kT}} \]

\[ \bar{U} = \frac{\Sigma q_i B_i e^{-m_i q_i B_i / kT}}{\Sigma e^{-m_i q_i B_i / kT}} \]

Yielding (after integrating constants)

\[ \bar{\rho}_m = q_i B_i \frac{\left( \frac{2}{2j+1} \right) \cosh \left[ \frac{(2j+1)x}{2} \right] - \cosh \left( \frac{x}{2} \right) }{\left( \frac{2}{2j+1} \right) \cosh \left[ \frac{(2j+1)x}{2} \right] + \cosh \left( \frac{x}{2} \right) } \]

For \( N \) atoms per unit volume:

\[ M = N \bar{\rho}_m \]

\[ \chi = \frac{M}{H} \]

Normal \( T \) and \( B \) (not very low \( T \) or very high \( B \))

\[ M = \frac{c}{T} \]

\[ c = N q_i^2 \beta (2j+1) B / 2k \]

\[ \chi = \frac{M}{H} = \frac{c}{T} \] (Curies Law)

GO TO TUESDAY
FREE ELECTRON THEORY (METALS) - BURCIE 1920

BULK VELOCITY $v_0$

MOBILITY $\mu = \frac{v_0}{E}$ \( \Rightarrow \) ELECTRIC FIELD

\[ \mathbf{J} \cdot \mathbf{E} = \rho \mathbf{E} \]

\[ \nabla \cdot \mathbf{J} = \rho \]

\[ \mathbf{E} \cdot \mathbf{J} = \mathbf{E} \cdot (\nabla \times \mathbf{B}) = 0 \]

OR $\mathbf{E} = \mathbf{J}$ (ANALOGOUS TO $\mathbf{V} = \mathbf{I}$)

$\mathbf{J} = \mathbf{E}$

$\mathbf{E} = \mu \mathbf{B}$

$\mathbf{V} = \mathbf{J} \times \mathbf{B}$

$\mathbf{E} = 0$, $\mathbf{J} = 0$

$\rho = \sigma \mathbf{E}$

$\sigma = \frac{\mathbf{J}}{\mathbf{E}}$

$\sigma = \frac{\mathbf{E}}{\mathbf{B}}$

$\sigma$: NUMBER OF FREE ELECTRONS

ON OIL DROP IN AIR:

$\Sigma \mathbf{E} = \mathbf{E}$ (FROM IA.1)

$\mathbf{E} = \frac{d\mathbf{V}}{dt}$

$\mathbf{E} = \frac{\mathbf{V}}{t}$

$\mathbf{V} = \mathbf{V}_0 e^{-t/\tau}$

SUPPOSE $E$ HAS BEEN ON $\Rightarrow \mathbf{V}_0(t)$

TURN OFF:

$\mathbf{V}_0 = \mathbf{V}_0 e^{-t/\tau}$

$\frac{d\mathbf{V}_0}{dt} + \frac{\mathbf{V}_0}{\tau} = 0$

$\mathbf{V}_0 = \mathbf{V}_0(0) e^{-t/\tau}$

$\mathbf{V}_0$ IS THE TIME FOR $\mathbf{V}_0$ TO DECREASE TO $\frac{1}{2}$ OF ITS ORIGINAL VALUE $\Rightarrow \frac{1}{2}$ OF THE ELECTRONS HAVEN'T COLLIDED AT END OF $\tau$ SECONDS.
\[ E = \frac{q}{m} V = \frac{d}{m} \frac{dV}{t} = 0 \]
\[ \Rightarrow E = \frac{q}{m} V = \frac{q}{m} (\frac{V}{t}) = (\text{mobility}) \]
\[ \text{AND} \quad \sigma = \frac{ne^2 \gamma}{m} \]

**For Thermal Conductivity**

\[
\begin{align*}
T_1 & \quad \quad \text{(KE)} \\
\text{and} & \\
T_2 & \quad \quad \text{(KE)}
\end{align*}
\]

\[ k = \frac{e^2}{3\pi^2} \cdot \frac{1}{m} \quad \text{thermal conductivity} \]

\[ \omega = \frac{e^2}{3\pi^2} \quad \text{bohr magneton constant} \]

\[ L = \frac{k}{e^2} = \left( \frac{e^2}{3\pi^2} \right) \frac{k}{e} = \text{orenberg number} \]

\[ = 2.45 \times 10^{-8} \text{ watt cm/deg} \]

**Specific Heat at High Temperatures:**

\[ C_v = 3R \quad \text{(clifford)} \]

For free q, classical says
\[ C_v = 3R + 3R \quad \text{(new degree of freedom)} \]
\[ & \quad \text{e}^{-K\infty} \]

\[ \text{not so} \]
\[ C_v = 3R \Rightarrow \text{something is inhibiting absorption of energy by free q} \]

**Paramagnetism of Free Electrons**

alignment of spin magnetic moments with magnetic field
\[ \Rightarrow \chi \text{ much larger} \]

Experimental: \( \chi \) only slightly increased by alignment of free electron magnetic moments
(something inhibiting moment alignments)

**Go To Fri., p. 53**
FREE ELECTRON THEORY

METAL CUBE EDGE.

IF ELECTRONS CANNOT BE Emitted (U ≤ 0) OUTSIDE, THE ALLOWED ELECTRON ENERGIES (FROM SCHRÖDINGER EQUATION ARE:)

\[ E_n = \frac{\hbar^2}{2m}(n_x^2 + n_y^2 + n_z^2) \]

\( n_x, n_y, n_z \text{ = INTEGERS} \geq 1 \)

IF \( U < 0 \)

\[ \begin{align*}
\text{if} \ A_x & = 0, \\
\text{and} \ U & = 0
\end{align*} \]

IF \( U \rightarrow \infty \), \( L = \infty \)

AGAIN \n
\[ E_n = \frac{\hbar^2}{2m}(n_x^2 + n_y^2 + n_z^2) \]

1) CAN'T DISTINGUISH ELECTRONS (PARTICLES ARE INDISTINGUISHABLE FROM EACH OTHER).

2) EXCLUSION PRINCIPLE: NO TWO PARTICLES ARE IN THE SAME STATE

\( n_x, n_y, n_z, m \rightarrow \text{STATE OF ELECTRONS} \)

YIELDS FERMI-DIRAC STATISTICS (TAKES PLACE OF BOLTZMANN STATISTICS).

PROBABILITY THAT THE STATE OF ENERGY \( E_n \) IS 'OCCUPIED' BY AN ELECTRON

(FERMI FUNCTION: \( f(E) = \left( e^{(E - E_n)/kT} + 1 \right)^{-1} \))

\[ f(E) \text{ is FERMI FUNCTION of ENERGY of STATE} \]

\[ f(E) \text{ having 50% chance of being occupied by an electron (low energies more likely to be occupied)} \]

\[ E \gg kT \]
\[ T = 0^\circ K \quad f(e) \]

**Finding \( E_p \)**

**Cubic Type Lattice, Each Point Represents Two States**

All points (states) inside \( R_{\text{MAX}} \) are occupied at \( T = 0^\circ K \)

\[ R_{\text{MAX}} = \left( \frac{n_x^2 + n_y^2 + n_z^2}{3} \right)^{\frac{1}{2}} \]

\[ R_{\text{MAX}} = \frac{L}{\pi} \quad \text{or} \quad R_{\text{MAX}} = \frac{2mE_p}{\hbar^2} \]

Number of occupied states having energy \( E_p \) to \( E_p + \Delta E \)

(Same as twice sphere section volume)

\[ = 2 \left( \frac{4}{3} \pi R_{\text{MAX}}^3 \right) \]

\[ = \frac{4}{3} \pi \left( \frac{2mL^2E_p}{\hbar^2} \right)^{\frac{3}{2}} \]

For \( N \) free electrons, \( N = \frac{4}{3} \left( \frac{2mL^2E_p}{\hbar^2} \right)^{\frac{3}{2}} \)

\[ \Rightarrow E_p = \frac{\hbar^2}{2m} \left( \frac{3N}{L^3} \right)^{\frac{3}{2}} \]

\[ = \frac{\hbar^2}{2m} \left( 3\pi^2n \right)^{\frac{3}{2}} \quad n = \text{free electron density} \]

\[ \approx 1 \times 10^{29} \text{ cm}^{-3} \]
Define \( S(E) \) as the number of states with energy between \( E \) and \( E + dE \).

And \( N(E) \) as the number of electrons having energy between \( E \) and \( E + dE \).

\[ f(E) S(E) dE = N(E) dE \quad \text{for any } T \]

\[ f(E) = 1 \text{ up to } E = E_0 \]

\[ f(E) = 0, \text{ above } E = E_0 \]

\[ N = \int_{-\infty}^{E_0} N(E) dE = \int_{-\infty}^{E_0} f(E) S(E) dE \]

Hence,

\[ \frac{L^3}{3\pi^2} \left( \frac{2\pi m E_0}{\hbar^2} \right)^{3/2} = \int_{-\infty}^{E_0} S(E) dE \]

\[ \delta(E) = \frac{L^3}{3\pi^2} \left( \frac{2\pi m}{\hbar^2} \right)^{3/2} \sqrt{E} = C \sqrt{E} \]

\[ \text{PARABOLA} \]

\[ \text{TEMPERATURE INDEPENDENT} \]

\[ E \]
ELECTRON ENERGY DISTRIBUTION

\[ T = 0^\circ \]

\[ N(E) \]

\[ \text{NO ELECTRONS} \]

\[ E = E_0, E_x, E_y \]

\[ T > T^* \]

FOR REAL HIGH TEMP, A

BOLTZMANN DISTRIBUTION

IS APPROACHED.

4.25-7.2 (KES) TEST FRE

FREE ELECTRON MODEL

\[ E = \left( k^2 \pi^2 / 2m^* \right) (n_x^2 + n_y^2 + n_z^2) \]

NO MORE THAN 1 ELECTRON PER STATE \( n_x, n_y, n_z = 0, 1, 2, 3, \ldots \)

DENSITY OF STATES:

\[ \xi(E) = \frac{E^2}{2m^*} \left( \frac{2m^*}{\pi h^2} \right)^{3/2} \]

\[ \xi(E) \] \( \text{DE} \) \( \text{NUMBER OF} \)

\[ \text{STATES HAVING ENERGIES} \]

\[ \text{WITH E AND E + DE} \]

\[ f(E) = \frac{1}{e^{(E - E_0)/kT} + 1} \]

\[ f(E) \]

\[ \text{SUPERPOSING } f(E) \text{ ON } \xi(E) \]

\[ N(E) \]

\[ E_F \]

\[ E \]
T = 0^\circ K \Rightarrow f(E) = 1 \quad 0 < E < E_F

\begin{align*}
E_F &= \frac{3}{2m} \frac{1}{(2\pi)^{3/2}} \\
N &= \int_{-E_F}^{E_F} N(E) dE = \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \\
N &= \int_{0}^{\infty} \int_{-E_F}^{E_F} N(E) dE = \int_{0}^{E_F} \sqrt{2m} E^{3/2} dE = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2}
\end{align*}

\text{AVERAGE ELECTRON ENERGY}

\begin{align*}
\langle E \rangle &= \frac{\int_{-E_F}^{E_F} E N(E) dE}{\int_{-E_F}^{E_F} N(E) dE} = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE \\
\langle E \rangle &= \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE
\end{align*}

\Rightarrow \langle E \rangle = \frac{3}{2} E_F

2) \quad T > 0^\circ K

\begin{align*}
N &= \frac{3}{2} CE_F^3/2 \quad \text{(From above)} \\
N &= \int_{-E_F}^{E_F} N(E) dE = \int_{0}^{E_F} \sqrt{2m} E^{3/2} dE
\end{align*}

\begin{align*}
\langle E \rangle &= \frac{\int_{-E_F}^{E_F} E N(E) dE}{\int_{-E_F}^{E_F} N(E) dE} = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE \\
\langle E \rangle &= \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE
\end{align*}

\Rightarrow \langle E \rangle = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE

\langle E \rangle = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE

\Rightarrow \langle E \rangle = \frac{E_F^3}{3}\sqrt{2} \pi^{3/2} \int_{0}^{E_F} \frac{\sqrt{2m}}{\pi^{1/2}} E^{3/2} dE

\text{increases a little with } T \text{, and } E_F \text{ decreases slightly.}
SPECIFIC HEAT

TOTAL ENERGY IN ELECTRONS:

\[ U = N E = N E(0) \left[ 1 + \frac{3}{2} \left( \frac{kT}{kT_0} \right)^2 \right] \]

\[ C_v = \frac{\partial U}{\partial T} = N E(0) \frac{3kT^2}{2E_0} \]

\[ \Rightarrow E(0) = \frac{3}{2} E_0 \]

\[ \Rightarrow C_v = \frac{NkT^2}{2E_0} \]

SUPPOSE 1 MOLE: \( N_A \) ATOMS WITH 1 \( \delta \)/ATOM FREE.

\[ \Rightarrow C_v = \frac{NkT^2}{2E_0} \approx \frac{3}{2} R \]

\[ \text{Slope of } A \]

\[ \beta = \frac{RkT^2}{2E_0} \]

\[ \text{MAY FIND } E_0 \]

IN COPPER:

\[ \beta = \frac{1.78 \text{ cal}}{\text{mole} \cdot \text{deg}} \] (EXPERIMENTAL)

\[ \beta = \frac{1.24 \text{ cal}}{\text{mole} \cdot \text{deg}^2} \] (THEORY)

\[ p = \hbar k = \text{ELEC \cdot MOMENTUM} \]

\[ p_x = \pi k_x \]

\[ p_y = \pi k_y \]

\[ p_z = \pi k_z \]

FERMI SURFACE IN \( k \) SPACE

SCATTERING BONE BY \( \Phi \) NEAR FERMI SURFACE

\[ E \text{ WILL SHIFT FERMI SURFACE} \]

SHIFTS M. V. \( \Phi \)
PARAMAGNETISM - MAGNETIC MOMENTS AND APPLIED FIELD

\[ \vec{P}_z \]

\[ \vec{P}_x \]

\[ \vec{P}_y \]

\[ \vec{P}_z \]

BOLTZMANN DISTRIBUTION: \( N = \frac{1}{\sqrt{\pi \cdot kT}} \)

The highest number of particles will be in state \( \sigma \) where \( P_z \) is largest in the direction of \( \vec{P}_z \).

\[ N_\sigma \]

\[ C \]

\[ E \]

SPACING BETWEEN ENERGY LEVELS: \( \Delta U = \hbar \beta \beta^* = \frac{1}{2} \hbar \)

EXPERIMENT

MICROWAVES OF FREQUENCY \( \gamma \)

PHOTONS OF ENERGY \( E = h \gamma \)

If \( \beta \) is increased gradually, increasing spacing between energy levels.

When \( \beta \) is \( \geq \beta^* \), there will be resonant absorption.

Measure the value of \( \beta \) for which you get a sudden increase in power input.

Can now compute \( \gamma \) for the solid.

This experiment is also used to determine internal fields, and is called electron paramagnetic resonance.
FERROMAGNETISM

SPONTANEOUS MAGNETISM WITH NO APPLIED FIELD
M VERY LARGE COMPARED WITH PARAMAGNETIC

\[ M \rightarrow M_0 \]

\[ \text{FERRO} \quad \text{PARA} \quad T_c \]

SUSCEPTIBILITY OF FERROMAGNETIC

\[ \chi \sim \frac{c}{T-T_c} \quad \text{CURIE-WEISS} \]

RECALL FOR PARAMAGNETIC: \( \chi = \frac{c}{T} \)

WEISS

COOPERATIVE EFFECT—MAGNETIC MOMENTS TEND TO LINE UP NEIGHBORING \( \hat{m} \) IN SAME DIRECTION.

AT THE POSITION OF THE ATOM:

\[ H_{\text{eff}} = H + \lambda M \quad \text{DUE TO ALIGNMENT} \]

ABOVE THE CRITICAL \( T_c \) IT'S A PARAMAGNETIC MATERIAL

\[ \Rightarrow \chi = \frac{M}{H_{\text{eff}}} = \frac{c}{T} \]

(NEIGHBORING MOMENTS BEGIN TO HAVE LESS EFFECT ON EACH OTHER PAST \( T_c \))

\[ \frac{M}{H + \lambda M} = \frac{c}{T} \quad \chi = \frac{H}{T-T_c} \]

\[ M = \frac{cH}{T-T_c} \]
WHAT CAUSES THESE MAGNETIC MOMENTS TO Align EACH OTHER?

"EXCHANGE" FORCE CAUSES NEIGHBORING SPIN MAGNETIC MOMENTS OF OUTER ELECTRONS IN CERTAIN ATOMS TO BE IN THE SAME DIRECTION.

LOOK AT THE HYDROGEN MOLECULE

2 POSSIBILITIES

1. THE ELECTRONS HAVE THE SAME SPIN. EXCLUSION PRINCIPLE TENDS TO FORCE APART.

2. THE TWO ELECTRONS HAVE OPPOSITE SPIN.

PARALLEL SPINS:

- CONSTANT PROBABILITY LINES OF ELECTRON LOCATION
- LOW PROBABILITY OF FINDING A "SHARED" ELECTRON

ANTI-PARALLEL SPINS:

- LOWEST COULOMB POTENTIAL ENERGY

IN FERROMAGNETIC MATERIALS, THE PARALLEL SPIN CONFIGURATION HAS LOWEST ENERGY. PARALLEL SPINS IN ADJACENT ATOMS (Fe, N, Co) DOMAINS IN WHICH M IS IN ONE DIRECTION.

Hysteresis

BOUNDARIES WON'T RE-ALIGN EXACTLY AS BEFORE THE FIELD IS APPLIED. (LEFT WITH A NET MAGNETIZATION)

Go to Wed. Read
PARAMAGNETISM : FREE ELECTRON

\[ \mu_0 = g \frac{e}{2m} \frac{1}{2} \]

\[ \mu = \frac{\mu_0}{2m} = g \frac{e}{2m} \frac{1}{2} \]

\[ \mathbf{\mu} \parallel \mathbf{B} \Rightarrow \mathbf{\mu} = \frac{1}{2} (\frac{e}{2m}) \]

\[ U = -\mathbf{\mu} \cdot \mathbf{B} = - (\mathbf{\mu}) \cdot \mathbf{B} \quad \text{(PAR. HAVE LOWEST ENERGY)} \]

\[ N, N_x, N_y, N_z, M = \frac{\mu}{2} \quad \text{M = S_x} \]

\[ N(E) \text{ at } T=0 \]

\[ \text{N}(E) \text{ PARALLEL} \quad \text{N}(E) \text{ ANTI-PARALLEL} \]

\[ 2N(E) = \text{NUMBER OF ELECTRONS WITH ENERGY BETWEEN } E_0 \text{ and } E_0 + \Delta E \]

\[ \text{WITH A FIELD } (\Theta T = 0 \text{ K}) \]

\[ \Delta \text{E = (E}/2m)B \]

THE NUMBER OF SPIN \( \mathbf{\mu} \) THAT CHANGED FROM ANTI-PARALLEL TO PARALLEL = \( \frac{1}{2} N(E_0) \Delta E \)

\[ \Delta E = \frac{(E_0)}{2m} \]
Excess Parallel fer Electron: \( N(E_F_\alpha) \Delta E \)

\[
N(E_F) \Delta E = C E^{-2/3} \frac{dE}{E_F} \frac{3/2}{2} \frac{1}{\sqrt{2}} \frac{1}{E_F} \Delta E
\]

\[\Rightarrow E - P/F = \frac{1}{2} \frac{C}{E_F} \left( \frac{2}{3} \times \frac{3/2}{2} \right) E_F^{1/2} (P_{\text{eff}}) \delta B \]

\( M = \text{Magnetic Moment per Unit Volume (M)} \)

\[
M = \frac{1}{2} \frac{C}{E_F} \left( \frac{2}{3} \times \frac{3/2}{2} \right) E_F^{1/2} (P_{\text{eff}}) \delta B \]

Assuming \( N/\text{unit volume} \)

\[\chi = \text{Susceptibility} = \frac{M}{H} \text{ and } \mu = \frac{M}{H} \]

\[\Rightarrow \chi = \frac{M}{H} = \frac{1}{\chi} \left[ \frac{2}{3} \times \frac{3/2}{2} \right] E_F^{1/2} (P_{\text{eff}}) \delta B \]

\[
\chi = \frac{2}{3} \frac{C}{E_F} (P_{\text{eff}})^{1/2} \delta B
\]

---

**Test Review**

**Description and Algebraic Derivation**

A) Atomic Diamagnetism

B) Atomic Ferromagnetism

1) Curie Law for Normal \( B \) and \( T \)

2) Paramagnetic Resonance

C) Ferromagnetism

1) Weiss Internal Field

2) Curie-Weiss Law in Paramagnetic Region

3) Exchange Forces

4) Spontaneous \( M \)

5) Domains

6) Hysteresis

D) Free Electron Theory

1) Model

2) Conductivity \( \sigma(\tau, m, e, \hbar) \)

3) In Quantum Mechanics

a) Determination of electron energy

- Defined electron state - exclusion principle, Fermi energy, Fermi surface in \( k \) (momentum space)

b) Determination of Fermi \( E_{\text{F}} \) at \( T = 0^\circ \text{K} \) as \( f(N_0/v) \)
3) DETERMINATION OF THE DENSITY OF STATES
\[ \varepsilon(E) = C E^{1/2} \]

4) AVERAGE ELECTRON ENERGY @ T=0K, DEPENDENCE ON T, AND ELECTRONIC SPECIFIC HT.

5) FREE ELECTRON PARAMAGNETISM - DETERMINATION OF SUSCEPTIBILITY @ T=0K

GO TO NEXT

FRI (4/21-78)

FREE ELECTRONS IN A METAL

\[ \text{ELECTRONS CONFINED TO BOX} \]

\[ V = 0 \text{ IN BOX}; V = \infty \text{ OUTSIDE} \]

\[ -\frac{\hbar^2}{2m} \Delta^2 \psi + U \psi = \varepsilon \psi \]

\[ \varepsilon = \frac{p^2}{2m} + \frac{1}{2} k^2 \]

\[ V = 0 \]

\[ \psi(x,y,z) = C \exp \left( \frac{\alpha x}{2m} \right) \exp \left( \frac{\beta y}{2m} \right) \exp \left( \frac{\gamma z}{2m} \right) \]

\[ E = \frac{\hbar^2}{2m} \left( \frac{\alpha^2}{\alpha^2} + \frac{\beta^2}{\beta^2} + \frac{\gamma^2}{\gamma^2} \right) \]

ONLY ALLOWED ENERGIES

THE STATE OF MOTION OF THE ELECTRONS DETERMINED BY N_x, N_y, AND N_z
\[ E = \frac{p^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} \]

\[ p_x = \hbar \pi x \quad p_y = \hbar \pi y \quad p_z = \hbar \pi z \]

The direction of the spin angular momentum in the presence of a magnetic field.

**Exclusion Principle**

No two electrons in the same system (cube) are allowed to have the same quantum numbers. No two electrons in the same state of motion \( \uparrow \) \( \downarrow \).

At \( T = 0 \) K, all states up to \( E_f \) are occupied by an electron each. No states above \( E_f \) are occupied.

\[ (C_v)_{\text{elect}} = \frac{3}{2} \theta \]

Exclusion principle causes \( C \) to be lower than usual.
NEW TEST

SAND THEORY

TREAT ALL ELECTRONS ALIKE

1) VIBRATING SIMPLE HARMONIC APPROXIMATION

\[ \frac{\partial^2}{\partial t^2} \psi + \frac{m}{2} \nabla^2 \psi = 0; \quad \psi = 0 \quad (E = \frac{p^2}{2m}) \]

2) NEARLY FREE ELECTRON APPROXIMATION

ELECTRONS IN A PERIODICALLY CHANGING POTENTIAL

1) TUNNELING

2) NEARLY FREE ELECTRON

PERFECTLY FREE ELECTRON

\[ \frac{\partial^2}{\partial t^2} \psi + \frac{m}{2} \nabla^2 \psi = 0; \quad \psi = 0 \quad (E = \frac{p^2}{2m}) \]

\[ k = \frac{p}{\hbar}; \quad \psi = \frac{e^{-kx}}{\sqrt{2\pi}} \]

IN ONE DIMENSION:

\[ \frac{\partial^2}{\partial x^2} \psi = k^2 \psi \]

\[ \Rightarrow \psi = c e^{\pm ikx} \]

\[ E = \frac{p^2}{2m} \]

\[ k = \frac{p}{\hbar} \] FOR MOTION TO THE RIGHT

\[ k < 0 \] FOR MOTION TO THE LEFT
\[ u(x+\alpha) = u(x) \]
\[ \nabla^2 \psi + \frac{2m}{\hbar^2} (E - U) \psi = 0 \]

**For the x direction**
\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} [E - U(x)] \psi = 0 \]
\[ \psi = u_k(x) e^{ikx} \] (Bloch functions)
\[ u_k(x+\alpha) = u_k(x) \]

**Modulation function**

\[ R_\alpha(\psi) \]

** Kronig-Penney model**

\[ U(x) = \begin{cases} 
0 & \text{for } 0 < x < a \\
2U_0 & \text{for } a < x < 0 \\
-2U_0 & \text{for } 0 < x < -a \\
0 & \text{for } -a < x < 0 
\end{cases} \]

\[ \psi = u_k(x) e^{ikx} \]

\[ \begin{align*}
U_1 &= A e^{i(k-a)x} + B e^{-(k-a)x} \\
U_2 &= C e^{i(k+b)x} + D e^{-(k+b)x} \\
U_0 &= U_2(-b) \quad \Rightarrow \quad x = 0 \\
U_0 &= U_2(b) \quad \Rightarrow \quad x = b 
\end{align*} \]

\[ \Rightarrow \frac{\beta^2}{\hbar^2} - E^2 = \omega \] with
\[ \beta h \sin \alpha + \frac{\omega}{\beta h} \cos \beta h \cos x = 0 \]

\[ \frac{a \hbar^2}{\hbar^2} = \frac{1}{\hbar^2} \] \( \alpha = \kappa \)

Let \( U_0 \to \infty; \beta \to 0 \)
ELECTRON IN A PERIODIC POTENTIAL
KRONIG-PENNY MODEL

\[ U(x) \]

SCHRÖDINGER EQUATION GIVES

\[ \psi_n(x) = \sqrt{\frac{2m}{\hbar^2}} \sin k a + \text{const} \left( \cos k (a + b) \right) \]

\[ \beta = \sqrt{\frac{2m}{\hbar^2} (a' - c)} \]

\[ \alpha = \sqrt{\frac{2m}{\hbar^2} \frac{e^2}{4\pi \epsilon_0}} \]

\[ \frac{\mu_0 b}{2} \sin^2 \frac{\alpha x}{a} = \cos^2 \frac{\alpha x}{a} \]

\[ \beta^2 = \mu_0 b / \hbar^2 \]

\[ P = \frac{\mu_0 b}{\hbar} \]

\[ \Rightarrow \frac{\mu_0 b}{\hbar} \sin^2 \frac{\alpha x}{a} + \cos^2 \frac{\alpha x}{a} \]

\[ \Rightarrow \text{lim} \frac{\sin^2 \frac{\alpha x}{a} + \cos^2 \frac{\alpha x}{a}}{a} \]

\[ \Rightarrow \text{lim} \frac{1}{a} \]

BUT RIGHT SIDE HAS LIMITS OF [-1, +1]
\[ \Rightarrow \text{CERTAIN VALUES OF } \alpha \text{ ONLY} \]

AS \[ \alpha \] INCREASES, GAP LENGTHS INCREASES
(FORBIDDEN GAPS DECREASE)
FREE ELECTRON

\[ E(k) = E(-k) \]

PARABOLIC

IN A PERIODIC POTENTIAL

\[ \frac{\pi}{q} \leq k \leq \frac{2\pi}{q} \]

\[ \omega = \frac{2\pi}{q} \]

FIRST ORDER BRAGG'S LAW

FIRST BRILLOUIN ZONE

SECOND "

\[ \not p \neq \not k \text{ ANYMORE} \]

\[ \not k = \text{CRYSTAL MOMENTUM (ENERGY OF FREE $e^-$)} \]

\[ \not k \text{ IS CONSERVED} \]

NUMBER OF STATES PER BAND

\[ N = 0, 1, 2, \ldots, q \]

\[ \psi(x) = \psi(x + L) \]

PERIODIC BOUNDARY CONDITIONS

NOW \[ \mu_k(x) = \mu_k(x + q) = \mu_k(x + Nq) \]

\[ \Rightarrow \psi_{\pm q}\psi_{Nq} = 1 \Rightarrow \psi_{Nq} = 2\pi \eta \quad \eta = \pm 1, \pm 2, \ldots, \pm \frac{N}{2} \]
N states per band
\( (x^2\text{ considering } \uparrow \text{ spin}) \)

Density of states:
\[ 1 \text{ state per } \Delta K = \frac{2\pi}{N} \quad \text{at } x = 0 \]
\[ \frac{N/2}{\pi/2} = \frac{1}{2\pi/N} \]
States per unit \( K \):
\[ \frac{\Delta K}{\pi/2} = \frac{N}{2\pi} \]

Go to Eq. (13) - E = 3.72 eV
5-5-72 (FRI)

\[ q = \frac{e}{m}; \quad q = \frac{e^2}{m^*} = \frac{1}{m^*} \text{ effective mass} \]
For \( E_1 \): \[ q = \frac{e^2}{m^*} \quad m^* = \frac{e^2}{\frac{1}{2}k^2} \]

Nearly full conduction band

\( \downarrow \) not occupied (hole)

Apply E field, acc to left

Empty state

Yields net electron
I) Quantum Mechanics Review (Double-Slit Experiment)

A) Dual Properties of Light:
- Matter (Photon)
  - Wave (Electromagnetic)
  
  \[ E = \hbar f \quad \text{(Energy is proportional to frequency)} \]
  \[ \mathbf{p} = \hbar \frac{\mathbf{k}}{\lambda} \quad \text{(Momentum inversely proportional to wavelength)} \]
  \[ \mathbf{p} = \hbar \mathbf{k} \quad \mathbf{k} = \frac{2\pi}{\lambda} \mathbf{e} \quad \text{is in direction of the wave front motion;} \quad f = \frac{1}{2\pi} \]

B) Wave Properties of Electrons:

\[ \text{From this experiment, one may determine:} \]

\[ \mathbf{p} = \hbar \frac{\mathbf{k}}{\lambda} \]

\[ E = \frac{p^2}{2m} + V \quad \text{V = potential energy} \]

Duality Nature of Waves and Particles:
- Light: \[ E = \hbar f \quad \mathbf{p} = \hbar \frac{\mathbf{k}}{\lambda} \]
- Matter: \[ E = \frac{p^2}{2m} \quad \mathbf{p} = \hbar \mathbf{k} \]

C) Heisenberg's Uncertainty Principle: One cannot simultaneously determine a position co-ordinate and the corresponding momentum co-ordinate to any greater precision than:

\[ \Delta x \Delta p \geq \hbar \]

The probability of finding a particle in the volume \( dV \) at position \( x, y, z \):

\[ P = \int |\psi|^2 dV \quad \psi \text{ is the wave function, valued at all points in space, may be real or complex} \]

D) Schrödinger's Equation (conservation of \( E \))

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = E \psi \quad \text{(Time independent)} \]

Example: The Vibrating Atom

\[ V = \frac{1}{2} k \mathbf{x}^2 \]

\[ \Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + \frac{1}{2} k \mathbf{x}^2 \psi = E \psi \]

Solution yields: \( E_n = \frac{n^2 \hbar f}{2} \)

Note: No solution for \( E = 0 \) \( \Rightarrow \) Atom is never at rest!
(Example 2) One electron atom: \[ V = \frac{1}{4 \pi \varepsilon_0} \frac{q^2}{r} \]

E\(n\) = \(-\frac{e^2}{\varepsilon_0} \frac{1}{n^2} \) \(n = 1, 2, 3, 4, 5, \ldots\) (Principle Quantum Number)

E) Quantum Numbers

1) Atom

\( L = \vec{P} \times \vec{\ell} \) (Angular Momentum)

Both paths have the same \( E \), but different \( \ell \)

\[ |\ell| = \left( L (L+1) \right)^{1/2} \hbar \]

\( L = n-1, n-2, \ldots, 0 \) (Same \( n \))

\( \ell \): Principle Quantum Numbers

\( \ell \): Azimuthal Quantum Numbers

2) Electron Spin Angular Momentum \( \frac{\hbar}{2} \)

\[ |S| = \sqrt{\frac{1}{4}} \hbar \]

3) In magnetic field, only certain directions are allowed for \( \ell \) and \( S \)

\( S_\ell = m_S \hbar \) \( m = 2, 1, 0, -1, -2 \)

(Sweeps a cone)

\( S_z = m_S \hbar \) \( m_S = \pm \frac{\sqrt{2}}{2} \)

\( S = \sqrt{S(S+1)} \hbar \)

4) Pauli-Exclusion Principle (Applies to Odd Half Integral Spin Particles): No Two Electrons in the Same Quantum-Mechanical System May Have Identical Sets of Quantum Numbers \((n, \ell, m, m_S)\)

\( n = 1 \)

\( n = 2 \)

\( n = 3 \)

\( \ell = m \hbar \) \( m = 2, 1, 0, -1, -2 \)

\( \ell = (0, 1, 2, 3) \) \( \hbar \)

\( m = (0, 1, 2, 3, 4) \) \( \hbar \)

\( m_S = \pm \frac{\sqrt{2}}{2} \)

\( \sqrt{1} = \sqrt{\frac{1}{2}} \hbar \)

Energy

\( L \): Orbital Angular Momentum

\( m \): Direction of \( L \)

\( m_S \): \( z \) Component of \( S \)

\( S = \pm \frac{1}{2} \)
II. SOLIDS AND FORCES 'TWIXT ATOMS IN 'EM
A) CLASSIFICATIONS OF SOLIDS
   1) AMORPHOUS SOLIDS: RANDOM ATOMIC ARRANGEMENT (VERY HAIRY TO ANALYZE)
   2) CRYSTALLINE SOLIDS: REGULAR ATOM ARRANGEMENT (THOSE, WE STUDY)
B) FORCES 'TWIXT ATOMS
   1) IONIC FORCES (SUCH AS Na⁺Cl⁻)
   2) COULOMB ATTRACTION OF IONS
   3) SUPER STRONG FORCE
      a) HIGH MELTING POINT
      b) LOW ELECTRICAL- THERMAL CONDUCTION
   4) COVALENT FORCE (SHARED ELECTRONS) (SUCH AS C₁₂)
      (C₁₂ SHARES 2 3P ELECTRONS)
      \[ \frac{1}{2} \text{ prob. of finding } e^- 'T WIXT ATOMS \]
      A FAIRLY STRONG FORCE
   5) METALLIC BOND-SHARED ELECTRONS 'TWIXT ALL ATOMS OF THE MATERIAL
C) VAN DER WAALS FORCE (MOLECULAR CRYSTALS)
   A VERY WEAK DIPOLE ATTRACTION FORCE
   THESE MATERIALS ARE SOLID ONLY AT TEMPERATURES NEAR 0⁰K
D) REPULSIVE FORCES (DUE TO EXCLUSION PRINCIPLE)
   \[ F_{\text{repulse}} \]
   \[ F_{\text{attract}} \]
   \[ r \to r_e \]

III. LATTICES AND CRYSTAL STRUCTURE
A) LATTICE POINT TO GET FROM ONE LATTICE POINT TO ANOTHER:
   \[ \bar{r} = m_1 \bar{a} + m_2 \bar{b} + m_3 \bar{c} \]
   \[ \exists m, m_2, m_3 \text{ are integers} \]
   VOLUME OF "UNIT CELL" = \( \bar{a} \times \bar{b} \times \bar{c} \) (PRIMITIVE UNIT CELL)
   OPTS. ONLY @ CORNERS
   SPACE LATTICE: REGULAR REPEATING ARRANGEMENT OF POINTS SUCH THAT THE ARRANGEMENT OF ATOMS ABOUT EACH POINT IS IDENTICAL
   PRIMITIVE UNIT CELL = UNIT CELL HAVING SMALLEST POSSIBLE VOLUME
   SINGLE CRYSTAL-LATTICE CONTINUES FROM ONE EDGE OF THE CRYSTAL TO THE OTHER WITH NO BREAKS
   POLYCRYSTALINE-BREAKS IN THE LATTICE
**SPACE LATTICE SYMMETRY**

1. **MIRROR PLANE**
2. **ROTATIONAL SYMMETRY (n-fold)**
   - Number of equal angles of rotation to get back to original configuration (each rotation must yield original configuration)
   - Example: Cubic crystals: 4-fold, 3-fold rotation axes

**B) MILLER INDICES (CRYSTAL CONFIGURATION)**

1. Find the plane intercepts with \( a \), \( b \), and \( c \) as integral multiples and reciprocate
2. Clear fractions, result: \((h, k, l)\)
   - Example: \((\infty, 1, \infty) \rightarrow (0, 1, 0)\)
   \((1, \infty, \infty) \rightarrow (1, 0, 0)\)
   \((\infty, 0, 1) \rightarrow (0, 0, 1)\)
   \((1, 1, \infty) \rightarrow (1, 1, 0)\)
   \((1, 1, 1) \rightarrow (1, 1, 1)\)

The plane will intersect the plane \(\frac{a}{h}, \frac{b}{k},\) and \(\frac{c}{l}\)

**SPACING BETWEEN PLANS CONTAINING LATTICE POINTS (EXAMPLES)**

\((1, 0, 0) ; d = a\)
\((1, 1, 0) ; d = a/\sqrt{2}\)
\((1, 1, 1) ; d = a/\sqrt{3}\)

Generally: \(d = a \left( h^2 + k^2 + l^2 \right)^{-1/2}\)

**C) X-RAY DETERMINATION (BY DIFFRACTION)**

**OF UNIT CELLS**

**X-RAY TUBE**

**BRAGG'S LAW FOR CONSTRUCTIVE INTERFERENCE:**

\(2d \sin \theta = n \lambda ; \) Constr. Inter.

**FOR PRIMITIVE CUBIC**

**INTENSITY**

\((100) \quad (110) \quad (111) \quad (100) \quad (210)\)

\(n = 1 \quad n = 1 \quad n = 1 \quad n = 2 \quad n = 2\)

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

\(\Rightarrow \sin \theta = \frac{n \lambda \sqrt{h^2 + k^2 + l^2}}{2d}\)

\(\Rightarrow \text{LATTICE CONSTANT: } a = \frac{n \lambda \sqrt{h^2 + k^2 + l^2}}{2 \sin \theta}\)
FOR BODY CENTERED CUBICS:

\[
\begin{align*}
\text{Intensity} & \quad \text{(knocks out every other peak)} \\
(110) & \quad (111) \\
\end{align*}
\]

\begin{align*}
\text{n.(hkl)} & \quad \text{Cubic primitive} & \quad \text{Cubic body center} & \quad \text{Cubic face center} \\
100 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
110 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
111 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
200 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
210 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
211 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
220 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
221 & \quad \checkmark & \quad \checkmark & \quad \checkmark \\
\end{align*}

Determination of crystal given \( \lambda \) and \( 2\theta \):

1) Assume first peak is (100)... compute \( q \) and see if the other peaks fit with \( q \) and some \( hkl \)

2) Assume BCC ⇒ first peak \( \in (110) \) ⇒ ...

3) Assume FCC ⇒ first peak \( \in (111) \) ⇒ ...

IV) IONIC CRYSTALS

\( \text{Na}^+ \text{Cl}^- \Rightarrow \text{cube of volume } R^3 \text{ contains } \frac{1}{2} \text{Na} \text{ and } \frac{1}{2} \text{Cl} \)

For \( N \) ion pairs: \( V = 2NR^3 \)

For other crystals:

\( V = CNR^3 \)

For 2 ions:

\( E = E_a \text{(attraction or Coulomb)} + E_r \text{(repulsion or exclusion)} \)

\[
E_a = \frac{q_1 q_2}{4\pi \varepsilon_0 R^2}
\]

Ion #1 (sodium in center)

\[
E_{a1} = \frac{1}{4\pi \varepsilon_0} \left( \frac{9.92}{12} + \frac{9.92}{8} + \frac{9.93}{8} + \frac{9.94}{14} + \ldots \right)
\]

\[
E_{r1} = \frac{\sigma^2}{4\pi \varepsilon_0 R} \left( \frac{1}{12} + \frac{1}{8} + \frac{1}{8} + \ldots \right)
\]

Including only the part of the atom inside the cube (Ehren method of cutting off the series):

\[
E_{c1} = \frac{\sigma^2}{4\pi \varepsilon_0} \left( \frac{3}{7} + \frac{3}{12} + \frac{1}{7} + \ldots \right)
\]

\[
= \alpha \sigma^2 / 4\pi \varepsilon_0 R
\]

\( \alpha = \text{modeling constant} (= 1.747 \text{ for NaCl}) \)
TOTAL P.E.:

\[ E_T = N \left[ -\frac{\alpha e^2}{4\pi\varepsilon_0 R} + \frac{A}{R^a} \right] \]

\[ \frac{\delta E}{\delta R} \bigg|_{R = R_e} = 0 \quad \Rightarrow \quad T = 0^\circ \text{K} \]

\[ \Rightarrow E_{T_e} = \frac{-N \alpha e^2}{4\pi\varepsilon_0 R_e} \left[ 1 - \frac{1}{n} \right] \]

\( n \) IS RELATED TO COMPRESSIBILITY (K)

\[ \frac{dW}{dV} = -p dV = dE \Rightarrow \frac{dE}{dV} = \frac{dE}{dV^2} \]

\[ K = -\frac{1}{V} \frac{dV}{dP} \Rightarrow K = -V \frac{dP}{dV} = V \frac{dE}{dV^2} \]

\[ \frac{d^2E}{d^2R} = \frac{dE}{dR} \frac{d^2R}{dV} + \frac{dR}{dV} \frac{dE}{dV} \frac{d^2R}{dV^2} = \frac{dE}{dR} \frac{d^2R}{dV^2} + \frac{d^2E}{dV^2} \left( \frac{dR}{dV} \right)^2 \]

\[ \Rightarrow \frac{1}{K_0} = V \frac{d^2E}{dR^2} \left[ \frac{dR}{dV} \right]^2 \]

VOLUME OF CRYSTAL: \( V = 4\pi CNR^3 \)

\[ \Rightarrow \frac{dV}{dR} = 3CNR^2 \]

\[ \Rightarrow \frac{1}{K_0} = CNR e^3 \frac{d^2E}{dR^2} \left[ \frac{1}{q c^2 N^2 R_e^4} \right] \]

\[ = \frac{1}{9CNR e} \left( \frac{d^2E}{dR^2} \right) \bigg|_{R = R_e} \]

\[ \Rightarrow \frac{d^2E}{dR^2} \bigg|_{R = R_e} = \frac{N \alpha e^2}{4\pi\varepsilon_0} \left[ \frac{n-1}{R_e^3} \right] \]

\[ \Rightarrow \frac{1}{K_0} = 9CNR e \left[ \frac{N \alpha e^2}{4\pi\varepsilon_0} \left( \frac{n-1}{R_e^3} \right) \right] \]

\[ = \alpha \varepsilon e^2 (n-1) / 36 \pi C \varepsilon_0 R_e^4 \]

SOLVE FOR \( n \).
Vibrations

1. Monotonic

\[ M_{n+1} = \beta (\mu_{n+1} - \mu_n) - \beta (\mu_n - \mu_{n-1}) \]
\[ M_{n+1} = \beta (\mu_{n+1} + \mu_{n-1} - 2\mu_n) \rightarrow \text{Wave equation} \]
\[ \omega^2 = \frac{4\beta}{M} \sin^2 \frac{kq}{2} \]
\[ \omega = \sqrt{\frac{4\beta}{M}} \sin \frac{kq}{2} \]

\[ V_p = \text{Phase speed} = \frac{f}{\lambda} = \frac{\omega}{k} \]
\[ V_g = \text{Group velocity} = \frac{6\omega}{6k} \]

2. Diatomic

\[ \rho_2n = \beta (\mu_{2n} + \mu_{2n+2} - 2\mu_{2n}) \]
\[ \rho_{2n+1} = \beta (\mu_{2n+1} + \mu_{2n+3} - 2\mu_{2n+1}) \]
\[ \text{Then } \omega^2 = \frac{4\beta}{M} \sin^2 \frac{kq}{2} \frac{1}{(\lambda + \lambda)^2} \]

Optical band

Acoustic band

Absorption resonance

\[ \omega = 2\pi f \]
Monatomic Lattice: Longitudinal Vibrations

\[ \delta \delta \delta \delta \delta \delta \ldots \delta \cdot \delta \ldots \delta \]

o and n are fixed

\[ \Rightarrow \sin kl = \sin kN_0 = 0 \Rightarrow kl = kN_0 \]

Standing Wave Equation:

\[ \mu = Re \left[ \mu e^{i\omega t} \sin kx \right] \]

\[ \therefore k = \frac{2\pi}{L}, \frac{4\pi}{L}, \frac{6\pi}{L}, \ldots, \frac{(2n-1)\pi}{L} \]

@ \[ k = \frac{2\pi}{L}, \mu = 0 \]

\[ \therefore \text{Discrete } k \& \omega \]

Test 1
V) SPECIFIC HT. ON INSULATORS

A) CLASSICAL STATISTICAL MECHANICS

1) PHASE SPACE: $dS = dx dy dp_x dp_y dp_z$

2) EQUILIBRIUM DISTRIBUTION = MOST PROBABLE DISTRIBUTION OF POINTS AMONG CELLS

EXAMPLE: 2 BOXES, 4 PARTICLES

a) ALL IN CELL A $\rightarrow$ 1 WAY
b) 3 IN A, 1 IN B $\rightarrow$ 4 WAYS
c) 2 IN A, 2 IN B $\rightarrow$ 6 WAYS

$P = \frac{N!}{N_1!N_2!} \frac{N_1^2 N_2^2}{N^2}$ $N_1 + N_2 = N$ AND $N_1 \leq N_2$

3) MAXWELL BOLTZMANN DISTRIBUTION:

$$dN \propto e^{-\frac{E}{kT}} d\Omega$$

FRACTION OF PARTICLES @ $P(\mathbf{p}_x, \mathbf{p}_y, \mathbf{p}_z)$ AND POSITION $x, y, z$ IN PHASE SPACE $d\Omega$

$$\frac{dN}{N} = e^{-\frac{E}{kT}} d\Omega / \int e^{-\frac{E}{kT}} d\Omega$$

$$E = \frac{\int e^{-\frac{E}{kT}} d\Omega}{\int e^{-\frac{E}{kT}} d\Omega} = 3kT$$

TOTAL E ON N VIBRATING ATOMS: $U = 3NkT$ FOR 3 GRAM MOLES:

$$U = 3N_0kT = 3RT$$

$N_0 = \text{AVOGADRO'S NUMBER}$

$R = \text{IDEAL GAS CONSTANT}$

4) SPECIFIC HT/PER MOLE = $C_V = \left. \frac{\partial U}{\partial T} \right|_V = \left. \frac{6U}{8T} \right|_V = 3R = 5.96 \text{ CALORIES/K MOLE}$

$C_V = \frac{\text{CLASSICAL}}{\text{EXPERIMENTAL}}$

FROM QUANTUM MECHANIC OSCILLATORS

$E = \frac{n + \frac{1}{2}}{\hbar} \hbar + \hdots \hbar; n = 0, 1, 2, \ldots$

B) EINSTEIN MODEL OF THE ATOM

1) ASSUMPTIONS

a) ALL ATOMS VIBRATE WITH SINGLE FREQUENCY $\omega$

b) EACH OSCILLATOR IS 3 LINEAR HARMONIC OSCILLATORS (MUTUALLY ___ VIBRATIONS)

c) N ATOMS $\rightarrow$ 3N LINEAR OSCILLATORS

d) BOLTZMANN DISTRIBUTION: $N_0 \propto e^{\frac{E}{kT}}$

WITH $U = 3N \propto E = \text{AVERAGE ENERGY}$
2) DERIVATION

\[ N_\lambda = e^{-E_\lambda/kT} \]

\[ E = \sum_{n=0}^{\infty} e^{-hf/kT} \]

\[ E = e^{-hf/kT} + \frac{1}{e^{-hf/kT}} \]

\[ E = \frac{1}{e^{-hf/kT}} + \frac{\sum_{n=0}^{\infty} nfh \exp\left(-\frac{nhf}{kT}\right)}{\sum_{n=0}^{\infty} e^{-nhf/kT}} \]

\[ = \frac{1}{2}h \sum_{n=0}^{\infty} e^{-nhf/kT} + \frac{\sum_{n=0}^{\infty} nfh \exp\left(-\frac{nhf}{kT}\right)}{\sum_{n=0}^{\infty} e^{-nhf/kT}} \]

\[ = \frac{1}{2}h + \frac{hfe^{-hf/kT} + 2hfe^{-2hf/kT} + 3hfe^{-3hf/kT} + \ldots}{1 + e^{-hf/kT} + e^{-2hf/kT} + \ldots} \]

\[ \Rightarrow E = \frac{1}{2}h + h f \left[ \frac{e^x + 2e^{2x} + 3e^{3x} + \ldots}{1 + e^x + e^{2x} + \ldots} \right] \]

\[ \Rightarrow U = 1 + e^x + e^{2x} + \ldots \Rightarrow \frac{dU}{dx} = 1 - e^x \]

\[ \text{NUMERATOR} \]

\[ \text{DENOMINATOR} \]

\[ \frac{dx}{1 - e^x} = \left(\frac{e^x}{1 - e^x}\right) \]

\[ \text{THUS:} \quad E = \frac{1}{2}h + h f \left(\frac{1 - e^x}{1 - e^x}\right) \]

\[ = \frac{1}{2}h + h f \left[ \frac{e^x}{1 - e^x} \right] = \frac{1}{2}h + h f \left[ \frac{e^x - 1}{e^{hf/kT} - 1} \right] \]

\[ \text{TOTAL ENERGY} \]

\[ U = 3N\overline{E} = \frac{3}{2}Nh + 3Nh f \left[ \frac{1}{e^{hf/kT} - 1} \right] \]

\[ C_V = \frac{\delta U}{\delta T} = 3Nh f \frac{A}{A} \left( \frac{e^{hf/kT} - 1}{e^{hf/kT} - 1} \right) \]

\[ = 3N \left[ \left( \frac{h f}{kT} \right)^2 \frac{e^{hf/kT}}{(e^{hf/kT} - 1)^2} \right] \]

\[ C_V = 3R \left[ \left( \frac{h f}{kT} \right)^2 \frac{e^{hf/kT}}{(e^{hf/kT} - 1)^2} \right] \]

@ \( T = \infty \), \( e^{hf/kT} = 1 \); \( \Rightarrow C_V = 3R \)

@ \( T = 0 \), \( C_V = 0 \)

\[ C_V \]

\[ 3R \]

\[ \text{EXPERIMENT} \]

\[ \text{EINSTEIN MODEL (LITTLE LOW)} \]
c) Debye Model

1) Assumptions
(a) 3N Linear Harmonic Oscillators
(b) Maxwell Distribution
(c) Frequency Assumptions
(i) Standing Waves of Continuous Medium
(ii) All Waves Travel at the Same Speed (Non-Dispersive Media)

\[ L = n \lambda/2 \quad \forall n = 1, 2, 3, \ldots \]
\[ f = \nu/\lambda \]

2) Derivation

Wave Equation: \[ \nabla^2 U = \frac{1}{\sqrt{\varepsilon}} \left( \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right) \]

\[ \Rightarrow \mu = \mu_0 \sin \left( \frac{n_x \pi x}{L} \right) \sin \left( \frac{n_y \pi y}{L} \right) \sin \left( \frac{n_z \pi z}{L} \right) \cos \left( 2\pi f t \right) \]
\[ \forall n_x, n_y, n_z = 1, 2, 3, 4, \ldots \]

Plugging back into the wave equation:

\[ -\left( \frac{n_x \pi}{L} \right)^2 \mu - \left( \frac{n_y \pi}{L} \right)^2 \mu - \left( \frac{n_z \pi}{L} \right)^2 \mu = \frac{1}{\sqrt{\varepsilon}} (2\pi f)^2 \mu \]

\[ \Rightarrow f = \text{Standing Wave Frequencies} \]
\[ = \frac{\nu}{2} \sqrt{n_x^2 + n_y^2 + n_z^2} = \frac{\nu}{2} R \]

Forms cubic "lattice" each point representing a standing wave node

\[ \Rightarrow R = \frac{2 \lambda f}{\nu} \text{ and } dR = \frac{2 \lambda}{\nu} df \]

Take a sphere shell

\[ dN = \frac{1}{3} (4\pi R^2) \, dR \]
\[ = \frac{4}{3} R^3 \, dR \]
\[ = \frac{4}{3} \left( \frac{4\pi R^2}{\nu^2} \right) (2\lambda df) \]
\[ = \frac{4\pi \lambda^2}{\nu^2} f^2 df \]
\[ = \frac{4\pi \lambda^2}{\nu^3} f^2 df \Rightarrow \boxed{V = \frac{\lambda^3}{3} = \text{Cube's Volume}} \]
3 VIBRATIONS
TWO TRANSVERSE, WITH VELOCITY $V_T$
ONE LONGITUDINAL, WITH VELOCITY $V_L$

$\Rightarrow dN = 4\pi \frac{x}{(\frac{2}{V_T} + \frac{1}{V_L})} f^2 df$

Now, $3N = \int f_0^d dN \Rightarrow f_0 = \text{CUT OFF FREQUENCY}$

$= 4\pi \frac{x}{(\frac{2}{V_T} + \frac{1}{V_L})} \int_0^{f_0} f^2 df$

$\Rightarrow f_0 = \left[ \frac{gN}{4\pi \frac{x}{(\frac{2}{V_T} + \frac{1}{V_L})}} \right]^\frac{1}{2}$

IF EACH OSCILLATOR HAS THE AVERAGE ENERGY OF EINSTEIN'S OSCILLATORS:

$E = hf / (e^{hf/kT} - 1)$

THEN TOTAL ENERGY

$U = \int f_0^d f_0 E dN$

$= \int_0^{f_0} \frac{hf}{e^{hf/kT} - 1} dN$

$= 4\pi \frac{x}{(\frac{2}{V_T} + \frac{1}{V_L})} \int_0^{f_0} \frac{hf^3}{e^{hf/kT} - 1} df$

SUBSTITUTING $\left(\frac{2}{V_L} + \frac{1}{V_T}\right)$ FROM EXPRESSION FOR $f_0$,

LETTING $x = hf/kT$ AND $x_0 = hf_0/kT$

$\Rightarrow N (\frac{hf_0}{hf})^3 KT \int_0^{x_0} \frac{x^3 dx}{e^x - 1} = U$

1 FOR HI $T$

$U = N (\frac{hf_0}{hf})^3 \int_0^{x_0} \frac{x^3 dx}{(x+1)-x}$

$\Rightarrow C_v = \frac{5U}{5T} \mid_v = 3R$

2 FOR LOW $T$ ($\Rightarrow$ HI $x_0 \approx \infty$)

$U = 5N (\frac{hf_0}{hf})^3 KT \int_0^{x_0} \frac{x^3 dx}{e^x - 1}$, But $\int_0^{x_0} \frac{x^3 dx}{e^x - 1} = \pi^4/15$

$\Rightarrow U = \frac{2}{5} \pi^4 N KT (\frac{f_0}{h})^3 \Rightarrow \Theta_0 = hf_0/k = \text{DEBYE TEMP}$

$\Rightarrow C_v = \frac{5U}{5T} \mid_v = \frac{R}{5} \pi^4 R (\frac{f_0}{h})^3$

A GOOD FIT OF EXPERIMENTAL RESULTS. $\Theta_0$ CHOSEN TO FIT CURVE, AND DEPENDS ON THE SUBSTANCE.
VI) DIELECTRICS
A) DEFINITIONS OF $\vec{P}$, $\vec{P}$, $\vec{D}$, $K$, $\alpha$

1) $\vec{P}$ = DIPOLAR MOMENT
   $$\vec{P} = \frac{q\vec{e}}{V}$$

2) $\vec{P}$ = POLARIZATION: $\vec{P} = \frac{\xi}{V}$ = DIPOLAR MOMENT
   UNIT VOLUME

3) $\vec{D}$ = DISPLACEMENT: $\vec{D} = \varepsilon_0\vec{E} + \vec{P}$
   ⇒ DIELECTRIC DECREASES $\varepsilon$ IF CHARGE ON
   THE PLATES IS THE SAME

4) $K$ = DIELECTRIC CONSTANT
   $$\varepsilon_k = \varepsilon_0 + \frac{P}{\varepsilon_0 E}$$

B) TYPES OF POLARIZATION

1) ELECTRONIC POLARIZATION
   SHIFT $e^-$ ORBITS RELATIVE TO
   NUCLEUS

2) IONIC POLARIZATION
   $\text{Na}^+ \text{O}^-$

3) ORIENTATIONAL POLARIZATION
   WATER: $\text{H}_2\text{O}^-$
   REORIENTATION OF PERMANENT
   DIPOLE DUE TO $\vec{E}$

C) LOCAL FIELDS DUE TO DIOPILES AND OTHER
   CHARGES AT THE ATOMIC POSITION

1) IN INSULATORS: $C_V = \left(\frac{8\pi}{5}\right)\varepsilon_{\text{Vir}}$

2) IN METALS: $C_V = \left(\frac{8\pi}{5}\varepsilon_{\text{Vir}} + \frac{8\pi}{5}\varepsilon_{\text{Elec}}\right)$
   $\Rightarrow C_V = C_{V_{\text{Vir}}} + C_{V_{\text{Elec}}}$

$P = \mu\chi \Rightarrow \chi = \frac{4\pi}{P}$; $P$: PHONON VIBRATION

IN DIELECTRIC

$$E_{\text{loc}} = \text{LOCAL FIELD AT POSITION OF ATOM}$$
DUE TO OTHER CHARGES

$E_1 = \text{E FIELD AT PT. DUE TO PLATES}$

$E_2 = \text{E FIELD AT PT. DUE TO OUTSIDE}$
PLATE POLARIZATION CHARGE $\Rightarrow E = E_1 + E_2$

$E_3 = \text{E FIELD DUE TO CHARGE ON CAVITY SURFACE}$

$E_4 = \text{E FIELD INSIDE THE CAVITIES}$
DUE TO INDIVIDUAL DIPOLES

$$E_{\text{loc}} = E_1 + E_2 + E_3 + E_4$$

$E = E_3 + E_4$
2) $E_3$: Due to cavity surface

Area = $R \, d\theta \, 2\pi R \cos \theta \sin \theta$

$\Rightarrow d\sigma = \cos \theta \, d\theta \cos \theta \, d\theta$

$\Rightarrow \sigma \, d\theta = \int_0^\pi \cos \theta \, d\theta \cos \theta \, d\theta$

$E_3 = \frac{-P}{2\varepsilon_0} \int_0^\pi \cos \theta \, d\theta \cos \theta \, d\theta$

$\Rightarrow E_3 = \frac{-P}{2\varepsilon_0} \frac{1}{3} \sqrt{\frac{3}{2}} \pi = \frac{P}{3\varepsilon_0}$

$\Rightarrow E_{10c} = E + \frac{P}{3\varepsilon_0} + E_4$

For a cubic lattice; $E_4 = 0$

For other lattice; $E_4 = \gamma \cdot P$

D) Atom in $\vec{E}$ field (Clausius-Mossotti)

Atomic polarizability; $\alpha_i = \frac{P}{\varepsilon_0 E_{10c}}$ P = dipole moment

For cubic lattice of identical atoms

$E_{10c} = E + \frac{P}{3\varepsilon_0}$

$\Rightarrow \frac{E_{10c}}{E} = \frac{(k+1)}{3} \Rightarrow k = 1 + \frac{P}{3\varepsilon_0} E$

$E_{10c} = E + \frac{(k-1)}{3} \varepsilon_0$

$\Rightarrow \frac{E_{10c}}{E} = \frac{(k-2)}{3} \Rightarrow k = 1 + \frac{P}{3\varepsilon_0} E_{10c}$

E) Ionic polarizability

Apply an $E$ field; sum shift of X ions relative to negative ions

Dipole moment: $\vec{P}_{10c} = \beta \vec{x} \Rightarrow \vec{x} = \frac{\vec{P}_{10c}}{\beta}$

$\vec{P}_{ionic} = N \vec{x} \vec{E}_{10c}$

$\Rightarrow \frac{k-1}{k+2} = \frac{P}{3\varepsilon_0 E_{10c}} = \frac{N \alpha_{10c} + N E_{10c} + N \beta^2 E_{10c}}{3\varepsilon_0 E_{10c}}$

$\Rightarrow \omega = \sqrt{\frac{P}{M}}$
F) ORIENTATIONAL POLARIZATION

ALIGNMENT OF PERMANENT DIPOLES WITH FIELD PRESENT TENDS TO LINE UP DIPOLES, WHILE INTERACTIONS 'TWIXT THE DIPOLES THEMSELVES TEND TO RANDOMIZE DIRECTION

\[ U = - \mathbf{P} \cdot \mathbf{E} = - P E \cos \theta \]
\[ U = \frac{1}{N} \int U dN \]
\[ = - \int P E \cos \theta e^{PE \cos \theta / KT} d\Omega \]
\[ = - \int P E \cos \theta / KT e^{PE \cos \theta / KT} d\Omega \]
\[ \Rightarrow E = - \frac{P E \cos \theta / KT}{d\Omega} \]

\[ d\Omega = \frac{dA}{R^2} \]

\[ d\Omega = \frac{1}{\pi} P E \cos \theta e^{PE \cos \theta / KT} 2 \pi \sin \theta d\theta \]

Now \[ dx = - \sin \theta d\theta \Rightarrow x = \cos \theta \]

\[ \Rightarrow \cos \theta = \frac{\int x e^a dx}{\int e^a dx} = \frac{e^a e^{-a}}{e^a - e^{-a}} = \frac{1}{2} \tanh \frac{a}{2} \]

\[ \tanh \frac{a}{2} \]

\[ \frac{\alpha}{\beta} \]

LANGEVIN FUNCTION

H1E, LOW T, OR BOTH

FOR NORMAL T & E, \( \alpha \ll 1 \), AND \( \cos \theta \approx \theta / 3 \)

THEN \[ P = NP \cos \theta \]

\[ N = \text{DIPOLES/VOLUME} \]

\[ = NP \frac{PE}{3KT} \]

NOW \[ K = 1 + P / \varepsilon_0 E = 1 + NP^2 / 3 \varepsilon_0 kT \]

IF OTHER POLARIZATION IS THERE

\[ K = K_0 + 1/T \] (CURIE LAW)

FOR H₂S

\[ K \]

\[ 20 \]

\[ 10 \]

STRUCTURE 2

STRUCTURE 1

LIQUID

104 K 185 K T(0K)
6) A-C Electric Fields in a Dielectric

\[ E = E_0 e^{i\omega t} \]

\[ \varepsilon E = m \frac{\partial^2 x}{\partial t^2} = q E_0 e^{i\omega t} - \beta x - \kappa \frac{dx}{dt} \]

- \( \beta \) = Restoring Coefficient
- \( \kappa \) = Fudge Factor
- \( m \frac{dx}{dt} \) = Radiation Loss

By magic:

\[ x = \frac{q E_0}{m} e^{i\omega t} \left[ \frac{\omega_0^2 - \omega^2 - i\kappa \omega}{(\omega_0^2 - \omega^2) + \kappa^2 \omega^2} \right] = \frac{q E_0}{m} e^{i\omega t} \left\{ \left[ \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2) + \kappa^2 \omega^2} \right] - i \left[ \frac{\kappa \omega}{(\omega_0^2 - \omega^2) + \kappa^2 \omega^2} \right] \right\} \]

Now \( P = qx \Rightarrow P = Nq x = \frac{Nq^2 E_0}{m} e^{i\omega t} \)

![Diagram showing E0, P_in (in phase with E), and P_out (out of phase with E).]

1) For a Slow Field \( (\omega << \omega_0) \)

\[ P_{in} = \frac{Nq^2 E_0}{m} e^{i\omega t} \left( \frac{1}{\omega^2} \right); (\kappa^2 \omega^2 \text{ is negligible}) \]

\( P_{out} = 0 \)

2) Near \( \omega = \omega_0 \)

\[ P_{in} = 0 \]

\[ P_{out} = \frac{Nq^2 E_0}{m + \kappa^2 \omega} e^{i\omega t} \]

Yielding:

\[ P_{in} \]

\[ P_{out} \]

![Diagram showing w, w0, w, and power input maximum at \( \omega = \omega_0 \).]

3) For \( \omega \gg \omega_0 \); \( P_{in} = \frac{Nq^2 E_0}{\omega} e^{i\omega t} \left( \frac{-\omega^2}{\omega^2 + \kappa^2 \omega^2} \right) \Rightarrow 0 \)

Similarly \( P_{out} \Rightarrow 0 \)

\[ \frac{d\varepsilon}{d\varepsilon} = FV; \]

Power Input Maximum \( \hat{\varepsilon} \) at \( \omega = \omega_0 \)

\[ K = 1 + \frac{\rho}{\varepsilon_0 E}; K' = 1 + \frac{P_{in}}{\varepsilon_0 E}; K'' = 1 + \frac{P_{out}}{\varepsilon_0 E} \]

- Orientational (Microwave)
- Ionic (Infrared)
- Electronic (Ultraviolet)
H) FERRO-ELECTRICITY
a) UNIT CELLS HAVE NO INVERSION CENTER OF SYMMETRY
b) ALTERNATING POSITIONS FOR SOME ATOMS IN UNIT CELL
c) DIPOLE IN ONE CELL IS STRONG ENOUGH TO PRODUCE DIPOLE IN NEXT, ETC. (CO-OPERATIVE PHENOMENON)
d) POLARIZATION WITH ALL DIPOLE MOMENTS IN A GIVEN REGION OF CRYSTAL (DOMAIN) ARE IN THE SAME DIRECTION

APPLYING E FIELD

\[ P(\text{FERRO ELECTRIC}) \]

\[ P_s \]

\[ E \]

REGIONS NOT WANTING TO LINE UP

REGIONS LINING UP WITH EACH OTHER

\[ P(\text{NORMAL}) \]

\[ K = 1 + \frac{dP}{\varepsilon_0 E} = 1 + \frac{1}{\varepsilon_0} \left. \frac{dP}{dE} \right|_{E=0} \]

\[ K = K_0 + \frac{C}{T - T_c} \]

\[ T_c = \text{CURIE TEMPERATURE} \]
III. ATOMIC DIAMAGNETISM AND ATOMIC FERROMAGNETISM

A) MAGNETIC PROCESSES

APPLICATION OF $\vec{H}$ TO A MATERIAL INDUCES A MAGNETIZATION $\vec{M}$

$$\vec{M} = \varepsilon \vec{p} m / V = \mu_0 \vec{H} + M = (\mu_0 + \chi) \vec{M}$$

WHERE $\chi = M / H =$ MAGNETIC SUSCEPTIBILITY

B) MAGNETIC MOMENTS

1) ORBITAL MAGNETIC MOMENT (FOR A CIRCLE)

$$\vec{p}_m = I \vec{A} \hat{n}$$

$$= \frac{2m}{2m} \sqrt{\pi \alpha^2} \hat{n} = \frac{2m}{2m} \left( -m \alpha \hat{n} \right)$$

$$= \frac{I}{2m} \hat{e}_x \hat{e}_z \rightarrow \vec{L} = \text{ORBITAL MAGNETIC MOMENT}$$

2) SPIN MAGNETIC MOMENT

$$\vec{p}_s = -\gamma \left( \begin{array}{c} \vec{E} \\ \vec{m} \end{array} \right) \gamma \vec{S} = \text{SPIN ANGULAR MOMENTUM}$$

$\gamma = \text{FUGGE FACTOR}$

C) DIAMAGNETISM DUE TO LARMOR PRECESSION OF ELECTRON ORBIT

\[ \text{Electron circle will change its tilt in time, much as would a top} \]

$$\gamma = \vec{p}_m \times \vec{B} = \frac{\vec{L}}{\varepsilon t}$$
2) *INDUCED ANGULAR MOMENTUM (DIAMAGNETIC EFFECT)*

- ALL IN ELECTRON'S ORBIT -

\[ L_{\text{ind}} = m \omega_L \rho^2 \]

\[ (P_m)_{\text{ind}} = \frac{\hbar}{2m} L_{\text{ind}} \]

\[ \Rightarrow \rho_{\text{ind}} = \left( \frac{\hbar}{2m} \right) m \omega_L \left( \frac{3}{2} \rho^2 \right) \]

Assume N atoms per unit volume

\[ M = N \rho_{\text{ind}} \]

\[ \chi = M / H = N \rho_{\text{ind}} / H \]

D) *ANGULAR MOMENTUM*

- \( l = (l+1) \frac{1}{2} \) \( \ell \) \( \ell \) ORBITAL ANGULAR MOMENTUM
- \( s = 1 \) \( s \) \( s \) SPIN ANGULAR MOMENTUM
- \( j = (j+1) \frac{1}{2} \) \( j \) \( j \) TOTAL ANGULAR MOMENTUM

E) *ENERGY LEVELS AND THE BOHR MAGNETRON*

- **T**otal **M**agnetic **M**oment:

\[ P_m = -\frac{\hbar}{2m} J \quad \exists \quad \ell, s, j = 1 + \frac{1}{2} j (j+1) \]

- **A**ppl**ication** of \( B \) **F**ield to **A**tom with **M**agnetic **M**oment

\[ J_2 = 2 \] component of \( J \)

\[ J_2 = m \quad \exists \quad m = j, j-1, j-2, \ldots, -j+1, -j \]

**Example:** Let \( J = 3/2 \)

\[ m = 3/2, 1/2, -1/2, -3/2 \]

Now \( U = -P_m \cdot B \) \( \exists \) \( U \) = **E**nergy

\[ (P_m)_{\text{ind}} = -\frac{\hbar}{2m} J \quad \Rightarrow \quad (P_m)_{\text{ind}} = -\frac{\hbar}{2m} m \hbar \]

\[ \therefore \quad U_1 = -P_m \cdot B = \frac{\hbar}{2m} \left( -\frac{3}{2} \right) \hbar B \]

\[ = -\frac{3}{2} \frac{\hbar}{2m} B \]

\[ \Rightarrow B = \left( \frac{\hbar}{2m} \right) \text{BOHR MAGNETRON} \]
F) Paramagnetism (Boltzmann Distribution)

1) \[ U = \frac{2ue^{-\frac{u}{kT}}}{2e^{-\frac{u}{kT}}} \]

\[ = e^{-\frac{u}{kT}} \sum m_0 g_0 B B e^{-m_0 g_0 B B / kT} / \sum m_0 g_0 B B e^{-m_0 g_0 B B / kT} \]

\[ \text{with cranked:} \]

\[ (P_m)_e = g_0 B J \left\{ \frac{(2j+1)}{2j} \coth \left( \frac{2j+1}{2j} \right) - \frac{1}{2j} \coth \left( \frac{1}{2j} \right) \right\} \]

\[ 3x = g_0 B B J / kT \]

\[ \text{for } N \text{ atoms per unit volume} \]

\[ \overline{M} = N (P_m)_e \]

\[ \text{for normal } T \text{ (not too low) and } B \text{ (not too high)} \]

\[ M = C' / T \quad C' = N g_0^2 B J (J+1) B / 2k \]

\[ \Rightarrow \chi = M / H = C' / T \quad \text{(Curie's Law)} \]

\[ \chi \quad \text{experiment} \]

2) The magnetic moments aid the applied field in paramagnetism. The largest number of particles will be where \( P_m \) is largest in the direction of \( B \) (state \( 1 \))

\[ \Delta U = g_0 B B \varepsilon \beta = \frac{e}{2m} \]

\[ N_2 \]

\[ \text{experiment} \]

3) Experiment

Microwaves of freq. \( f \), photons of energy \( E = hf \), increasing \( B \) increases \( \Delta U \)

At the point where \( g_0 B B = hf \), there will be resonant absorption, at which point \( g_0 \) may be computed.

(Known as electron parametric resonance)
VIII) Ferromagnetism

(Spontaneous magnetism with no applied field)

A) \( M \) very large compared with paramagnetic

\[
\begin{align*}
M & \quad \text{Ferromagnetic} \\
N_s & \quad \text{Paramagnetic}
\end{align*}
\]

Susceptibility of Ferromagnetic

\[
\chi = \frac{C}{T - T_c}
\]

\[
\chi_{\text{Ferromagnetic}} = \frac{C}{T - T_c}
\]

\[
\chi_{\text{Paramagnetic}} = \frac{C}{T}
\]

B) Weiss

Cooperative effect: magnetic moments tend to line up neighboring \( \mathbf{P}_n \) is same direction

\[
H_{\text{eff}} = H + \lambda M \quad (\lambda M \text{ due to alignment})
\]

Above the critical \( T_c \), ferrom become param

\[
\chi = \frac{M}{H_{\text{eff}}} = \frac{C}{T}
\]

Due to decrease of the cooperative effect above \( T_c \)

\[
\Rightarrow \frac{C}{T} = \frac{M}{H_{\text{eff}}}
\]

\[
\Rightarrow M = \frac{C}{T} (H + \lambda M) \Rightarrow \chi = \frac{M}{H} = \frac{C}{T - T_c} \quad \Rightarrow T_c = \frac{C}{\lambda}
\]

C) Cause of magnetic moment alignment (hysteresis)

- Exchange force causes neighboring atoms spin magnetic moments of outer electrons in certain atoms to be in the same direction.

- Example: the hydrogen molecule

Two possibilities

1. The electrons have the same spin. Exclusion principle tends to force them apart, anti-source.
2. The electrons have the same spin, opposite spin (anti-parallel).

In ferrom, the parallel configuration has the lowest energy. \( \parallel \) spins in adj. atoms (\( F, N, C \))

Boundaries won't re-align exactly as before the field is applied (left with a net magnetization)

Hysteresis
IV) FREE ELECTRON THEORY
DEVELOPED BY DRUDE IN 1900

A) TRANSIENT ANALYSIS MODEL

\[ \mathbf{V} = \mathbf{I} / \mathbf{A} = \left[ \frac{ne}{\mu} \right] \, \text{(UNIT AREA)} \, \mathbf{E} = \text{NUMBER OF FREE ELECTRONS} \]

OHM'S LAW:
\[ V = IR = \frac{\rho J}{A} \]

\[ E = V / A = \rho J \Rightarrow \mathbf{E} = \rho \mathbf{J} \] (ANALAGOUS TO \( V = IR \))

\[ \rho = \text{RESISTIVITY} \]
\[ \sigma = \frac{1}{\rho} = \text{CONDUCTIVITY} \]

\[ \sigma = \frac{J}{E} \]
\[ = \frac{n e \mathbf{v}_0}{E} \]
\[ = \frac{n e \mathbf{v}_0}{E} \] (\( \mu = \text{MOBILITY} \))

B) TRANSIENT ANALYSIS

1) DIL DROP IN AIR (?)

\[ \sum F = \Delta \mathbf{E} = \left( \frac{m}{\mu} \right) \mathbf{v}_0 = m \frac{d \mathbf{v}_0}{d t} \]

2) SUPPOSE \( \mathbf{E} \) HAS BEEN ON \( \rightarrow \mathbf{v}_0(0) \)
   TURN IT OFF

\[ m \frac{d v}{dt} + \frac{q}{m} \mathbf{v}_0 = 0 \Rightarrow \mathbf{v}_0 = v(0) e^{-t/\gamma} \]

\( \gamma \) IS TIME FOR THE DRIFT VELOCITY TO DROP \( \mathbf{v}_0 \) OF IT'S INITIAL VALUE

(\( \mathbf{v}_0 \) OF THE ELECTRONS HAVEN'T COLLIDED AFTER \( \gamma \) SECONDS)

3) WITH FIELD ON

\[ \Delta \mathbf{E} = \frac{q}{m} \mathbf{v}_0 = m \frac{d \mathbf{v}_0}{d t} = 0 \]

\[ \Rightarrow \Delta \mathbf{E} = \frac{q}{m} \mathbf{v}_0 \]

\[ \mathbf{v}_0 \]

\[ \mathbf{v}_0 = \frac{q}{m} \gamma - \mathbf{v}_0 \]

\[ \Rightarrow \mathbf{v}_0 = \frac{q}{m} \gamma / \mathbf{E} \]

\[ \sigma = \frac{n e^2 \gamma}{m} \]
C) Specific heat at high temperatures

For free electrons, classical mechanics says
\[ C_v = 3R + \frac{3}{2} R \frac{V}{T} e^{-\frac{V}{kT}}. \]

Not so! The free electron contributes very little specific heat to the system. Something is inhibiting the absorption of the free electrons. (Inhibiting the moment alignments)

E) Free electrons in a metal

Electrons confined to a box
\[ U = 0 \text{ inside} \]
\[ U = \infty \text{ outside} \]

\[ \frac{\hbar^2}{2m} \Delta^2 \Psi + U \Psi = \epsilon \Psi \text{ for time independent } \Psi \]

\[ \epsilon = \frac{\hbar^2 \pi^2}{8x^2} + \frac{\hbar^2 \pi^2}{8y^2} + \frac{\hbar^2 \pi^2}{8z^2} + \frac{2m}{\hbar^2} E \Psi = 0 \]

\[ \Psi = C \sin \left( \frac{n_x \pi x}{L} \right) \sin \left( \frac{n_y \pi y}{L} \right) \sin \left( \frac{n_z \pi z}{L} \right) \]

\[ \left( \frac{n_x \pi}{L} \right)^2 \Psi - \left( \frac{n_y \pi}{L} \right)^2 \Psi - \left( \frac{n_z \pi}{L} \right)^2 \Psi = -\frac{2mE}{\hbar^2} \Psi \]

\[ E = \frac{\hbar^2 \pi^2}{2mL^2} \left( n_x^2 + n_y^2 + n_z^2 \right) \]

The \[ \Psi \text{ motion determined by } n_x, n_y, n_z \geq 1 \]

Also \[ E = \frac{P^2}{2m} = \frac{p_x^2 + p_y^2 + p_z^2}{2m} \]

Then \[ p_x = \frac{n_x \pi}{L} \]
\[ p_y = \frac{n_y \pi}{L} \]
\[ p_z = \frac{n_z \pi}{L} \]

F) Fermi-Dirac statistics and Fermi function

1) Assumptions

a) Can't distinguish one electron from another (as opposed to Boltzmann)

b) Exclusion principle

2) Fermi function: Probability that the state of energy \( E_i \) is occupied by an electron:

\[ f(E_i) = \frac{1}{e^{(E_i - E_F)/(kT)} + 1}, \quad E_i \gg kT \]

\( E_F \) = energy of state having 50% chance of being occupied.
CUBIC TYPE LATTICE; EACH POINT REPRESENTING 2 STATES. ALL POINTS INSIDE R_max ARE OCCUPIED @ T=0°K

\[ R_{\text{max}} = \left( n_x^2 + n_y^2 + n_z^2 \right)^{\frac{1}{2}} = \frac{L \sqrt{2mE_{fo}}}{\hbar} \]

OR \[ R_{\text{max}}^2 = \frac{2mL^2E_{fo}}{\hbar^2\pi^2} \]

THE NUMBER OF OCCUPIED STATES HAVING ENERGY LESS THAN \( E_{fo} \)

\[ = 2 \left[ \frac{1}{8} \left( \frac{4}{3} \pi R_{\text{max}}^3 \right) \right] \]

\[ = \frac{\pi}{3} \left( \frac{2mL^2E_{fo}}{\hbar^2\pi^2} \right)^{3/2} \]

FOR \( N \) FREE ELECTRONS; \( N = \frac{L^3}{2m} \left( \frac{3\pi^2N}{L^3} \right)^{2/3} \)

\[ E_{fo} = \frac{\pi^2}{2m} \left( \frac{3\pi^2N}{L^3} \right)^{2/3} \quad \text{\( N \) = FREE \( \theta^- \) DENSITY ~1 TO 10 ELECTRON VOLTS}

G) \( g(E) \) AND \( N(E) \)

1) \( g(E) \) = NUMBER OF STATES WITH ENERGY TWIXT E AND E+\( \Delta E \)

\( N(E)dE \) = NUMBER OF ELECTRONS WITH ENERGY TWIXT E AND E+\( \Delta E \)

\[ \Rightarrow f(E)g(E)dE = N(E)dE \]

2) @ T=0°K, \( f(E) = 1 \) FOR \( 0 \leq E \leq E_{fo} \)

\[ \Rightarrow \int_0^{E_{fo}} N(E)dE = N = \int_0^{E_{fo}} g(E)dE \]

\[ N = \frac{L^3}{3\pi^2} \left( \frac{2mE_{fo}}{\hbar^2} \right)^{3/2} \]

\[ \Rightarrow g(E) = CE^{3/2} \quad \text{\( C = \frac{L^3}{3\pi^2} \left( \frac{2m}{\hbar^2} \right) \)} \]
For $T > 0$:

$\langle E \rangle_0$ approaches a Boltzmann distribution:

$\langle E \rangle = \frac{\int_{E_0}^{E^*} E N(E) dE}{N}$

$\Rightarrow \langle E \rangle = \frac{1}{N} \int_{E_0}^{E^*} E N(E) dE$

$\Rightarrow \langle E \rangle = \langle E \rangle_0 \left[ 1 + \frac{5T^2}{12} \left( \frac{kT}{E_0} \right)^2 \right]$

$\Rightarrow$ Energy increases a little with increasing $T$.

H) Specific Heat:

$U = NE = N \langle E \rangle_0 \left[ 1 + \frac{5T^2}{12} \left( \frac{kT}{E_0} \right)^2 \right]$

$C_v = \frac{dU}{dT} = N \langle E \rangle_0 \frac{5T^2}{12} \left( \frac{kT}{E_0} \right)^2$

For 1 mole:

$(C_v)_{\text{Elec}} = \frac{RkT}{2} \frac{n^2}{2} E_0 \ll \frac{3}{2} R$

$\Rightarrow C_v = (C_v)_{\text{Vib}} + (C_v)_{\text{Elec}}$

$\Rightarrow C_v/T = AT^3 + BT$ (at low $T$)

$\Rightarrow$ slope of $A = \frac{RkT}{2} E_0$

$\Rightarrow$ may thus experimentally compute $E_0$.
I) K SPACE AND THE FERMI SURFACE
\( \rho = \frac{4}{3} \pi k^2 \text{ELEC. MOMENTUM} \)

- **Fermi-Surface in K Space**
- **The applied E field will shift the Fermi surface**

II) Paramagnetism of Free Electron
\[ p_m = q \left( \frac{\hbar}{2m} \right)^3 \]
\[ (p_m)_x = g \left( \frac{\hbar}{2m} \right) S_x \geq \frac{1}{2} \pi \text{ and } g \geq 2 \]

\[ \Rightarrow \ (p_m)_z = \pm \left( \frac{\hbar q}{2m} \right) \]

\[ U = p_m \cdot B = -(p_m)_z B \quad \text{(Low Energy)} \]

K) Determination of Susceptibility @ \( T = 0^\circ K \)

\[ N(E) @ T = 0^\circ K \]

\[ \frac{\text{Excess Par. \( \rho \)}}{\text{N(E)E}} = \frac{1}{2} \frac{\pi^2 \left( \frac{\hbar}{2m} \right)^3}{\frac{q}{2m}} E_{fo} \cdot \frac{1}{2} \pi^2 p_m B \]

\[ \xi; \text{Crank:} \]
\[ \chi = \frac{3\pi^2}{4} \frac{p_m^2}{2E_{fo}} \]
2. Briefly explain the nature of the following forces between atoms:

(a) covalent forces

Covalent bonding arises when atoms share electrons, the diatomic gases being an example ($\text{H}_2$). What is the nature of this force?

(b) the repulsive force

The repulsive force arises from the exclusion principle: no two quantum particles in a quantum system may have the same quantum number $(\gamma: s = \pm \frac{1}{2})$.

2. Is a crystal held together by Van der Waals forces likely to have a higher or lower melting point than an ionic crystal? Why? (Note: the Van der Waals crystal would have the lower melting point, in that Van der Waals forces act effectively only on materials boiling which solidify near $0^\circ \text{K}$.)
3. Given a powder whose crystals are known to have a primitive cubic structure with lattice constant \( a = 2.0 \text{ Å} \).

(a) Determine the Miller indices of all planes parallel to the one shown. The plane will intersect at \( \frac{3}{4}h, \frac{1}{2}k, \frac{1}{2}l \) so \( 4h, 2k, 0 \Rightarrow (2, 1, 0) \).

(b) If this polycrystalline solid is irradiated at various angles \( \theta \) with X-rays of wavelength \( \lambda = 1.0 \text{ Å} \), what are the values of \( \sin \theta \) for the first 4 diffraction peaks (starting at \( \theta = 0 \)), and what lattice planes (Miller indices) give rise to each peak?

\[ 2d \sin \theta = n \lambda \] (BRAGG'S LAW)

\[ \sin \theta = \frac{n \lambda}{2d} \]

\[ d = \sqrt{h^2 + k^2 + l^2} \]

2/14
4. The expression for the total potential energy of an insulating crystal containing \(2N\) ions was:

\[
E = N \left( -\frac{\alpha e^2}{4\pi \varepsilon_0 R} + \frac{A}{R^2} \right) \quad (1)
\]

which at absolute zero (\(0^oK\)) becomes

\[
E = -\frac{N\alpha e^2}{4\pi \varepsilon_0 R_e} \left( 1 - \frac{1}{n} \right) \quad (2)
\]

Born has suggested that the second term \(\frac{A}{R^2}\) in equation (1), representing the repulsive force between neighboring atoms, should be replaced by \(A e^{-\frac{R}{n}}\).

Derive the corresponding new equation (2),

\[
E = N \left( \frac{\alpha e^2}{4\pi \varepsilon_0 R_e} + A e^{-\frac{R}{n}} \right)
\]

\[
\left. \frac{\delta E}{\delta R} \right|_{R=R_e} = 0 = N \left( \frac{\alpha e^2}{4\pi \varepsilon_0 R_e^2} - \frac{A}{n} e^{-\frac{R}{n}} \right) \quad ; \quad T=0^oK
\]

\[
\frac{\alpha e^2}{4\pi \varepsilon_0 R_e} = \frac{A}{n} e^{-\frac{R}{n}}
\]

\[
\frac{\alpha e^2}{4\pi \varepsilon_0 R_e} \cdot 2 \ln R_e = 0 \quad \text{nK}
\]

\[
\Rightarrow A = \frac{n \alpha e^2}{4\pi \varepsilon_0 R_e} e^{\frac{R}{n}}
\]

\[
E = N \left( \frac{-\alpha e^2}{4\pi \varepsilon_0 R_e} + \frac{\alpha e^2}{4\pi \varepsilon_0 R_e^2} e^{\frac{R}{n}} \right)
\]

\[
= N \frac{\alpha e^2}{4\pi \varepsilon_0 R_e} \left( \frac{ne^{\frac{R}{n}}}{R^2} - 1 \right)
\]

\[13/17\]
5. Suppose a rod contains a line of atoms, 0.01 meters long, with the end atoms fixed, and suppose the mass of the atom $M = 10^{-26}$ kg, the spacing between atoms $a = 4 \times 10^{-10}$ meters, and the force constant between neighboring atoms is $\beta = 10^{-10}$ at m.

(a) Draw a figure showing the relationship between the frequency of waves traveling along this line of atoms and the wavelength of these waves (graph of $w = 2\pi f$ versus $k = 2\pi/a$).

\[ \omega = \frac{2\pi}{2 \times 10^{-10}} = 5 \times 10^8 \text{ rad/s} \]

\[ \frac{2\pi}{a} = \frac{2\pi}{4 \times 10^{-10}} = 200\pi \text{ rad/m} \]

(b) Do higher or lower frequency waves travel faster?

\[ V_g = \frac{6\mu k}{8k} = \frac{1}{2} \sqrt{\frac{15}{4m}} \cos \frac{k \rho}{2} \]

$V_g \text{ max} \text{ is at } k = 0 \Rightarrow$ FASTER AT LOWER FREQUENCIES

(c) What are the frequencies $f$ of the lowest frequency and highest frequency standing wave for this line of atoms?

For standing wave: $\sin(kd) = 0$

$\Rightarrow kd = \pi, 2\pi, \ldots, \frac{(n-1)\pi}{2}$

$\Rightarrow k = \frac{\pi}{2}, \frac{2\pi}{2}, \ldots, \frac{(n-1)\pi}{2}$

$w = \sqrt{\frac{\beta}{M}} \sin \frac{(n-1)\pi}{2} \frac{\pi}{2}$

LOWEST FOR $n = 1 \Rightarrow k = \frac{\pi}{2}$
I. In the Einstein model of a solid, from which he calculated an expression for the specific heat of an insulator:

A. What assumptions are built into this model?

1) The atoms vibrate at a single frequency
2) Assumption of Boltzmann distribution
3) Each atom acted as 3 mutually perpendicular oscillators
   (i.e., N atoms \( \Rightarrow \) 3N oscillators)

B. What are the vibration energies allowed the oscillatory atoms?

\[ E_h = (n + \frac{1}{2}) \hbar \nu; \quad n = 0, 1, 2, 3, \ldots \]

6/6

C. Set up an expression for the average oscillation energy of vibrating atoms:

\[ E = \frac{\hbar \nu}{e^{\frac{-E_h}{kT}} - 1} \]

\[ E = \sum_{n=0}^{\infty} E_h \cdot e^{-E_h/kT} \]

10/10
D. Outline, without all the mathematical details, the procedure for determining an expression for the specific heat $C_v$ from the average vibrational energy.

1. Substitute $E_x$ into $E$ expression
2. Cancel exponents in both numerator and denominator.
3. Let $x = h\nu/kT$
4. Expand numerator and denominator, noticing that the numerator is its derivative, and substitute in integral.
5. $u = 3N\nu$, so multiply $E$ by $3N$ to obtain $u^o$ evaluate integral.
6. $C_v = \frac{\mu}{8T}$

E. How did Einstein's $C_v$ compare with the experiment at low temperature, and what might be done to get better agreement?

Einstein's model dropped off a little too fast at the origin and could have been improved by considering more than just a single frequency (as did Debye). He might have tried other distributions. Also, some of the parameters taken outside the integral, the sign in the derivation was not found. Indeed, the variable $S$...
II. Polarization of a Dielectric

A. Describe the three kinds of polarization processes which occur in dielectrics and cause a reduction in the electric field:

1) ORIENTATIONAL - DUE TO THE GEOMETRY OF A MOLECULE, IT IS LOPSIDED IN THE SENSE OF CHARGE, SUCH AS WATER:

\[ \text{H-O-H} \]

2) ELECTRIC - DUE TO NON-SYMMETRIC ROTATION OF ELECTRONS ABOUT THEIR NUCLEUS:

\[ \text{H-O-H} \]

3) IONIC - RISES FROM ATTRACTION OF IONS, EX: \( \text{Na}^+ \text{Cl}^- \)

\[ \text{Na}^+ \rightarrow \text{Cl}^- \]

Shift of ions due to applied field

B. Given a dielectric which has a cubic lattice structure of one type of atom only. Starting with the general relationship between the dielectric constant \( \varepsilon \) and polarization \( P \), and the equation relating the local field at the position of an atom to the macroscopic field \( E \) in this dielectric, derive the expression relating its dielectric constant to the electronic polarizability of the atom (Classen-Mosotti equation).
\[ D = \varepsilon_0 E + P = K \varepsilon_0 E \Rightarrow K = \frac{\varepsilon_0 E + P}{\varepsilon_0 E} = 1 + \frac{P}{\varepsilon_0 E} \]

\[ E_{\text{loc}} = E_1 + E_2 + E_3 \approx \frac{E}{30} \text{ (Cubic)} \]

\[ E_3 = \ldots \frac{P}{360} \]

\[ \alpha = \frac{P}{E_{\text{loc}}} \]

c. Explain briefly the following graph showing the dielectric constant of solid HCl as a function of temperature

(i.e., why the sudden change at

\( \sim 100^\circ \text{K} \) and why the decrease at

higher T?)

For some reason, dipoles suddenly become aligned at

100°K and as temperature increases, molecular

and thus, dipole vibration increases, delining the
dipoles to the limit of randomness again from

whatever the prevailing polarizability of HCl is.
I. Magnetism in Solids (Insulators)

A. An electron in orbit about a nucleus has an angular momentum \( \vec{L} \) causing a magnetic moment \( \vec{p}_m = -\left(\frac{e \vec{L}}{2m}\right) \). Show that the application of a magnetic field \( \vec{B} \) making angle \( \phi \) with the direction of \( \vec{L} \) causes the orbit to precess about the direction of \( \vec{B} \) with angular frequency \( \omega = \left(\frac{e}{2m}\right) \vec{B} \) (rad/sec).

\[
\vec{p}_m = -\left(\frac{e \vec{L}}{2m}\right)
\]

\[
\tau = \vec{p}_m \times \vec{B} = \frac{d\vec{L}}{dt}
\]

Let \( \omega = \frac{d\theta}{dt} \)

Now \( d\vec{L} = \vec{p}_m \times \vec{B} \, dt \)

\[
= P_m \sin \phi \, B \, dt
\]

\[
dL = \frac{e}{2m} (L \sin \phi) \, d\theta
\]

\[
P_m \sin \phi \, B \, dt = L \sin \phi \, d\theta
\]

\[
\omega = \frac{d\theta}{dt} = \frac{P_m B}{L} = \frac{(\frac{e}{2m})L \sin \phi}{L} = \frac{e}{2m} \vec{B}
\]

\[
a bit of sign difficulty
\]
D. Suppose that some of the atoms in a particular solid have magnetic moments. Explain briefly how it happens that these atoms will contribute a paramagnetic effect when a magnetic field is applied to the solid.

There will be an additional _angular momentum_ induced in the system, due to _orbital_ and _spin_.

\[ \vec{p}_m = \frac{e}{2m} \vec{L} \quad \text{and} \quad \vec{L} = [L(L+1)]^{1/2} \hbar \]

\[ \vec{B} = \mu_0 \vec{H} + \lambda \hat{m} \quad \text{due to } \text{eff.} \]
II. Free Electron Theory of Metals

A. What is the meaning of the letter $\tau$ in the expression for the electrical conductivity $\sigma = \frac{ne^2\tau}{m}$ and what effect does changing the temperature have on it?

$\gamma$ is the time (in transient analysis) for initial drift velocity to reduce by a factor of $1/e$. (In the case of shutting off an established field)

The higher the temperature, the larger $V_0$, (the electrons move faster) and thus the greater chance for collision.

Ergo, the smaller $\tau$
B. Given the expression for the energy allowed a free electron in a metal cube, \( E = \left( \frac{k^2 q^2}{2m} \right) (n_x^2 + n_y^2 + n_z^2) \), show that the Fermi energy at \( T = 0 \) K is related to the number \( N \) of free electrons per unit volume \( L^3 \) by:

\[
\frac{N}{L^3} = \frac{\pi}{3} \left( \frac{2m E_{F0}}{k^2 \pi^2} \right)^{3/2}
\]

\[
R_{\text{MAX}} = (n_x^2 + n_y^2 + n_z^2)_{\text{MAX}} = \frac{2m L^2 E_{F0}}{k^2 \pi^2}
\]

Each point represents 2 states,

\[
\Rightarrow N = \frac{1}{8} \left[ 2 \left( \frac{4}{3} \pi R_{\text{MAX}}^3 \right) \right]
\]

\[
= \frac{\pi}{3} R_{\text{MAX}}^3
\]

\[
= \frac{\pi}{3} \left( \frac{2m L^2 E_{F0}}{k^2 \pi^2} \right)^{3/2}
\]

\[
= \frac{\pi}{3} L^3 \left( \frac{2m E_{F0}}{k^2 \pi^2} \right)^{3/2}
\]

\[
\therefore \frac{N}{L^3} = \frac{\pi}{3} \left( \frac{2m E_{F0}}{k^2 \pi^2} \right)^{3/2}
\]
Draw a graph showing the approximate energy distribution of free electrons in a solid at room temperature
(i.e., show how the number of electrons in an energy interval of size \( dE \) depends on the energy \( E \)).

\[ N(E) \]

\[ f(E) \approx \frac{N(E)}{dE} \]

1. Mark the "Fermi energy" on the graph and explain what it meant by the term "Fermi energy.

   THE FERMI ENERGY \( (E_F) \) IS THE ENERGY AT WHICH THE PROBABILITY OF OCCUPANCY OF AN ENERGY LEVEL BY AN ELECTRON IS 50%.

2. Give two energy intervals \( dE \) at low energies \( E_1 \) and \( E_2 \) where \( E_2 = 2E_1 \). What is the ratio of the number of particles in the higher energy interval to that in the lower?

   FOR LOW ENERGIES: \( \frac{CVE_2}{CVE_1} = \frac{V2E_2}{VE_1} = \sqrt{2} \)
1. The figure shows the first two Brillouin zones for electron wave vectors in a cubic lattice (unit cell cube edge a).

(a) What is likely to happen to an electron having a propagation wave vector as shown? Justify your answer mathematically. (14)

**Bragg's Law Yields**

\[ \lambda = 2a \sin \theta \]  
\[ k = \frac{2\pi}{\lambda} \]

\[ \frac{2\pi}{k} = 2a \sin \theta \Rightarrow k = \frac{2\pi}{2a \sin \theta} \]

(b) Suppose that this crystal has the same number of electrons as it has electron states per band. What determines whether it will be a metal, semiconductor, or insulator? Which of the bands filled first? (13)
\[ \dot{\varepsilon} = \varepsilon_0 \varepsilon' + \varepsilon = K \varepsilon_0 \varepsilon \Rightarrow K = \frac{\varepsilon_0 \varepsilon + \varepsilon}{\varepsilon_0 \varepsilon} = 1 + \frac{\varepsilon}{\varepsilon_0 \varepsilon} \]

\[ E_{\text{loc}} = E_1 + E_2 + E_3 + E_4 \]

\[ E = E_1 + E_3 \]

\[ E_3 = \frac{\varepsilon}{\varepsilon_0} = \frac{P}{360} \]

\[ \alpha = \frac{P}{E_{\text{loc}}} \]

C. Explain briefly the following graph showing the dielectric constant of solid HCl as a function of temperature (i.e., why the sudden change at \( \approx 100^\circ K \) and why the decrease at higher \( T \)?)

For some reason, dipoles suddenly become aligned at \( 100^\circ \) and as temperature increases, molecular and thus dipole vibration increases, delining the dipoles to the limit of randomness again from whatever the prevailing polarizability of HCl is.
(2) An electron is moving in the $x$ direction in a periodic lattice and is being acted upon by an electric force $\vec{F}$. Derive an expression for its acceleration as a function of $\vec{F}$ and the $E$ vs. $k$ curve for motion along this axis (assuming force $\vec{F}$ is along the $x$ axis).
The conductivity of an intrinsic semiconductor increases with temperature while that of a metal decreases. Explain.

**THE INCREASE IN CONDUCTIVITY OF AN INTRINSIC SEMICONDUCTOR AS DERIVED IN 4b)**

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Explain.

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4. From the expression $n = N_c e^{-(E_c - E_F)/kT}$ for the number of electrons per unit volume in the conduction band, and $p = N_v e^{-(E_F - E_v)/kT}$ for the number of holes per unit volume in the valence band.

(a) derive an equation relating the conductivity of an intrinsic semiconductor to the energy gap and temperature (among other things), $\sigma = n^2 p$
\( n = N_e e^{-(E_e - E_f)/kT} \)
\( p = N_v e^{-(E_v - E_f)/kT} \)
\( e = n e^{-\mu_n} + p e^{-\mu_p} \)
\( = (N_e e^{-\mu_n} + N_v e^{-\mu_p}) e^{-(E_e - E_f)/kT} \)
\( = e^{-\mu_n} e^{-(E_e - E_f)/kT} + N_v e^{-\mu_p} e^{-(E_v - E_f)/kT} \)

(b) Briefly explain how the result of part (a) allows one to measure the energy gap by measuring conductivity as a function of temperature.

\[ \text{DERIVED EQUATION (WHICH IS WRONG)} \]

\[ \text{Slope} = - \frac{E_g}{2k} \]

\( \text{Slope proportional to } E_g \)

5) What is the "Meissner effect" in superconductors?

\( \text{Superconductor} \)

\( \text{Cut-off sharpens w/ added impurities} \)

\( \text{Twin pairs} \)

\( \text{Opposite } E \text{ at } T \)
b) Derive an expression for the electric field intensity $E$ at any position $x$ along the positive $x$ axis, starting from the expression for $V$ found in part (a). (12)
Solids, like gases, are made up of large numbers of interacting particles. In the absence of any information about individual particles one can still predict with accuracy many properties of such an assembly, using the laws of probability and statistics. One of the central problems of statistical mechanics is concerned with the prediction of the most probable energy distribution of a large number of interacting particles. This distribution, called the "equilibrium" distribution, has been found to have such a high probability of occurrence when the number of particles is large, that significant deviations from this distribution are very unlikely (but not impossible).

The energy $E$ of an individual particle is the sum of its kinetic energy and its potential energy. The kinetic energy depends only on the particle's momentum and the potential energy only on its position so that its energy is completely specified by six quantities, three momentum components (e.g., $p_x, p_y, p_z$) and three position coordinates (e.g., $x, y, z$). At any instant, each particle of the assembly will have six values associated with it, one for each of the quantities mentioned above. The task of finding the energy distribution then becomes one of finding the numbers of particles having values between $x, y, z, p_x, p_y, p_z$ and $x + \Delta x, y + \Delta y, z + \Delta z, p_x + \Delta p_x, p_y + \Delta p_y, p_z + \Delta p_z$.

For example, suppose the particles are free so that the potential energy $U = 0$ for all particles (an ideal gas). In this case the energy of the particle is completely specified by its momentum components; it may be represented by a point in "momentum space" as shown below.
One may think of this momentum space as being divided into "cells" of dimensions $\Delta p_x$, $\Delta p_y$, $\Delta p_z$ and then try to find the most probable distribution of points among the cells in order to determine the energy distribution. In general, $U \neq 0$ and the cells are six dimensional cells in a six dimensional "phase space".

Suppose now that one has $N$ particles and wishes to determine the most probable distribution of them among cells of energy $E_1$, $E_2$, $E_3$, etc. The probability of a particular distribution is proportional to the number of ways $W$ of making the distribution, and it can be shown that if the particles are distinguishable from each other

$$W = \frac{N!}{N_1! N_2! N_3! \cdots}$$  \hspace{1cm} (1)

where $N_1$ = number of particles in cell 1, etc.

**Example:** Suppose there are 4 particles to distribute between 2 cells.

(possibility 1): all 4 in cell 1; only one way to do it

$$W = \frac{4!}{4! 0!} = 1$$

(possibility 2): 3 in cell 1, 1 in cell 2; four ways to do it...

$$W = \frac{4!}{3! 1!} = 4$$

(possibility 3): 2 in each cell; six possible combinations

............ identify them yourself

$$W = \frac{4!}{2! 2!} = 6$$

(possibility 4): 3 in cell 2; similar to possibility 2

(possibility 5): all 4 in cell 2; similar to possibility 1

In this case possibility 3 describes the equilibrium distribution and it is not much more probable than possibilities 2 or 4 (this would not be the case if there were a large number of particles and cells).

In order to obtain a general expression for the equilibrium energy distribution, one maximizes $W$ (equation 1) with respect to variable $N_1$, $N_2$, .......

(LaGrange's method of undetermined multipliers) with the restrictions

$$N = N_1 + N_2 + N_3 + \cdots \cdots = \sum N_i$$
\[ E = N_1 E_1 + N_2 E_2 + \ldots = \sum N_i E_i \]

and gets the most probable energy distribution
\[ N_i \propto e^{-E_i/kT} \]  \hspace{1cm} (2)

where \( N_i \) is the number of particles having energy \( E_i \). This expression is directly useful only where energies are discrete so that a particular energy \( E_i \) is associated with each cell. If the energy is continuous the cells must be considered infinitesimal and of volume \( d\Omega \) in six dimensional phase space (e.g. in cartesian coordinates \( d\Omega = dp_x dp_y dp_z dx dy dz \)). The number of particles per infinitesimal cell is then
\[ dN \propto e^{-E/kT} d\Omega \]  \hspace{1cm} (3)

Equations (2) and (3) represent the classical Maxwell-Boltzmann equilibrium distribution.

One of the difficulties with the above analysis is that particles can't be labeled \( a, b, c, \ldots \) they are indistinguishable. Thus in the example given concerning the distribution of 4 particles between 2 cells, there are not actually four distinct ways to put three particles in cell 1 and one in cell 2; the expression (1) for \( W \) is incorrect. Also, according to quantum mechanics, the position and momentum of a particle can be determined simultaneously only with uncertainty
\[ p_x \Delta x > \hbar/2 \]  \hspace{1cm} etc.

and therefore the cell volume can't be infinitesimal but must be of the order \( \hbar^3/8 \) or greater to ensure knowledge of when a particle is in a particular cell. When these facts are taken into account, an analysis similar to the above yields for the equilibrium number of particles in a state of energy \( E_i \)
\[ N_i \propto \frac{1}{B e^{E_i/kT} - 1} \]  \hspace{1cm} (4)

which is the Bose-Einstein distribution function.

In the case of particles having half integral values of spin (e.g. electrons, protons, neutrons) there is also a restriction on the number of particles that can go into a particular state. In a given system, only one particle is allowed to occupy a state having a given set of quantum numbers. One determines the probability \( f(E_i) \) that a state of energy \( E_i \) is occupied rather than the number of particles in the state. The equilibrium result is
\[ f(E_i) = \frac{1}{B e^{E_i/kT} + 1} \]  \hspace{1cm} (5)
where the probability function $f(E_i)$ is called the Fermi function. The quantity $B$ is not temperature independent and may be written

$$B = e^{-E_F/kT}$$

resulting in

$$f(E_i) = \frac{1}{1 + e^{(E_i-E_F)/kT}}$$

where $E_F$ is called the Fermi energy of the system and is almost, but not quite, temperature independent. The Fermi energy $E_F$ is defined as the energy of that state which has a 50% chance of being occupied by some particle, since when $E_i = E_F$, $f = 1/2$. States having lower energies ($E_i < E_F$) are more likely to be occupied ($f > 1/2$), and states of higher energy ($E_i > E_F$) less likely to be occupied ($f < 1/2$).
II. Specialized Solution

A. Equation

only no variation
frequency function \( C \nu \)

\[ \nu \to \nu \text{ as } T \to 0 \]

\[ C \nu \to 0 \text{ as } T \to 0 \]

\[ \nu = \frac{1}{2} \sqrt{\frac{E}{\rho}} \]

B. Poles

\[ \text{WI IX different frequencies of vibration} \]

\[ \text{the standing}
\]

\[ \text{more frequent of a continuous medium with fixed}
\]

\[ \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} = \frac{1}{\nu^2} \frac{\partial^2 w}{\partial T^2} \]

\[ w = \text{the sum} \left( \frac{m \nu^2}{2} \right)^{\text{th}} \text{wave} \left( \frac{m \nu^2}{2} \right)^{\text{th}} \text{wave} \left( \frac{m \nu^2}{2} \right)^{\text{th}} \text{wave} \]

\[ \nu_1, \nu_2, \nu_3, \nu_4, \ldots \]

\[ \text{Substitute} \]

\[ \left[ \frac{\partial^2 w}{\partial x^2} \right] \left[ \frac{\partial^2 w}{\partial y^2} \right] \left[ \frac{\partial^2 w}{\partial z^2} \right] \left[ \frac{\partial^2 w}{\partial T^2} \right] \]

\[ = \int \left( \frac{\partial^2 w}{\partial x^2} \right) \left( \frac{\partial^2 w}{\partial y^2} \right) \left( \frac{\partial^2 w}{\partial z^2} \right) \left( \frac{\partial^2 w}{\partial T^2} \right) \]

\[ \rightarrow \left( \frac{\omega^2}{\rho} \right)^2 = \frac{E}{\rho} \to \text{standing} \]

\[ \left( \frac{\omega^2}{\rho} \right)^2 \]
Natural frequencies $\omega = \sqrt{\frac{1}{2} \text{constant}}$

Part with total number of "particles"

- $x$, $y$, $z$... coordinates
- In particular, oscillation modes

\[
\begin{align*}
\text{let } R^2 &= x^2 + y^2 + z^2 = \frac{V^2}{2} \\
R &= \frac{2K}{\gamma} = \text{distance from origin of any point}
\end{align*}
\]

\[
\frac{dR}{d\gamma} = \frac{2K}{\gamma}
\]

- Integrate across for determination of volume
  - Volume per unit volume

\[
\text{between } R \text{ and } R + dR, \text{ volume } = \frac{1}{2} (4\pi R^2 dR) = \frac{2\pi R^2}{3} dR
\]

No. of mole $\Theta$ between corresponding pressures $\gamma$ and $\gamma + d\gamma$

\[
\begin{align*}
dN &= \frac{\Theta}{R^2} \left( \frac{4\pi R^2}{2} \right) \left( \frac{3R^2}{2} d\gamma \right) = \frac{4\pi \Theta}{5} \frac{R^2}{2} d\gamma = \frac{16\pi \Theta V}{5} + \gamma^3
\end{align*}
\]

Actually, there are two temperature and one longitudinal mode

- For each point in reservoir $\gamma$ and $\Theta$ are temperature dependent

\[
\left\{ \begin{array}{l}
dN = 4\pi V \left( \frac{2}{\gamma^3} + \frac{1}{\gamma^2} \right) + \gamma^2 d\gamma \\
\end{array} \right.
\]

Cut off frequencies such that

\[
\int_0^{\gamma_0} dN = 3N
\]
14. $\lambda = 2500\text{Å}, \quad V_0 = 3.06\text{eV}$

**Work Function:**

$E_w = E_b - E_e$

$E_b =$ Energy of light $= h\frac{c}{\lambda}$

$E_e =$ Energy of electrons $= eV_0$

$E_b = 1.24 \times 10^{-3} \text{eV}\cdot\text{Å} = 4.0\text{eV}$

$E_e = (1.602 \times 10^{-19} \text{C})(3.06\text{eV}) = 5.08 \times 10^{-18} \text{J}$

$= 3.06\text{eV}$

$\Rightarrow E_w = 1.09\text{eV}$
\[ \frac{d\xi}{dt} = -\frac{2e^2}{3}\frac{(r)^3}{C^3} \]

\[ r = a \sin \omega t \]

\[ \Rightarrow r' = a \omega^2 \sin \omega t \]

\[ \Rightarrow \frac{d\xi}{dt} = -\frac{2e^2 a \omega^2}{3C^3} \sin \omega t \]

\[ \xi = -\frac{2e^2 a \omega^2 t}{3C^3} \left[ \frac{1}{2} t - \frac{1}{4 \omega} \sin 2\omega t \right] \]

\[ \frac{d\xi}{dt} = -2e^2 a \omega^2 \frac{t}{C^3} \]

\[ \frac{d^2\xi}{dt^2} = -2e^2 a \omega^2 \frac{1}{C^3} \]

**FOR HARMONIC OSCILLATOR:**

\[ \omega^2 = \frac{2e^2 a}{m} \quad \alpha^2 = \frac{2e^2}{m} \]

\[ \Rightarrow \omega^2 \alpha^2 = \frac{2e^2}{m} \]

\[ \Rightarrow \frac{d^2\xi}{dt^2} = -\frac{2e^2 \omega^2}{3m \alpha^2} \]

A differential equation of the form \[ \frac{dv}{dt} = -\frac{1}{v} \]

HAS SOLUTION \[ v = e^{-\frac{t}{\tau}} \quad \tau = \text{DECAY CONSTANT} \]

**APPLYING THIS ANALOGY TO THE ABOVE RELATIONSHIP:**

\[ \gamma = \frac{2e^2 \omega^2}{2m \alpha^2} \]

\[ = \frac{3(3.14 \times 10^{-9} \text{ C} \cdot \text{m})^2 (3.00 \times 10^{10} \text{ m/s}^2)}{2(4.82 \times 10^{-7} \text{ C} \cdot \text{m})^2} \quad \text{(in m/s)} \]

\[ = 1.60 \times 10^{-9} \]

\[ \omega = 10^{15} \text{ rad/} \text{sec} \times \frac{1 \text{ cycle}}{2\pi \text{ rad}} = \frac{10^{15} \text{ cycle}}{2\pi \text{ sec}} \]

\[ \Rightarrow \gamma = 6.32 \times 10^{-7} \text{ sec}^{-1} \]

\[ \omega = \frac{10^{15} \text{ cycle}}{2\pi \text{ sec}} \]

\[ \Rightarrow \gamma = 6.32 \times 10^{3} \text{ sec}^{-1} \]
1.7, \[ V = \frac{1.24 \times 10^4}{\lambda (\text{cm}^2)} \] \hspace{1cm} \text{Eq. 1.7}

\[ \lambda = R_h \left( \frac{1}{k^2} - \frac{1}{n^2} \right) \]

For ionization: \[ \frac{1}{\lambda} = R_h = 1.09677 \text{ cm}^{-1} \]

\[ V = \frac{1.24 \times 10^4 \times 1.09677}{\text{cm} \times 10^9 \text{ cm}^{-1}} = \]

\[ = 13.6 \text{ GeV} \]

\[ V = 1.2 \times 10^9 \text{ cm}^{-1} \]

\[ \frac{1}{\lambda} = R_h \left( \frac{1}{k^2} - \frac{1}{n^2} \right) \]

\[ V = \frac{1.24 \times 10^4}{\lambda (\text{cm}^2)} \]

\[ \Rightarrow \frac{V}{\lambda (\text{cm}^2)} = 1.24 \times 10^4 = R_h \left( \frac{1}{k^2} - \frac{1}{n^2} \right) \]

\[ R_h = \frac{1.09677 \text{ cm} \times 10^9 \text{ cm}^{-1}}{1.24 \times 10^4} = 1.09677 \times 10^5 \text{ cm} \]

\[ \Rightarrow \frac{1}{k^2} - \frac{1}{n^2} = \frac{1.24 \times 10^4 \times (1.09677 \times 10^5)}{1.24 \times 10^4} = 1.389 \]

This relationship is satisfied for:

\[ k = 2 \text{ and } n = 3 \]

\[ \Rightarrow \text{The current drop represents} \]

\[ \text{an electron changing from its} \]

\[ \text{second to its third lowest} \]

\[ \text{energy level}. \]
\[ \lambda - \lambda_0 = \frac{h (1 - \cos \theta)}{m_0 c} \quad \text{Eq. 1.12} \]
\[ \rho^2 = h^2 (k_0^2 + k^2 - 2k_0 k \cos \theta) \quad \text{Eq. 1.11} \]
\[ k = \frac{2\pi}{\lambda}, \quad \nu = \frac{\nu_0}{\lambda} \]
\[ h \nu_0 + m_0 c^2 = h \nu + (m_0 c^2 + \rho^2 c^2)^{1/2} \quad \text{Eq. 1.9} \]

Solving for \( \rho^2 \) in Eq. 1.9:
\[ \rho^2 = \frac{1}{c^2} \left[ (h \nu_0 + m_0 c^2 - h \nu)^2 - m_0 c^4 \right] \]

Equating with Eq. 1.11:
\[ c^2 h^2 [k_0^2 + k^2 - 2k_0 k \cos \theta] = (h \nu_0 + m_0 c^2 - h \nu)^2 - m_0 c^4 \]
\[ = c^2 h^2 \left( \frac{\nu_0}{\lambda} + \frac{\rho^2}{\lambda^2} - \frac{2 \rho \nu_0 \cos \theta}{\lambda^2} \right) = c^2 h^2 \frac{\lambda^2 - \lambda_0^2 - 2 \lambda_0 \rho \cos \theta}{\lambda_0^2} \]

Now, since \( \nu = \frac{\nu_0}{\lambda} \):
\[ \left( \frac{h c}{\lambda_0} + m_0 c^2 - \frac{h c^2}{\lambda_0} \right)^2 - m_0 c^4 = \left[ h c \left( \frac{1}{\lambda_0} - \frac{\rho}{\lambda^2} \right) + m_0 c^2 \right]^2 - m_0 c^4 \]
\[ = h^2 c^2 \left( \frac{\lambda_0^2 - \lambda^2 - 2 \lambda_0 \rho \cos \theta}{\lambda_0 \lambda^2} \right) \]
\[ = c^2 h^2 \frac{\lambda^2 - \lambda_0^2 - 2 \lambda_0 \rho \cos \theta}{\lambda_0 \lambda^2} \]

Or:
\[ h^2 c^2 - \frac{2 \lambda_0 c^2 h (\lambda - \lambda_0)}{\lambda_0} = \frac{2 \rho \lambda \cos \theta}{\lambda_0^2} \]
\[ m_0 c^2 h (\lambda - \lambda_0) = \frac{c^2 h^2 (1 - \cos \theta)}{\lambda_0} \]
\[ \Rightarrow \lambda - \lambda_0 = \frac{h (1 - \cos \theta)}{m_0 c} \]
1.15. \( V(t) = V_0 \text{rect} \left( \frac{t}{T} \right) \)

\[ G(\omega) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} V(t) \cos \omega t \, dt \]

\[ = \sqrt{\frac{2}{\pi}} \int_{0}^{T} V_0 \cos \omega t \, dt \]

\[ = \sqrt{\frac{2}{\pi}} V_0 \sin \omega T \bigg|_0^T \]

\[ = V_0 \sqrt{\frac{2}{\pi}} \sin \omega T \]

\[ G(\omega) = \frac{V_0 \sqrt{2}}{\pi} \]

(Traced from Fig 1.26)

Define \( \Delta \omega \) such that

\[ G \left( \frac{\Delta \omega}{2} \right) = \left( \frac{2}{\pi} \right) G(0) \]

\[ = V_0 \sqrt{\frac{2}{\pi}} \frac{\sin \omega \Delta T/2}{\omega \Delta T/2} = \left( \frac{2}{\pi} \right)^{3/2} V_0 \gamma \]

\[ \frac{\Delta \omega}{\Delta T} = \frac{\pi}{2} \gamma \]

Define \( \Delta V = \frac{\Delta \omega}{2\pi} \) or \( \Delta \omega = 2\pi \Delta V \)

\[ \frac{\gamma \Delta V \Delta T}{\Delta \omega} = \frac{\pi}{2} \]

or \( \Delta V = \Delta \gamma \)

Define \( \Delta t = 2 \gamma \)

\[ \frac{\gamma \Delta V \Delta t/2}{\Delta \omega} = \Delta \gamma \]

or \( \Delta \omega \Delta V \Delta t = \Delta \gamma \Delta t \)

This relationship is valid only for \( \Delta V \Delta t = 0 \) (which is a no-no solution) or

\[ \Delta V \Delta t = 1 \]
\[ E_n = -\frac{13.6\, \text{eV}}{n^2} \]

\[ E_n = -1.5\, \text{eV} \]

\[ E_n = 0.5\, \text{eV} \]

\[ E_n = 0.38\, \text{eV} \]

\[ E_n = -1.5\, \text{eV} \]

\[ E_n = -5.1\, \text{eV} \]
A. Electron is in state \( j \)
Assume 1 electron per acceptor
\( f_j = P[\text{Hole is in state } j] \) (\( \text{P} \) has energy \( E_j \))

\[
f_j = \left[ 1 + e^{\frac{E_j - E_0 - E_{0j}}{kT}} \right]^{-1}
\]

\[
f_j = \left[ 1 + \frac{1}{1 + e^{\Delta E_j/kT}} \right]^{-1}
\]

\[
f_j = \left[ 1 - \frac{1}{1 + e^{\Delta E_j/kT}} \right]^{-1}
\]

\[
F^+ = P[\text{acceptor atom has no hole}]
\]

\[
\frac{dF^+}{dE_0} = \frac{dF_0}{dE_0}
\]

\[
F_0 + F^+ = 1 \Rightarrow F_0 = P[\text{acceptor has a hole}]
\]

\[
F^+ \left( 1 + e^{-\Delta E_j/kT} \right) = 1
\]

\[
\Rightarrow F^+ = \frac{1}{1 + e^{-\Delta E_j/kT}} = \frac{F_0}{F_0 + F^+}
\]

\( N_A \) = number of holes in conduction band from acceptors
\( N_A \) = concentration of acceptor atoms

To include degeneracy, let \( E_0 \) = states \( \leq E_0 \)

\[
\Rightarrow F^+ = \left[ 1 + \frac{e^{-\Delta E_j/kT}}{1 + e^{-\Delta E_j/kT}} \right]^{-1}
\]

\[
= \left[ 1 + \frac{1}{1 + e^{\Delta E_j/kT}} \right]^{-1}
\]

\[
\Rightarrow F_0 = 1 - F^+ = 1 - \frac{1}{1 + e^{\Delta E_j/kT}}
\]

\[
F^+ = \left[ 1 + \frac{e^{-\Delta E_j/kT}}{1 + e^{-\Delta E_j/kT}} \right]^{-1}
\]

\( F^+ \) = \( \frac{1}{1 + e^{\Delta E_j/kT}} \)

ETC.
**Effective Mass in 3 Dimensions**

\[
\frac{\partial V}{\partial k} = m^{-1} \frac{\partial E}{\partial k}
\]

\[
m^{-1} = \text{Reciprocal Effective Mass Tensor}
\]

\[
\frac{\partial V}{\partial k} = m^{-1} \frac{\partial E}{\partial k}
\]

\[
\Rightarrow m^{-1} = \frac{E}{\partial E/\partial k}
\]

Now

\[
V = \nabla_k \omega \Rightarrow \nabla_k = \frac{\partial V}{\partial E} = \frac{E}{\partial E/\partial k}
\]

\[
\omega = \frac{E}{\partial E/\partial k}
\]

\[
\Rightarrow \frac{\partial V}{\partial k} = \frac{1}{h^2} \frac{\partial E}{\partial k}
\]

\[
\frac{\partial V}{\partial k} = \frac{1}{h^2} \frac{\partial E}{\partial k}
\]

\[
\frac{\partial V}{\partial k} = \frac{1}{h^2} \frac{\partial E}{\partial k}
\]

\[
\Rightarrow m^{-1} = \frac{1}{h^2} \frac{\partial^2 E}{\partial k^2}
\]

\[
m^{-1} = \frac{1}{h^2} \frac{\partial^2 E}{\partial k^2}
\]

\[
\begin{pmatrix}
m_{xx} & m_{xy} & m_{xz} \\
m_{yx} & m_{yy} & m_{yz} \\
m_{zx} & m_{zy} & m_{zz}
\end{pmatrix}
= \frac{1}{h^2}
\begin{pmatrix}
\frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} & \frac{\partial^2 E}{\partial k_x \partial k_z} \\
\frac{\partial^2 E}{\partial k_y \partial k_x} & \frac{\partial^2 E}{\partial k_y^2} & \frac{\partial^2 E}{\partial k_y \partial k_z} \\
\frac{\partial^2 E}{\partial k_z \partial k_x} & \frac{\partial^2 E}{\partial k_z \partial k_y} & \frac{\partial^2 E}{\partial k_z^2}
\end{pmatrix}
\]
\[
\frac{dV}{dt} = \frac{m^{-1} F}{E} \equiv \frac{1}{m^{*}} = \text{RECIPROCAL EFFECTIVE MASS TENSOR}
\]

\[
\frac{dV}{dt} = \frac{m^{-1} \dot{E} \varepsilon}{E} \equiv \frac{1}{m^{*}} = \text{RECIPROCAL EFFECTIVE MASS TENSOR}
\]

\[
\frac{dV}{dt} = \frac{\varepsilon}{E} \frac{\varepsilon}{E} \Rightarrow m_{xy}^{-1} = \frac{1}{h^{2}} \frac{\varepsilon}{E} \frac{\varepsilon}{E}
\]

\[
E = \hbar \varepsilon
\]

\[
\Rightarrow \dot{V} = \frac{1}{h^{2}} \nabla_{E} \varepsilon
\]

\[
\varepsilon = \frac{1}{h} \frac{\varepsilon}{E} \frac{\varepsilon}{E} \Rightarrow m_{xy}^{-1} = \frac{h^{2}}{\varepsilon_{xy} \varepsilon_{xy}}
\]

\[
\Rightarrow M_{xy} = \frac{h^{2}}{\varepsilon_{xy} \varepsilon_{xy}}
\]

\[
\begin{bmatrix}
\frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\
\frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\
\frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}}
\end{bmatrix} = \frac{1}{h^{2}}
\begin{bmatrix}
\frac{\varepsilon_{xx}}{E} & \frac{\varepsilon_{xy}}{E} & \frac{\varepsilon_{xz}}{E} \\
\frac{\varepsilon_{yx}}{E} & \frac{\varepsilon_{yy}}{E} & \frac{\varepsilon_{yz}}{E} \\
\frac{\varepsilon_{zx}}{E} & \frac{\varepsilon_{zy}}{E} & \frac{\varepsilon_{zz}}{E}
\end{bmatrix}
\]
TWO DIMENSIONAL DENSITY OF STATES

\[ d n^{(2)} = \frac{1}{2\pi} \int \frac{d\mathbf{p}}{\mathbf{p}_T} \int dE \frac{1}{\sqrt{E}} \text{ for } E > 0 \]

IN THREE DIMENSIONS

\[ d n^{(3)} = \frac{1}{6} (4\pi n^2) \int d\mathbf{p} \int dE \frac{1}{\sqrt{E}} \text{ for } E > 0 \]

\[ = \frac{1}{6} (4\pi \frac{2m^2}{h^2} \frac{E}{\hbar^2} \frac{1}{\sqrt{E}}) \int dE \frac{1}{\sqrt{E}} \]

\[ = \frac{1}{6} m^2 \frac{1}{\hbar^2} \frac{1}{\pi^2} \int dE \frac{1}{\sqrt{E}} \]

\[ = \frac{1}{6} \left( \frac{m^2}{\hbar^2} \right)^3 \int dE \frac{1}{\sqrt{E}} \]

IN TWO DIMENSIONS

\[ d n^{(2)} = \frac{1}{4} (2\pi n) \int d\mathbf{p} \int dE \frac{1}{\sqrt{E}} \text{ for } E > 0 \]

\[ = \frac{1}{4} (2\pi \frac{\sqrt{2m}}{\hbar} \frac{1}{\sqrt{E}}) \int dE \frac{1}{\sqrt{E}} \]

\[ = \frac{1}{4} \frac{\sqrt{2m}}{\hbar} \int dE \frac{1}{\sqrt{E}} \]

\[ \Rightarrow d n^{(2)} = \frac{m}{\hbar} \left( \frac{1}{\hbar} \right)^2 \int dE \frac{1}{\sqrt{E}} \]
\[ n(E) = A \int_{E_c}^{\infty} e^{-\frac{(E-E_c)}{kT}} \, dE \]

where \( A \) is constant.

\[ n(E) = A \int_{E_c}^{\infty} e^{-\frac{E}{kT}} \, dE = \frac{A}{kT} \left( e^{-\frac{E_c}{kT}} - e^{-\frac{E}{kT}} \right) \]

Let \( \frac{E}{kT} = \varphi \)

\[ d\varphi = \frac{dE}{kT} \Rightarrow dE = kT \, d\varphi \]

\[ n(E) = 2kTA \int_{E_c}^{\infty} e^{-\varphi} \, d\varphi \]

\[ n(E) = 2kTA \left( e^{-\varphi} \right) \bigg|_{E_c}^{\infty} = \frac{2kTA}{e^{\frac{E_c}{kT}}} \]

\[ A = \frac{1}{2} \left( \frac{2kT}{Z} \right)^{3/2} \]
At the Brillouin zone boundary,

\[ K = \frac{2\pi}{2d} = \frac{2\pi}{\lambda} \]

For \( d = \frac{1}{2} \lambda = 0.5 \times 10^{-8} \text{cm}, \)

\[ K = \pi \times 10^8 \frac{\text{rad}}{\text{cm}} \quad (\lambda = 5 \times 10^{-7} \text{cm}) \]

1. \( E = 50 \text{ meV} \)

\[ E = h \nu = \frac{h c}{\lambda} = \frac{50 \times 10^{-3} \text{eV}}{1.054 \times 10^{-37} \text{ergs sec} \cdot \text{cm} / \text{sec} \cdot \text{J} \times \left( \frac{1.6 \times 10^{-19} \text{J}}{1 \text{eV}} \right)} \]

\[ = 7.590 \frac{\text{rad}}{\text{cm}} = 2502 \frac{\text{rad}}{\text{cm}} \]

2. \( E = 3 \text{ eV} \)

\[ E = \frac{h \nu}{k} = \frac{1.054 \times 10^{-37} \text{ergs sec} \cdot \text{cm} / \text{sec} \cdot \text{J}}{1.6 \times 10^{-19} \text{J}} \]

\[ = 4.54 \times 10^5 \frac{\text{rad}}{\text{cm}} \]

\[ = 1.52 \times 10^5 \frac{\text{rad}}{\text{cm}} \]
\[ w^2 = u'' \left[ \frac{2}{m} \pm \sqrt{\left( \frac{2}{m} \right)^2 - \left( \frac{2}{m^2} \lambda m \right)^2} \right] \]

\[ m_1 = m_2 = m \]

\[ w_1^2 = \frac{2}{m} \left[ 1 \pm \cos k_0 \right] \]

\[ w_2^2 = \frac{2}{m} \left( 1 \pm \cos k_0 \right) \]

\[ w_+ = \frac{2}{m} \left[ 1 - \cos k_0 \right] \]

\[ w_- = \frac{2}{m} \left[ 1 + \cos k_0 \right] \]

\[ \omega = \frac{2}{m} \sin \frac{k_0}{2} \]

\[ \omega = \frac{2}{m} \cos \frac{k_0}{2} \]

\[ V_g = \text{GROUP VELOCITY} = \frac{dw}{d\omega} \]

**OPTICAL BRANCH:**

\[ V_g^+ = \pm \frac{4}{m} \sin \frac{k_0}{2} \]

**ACOUSTIC BRANCH:**

\[ V_g^- = \pm \frac{4}{m} \cos \frac{k_0}{2} \]
\[ H_0 = 2 \int_{-\infty}^{\infty} e^{-x^2} \, dx = \sqrt{\pi} \]

\[ H_1 = 2 \int_{-\infty}^{\infty} x e^{-x^2} \, dx = 0 \]

\[ H_2 = 2 \int_{-\infty}^{\infty} x^2 e^{-x^2} \, dx = 2 \int_{-\infty}^{\infty} (4e^{-x^2} - 2x^2 e^{-x^2}) \, dx = 2 \int_{-\infty}^{\infty} e^{-x^2} \, dx = \sqrt{\pi} \]

\[ H_3 = 2 \int_{-\infty}^{\infty} x^3 e^{-x^2} \, dx = 2 \int_{-\infty}^{\infty} (8e^{-x^2} - 12xe^{-x^2}) \, dx = 2 \int_{-\infty}^{\infty} e^{-x^2} \, dx = \sqrt{\pi} \]

\[ \cdots \]

\[ H_n = (2n)! \int_{-\infty}^{\infty} x^n e^{-x^2} \, dx = 2^n n! \sqrt{\pi} \]

\[ \text{It follows that} \]

\[ \int_{-\infty}^{\infty} x^n e^{-x^2} \, dx = 2^n n! \sqrt{\pi} \]

\[ \int_{0}^{\infty} x^n e^{-x^2} \, dx = \frac{2^{n/2} n!}{(n+1)!} \sqrt{\pi} \]

\[ \int_{0}^{\infty} x^n e^{-x^2} \, dx = \frac{2^{(n+1)/2} n!}{(n+1)!} \sqrt{\pi} \]
WHAT IS \( C_v \) AT LARGE TEMP.?

\[
C_v = \frac{\delta S}{\delta T} = N K \left( \frac{\hbar w}{K T} \right) \left( \frac{e^{\frac{\hbar w}{K T}}}{e^{\frac{\hbar w}{K T}} - 1} \right)^2
\]

CONSIDER:

\[
e^{\frac{\hbar w}{K T}} = 1 + \frac{\hbar w}{K T} + \frac{1}{2!} \left( \frac{\hbar w}{K T} \right)^2 + \ldots
\]

FOR LARGE \( T \) (AND SINCE \( h \) IS SMALL)

\[
e^{\frac{\hbar w}{K T}} \approx 1 + \frac{\hbar w}{K T}
\]

AND:

\[
e^{\frac{\hbar w}{K T}} - 1 \approx \frac{\hbar w}{K T}
\]

SUBSTITUTING BACK IN

\[
C_v = N K \left( \frac{\hbar w}{K T} \right) \frac{1 + \frac{\hbar w}{K T}}{\left( \frac{\hbar w}{K T} \right)^2}
\]

\[
= N K \left( \frac{K T}{\hbar w} \right) \left( 1 + \frac{\hbar w}{K T} \right)
\]

\[
= N K \left( \frac{K T}{\hbar w} + 1 \right)
\]

BUT UNDER THE ASSUMPTIONS: \( \frac{\hbar w}{K T} \ll 1 \)

THUS \( \frac{K T}{\hbar w} \gg 1 \)

\[
\therefore C_v \approx \frac{N K K T}{\hbar w} \] AT VERY HIGH TEMPERATURES
\[
P(x) = 4 \int_{-\frac{1}{2}}^{\frac{1}{2}} \sqrt{(E - \epsilon)^2 - \frac{1}{4}} \, d\epsilon
\]

\[
\lim_{x \to \frac{1}{2}} \frac{A_{n+1}}{A_n} = \frac{4}{\pi}
\]

\[
P(x) = 4 \int_{-\frac{1}{2}}^{\frac{1}{2}} \sqrt{(E - \epsilon)^2 - \frac{1}{4}} \, d\epsilon
\]

\[
\Rightarrow P(x) = \frac{4}{\pi} \int_{-\frac{1}{2}}^{\frac{1}{2}} \sqrt{(E - \epsilon)^2 - \frac{1}{4}} \, d\epsilon
\]
Given $r_0 = \sqrt{6}$

$$r^*= r \left(1 + i \lambda \right)$$

$$r = \frac{r_0}{\sqrt{2}} \left[ \varepsilon + \left( \varepsilon^2 + \frac{16 \pi^2 \omega^2}{\omega^2} \right)^{\frac{1}{2}} \right] \frac{1}{2}$$

$$\gamma = \sqrt{1 - \frac{\varepsilon}{r^2}} \quad \lambda = 5000 \text{A}$$

Find $\sigma$ such that

$$\left| \frac{r^*}{r_0} \right| = \frac{1}{10}$$

$$\left| \frac{r^*}{r_0} \right| = \frac{r^*}{r_0}$$

$$\left| \frac{r^*}{r_0} \right| = \frac{\sqrt{6}}{10}$$

$$\left| \frac{r^*}{r_0} \right| = (\frac{\sqrt{6}}{10})^2 r_0^2$$

$$r^2 = (\frac{\sqrt{6}}{10})^2 \varepsilon$$

$$\text{ONWARD: } \left| r^* \right|^2 = r^2 (1 + \lambda^2)$$

$$= r^2 (1 + \left(1 - \frac{\varepsilon}{r^2}\right))$$

$$= r^2 (2 - \frac{\varepsilon}{r^2})$$

$$= 2r^2 - \varepsilon$$

Thus:

$$2r^2 - \varepsilon = (\frac{\sqrt{6}}{10})^2 \varepsilon$$

$$2r^2 = \left[ 1 + (\frac{\sqrt{6}}{10})^2 \right] \varepsilon$$

$$r^2 = \frac{1}{2} \left[ 1 + (\frac{\sqrt{6}}{10})^2 \right] \varepsilon$$

$$\frac{1}{2} \left[ \varepsilon + \left( \varepsilon^2 + \frac{16 \pi^2 \omega^2}{\omega^2} \right)^{\frac{1}{2}} \right] = \frac{1}{2} \left[ 1 + (\frac{\sqrt{6}}{10})^2 \right] \varepsilon$$

$$\varepsilon + \left( \varepsilon^2 + \frac{16 \pi^2 \omega^2}{\omega^2} \right)^{\frac{1}{2}} = \left[ 1 + (\frac{\sqrt{6}}{10})^2 \right] \varepsilon$$

$$\varepsilon + \frac{16 \pi^2 \omega^2}{\omega^2} = \left( \frac{\sqrt{6}}{10} \right)^4 \varepsilon$$

$$\varepsilon^2 + \frac{16 \pi^2 \omega^2}{\omega^2} = \left( \frac{\sqrt{6}}{10} \right)^4 - 1 \varepsilon^2$$

$$\sigma^2 = \frac{\omega^2}{4 \pi^2} \left[ \left( \frac{\sqrt{6}}{10} \right)^4 - 1 \right] \varepsilon^2$$

$$\sigma = \frac{\omega}{4 \pi} \left[ \left( \frac{\sqrt{6}}{10} \right)^4 - 1 \right] \varepsilon$$

$$\omega = \frac{2 \pi \varepsilon}{\lambda}$$

$$\Rightarrow \sigma = \frac{1}{4 \pi} \left( \frac{2 \pi \varepsilon}{\lambda} \right) \sqrt{\left( \frac{\sqrt{6}}{10} \right)^4 - 1} \varepsilon$$

$$\Rightarrow \frac{\varepsilon \omega}{2 \pi} \sqrt{\left( \frac{\sqrt{6}}{10} \right)^4 - 1} \varepsilon \text{ NEED TO KNOW } \varepsilon$$
Reflection Coefficient Derivation

\[ \begin{align*}
E_i & = E_{i0} e^{-i \omega t r_1 + \phi_1} \\
H_i & = H_{i0} e^{-i \omega t r_1 + \phi_1}
\end{align*} \]

\[ \begin{align*}
E_r & = E_{r0} e^{+i \omega t r_2 + \phi_2} \\
H_r & = H_{r0} e^{+i \omega t r_2 + \phi_2}
\end{align*} \]

Reflected
\[ \begin{align*}
E_r & = E_{r0} e^{+i \omega t r_2 + \phi_2} \\
H_r & = H_{r0} e^{+i \omega t r_2 + \phi_2}
\end{align*} \]

"Sign since pointing vector is to left"

Boundary Conditions:
1. \[ E_i(0) = E_0(0) + E_r(0) \Rightarrow E_{i0} = E_{r0} + E_{r0} \]
2. \[ H_i(0) = H_0(0) + H_r(0) \Rightarrow H_{i0} = H_{r0} + H_{r0} \]

Then, \[ E_{r0} = \frac{r_1^*}{r_2^*} (E_{i0} + E_{r0}) \]

Substituting into 1:
\[ E_{i0} = E_{r0} + \frac{r_1^*}{r_2^*} (E_{r0} + E_{i0}) \]
\[ E_{i0} (1 - \frac{r_1^*}{r_2^*}) = E_{r0} (1 + \frac{r_1^*}{r_2^*}) \]

\[ \frac{E_{i0}}{E_{r0}} = \frac{1 - \frac{r_1^*}{r_2^*}}{1 + \frac{r_1^*}{r_2^*}} = \frac{r_2^* - r_1^*}{r_2^* + r_1^*} \]

\[ R = \left| \frac{E_{i0}}{E_{r0}} \right|^2 = \left| \frac{r_2^* - r_1^*}{r_2^* + r_1^*} \right|^2 \]
\[ = \left( \frac{r_1 - r_2 + i(r_1 \delta_1 - r_2 \delta_2)}{r_1 + r_2 + i(r_1 \delta_1 + r_2 \delta_2)} \right)^2 \]
\[ = \frac{(r_1 - r_2)^2 + (r_1 \delta_1 - r_2 \delta_2)^2}{(r_1 + r_2)^2 + (r_1 \delta_1 + r_2 \delta_2)^2} \]
**SPECIAL CASE: $\sigma = 0$**

$\Rightarrow \gamma_1 = \sqrt{\epsilon_1} \quad , \quad \gamma_2 = \sqrt{\epsilon_2}
\gamma_1 = 0 \quad , \quad \gamma_2 = 0.$

$\therefore R = \left(\frac{\sqrt{\epsilon_1} - \sqrt{\epsilon_2}}{\sqrt{\epsilon_1} + \sqrt{\epsilon_2}}\right)^2$

**SPECIAL CASE: VACUUM/METAL INTERFACE**

**MEDIUM 1:** VACUUM: $\gamma_1 = \sqrt{\epsilon_1} \quad , \quad \gamma_1 = 0, \quad \gamma_1 = 0$

**MEDIUM 2:** METAL: $\epsilon_2, \sigma_2$

$\gamma_2 = \sqrt{1 - \epsilon_2 / 1} \quad , \quad \gamma_2 = \sqrt{\epsilon_2}
\gamma_1 = \sqrt{2} \sqrt{\epsilon_1 + \left(\frac{\pi^2 \sigma_2^2}{\epsilon_2}\right)^2}

AND

$R = \left(\frac{\sqrt{\epsilon_1} - \gamma_2}{\sqrt{\epsilon_1} + \gamma_2}\right)^2 + \left(\frac{\gamma_2 \delta_2}{\sqrt{\epsilon_1}}\right)^2$
IN A HOMOGENEOUS ISOTROPIC MEDIA
OF PERMITTIVITY, DIELECTRIC CONSTANT $\varepsilon$, AND CONDUCTIVITY $\sigma$, TWO OF MAXWELL'S
EQUATIONS ARE
\[
\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J},
\]
\[
\nabla \times \mathbf{E} = -\frac{\varepsilon}{\mu} \frac{\partial \mathbf{H}}{\partial t}.
\]

BUT \( \mathbf{J} = \sigma \varepsilon \mathbf{E} \) AND \( \mathbf{B} = \mu \mathbf{H} \)

\[
\Rightarrow \nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \sigma \varepsilon \mathbf{E} \quad (1)
\]
\[
\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \quad (2)
\]

TAKING THE CURL OF (2): (WITH VECTOR IDENTITY)
\[
\nabla \times (\nabla \times \mathbf{E}) = \nabla (\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E}
\]

ASSUMING NO FREE CHARGE IN CONDUCTOR: \( \nabla \cdot \mathbf{E} = 0 \)
\[
\Rightarrow \nabla \times (\nabla \times \mathbf{E}) = -\nabla^2 \mathbf{E} = -\frac{1}{\varepsilon} \frac{\partial}{\partial t} \nabla \times \mathbf{H}
\]
\[
\Rightarrow \frac{\partial}{\partial t} \nabla \times \mathbf{H} = \frac{1}{\mu} \nabla^2 \mathbf{E} \quad (3)
\]

FROM (1):
\[
\frac{\partial}{\partial t} \nabla \times \mathbf{H} = \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \sigma \varepsilon \mathbf{E} \quad (4)
\]

EQUATING (3) AND (4):
\[
\frac{1}{\mu} \nabla^2 \mathbf{E} = \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \sigma \varepsilon \mathbf{E}
\]
\[
\nabla^2 \mathbf{E} = \varepsilon \mu \frac{\partial^2 \mathbf{E}}{\partial t^2} = \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2}
\]

BUT \( \frac{1}{\varepsilon} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \sigma \varepsilon \mathbf{E} \)
\[
\Rightarrow \nabla^2 \mathbf{E} = \frac{1}{\varepsilon} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \varepsilon \mu \frac{\partial^2 \mathbf{E}}{\partial t^2}
\]

THIS IS THE DESIRED RESULT.
TIGHT BINDING APPROXIMATION FOR ELECTRONS IN METALS

The tight binding approximation is good for the outer electrons of metals, but not particularly good for conduction electrons. Roughly, the method starts with the wave functions of a number of free neutral atoms, as the atoms move towards each other (in a mental picture), the wave functions overlap. One then looks at all linear combinations of these bound atom's wave functions and computes the resulting allowable energy levels.

As an example, consider the following sketch of two identical atoms with corresponding wave functions:

\[ \psi_1 \quad \psi_2 \]

Such a representation is characteristic of, say, two hydrogen atoms at the ground state. As the atoms move closer together, the wave functions overlap to give two possible wave function combinations:

\[ \phi = \psi_1 + \psi_2 \]
\[ \phi = \psi_1 - \psi_2 \]

\( \phi \) is read "proportional to" (proportionality constant determined via normalization)
EXTRA

DISCUSSION OF EXCHANGE TERM

First, Hartree's two-electron wave function: \( \Psi_{\text{H}}(x_1, x_2) = \Phi_1(x_1) \Phi_2(x_2) \). This relationship assumes two states \( \Phi_1, \Phi_2 \) and two electrons respectively at "positions" \( x_1 \) and \( x_2 \). It assumes the electrons are distinguishable. That is, electron one is always in state \( \Phi_1 \) and electron two is always in state \( \Phi_2 \). The choice of this product form does not allow one to take into account the correlation in the in the motion of the electrons. Fock's method allows such a treatment. We have:

\[
\Psi_{\text{F}}(x_1, x_2) = \frac{1}{2} \left[ \Phi_1(x_1) \Phi_2(x_2) - \Phi_1(x_2) \Phi_2(x_1) \right]
\]

Here, we take into account all possible arrangements, electron one in state one and electron two in state two, or electron two in state one and electron one in state two, but not both at once (this, of course, is due to Pauli's exclusion principle). In a very rough sense, Fock's expression is the probabilistic sum on mutually exclusive events, discarding terms such as \( \Phi_1(x_1) \Phi_1(x_2) \) which violate the exclusion principle and terms such as \( \Phi_1(x_1) \Phi_2(x_1) \) which violate reason.
Tight Binding Approximation for Electrons in Metals

The tight binding approximation is good for the inner electrons of atoms, but not particularly good for conduction electrons. Roughly, the method starts with the wave functions of a number of free neutral atoms. As the atoms move towards each other (in a mental picture), the wave functions overlap. One then looks at all linear combinations of the bound atom's wave functions and computes the resulting allowable energy levels.

As an example, consider the following sketch of two identical atoms with corresponding wave functions:

\[ \psi_1 \quad \psi_2 \]

Such a representation is characteristic of, say, two hydrogen atoms at the ground state. As the atoms move closer together, the wave functions overlap to give two possible wave function combinations:

\[ \psi_+ = \psi_1 + \psi_2 \]
\[ \psi_- = \psi_1 - \psi_2 \]

"\( \psi_+ \) is zero proportional to " (proportionality constant determined via normalization)
SKETCHES OF THESE FUNCTIONS ARE ROUGHLY

\[ \phi^+ \quad \phi^- \]

CONSIDER FIRST, \( \phi^+ \), THE ELECTRON WILL SPEND MUCH OF ITS TIME MIDWAY BETWEEN THE ATOMS AT A LOWER ENERGY AS COMPARED TO \( \phi^- \), WHERE THE ELECTRON IS NEVER AT THE MIDPOINT, THUS \( \phi^- \) HAS A LOWER CORRESPONDING ENERGY THAN \( \phi^- \).

EXTENSION OF THIS METHOD THEN, TO A LARGE NUMBER OF ATOMS, IS THE TIGHT BONDING APPROXIMATION. AS N ATOMS ARE Brought CLOSE TOGETHER, THERE WILL RESULT N ENERGIES EACH ASSOCIATED WITH ONE OR MORE ENERGY BANDS. ONE MUST GENERALLY ALLOW FOR VARIOUS ORBITALS, ENERGY SPITTING, AND OTHER STUFF IN SUCH A COMPUTATION.

AS MENTIONED, THE TIGHT BAND APPROXIMATION IS "THOUGHT" TO BE QUITE GOOD FOR INNER ELECTRONS OF ATOMS, SUGGESTING THAT COMPUTATION AND THEORY
For this case historically agree. A similar statement holds for its less successful role in describing conduction electrons. It has been employed to approximately describe the d bands of transition metals, and the valence bands of inert gas crystals.

Ref: Kittel, Introduction to Solid State Physics.
Ebers-Moll Model of Transistor Current

We will here consider a PNP (Junction) Transistor formed by joining two diodes at their N junctions. Bias is appropriately applied.

Consider, first, the forward biased emitter which increases the number of holes in the N-doped material at the emitter-base junction. The totality of these holes may be determined by a Boltzmann factor:

\[ P_{\text{tot}} = P_n \left(1 + e^{\frac{V_E}{kT}}\right) \]  \( (1) \)

Where \( P_n \) is the junction's intrinsic hole density. We may write equivalently

\[ \Delta P_E = P_n \left(e^{\frac{V_E}{kT}} - 1\right) \]  \( (2) \)

Where \( \Delta P_E \) is the "excess" hole
Density resulting from the forward bias voltage $V_b$.

In a similar fashion, the excess hole density at the collector junction is

$$\Delta P_c = P_n \left( e^{eV_b/kt} - 1 \right)$$

(3)

Note, however, that $V_c < 0$, and, accordingly, $\Delta P_c < 0$.

Now, a portion of the holes at the emitter junction will stray from the junction and undergo some recombination during their diffusion. The electrons required for this recombination are supplied externally by the base. Thus, controlling the base current controls the available recombination electrons, and the number of holes reaching the collector is controlled by the base current.
ASSUMING THE VOLTAGE DROP OCCURS PRIMARILY ACROSS THE JUNCTION, ONE MAY USE BOLTZMANN FACTOR REASONING TO WRITE

\[ I_c = -\alpha I_{E0} \left( e^{\frac{V_E}{kT}} - 1 \right) - I_{C0} \left( e^{\frac{V_C}{kT}} - 1 \right) \]

HERE, THE PROPORTIONALITY CONSTANT IS

\[ \alpha = \text{FORWARD CURRENT TRANSPORT FACTOR (CURRENT GAIN)} \]

\[ \text{EXCESS COLLECTOR CURRENT} \]

\[ = \text{EMITTER CURRENT} \]

FOR LARGE VALUES OF BIAS

\[ -I_c = \alpha I_E + I_{C0} \]

SIMILARLY THE BASE CURRENT:

\[ -I_B = (1 - \alpha) I_E - I_{C0} \]

THE TRANSISTOR \( \beta \) IS FOUND FROM

\[ -I_c = \beta I_B + \frac{I_{E0}}{1 - \alpha} \]

\[ \beta = \frac{\alpha}{1 - \alpha} \]

WE HAVE NOTED THAT A LARGE COLLECTOR CURRENT IS CONTROLLED BY A SMALL BASE CURRENT. THIS BECOMES SMALLER AS \( \alpha \) NEARS 1.

IT CAN BE SHOWN THAT, FOR A NARROW BASE REGION (\( w_B < L_p \)):

\[ \alpha = 1 - \left( \frac{w_B}{L_p} \right)^2 \]
1. Set up an expression for the number of holes in the valence band of a semiconductor, assuming pure material. Describe each term.

2. What is the Fermi energy? How is it determined? What is the effect of doping?

3. Describe qualitatively the phonon and electron energy level structure of a solid.

4. Solve the Schrödinger equation for \( V = \infty \), \( V = 0 \), \( V \), and obtain an energy formula.
1. \( n = \text{holes in the valence band} \)
   \[ = N \nu \left[ e^{-(E_f - E_V)/kT} \right] \text{ for small } T \]
   \[ \text{from } \frac{h}{c} = \int_{-\infty}^{\infty} \frac{n(E)dE}{\mu - E} \]
   \[ h = c \int_{\text{valence band}} \frac{n(E)dE}{E - E_f/kT} \]
   \[ c = \text{const} \]
   \[ h = c \int_{\text{valence band}} e^{-(E - E_f)/kT} \text{ for small } T \]

\( n(E) = \text{dens. of states} \)
\( f(E) = \text{Fermi distribution} \)
\[ n(E) = \left[ 1 - f(E) \right] \rho(E) \]
\( \rho(E) = \# \text{holes as a function of } E. \)
2. The Fermi energy is the energy of a solid which at 0°K, all energy is below it. At 0°K, the Fermi level is at the mean energy levels. Doping changes the Fermi energy level. Donor doping will increase it and acceptor doping will decrease it.
3. Electrons may only have quantized energy. Roughly, an electron can be
1. In the valence band (why aren't e's are)
2. Within an acceptor
3. In the conduction band
   Conduction Band
   Acc. Level

Similarly, a hole can lie at the top of the valence band (instead of acceptor)
An electron in the conduction band may combine with a hole in the valence band, producing a phonon and a photon.

Before

\[ E \text{ in electron band} \]

After

\[ E \text{ in photon} \]

That is:

\[ h\nu + E_{\text{CB}} = P_{\nu} + \text{PHONON} \]

In this interaction, momentum must be conserved. The phonon velocity is very low and the light \( \nu \) is very high.
\[
\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{2mE}{\hbar^2} \psi = 0
\]

\[
\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - k^2 \psi = 0 \quad k^2 = \frac{2mE}{\hbar^2}
\]

\[
\psi = A \cos kx + B \sin kx
\]

\[
y(0) = 0 \Rightarrow A = 0
\]

\[
y = B \sin kx
\]

\[
y(0) = 0 \Rightarrow k = \frac{\pi n}{a}
\]

\[
\Rightarrow \psi = B \sin kx
\]

Set \( B \) from \( \int_0^a B^2 \sin^2 \frac{\pi n x}{a} dx = 1 \)

Anyway
\[
k^2 = \frac{\pi^2 n^2}{a^2} = \frac{2mE}{\hbar^2}
\]

\[
\Rightarrow E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2}
\]
Solve 4 only

\[ \sqrt{\text{give as complete a derivation as possible, making necessary assumptions, of the Wiedemann-Franz ratio for metals}} \]

\[ \frac{K}{\sigma T} = \frac{\pi^2}{3} \frac{k^2}{e^2} \]

(2) Consider a lattice of atoms with nearest neighbors at \( a(1,1,1), a(1,-1,-1), a(-1,-1,1), a(-1,1,-1) \). Assuming an interaction between nearest neighbors only (for electrons tightly bound), obtain an expression for \( \varepsilon(k) \).

Let \( V = 1 \) for nearest neighbors.

(3) For a solid with atomic polarizability \( \alpha \) and \( \eta \text{ atoms/mo} \), the Clausius-Mosotti equation relates \( \frac{\varepsilon-1}{\varepsilon+2} = \frac{4.17 N \alpha}{3} \).

(4) Describe heat conduction in an insulator.
5) Derive a dispersion relation for a one-dimensional lattice of atoms, mass m, connected by springs, spring constant k, and separated by d.

6) What would the effect of a light impurity be on the vibrational structure of a solid? Assume a impurity, mass m, in place of an atom of a monoatomic solid, mass M, with \( m \ll M \).

7) What atoms would you expect to be donors and acceptors in Si?
1. One starts with the Boltzmann Transport Equation (2-dimensional time variant probability density function \( \rho \))

\[
\n\n\frac{\nabla \cdot \mathbf{J}}{\rho} + \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{v} = -\frac{\partial \rho}{\partial t}/\tau
\]

where \( \mathbf{J} \) is the current density and \( \mathbf{v} \) is the Fermi velocity. One then finds \( n(x) \), the equilibrium density, from

\[
n(x) = \int \rho(x, y, z, v_x, v_y, v_z) \, dv_x \, dv_y \, dv_z
\]

where \( \rho(x, y, z, v_x, v_y, v_z) \) is the equilibrium PDF. The Widom-Maxwell-Ferry ratio employs the Fermi-Dirac distribution for \( \rho \)

\[
n(x) = \left[ 1 + e^{(E - EF)/kT} \right]^{-1}
\]

where \( E = \frac{p^2}{2m} + \mu \) and \( E_F \) is the Fermi energy. You then find \( J_x \), the current density.

\[
J_x = \int \rho(x, y, z, v_x, v_y, v_z) \, v_x \, dv_x \, dv_y \, dv_z
\]

This gives you something like

\[

\frac{\partial \rho}{\partial t} = \nabla \cdot \mathbf{J}
\]

The thermal current density \( C_x \) is analogously computed.

\[
C_x = \int \rho(x, y, z, v_x, v_y, v_z) \, v_x \, dv_x \, dv_y \, dv_z
\]

Free electrons are assumed.

\( \tau \) is the relaxation time. The resulting thermal conductivity \( K \) is

\[
K = \frac{\pi^2 k^2}{3} n \tau (E_F)
\]

Taking the ratio gives the W-F ratio

\[
\frac{K}{\sigma T} = \frac{\pi^2 k^2}{3} \frac{k^2}{\rho^2}
\]
4. The diffusion of heat is described by the differential equation:
\[
\nabla^2 T = \frac{C}{\rho c} \frac{\partial T}{\partial t}
\]
where \( \rho \) is the density, \( c \) is the specific heat, and \( k \) is the thermal conductivity. An example (derived in class) describing heat diffusion was illumination of a material with a Gaussian beam \( I = I_0 e^{-r^2/2R^2} \) for a short time, and watching how the temperature changed. 0 radially and 2 in the \( z \) direction.

\[
J(\mathbf{r}, t) = -\alpha \frac{\partial T}{\partial z}
\]
where \( \alpha = \left( 1 + \frac{2KT}{\rho c \sigma^2} \right)^{-1} \)
that is, the temperature spread outward (in r) at an inward exponential manner determined by the material's intrinsic constants. We noted that:

1. \( T(r, t) = T_0 e^{-r^2 / 2\sigma^2 t} \)

2. For the \( r = 0 \) direction, after going through some Fourier cosine x form stuff, we found that:

\[
T(0, t) = T_0 e^{-r_0^2 \sigma^2 t}
\]

where \( r_0 \) was an initial condition parameter:

\[
T(0, \sigma) = r_0
\]

Here again, describing is governed solely by the intrinsic behavior of the material.
\[ F = k u \quad k = \text{spring constant} \]

One considers, to an approximation, the interaction of atom \( n \) with atoms \( n-1 \) and \( n+1 \) (i.e., only with the nearest neighbors).

This gives one to two simultaneous differential equations with two arbitrary constants. Taking the determinate and setting to zero will give these constants and leaves one with something proportional to \( \sin k a \).

To the first Brillouin zone.

This also gives a light band. The mass \( m \), determines the curve's intersection at the Brillouin boundaries.
1. A donor in Si would be an element with five electrons in its conduction shell. Similarly, an acceptor should have three electrons in its conduction shell.
WANG: SOLID STATE ELECTRONICS (TEXT)

Kittel: SOLID STATE PHYSICS

P. Bube: ELECTRONIC PROPERTIES OF CRYSTALLINE SOLIDS

J.C. Phillips: BONDS AND BANDS IN SEMICONDUCTOR SOLIDS. AREAS:

- DEVICES: JUNCTION, FETS, D.C., LEDS, LEDs, IMPATT, SWITCHES, ETC.
- PROPERTIES OF SOLIDS: MAGNETICS, LUMINESCENCE, ELECTRICAL, OPTICAL
- QUANTUM ELECTRONICS: SOLID STATE LASERS, Q-SWITCH, OPTICAL THIN FILMS, INTEGRATED OPTICS
- FUNDAMENTAL PROPERTIES: LATTICE RESONANCES, BAND STRUCTURE, LINEAR AND NONLINEAR INTERACTIONS OF LIGHT WITH MATTER
- DEFECTS AND IMPURITIES: LOOPS, ACCEPTORS, ATR ACTIONS, BURL, EXTRONS
- SUPERCONDUCTIVITY: BCS THEORY OF JOSEPHSON JUNCTION
- SURFACE PROPERTIES
- THERMAL PROPERTIES
- METHODS OF STUDY

H.W. READ TO PG. 12, IN TEXT
WAVE AND PARTICAL NATURE OF MATTER

\[ \text{Einstein: } E = h \nu \]
\[ h = \text{Planck's constants} \]
\[ \nu = \frac{c}{\lambda} \]

Schrödinger's Eq'n

\[ \frac{-h^2}{2m} \nabla^2 \psi + \nu(\nu) \psi = E \psi \]

9-5-75 (THURS)

COMPTON EFFECT

\[ \begin{array}{c}
\text{\(E_{\text{photon}} = h \nu = \hbar \omega\)} \\
\text{\(P_{\text{photon}} = \hbar \mathbf{k} \)} \\
\text{\(\hbar = \frac{h}{2\pi} \)} \\
\text{\(k = \frac{\lambda}{\hbar} \)} \\
\text{\(\lambda = \text{wavelength} \)} \\
\text{\(k = \text{Boltzmann's constant} \)} \\
\text{\(h = \text{Planck's constant} \)} \\
\text{\(\omega = 2\pi \nu \)}
\end{array} \]

To solve, use RELATIVISTIC KINEMATICS.

\[ \text{4. Momentum} \]

\[ \text{For electron, } [E, P_x, P_y, P_z] \]
\[ [E, P_x, P_y, P_z] \cdot [E, P_x, P_y, P_z] = E^2 - P^2 \]
\[ = E^2 - m^2 \]

Here, \( c \approx 1 \)
\[ E = m \]
\[ \Rightarrow E^2 - P^2 = m^2 - P^2 \]

Back to problem:

\[ k_1 = [\omega_1, 0, 0, 0] \]
\[ P_1 = [m, 0, 0, 0] \]
\[ k_2 = [\omega_2, 0, 0, 0] \]
\[ P_2 = [E_2, 0, 0, 0] \]

Now, to conserve energy:

\[ P_1 + k_1 = P_2 + k_2 \]
\[ \Rightarrow P_2 = P_1 + k_1 - k_2 \]
\[ P_2^2 = (P_1 + k_1 - k_2)^2 \]
\[ = P_1^2 + k_1^2 + k_2^2 + 2P_1 \cdot k_1 - 2P_1 \cdot k_2 \]
\[ = -2k_1 \cdot k_2 \]
\[ m^* = m_e + \alpha + 2\beta \cdot \vec{k} = 2 \beta \cdot \vec{k} - 2 \beta \cdot \vec{k} = \alpha \]

\[ \Rightarrow \vec{q} \cdot \vec{k} = \beta \cdot \vec{k} + \beta \cdot \vec{k} = m_e \vec{u} + m_e \vec{u} [1 - \cos \theta] \]

\[ \vec{u}_2 - \vec{u}_1 = \frac{1}{m} [1 - \cos \theta] \Rightarrow \text{Compton Scattering} \]

**The Bohr Atom**

**Hydrogen Spectra**

\[ \text{Characteristic Frequencies} \]

**Method of Attack**

- **Electron**
- **Einstein Equation**
- **Angular Momentum**

\[ E = \frac{1}{2} m \nu^2 + \frac{2 e^2}{r} \]

K.E. Potential

Coulomb Force must equal Mechanical Force

\[ \frac{m \nu^2}{r} = \frac{2 e^2}{4 \pi \varepsilon_0 r^2} \]

- **Angular Momentum**

\[ L = \text{Angular Momentum} = m \nu \times \nu = m \nu \nu (= r \hat{r}) \]

From Planck's Work, Bohr knew light of freq. y had energy \( E = h \nu \)

And from discrete orbits assumption: \( E_2 - E_1 = h \nu \)

\[ \Rightarrow L = \frac{\hbar}{\nu} \]
So, important equations:

\[ E = \frac{h}{m} \cdot \frac{1}{r^2} + \frac{Z}{r} \quad \text{Energy of E} \]
\[ \frac{1}{r} = \frac{Z}{e} \quad \text{Force} \]
\[ L = \frac{h}{2\pi} \quad \text{Angular momentum assumption} \]
\[ E_n - E_1 = \hbar \]

Solving for \( E \) gives:

\[ E_n = \hbar \left( \frac{\pi^2}{32} \right) \quad \text{Orbital energy} \]

\[ E_n - E_m = E = \text{Photon energy} \]
\[ n = \frac{mZ^2e^4}{32\pi^2\hbar^2} \left( \frac{1}{n^2} - \frac{1}{m^2} \right) \]

9-8-75 (Mon)

Homework: Due Mon 9-15-75

Text problems: 1.4, 1.5, 1.7, 1.11, 1.15

(4) Make an energy level diagram for the Bohr atom.

Notes: \( E = h\nu = R \left( \frac{1}{n^2} - \frac{1}{m^2} \right) \quad n, m > 0, n, m \in \text{integer} \quad n < m \)

Ionization energy \( \Rightarrow n = 1, m = \infty \)

Then \( E_{\text{max}} = 13.6 \text{ eV} \) \( \Rightarrow \) \( 108,000 \text{ cm}^{-1} \)

Where \( \text{cm}^{-1} \) is a unit of energy.

1 micron = 10^{-6} m (Infrared \( \Rightarrow \) 7.6 x 10^{3}

10,000 Å = 1 μm

Now, \( E = h\nu = h\frac{c}{λ} \)

15,000 Å = # of cm^{-1}

Intensity (Conc. extra electron)

\[ E_{\text{init}} = 13.6 \text{ eV} \times \left( \frac{e^2}{100} \right) \]

\[ E_{\text{final}} = \frac{E_{\text{init}}^2}{2m} \]

\[ E_{\text{final}} \approx 10 \text{ eV} \]
SCHROEDINGER'S EQUATION

ENERGY EQUATION

\( (k.e. + p.e.) \psi(x) = E \psi(x) \)  EIGENVALUE FORM

\( \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) = E \psi(x) \)

GIVES SCHROEDINGER'S EQUATION AS

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi = E \psi \]

WILL GIVE ALLOWED ENERGY STATES IN SOLIDS

SIMPLIEST SOLUTION IS EQU. \( V(r) = 0 \)

CONSIDER IN ONE DIMENSION:

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \]

\[ \frac{d^2 \psi}{dx^2} - \left( \frac{2mE}{\hbar^2} \right) \psi = 0 \]

\[ \frac{d^2 \psi}{dx^2} + k^2 \psi = 0 \]

\[ k^2 = \frac{-2mE}{\hbar^2} \]

TWO SOLUTIONS:

\[ \psi = A e^{ikx} + B e^{-ikx} = A' \cos(kx) + B' \sin(kx) \]

\( k \) CORRESPONDS TO MOMENTUM \( \psi = \frac{hk}{\sqrt{2m}} \)

\[ k = \sqrt{\frac{2mE}{\hbar^2}} \]

Probability if the particle being at point \( x \):

\[ |\psi(x)|^2 \text{ AND } \int |\psi(x)|^2 \, dx = 1 \]

UNCERTAINTY PRINCIPLE: \( \Delta x \Delta p \approx \frac{\hbar}{2} \)
Potential well with infinite walls

\[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \]

For \( V = \infty \), \( \psi = 0 \Rightarrow \psi = 0 \) for \( x \leq 0, x \geq a \)

So boundary conditions are

\[ \psi(0) = \psi(a) = 0 \]

\[ \frac{d\psi(0)}{dx} = \frac{d\psi(a)}{dx} = 0 \] (not valid for of walls)

For \( 0 < x < a \), \( \psi(x) = A\sin(kx) + B\cos(kx) \)

\[ \psi(0) = 0 \Rightarrow B = 0 \]

\[ \psi(a) = 0 \Rightarrow A\sin(ka) = 0 \Rightarrow ka = n\pi \Rightarrow k = \frac{n\pi}{a} \]

(Note that \( E \) can be here solved for specifically,

\[ E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \]

\[ \Rightarrow A^2 \int_0^a \sin^2 kx \, dx = 1 \] gives \( A \)

9-10-75 (Wed)

Energy level structure of a solid

Energy typically 0.0005 eV < E < 5 eV

\[ E \]

Electronic states for electrons

\[ \text{Metal} \]

\[ \text{Empty} \]

\[ \text{Not filled completely} \]

\[ 2-5 \text{ V} \]

\[ \text{Insulator} \]

\[ \text{Filled} \]
SEMICONDUCTOR

(Conduction Band)

Empty

\( \Delta E \) (Small Gap)

Full

Valence Band

\[ E_{\text{gap}} = h \nu_0 \]

Parking Lot Examples of Poles

E Field

\( \Delta E \) (Ex: Avalanche to m\text{g}h)

HOLE POLES

Reason for poles is IMPURITIES

Forbidden Energy Gap

IMPURITY (DONOR):

\( E_{\text{gap}} \) (GAP)

HOLE BAND (< An BAND)
Semiconductor Classes:

IV \text{ III I I V V}

II-V

Cd Ge Ga P S

Zn Sb S As Tl

Se

\[ w = \sqrt{\frac{k}{m}} \]

In crystal

9-12-75 (FRI)

Schrodinger

HARMONIC OSC.: \[-\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{m \omega^2}{2} \psi = E \psi \]

For hydrogen:

\[-\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{e^2}{4 \pi \epsilon_0 r} \psi = E \psi \]

For general atom:

\[-\frac{\hbar^2}{2m} \nabla^2 \psi - \sum_{\alpha} \frac{e^2}{4 \pi \epsilon_0 r_{\alpha}} \psi \]

+ \frac{1}{2} \sum_{\alpha} \frac{e^2}{4 \pi \epsilon_0 r_{\alpha}} \nabla \cdot \nabla \psi = E \psi \]

MATHEW'S EQUATION:

\[ \psi'' + \left( N + \chi \cos 2x \right) \psi = 0 \quad \text{GOOD FOR PERIODICITY} \]

ONE-DIMENSIONAL HARMONIC OSCILLATOR

\[ \text{ACTUAL } V(r) \]

\[ \text{Coulomb FORCE} \]

\[ \text{APPROXIMATE} \]

\[ V(r-r_0) \approx V \left( x \right) \frac{5V}{r_0^3} \left( r-r_0 \right)^3 + \frac{\hbar^2}{2m} \frac{5V}{r_0^3} \left( r \right)^3 \]

\[ V(x) = V_0 + \chi \left( x \right) \frac{5V}{r_0^3} \left( r_0 + \frac{1}{2} \frac{\hbar^2}{m} \frac{5V}{r_0^3} \left( x \right)^3 \right) \]

CONT
\[ V_0 \text{ is a constant (no problem to calculate)} \]
\[ \frac{d^2}{dx^2} \underbrace{X^2}_{\text{minimum}} = 0 \]
\[ \frac{\frac{d^2}{dx^2}}{2} = \underbrace{X^2}_{\text{maximum}} ; \text{ Let } m\omega^2 = \text{constant} = \frac{\hbar^2}{2m} \]
gives:
\[ V(x) = \frac{1}{2} m\omega^2 x^2 \]

\[ \text{approximate well with a parabola} \]
\[ \frac{1}{2} \frac{\hbar^2}{2m} x^2 \text{ is sometimes used.} \]

Schrödinger's eq. for harmonic osc.
\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 = E \chi \]

9-17-75 (Wed) Read chapter 2 up to 2.5

Phase velocity \( \rightarrow k = \frac{\omega}{v_A} \) dispersion \( x^2 \)

Group velocity

Localized particle
\[ \phi(x) = e^{ikx} \]

Group velocity \( \rightarrow \text{velocity} = \frac{dk}{dE} \)

Fermi energy \( \rightarrow \f(E) \) (electrons, Fermi temperature)

Pauli exclusion principle

\[ \f(E) \text{ is velocity of state} \]
\[ \text{as a function of energy} \]
\[ \text{rate of transition} = \frac{1}{\hbar} \iint \phi^* \phi \frac{dE}{\f(E)} \]
EFFECTIVE MASS OF A CRYSTAL

\[ p = E k \]
\[ E = F v \]
\[ F = \frac{m_0}{dE} = q_0 E \]
\[ E = \frac{1}{2m} \frac{v^2}{k^2} \]

\[ F = \frac{dp}{dE} = \frac{dF}{dk} = m \star \frac{dV}{E} = m \star \frac{d}{dk} \frac{dE}{dk} \]
\[ \frac{v^2}{k^2} \frac{dE}{dk} = m \star \frac{d}{dk} \frac{dE}{dk} \]

in 3-d:
\[ m \star g = \frac{\frac{\partial}{\partial r} \cdot E}{\varepsilon r^2} \]

This effective mass is related to intrinsic crystal properties

HARMONIC OSCILLATOR SOLUTION
\[ \frac{\partial^2 u}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi \]
\[ \psi = e^{-\frac{x^2}{2}} \]

Assume solution \( U = \sum \xi_n x^n \)

End up with \( \sum (\xi_0 + \beta \xi_{n+2}) \xi_n = 0 \)
\[ U(x) = 0 \sum \xi_n x^n \]

Get \( \alpha \) \& \( \beta \) normalization

Solution is HERMITE POLYNOMIALS

Turns out \( E_n = (n + \frac{1}{2}) \hbar \omega \)

\[ \frac{E}{\hbar \omega} = \frac{1}{2} \text{ FROM } V = \frac{1}{2} k x^2 \]
9-19-75 (FBZ)

WAVE PROPAGATION IN PERIODIC STRUCTURES
BY L. BRILLOUIN (Dover Paperback)

BRILLOUIN ZONE

PROBLEMS OF WHICH THE BZ IS AN ASPECT
1. PHONON (SOUND: LATTICE VIBRATIONS)
2. ELECTRONIC ENERGY STRUCTURE

LAGRANGE (1759)

PLANE FUNCTIONS

\[
\text{V} = V_0 \left(1 - \frac{x}{a}\right) \quad \text{for} \quad -a \leq x \leq a
\]

\[
\text{V} = 0 \quad \text{for} \quad |x| > a
\]
**Transverse Displacement**

\[ y = \text{displacement of } n^{th} \text{ mass} \]

\[ y = A \cos \left( \omega t - k y \right) \]

\[ k = \frac{2\pi}{\lambda}, \quad A = \text{constant} \]

Replace \( k \) by \( k + \frac{2\pi}{\lambda} \) gives

The same thing:

\[ k = \frac{2\pi}{\lambda} \Rightarrow \frac{2\pi}{\lambda} + \frac{2\pi}{\lambda} \]

(not of Brillouin zone)

\[ y = y(\alpha = \frac{2\pi}{\lambda}) = \text{constant} \]

\[ \text{Ymax} \]

\[ -\frac{1}{y} d y \quad \frac{1}{y} d y \quad \frac{1}{y} d y \quad \frac{1}{y} d y \]

**First Brillouin Zone**

(Dispersion curve)
\[ \frac{1}{2} d = \frac{1}{12} d + \alpha \Rightarrow \text{INTEGRAL ADJOINING OF } \frac{1}{2} \text{ \ AND } \alpha \text{ \ RESTRICT } -\frac{1}{2} d < 0 \leq \frac{1}{2} d \]

As \( d \to \infty \), \(-\infty < 0 < \infty \) (as in a string)

LOADING COEFFICIENT \( \Lambda \)

ATTENUATION \( y = y_0 \) (akin to roll-off filter)

FOR UNEQUAL MASSES:

\[ M \quad 0 \quad \cdots \quad 0 \quad \cdots \quad 0 \quad 0 \quad M \]

DISPERSION CURVE
<z will have
stop band>

\[ \frac{1}{c} \text{ or } \frac{1}{\sqrt{2LC}} \]

9-22-75 (Mon)

Could have

\[ \frac{1}{\sqrt{2LC}} \text{ or } \frac{1}{\sqrt{4LC}} \]

\[ \text{Unatonic dispersion curve (periodic)} \]

\[ \text{Optic branch} \]

\[ \text{Acoustic branch} \]
OPTIC BRANCH (PRODUCES DIPOLAR MOMENT)

Two transverse and two long. modes

1. Long. → direction of propagation
2. Trans. → normal to longitudinal

Lattice spacing: \( y_n = A e^{i(\omega t - nkd)} \)

\( k = \frac{2\pi}{\lambda} \)

\( V = \text{frequency}, \; \omega = 2\pi V, \; A = \text{wave amplitude} \)

\( t = \text{time}, \; d = \text{lattice spacing} \)

\( n = \text{integer}, \; \lambda = \text{constant amplitude} \)

\( k' = k + 2\pi n/d \leq \text{may reduce to 1st zone} \)

\( \omega \) is periodic in \( kd \)

\( f(\lambda) = \text{even functions} \)
IF FOR EACH IS, 3 N DEGREES OF FREEDOM, THEN THERE ARE K BRANCHES.

1D LATTICE, 2 ATOMS PER CELL:

PROBLEM:

\[ i_{2n} - i_{2n+1} = \frac{\partial}{\partial t} Q_{2n} \]
\[ i_{2n+1} - i_{2n+2} = \frac{\partial}{\partial t} Q_{2n+1} \]

\[ L_1 \frac{d^2 i_{2n+1}}{dt^2} = \frac{Q_{2n}}{C_1} - \frac{Q_{2n+1}}{C_2} \]
\[ L_2 \frac{d^2 i_{2n}}{dt^2} = \frac{Q_{2n-1}}{C_2} - \frac{Q_{2n}}{C_1} \]

GET THE SECOND ORDER EQUATIONS:

\[ \begin{cases} 
L_1 \frac{d^2 i_{2n+1}}{dt^2} = \frac{i_{2n} - i_{2n+1} - i_{2n+1} - i_{2n+2}}{C_1} \\
L_2 \frac{d^2 i_{2n}}{dt^2} = \frac{i_{2n-1} - i_{2n} - i_{2n} - i_{2n+1}}{C_2} 
\end{cases} \]

USE \[ i_{2n} = A_2 e^{i(\omega t - 2nkx)} \]
\[ i_{2n+1} = A_1 e^{i(\omega t - (2n+1)kx)} \]

PLUGGING BACK IN GIVES

\[ (L_1 \omega^2 + \frac{1}{C_1} + \frac{1}{C_2})A_1 - \left( \frac{e^{i k x}}{C_1} + \frac{e^{-i k x}}{C_2} \right) A_2 = 0 \]
\[ (L_2 \omega^2 + \frac{1}{C_1} + \frac{1}{C_2})A_2 - \left( \frac{e^{i k x}}{C_2} + \frac{e^{-i k x}}{C_1} \right) A_1 = 0 \]
FOR A SOLUTION TO EXIST, $|\lambda| = 0$

$$[-1, e^{ikx} + e^{-ikx}] = 0$$

\[\begin{align*}
&\left[-1, e^{ikx} + e^{-ikx}\right] \neq 0 \\
&-\left(\frac{e^{ikx}}{c_1} + \frac{e^{-ikx}}{c_2}\right) \neq 0 \\
&\omega^4 - \omega^2 (\frac{1}{c_1} + \frac{1}{c_2}) + \frac{4 \lambda^2 k x}{L_1 L_2 c_1 c_2} = 0
\end{align*}\]

\[\Rightarrow \omega = \frac{1}{2} (\frac{1}{c_1} + \frac{1}{c_2}) \pm \frac{1}{2} \sqrt{4 (\frac{1}{c_1} - \frac{1}{c_2})^2 (\frac{1}{c_1} + \frac{1}{c_2}) - \frac{4 \lambda^2 k x}{L_1 L_2 c_1 c_2}}\]

ATTENUATION

\[\sim \omega \left(\frac{k a^d}{c}\right)\]

$L_1 = mL_2$

\[\omega = \frac{1}{2} \left(\frac{a^d}{c}\right) \pm \frac{1}{2} \sqrt{4 (\frac{1}{c_1} - \frac{1}{c_2})^2 (\frac{1}{c_1} + \frac{1}{c_2}) - \frac{4 \lambda^2 k x}{L_1 L_2 c_1 c_2}}\]

\[U_{nm} = U(1 x_{n+m} - X_n) \Rightarrow \text{potential energy}
\]

\[U_{\text{total}} = \sum_{n,m} U(4 x_{n+m} - X_n) \leq \text{new, make an expansion}
\]

\[U_{(1 x_{n+m} - X_n)} \sim U_{(md)} + \frac{(y_{n+m} - y_0) U'(md)}{2} + \frac{1}{2} (y_{n+m} - y_0)^2 U''(md)
\]
9-24-75 (Wed)

Review:

Developing Dimension Curve 1st 2nd 3rd 4th Order

\[ C : \quad M_1 \quad M_2 \quad M_3 \quad C \]

\[ x_{n+1} \quad x_n \quad x_{n-1} \]

\[ U[x_{n+1}, x_n] = U_{md} + \left( y_{n+1} - y_n \right) U'(md) + \frac{1}{2} \left( y_{n+1} - y_n \right)^2 U''(md) + \cdots \]

\[ U = \sum_{m > 0} \left[ U_{md} + y_n - y_m \right] U'(md) + \frac{1}{2} \left( y_n - y_m \right)^2 U''(md) \]

\[ F_p = - \frac{\Delta p}{\Delta y} \exp \left( -\frac{y_{n+1} - y_n}{m>0} \sum \left[ \frac{\Delta y}{m>0} \right] \frac{\left( y_{n+1} - y_k \right) U'(md) + \frac{1}{2} \left( y_{n+1} - y_k \right)^2 U''(md)}{m>0} \right] \]

\[ + \left( y_n - y_{p-m} \right) U'(md) + \frac{1}{2} \left( y_n - y_{p-m} \right)^2 U''(md) \]

\[ = - \sum \left[ -U'(md) - \left( y_n - y_{p-m} \right) U'(md) \right] \]

\[ - \left( y_{n+1} - y_n \right) + \left( y_n - y_{p-m} \right) U'(md) + U'(md) \]

\[ = \sum_{m>0} U''(md) \left[ y_{p+m} + y_{p-m} - 2y_n \right] \]

Ignoring higher terms:

\[ \begin{align*}
F_{2n} &= U'' \left( y_{2n-1} + y_{2n+1} - 2y_n \right) = M_2 \frac{d^2 y}{d^2 x} \\
F_{2n+1} &= U'' \left( y_{2n} + y_{2n+2} - 2y_{2n+1} \right) = M_1 \frac{d^2 y}{d^2 x}
\end{align*} \]

Assume solution forms:

\[ y_{2n} = A_n e^{i(\omega t - n \pi k d)} \quad k = \frac{3\pi}{A} \]

\[ y_{2n+1} = A_n e^{i(\omega t - (n+1) \pi k d)} \]

Plugging in gives:

\[ \begin{align*}
\left( M_2 (-A_2 \omega^2) = U'' \left[ A_1 e^{i(\omega t - n \pi k d)} + A_1 e^{i(\omega t - (n+1) \pi k d)} - 2A_2 \right] \\
( -A_1 \omega^2) = U'' \left[ A_2 e^{i(\omega t - n \pi k d)} + A_2 e^{i(\omega t - (n+1) \pi k d)} - A_1 \right]
\end{align*} \]

\[ \begin{align*}
( A_2 (M_2 \omega^2 - 2U'')) + 2A_1 U'' \cos \frac{kd}{2} = 0 \\
( A_1 (M_1 \omega^2 - 2U'')) + 2A_2 U'' \cos \frac{kd}{2} = 0
\end{align*} \]

Take a look now of the det. of coefficients.
\[
\begin{align*}
\text{REQUIRE} & \quad \ddot{u} + \frac{4}{M_1 M_2} \frac{u}{u} = 0 \\
\Rightarrow & \quad u''(M_1 + M_2) + \frac{4 u}{M_1 M_2} u = 0
\end{align*}
\]

GIVES:

\[
\begin{align*}
u^2 & = u'' \left[ \frac{1}{M_1} + \frac{1}{M_2} \right] \pm \sqrt{ \left[ \frac{1}{M_1} + \frac{1}{M_2} \right]^2 - \frac{4 u}{M_1 M_2}} - \frac{u}{M_1 M_2}
\end{align*}
\]

\text{PROBLEM: ANALYZE THE CASE } M_1 = M_2.

\text{FIND THE VELOCITIES OF A PROPAGATION VELOCITY V(k).}

\text{TURN IN NEXT TUESDAY.}

\text{NEW: } u^2 = M_1 M_2 \left[ M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2 M_1 M_2 \cos k d} \right] - k d

\text{ASSUME THAT } M_1 > M_2 \text{ FOR LONG WAVELENGTHS } (\lambda > 2 d) \text{ AND } 1 < k d < \frac{1}{d}

\Rightarrow \quad k d \leq 1 \implies u = k d \sqrt{\frac{1}{M_1 M_2} - \frac{k d^2}{M_1 M_2}}

\text{AT ZONE BOUNDARY, } u = k d \sqrt{\frac{1}{M_1 M_2} - \frac{k d^2}{M_1 M_2}}

\text{IN PHASE: } A_1 = -M_1 \frac{1}{M_2} \left[ - \frac{k d^2}{M_1 M_2} \right] - M_2 \frac{k d^2}{M_1 M_2}

\text{IN AMPLITUDE: } A_2 = \frac{1}{M_2} \left[ - \frac{k d^2}{M_1 M_2} \right] - M_2 \frac{k d^2}{M_1 M_2}

\text{Then:}

\begin{align*}
\frac{\partial^2 E}{\partial A_2^2} & = -M_1 \frac{1}{M_2} \left[ - \frac{k d^2}{M_1 M_2} \right] - M_2 \frac{k d^2}{M_1 M_2} \\
\frac{\partial^2 E}{\partial A_2} & = -M_1 \frac{1}{M_2} \left[ - \frac{k d^2}{M_1 M_2} \right] - M_2 \frac{k d^2}{M_1 M_2}
\end{align*}

\text{WHERE}

\begin{align*}
\alpha & = M_1 M_2 \left[ \frac{1}{M_1} + \frac{1}{M_2} \right] \\
\beta & = \frac{k d^2}{M_1 M_2}
\end{align*}

\text{AND}

\begin{align*}
u^- & = \sqrt{\frac{u''}{M_1 \frac{1}{M_2} - \frac{k d^2}{M_1 M_2}}} \\
\nu^+ & = \sqrt{\frac{u''}{M_1 \frac{1}{M_2} + \frac{k d^2}{M_1 M_2}}}
\end{align*}
1. \[ u^2 \left( \frac{m_1 + m_2}{2} - \frac{w^2 m_1 m_2}{4 u^2} \right) = \sin^2 \frac{k d}{2} \geq 1 \]

To include forbidden zone, must employ imaginary arguments.

2. \[ k d = \alpha + i \beta \text{ then} \]

\[ \sin \frac{k d}{2} = \sin \frac{\alpha}{2} \cosh \frac{\beta}{2} + i \cos \frac{\alpha}{2} \sinh \frac{\beta}{2} \]

\[ \frac{\alpha}{2} = \pi \]

\[ w^2 < 0 \Rightarrow \text{Im} \ w \]

\[ \Rightarrow \text{Re} \ \sin \frac{k d}{2} = 0 \]

\[ \sin \frac{\alpha}{2} \cos \frac{\beta}{2} = 0 \]

\[ \Rightarrow \beta = 0 \Rightarrow k = \frac{\omega}{c} \]

Case 2: Evanescent

Electronic Band Structure

Photon in Space

\[ \text{CASE 2} \]
Photon in free space:

\[ w = \text{slope} \quad C \]

\[ \text{with} \quad k \]

**1. WHAT IS \( n \) AT THE \( k \)-TH N-ZONE SHOWING \( \text{EQN} \) \( \frac{\partial n}{\partial \theta} \) IN \( \text{cm}^{-1} \)?

**FOR A PHONON, WHAT IS \( k \) FOR A 500-MEV LIGHT WAVE? FOR 3000 MEV?**

**9-26-75 (PRI)**

\[ \frac{\partial n}{\partial \theta} = \text{H}_\text{n} = E, \text{TH} \]

**AND A PERTURBATION \( \Rightarrow \) \( \frac{\partial n}{\partial \theta} \) \( = (H+V) \) \( \text{TH} \)

**WITHOUT PERTURBATION, \( \text{V} = 0, 2 \) \( \text{TH} \)**

**ASSUME, FOR PERTURBATION \( a = 2 \text{ TH} \)**

**PLUG INTO PERTURBED WAVE EQN:**

\[ \begin{align*}
\iota \frac{\partial}{\partial \theta} [\frac{\partial n}{\partial \theta} & \phi_0(x) e^{-\frac{1}{\hbar}E_\theta t} + \sum \phi_n(x) e^{-\frac{1}{\hbar}E_\theta t}] \\
& = [H+V] \sum \phi_n(x) e^{-\frac{1}{\hbar}E_\theta t}
\end{align*} \]

**MULTIPLY BOTH SIDES BY \( \phi^*_\text{TH} (x) \) AND INTEGRATE**

\[ \begin{align*}
\iota \frac{\partial}{\partial \theta} e^{\frac{1}{\hbar}E_\theta t} + E_\text{os} \text{as} e^{\frac{1}{\hbar}E_\theta t}
& = E_\text{os} \text{as} e^{\frac{1}{\hbar}E_\theta t} + \sum \int \phi^*_\text{TH} \phi_\text{TH} e^{\frac{1}{\hbar}E_\theta t} dx \\
& \Rightarrow \frac{\partial n}{\partial \theta} = \frac{\hbar}{\iota} \sum a_n V_{sn} \text{os} e^{\frac{1}{\hbar}E_\theta t} \text{TH}
\end{align*} \]

\[ V_{sn} = \int \phi^*_\text{TH} \phi_\text{TH} dx \]
\[ E_0 = -\frac{A}{2} \Sigma_{\alpha \beta} V_{\alpha \beta} (E_0 - E_\alpha) \]

Recall \( E_\alpha \) and \( E_\beta \) are different.

\[ \frac{1}{2} \Sigma_{\alpha \beta} V_{\alpha \beta} \]

\[ \text{A COUPLING T-NUMBER DIVISION} \]

\[ \frac{1}{2} \Sigma_{\alpha \beta} V_{\alpha \beta} \]

\[ \rightarrow \] FORMAL PRECEDENCE

\[ \uparrow \quad \downarrow \]

USUALLY MEASURE \( V_{SN} \).

CONSIDER THE SPECIAL CASE WHERE

\[ E_0 = E_0 \quad \Rightarrow \quad \frac{\Sigma_{\alpha \beta} V_{\alpha \beta}}{A} = \frac{1}{2} \Sigma_{\alpha \beta} a_{\alpha \beta} V_{SN} \]

(SECOND VOLUME OF FERMIAN LECTURES).

ELECTRONS IN A SOLID

\[
\begin{array}{cccc}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{array}
\]

ASSUME \( a = e^{i\omega d} \)

\[ \Rightarrow \pi a_{\alpha \beta} = \frac{\Sigma_{\alpha \beta} a_{\alpha \beta} V_{SN}}{E_0 = V_{SN}} \]

\[ E_0 = V_{SN} \]

\[ E_{\alpha \beta} = E_0 a_{\alpha \beta} + V_{SN, \alpha, \beta} a_{\alpha \beta} + V_{SN, \alpha, \beta} a_{\alpha \beta} \]

ASSUME ELECTRON WILL JUMP ONLY TO AN ADJACENT ATOM.

THIS GIVES

\[ E_{\alpha \beta} = E_0 a_{\alpha \beta} - V_{SN, \alpha, \beta} a_{\alpha \beta} - V_{SN, \alpha, \beta} a_{\alpha \beta} \]

Thus
\[(E-E_0)\sigma = -V(\sigma_{s1} + \sigma_{s+1})\]

Let
\[\sigma_{s+n} = e^{i kn d} \Rightarrow \sigma_{s-n} = e^{-i kn d}\]

Gives
\[E - E_0 = -V_1 [ e^{i kn d} + e^{-i kn d} ]\]
\[= -2V_1 \cos kd\]

\[\Rightarrow E = E_0 - 2V_1 \cos kd\]

Graph it's dispersion curve.

\[\cos kd = 1 - k^2 d^2 / 2\]

\[\Rightarrow E = E_0 - 2V_1 + V_1 d^2 k^2 \leq \text{Parabola}\]

Recall, from electron in free space:
\[E = \frac{\hbar^2 k^2}{2m} \Rightarrow \frac{\hbar^2}{2m} \text{effective mass}\]

\[(E - E_0) = -V_1 \cos kd + V_2 \cos^2 kd\]

From earlier,
\[\sigma_{s+2} - \sigma_{s-2} + V_{s+2} \sigma_{s+2}\]

thrown away previously.
\[ 1 + \frac{B_{q_{1,2}^a}}{S_{q_{1,2}^a}} = E_0 G_{q_{1,2}^a} + \sum_{n=1,2} V_{5+n} G_{5+n} \]

**ASSUMED:** \[ G = e^{-\sqrt{k} x} \]

**Gives:** \[ E = E_0 - 2V_1 \cos k d \]

**Consider 2-O Solid**

**Gives:** \[ E = E_0 - 2V_1 \cos^2 k d + 2V_2 \cos^2 k \sqrt{\frac{4}{k} d} \]


- Gallium Phosphides
MILLER INDICES (TO SPECIFY DIRECTIONS)

IS DISTANCE TO A PLANE

\( (x, y, z) \)

DISTANCE TO NEXT PLANE

\( \frac{1}{4}, \frac{1}{2}, \frac{1}{2} \) = \( 1, 1, 0 \) - 1

\( 1, 1, 1 \)

\( 1, 0, 0 \)

GOING BACKWARDS

G.F. KOESTER "SPACE GROUPS AND THEIR REPRESENTATIONS", AG. PRESS
\[ E_{CB} + h\nu \rightarrow (e, h)^{VB} + h\nu (E_{CB} - E_{VB}) \]

\[ k = \frac{E}{h} \]

MOMENTUM CONSERVATION: \[ k_0 + k_e \rightarrow 0 + k \]

DIRECT GAP (GaAs)

GaAs

\[ E_{gap} = 2.35\, eV \]

\[ E_{gap} = 1.14\, eV \]

EXTRINSIC \[ L, I, s, \ldots \]

\[ k = 0 \]

\[ x \]
10-1-75 (WED)

ON HOMEWORK

FIRST PROBLEM

Get \( w = \frac{5d}{2} \) and \( w = 2d - \frac{1}{2} \)

\[ w = \sqrt{\frac{d}{2}} \]

**EFFECTIVE MASS**

\[ v_b = \frac{\partial w}{\partial k} \quad k = \frac{2\pi}{\lambda} \]

ACCELERATION OF \( v_b = \frac{F}{m^*} = \frac{\partial v_b}{\partial E} \)

\[ E = h\omega \Rightarrow v_b = \frac{h\omega}{k} \Rightarrow k = \frac{h\omega}{v_b} \]

thus \( \text{ACCEL} = \frac{d^2 v_b}{dt^2} = \frac{h^2 \omega^2}{v_b^2} \)

\( P = \frac{hv}{k} \)

\[ F = \frac{\partial P}{\partial k} = \frac{h}{v_b} \frac{\partial v_b}{\partial E} = \frac{m^*}{k} \]

\( \frac{\partial k}{\partial E} = \frac{h^2 \omega^2}{v_b^2} \)

\[ \Rightarrow m^* = \frac{h^2}{E} \]

**PARABOLIC BAND**

\[ E = \frac{1}{2} m v^2 \]

\[ A = \frac{1}{2} + \frac{1}{2} k^2 \]

\[ \frac{S^2 E^2}{E^2} = T \frac{\partial}{\partial m} \]

\[ k = 0 \]

**PARABOLIC BAND**

**(QUASI FREE ELECTRON)**
PROBLEM: EXTEND \( m^* \) DERIVATION TO 3-D. (EFFECTIVE MASS)

HOW TO MEASURE \( m^* \).

\[ F_y = qV_x B = m^* \frac{\dot{y}}{\dot{z}} \]
\[ F_x = -qV_y B = m^* \frac{\dot{x}}{\dot{z}} \]

Assuming \( m^x = m^z \) (not always true):

\[ m(\dot{y}^2 + \dot{z}^2) = qB(\dot{x}^2 - \dot{y}^2) \]

Assume \( x = \sin \omega_0 t \), \( y = \cos \omega_0 t \)

Gives \( \omega_0^2 = \left( \frac{qB}{m^*} \right) \)

ABSORPTION MEASUREMENTS

(SCANNING MONOCHROMAT) SOURCE

SPECTRUM

PHOTOMULTIPLIER

FAR IR

USE GOLAY CELL

\[ E_g = h \omega_0 \]
10^{-3} - 7.5 \text{ (Pet)}

![Diagram of electron transitions and energy levels]

- **Phonon Assisted Transitions**
- **Pumping Electron from Level**
- **Conduction Band**

E_{binding} \approx \begin{cases} 2.3 \text{ eV (GaP)} \\ \approx 2.5 \text{ (CdS, HgSe)} \end{cases}

- **Exitons**
- **Donor**
- **Acceptor**

**Exitons in an Indirect Gap Material**

 UR \quad \text{FRE} \quad R \quad G

10 - 122 \text{ mev} \rightarrow \text{Bound Exiton Bound to Impurity (Si, Ge, Zn, Cd)}

\text{Free}
$10^9 K \approx 1 \text{ mK}$

**NEP = Noise Equivalent Power = \int_\gamma \delta E (\text{DISTRIBUTION})**

$$h\nu \rightarrow e + h + \text{PHONON}$$

$$h\nu = \hbar k_e + \hbar k_h + \hbar k_{\text{photon}},$$

**Gap**

$$\text{Exiton Wave Function: } \psi$$

$$\psi(x) = \sum_k \alpha_k e^{i k x}$$

**In K Space**

$$\int \psi^*_k \psi_i (r) \, dx = \int e^{-ikx} (\psi^*_k e^{ikx})$$

$$\int e^{2\pi i (\vec{k}_f - \vec{k}_i) \cdot \vec{x}} \, dx = \delta(\vec{k}_f - \vec{k}_i)$$

**Final and Initial K Must Be Equal (Cons. of Momentum)**
USE FOURIER ANALYSIS LIBERTY.
MAKING MEASUREMENTS (ABSORPTION)
CAN GIVE BINDING ENERGY.

FERMI-VIRAS DISTRIBUTION

\[ N = \int n(E) \, dE = \int P \, dE \]

1) ASSUME THERMAL EQUILIBRIUM
2) ELECTRON PROPERTY (PAULI EXCLUSON
PRINCIPAL) NOT MORE THAN ONE
ELECTRON CAN HAVE A GIVEN
SET OF QUANTUM N\#S, \( E, L, S, \text{ETC.} \)
ANS. N\#M = \( \frac{1}{2} \)}
10-6-75 (Mon)

Fermi-Dirac Distribution

\[ \Delta E = \frac{n}{N} \approx e^{\frac{-\Delta E}{kT}} = \text{Boltzman factor} \]

\[ \begin{align*}
\text{E} & \quad \text{SYSTEM} \\
\text{E} & \quad \text{E+}\Delta \\
\text{E} & \quad \text{E+}\Delta \\
\text{E} & \quad \text{E+}\Delta \\
\text{E} & \quad \text{E+}\Delta \\
\text{E} & \quad \text{E+}\Delta \\
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WHAT IS \( f(E) = \text{FERMI-Dirac dist. func.} \)

\[
f(E) = \frac{1}{e^{\frac{E-E_F}{kT}} - 1}
\]

1. WHAT IS \( n(E) \)?
2. WHAT IS \( n \)?

\[n(E) = \# \text{ELECTRONS WITH ENERGY } E\]

\[= \rho_{\text{LEVEL}} \text{ CAN HAVE EN. } E \int d\mathbf{\mathbf{r}} = e^{-\frac{E}{kT}} \int d\mathbf{\mathbf{r}}
\]

\[n = \int_{\text{BAND}} n(E)\, dE
\]

DENSITY OF DONOR STATES

\[N_d^+ = N_0 \left[ 1 - f(E_0) \right]
\]

IN CONDUCTION BAND, \( E^- \) ACTS FREE.

DENSITY OF STATES FOR A FREE PARTICLE.

![Diagram of One Dimension (Free Particle in a Box)](image)

LOWEST \( E \rightarrow \) LONGEST \( \lambda \)

<table>
<thead>
<tr>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
</tr>
<tr>
<td>( 2L )</td>
</tr>
<tr>
<td>( \frac{3L}{2} )</td>
</tr>
</tbody>
</table>

\( E = \frac{p^2}{2m} \)

\( E = \frac{p^2}{2m} \frac{1}{2mL^2} \)

\( E = \frac{p^2}{2m} \frac{1}{2mL^2} \)

\( E = \frac{p^2}{2m} \frac{1}{2mL^2} \)
\( d N^{(1)} = \text{# OF STATES} / \text{TWIXT } h^2 / 2mL^2 = M \)

\( E_n = n^2 \left( \frac{h^2 \pi^2}{2mL^2} \right) \)

\[ n = \sqrt{\frac{2mEL^2}{h^2 \pi^2}} \Rightarrow dN = \frac{1}{2} \left( \frac{2mL^2}{h^2 \pi^2} \right) \frac{dE}{\sqrt{E}} \]

IN 3D WE GET

\[ \frac{1}{8} \left( \frac{4 \pi m^2}{h^2} \right) dE \nabla dN \]

GETS FIRST OBTAIN OF A SPHERE SINCE \( n > 0 \)

\[ dN^{(3)} = 3 \left( \frac{2mL^2}{h^2 \pi^2} \right) E \frac{1}{2} \left( \frac{2mL^2}{h^2 \pi^2} \right)^{1/2} \frac{dE}{\sqrt{E}} \]

STUCK IN TO ALLOW FOR

2 SPIN STATES / ENERGY STATE

\[ = \left( \frac{2mL^2}{h^2 \pi^2} \right) \sqrt{E} \frac{dE}{E} \]

HOMWORK: SOLVE FOR DENSITY IN

TWO DIMENSIONS.

(FREE PARTICLE IN A LXL BOX).

NOW

\[ \nabla(E) = \frac{1}{2} \left( \frac{2mL^2}{h^2 \pi^2} \right)^{3/2} \sqrt{E} \frac{1}{E^{1/2} + 1} \frac{dE}{E} \]
\[ n(E) \, dE = \text{const.} \frac{\sqrt{E-E_c}}{1 + e^{(E-E_F)/K_T}} \]

Find top of conduction band:

\[ n = \int_{E_c}^{\infty} n(E) \, dE \]

\[ n = \text{const.} \int_{E_c}^{\infty} \frac{\sqrt{E-E_c}}{1 + e^{(E-E_F)/K_T}} \, dE \]

\[ E_F = 2.4 \text{ eV} \]

\[ K_T \text{ at room temp.} = 0.026 \text{ eV} \]

\[ \Rightarrow n = \text{const.} \int_{E_c}^{\infty} \sqrt{E-E_c} \, e^{-(E-E_F)/K_T} \, dE \]

\[ n = 2 \left( \frac{2\pi m^* K_T}{h^2} \right) \frac{e^{-(E_c-E_F)/K_T}}{K_T} \]

Effective density of states:

\[ n = N_c e^{-(E_c-E_F)/K_T} \]

\[ P = \# \text{ holes in the valence band} \]

\[ P = 2 \left( \frac{2\pi m^* K_T}{h^2} \right) \frac{e^{-(E_F-E_V)/K_T}}{K_T} \]

\[ = N_v e^{-(E_F-E_V)/K_T} \]

**Mass Action Law**

\[ np = N_c N_v e^{(-E_F + E_V - E_c + E_F)/K_T} \]

\[ = N_c N_v e^{-E_g/K_T} \]

\[ E_g = \text{energy gap} \]

\[ np = N_c^2 \]
SUMMATION

\[ f(E) = \frac{1}{E} \]

ELECTRONS

\[ 1 - f(E) \]

HOLMES

\[ \rho(E) \text{ FOR HOLES (DENSITY OF STATE)} \]

\[ n(E) = (1 - f(E)) \rho(E) \text{ FOR HOLES} \]

\[ n(E) = f(E) \rho(E) \text{ FOR ELECTRONS} \]

HOMWORK: FIND SOME STUFF

YOU CAN CALCULATE

WITH REAL NUMBERS

"RELATE RESULTS TO REAL NUMBERS. WHAT KIND OF THINGS CAN YOU CALCULATE?"
10-10-75  (FERI)

Impurity Distribution Function
(Donors: Acceptors for homework)

\[ f_j \triangleq P[ \text{Electron is in state } j \text{ (or the donor semiconductor complex)}] \]
Assume 1 electron (\(e^-\)) on donor.

\[ f_j = P[\text{No electron is already bound to the donor}] \times P[\text{An electron has energy } E_j] \]

Some define this as \(E_j\) \text{, but we don't.}

\[ E_j \]

\[ E_x \]

\[ E_g \]

\[ 1 \]

\[ \frac{1}{kT} \]

\[ \frac{1}{kT} + e^{\frac{(E_0 + E_j - E_F)}{kT}} \]

Define \( (E_0 + E_j - E_F)/kT = \phi \)

For an acceptor:
\( (E_F - E_A - E_j)/kT = \phi_j \)
\[ f'_f = \left[ 1 + f'_i - \frac{\Xi}{\alpha} f'_i \right] \left( \frac{1 + e\phi}{1 + e\phi} \right) \]

\[ f'_f = \frac{1}{1 + e\phi} \left( 1 - \frac{1}{1 + e\phi} \right) = f'_f \left( \frac{e\phi}{1 + e\phi} \right) = F^+ \left( \frac{1}{1 + e\phi} \right) \]

WHERE \[ F^+ = P[\text{DONOR ATOM HAS NO ELECTRON (ORIZATION)}] \]

\[ f'_f = F^+ e^{-\phi} \]

\[ F^+ + F_0 = 1 \quad \text{REQUIREMENT} \]

WHERE \[ F_0 = P[\text{DONOR HAS AN ELECTRON}] \]

\[ F_0 = \frac{\Xi}{\alpha} f'_i \]

\[ F_0 = F^+ \sum_i e^{-\phi} \]

\[ = (1 - F^+) \]

GIVES \[ F^+ (1 + \Xi e^{-\phi}) = 1 \]

\[ F^+ = \frac{1}{1 + \Xi e^{-\phi}} = \frac{n_0}{N_0} \]

\[ n_0 = \# e^- \text{ IN } \text{CONDUCTION BAND} \]

FROM DONORS

\[ N_0 = \text{CONCENTRATION OF DONOR ATOMS.} \]
To include degeneracy

\[ F^+ = \frac{1}{1 + \frac{S_0 \cdot e^{-\frac{E_0 - E}{kT}}}{\sum \text{ENERGY}} } \]

\[ F^+ \approx \left[ 1 + S_0 \cdot e^{-\frac{E_0 - E}{kT}} \right]^{-1} \]

Thus

\[ F^0 = 1 - F^+ \]

\[ F^0 = 1 + \frac{S_0 \cdot e^{-\frac{E_0 - E}{kT}}}{S_0} \]

\[ = 1 + \frac{e^{-\frac{E_0 - E}{kT}}}{1} \]

For one state

\[ F^0 = 1 + \frac{E_0 - E}{kT} \]

End

\[ F^+ = 1 + S_0 \cdot e^{-\frac{E_0 - E}{kT}} \]

On top of page, we approximate:

\[ F^+ \approx 1 + S_0 \cdot e^2 \]

\[ F^0 = 1 + \frac{S_0 \cdot e^0 \cdot e^{-\frac{E_0 - E}{kT}}}{S_0} \]

\[ \text{lord} = E_0 - E_\text{f} \]

\[ \text{g}_1 = E_0 - E_\text{f} + E_+ \]

Neglect the higher order terms which are small.

Problem: Derive for acceptors.
EFFECTS OF DOPING ON FERMI ENERGY

\( n = \# \text{ of} \ \text{ELECTRONS IN CONDUCTION BAND} \)

\[ n = \frac{N_e}{e} \left( \frac{E_c - E_F}{kT} \right) \]

NEUTRALITY DICTATES
\( N_d = N_d^0 \Rightarrow \# \ \text{DONORS} \ \text{IONIZED} \)

\[ n = (N_d - N_d^0) + p \quad n \gg p \]

\( p = \text{ACCEPTOR CONCENTRATION} \)

\[ \Rightarrow n \approx N_d - N_d^0 \]

\[ N_c e^{-\frac{(E_c - E_F)}{kT}} = N_d \left[ 1 - 1 + \frac{1}{8} e^{\frac{(E_F - E_0) / kT}{kT}} \right] \]

\[ = N_d \left( 1 + e^{\frac{(E_F - E_0)}{kT}} \right) \]

NORMALLY SOLVE FOR \( E_F \), CONSIDER SOME CASES

1. HIGH TEMP

\[ \Rightarrow \frac{N_d e^{\frac{(E_c - E_F)}{kT}}}{N_c e^{-\frac{(E_0 - E_F)}{kT}}} \ll 1 \]

\[ \Rightarrow E_F \approx E_c - kT \ln \frac{N_c}{N_d} \]

2. LOW TEMP.

\[ \frac{N_d e^{\frac{(E_c - E_F)}{kT}}}{N_c e^{-\frac{(E_0 - E_F)}{kT}}} \gg 1 \]

\[ E_F \approx E_c - \frac{kT}{2 \ln \left( \frac{N_c}{N_d} \right)} \]

GENERAL EXPRESSION FOR FERMI ENERGY

\[ N_c e^{-\frac{(E_c - E_F)}{kT}} = 1 + \sum_{\text{all}} e^{\frac{(E_0 - E_F - E_i) / kT}{kT}} \left( \frac{N_c}{N_d} \right) \]

\[ e^{-\frac{(E_c - E_F)}{kT}} \]
END OF MATERIAL COVERED ON TEST 1, 10-13-75 (MON)
SEMINAR @ 3:30 TODAY
ON RESONANCE RAMAN EFFECT.
RAMAN EFFECT
INFRARED ABSORPTION / RAMAN EFFECT

\[ \text{Light Source} \rightarrow \text{Sample} \rightarrow \text{Chromatograph} \rightarrow \text{Recording} \rightarrow \text{Photo Multiplier or Infra-red Detector} \]

\[ \text{Consider: } HCl \]

\[ \text{C} + \text{H}_2 \rightarrow \text{C} + \text{H}_3 \]

\[ \text{Light (V)} \]

\[ \text{Absorption} \]

\[ \text{Normal Mode} \]

\[ \mathbf{P} = \chi \cdot \mathbf{E} \quad \chi = \text{Tensor Dipole Moment} \]

\[ \alpha_{xy} = \alpha_{xy0} + \sum \alpha_{xyi} V_i + \frac{1}{4} \sum \alpha_{xyij} V_i V_j + \ldots \]

\[ \mathbf{U} = \text{Normal Mode} = \]

\[ \mathbf{P} = \text{Induced Polarization, } \mathbf{E} = \text{Applied E Field} \]

\[ \text{Suppose: } \mathbf{E} = E_0 \cos (\omega t + \phi) \]

\[ \mathbf{P} = [\alpha_{xy0} + \sum \alpha_{xyij} V_j \frac{V_0}{2} \cos (\omega t + \phi)] \cdot E_0 \cos \omega t \]

\[ \text{Gives: } \]

\[ \mathbf{P} = \alpha_{xy0} E_0 \cos \omega t + \frac{E_0}{2} \sum \alpha_{xyij} V_j \]

\[ \cos (\omega t + \phi) + \cos \left( \frac{\omega t}{2} + \phi \right) \]

\[ + \cos \left( \frac{\omega t}{2} - \phi \right) \]

\[ \rightarrow \text{Raman Effect} \]
First order: $P^{(1)}(w) \approx \coth w t$ if $\alpha_{x'y'} \neq 0$

Second order: $P^{(2)}(w \pm w_f) = \alpha_{x'y'} [\cos (w \pm w_f) t]$

If $\alpha_{x'y'} \neq 0$

$\text{Intensity} \sim w^4 \Rightarrow \text{Why the sky is blue}$

$w - w_f \quad w \quad w + w_f$

$\hbar \omega_{in} - \hbar \omega_f = \hbar \omega_{out}$

When does Raman scattering occur?

$P(w - w_f) = \delta \left[ E(w) E(w_f) \right]$ from intrinsic material properties

$-P = d \left[ -E(w) \right] \left[ -E(w_f) \right]$ if the crystal (gas) has inversion symmetry, then $d = d'$, then $d = 0$ and

$P(w - w_f) = -P(w - w_f)$

$\alpha_{x'y'} = 0$
APPLICATION TO CO$_2$

WHICH NORMAL MODES OF CO$_2$ ARE RAMAN ACTIVE

MODES:

1. $\text{O} \to \text{O} \to \text{O}$  $\to \text{O}$ $\to \text{O}$  $\to \text{O}$ $\to \text{O}$  $\to \text{O}$ $\to \text{O}$  $\to \text{O}$

1) CHANGE PHASE BY 180°

AND REFLECT THROUGH OR $\text{O}$

2) FOR RAMAN SCATTERING,

MOLECULE MUST BE DIFFERENT

FOR $\text{O} \to \text{O}$ (RAMAN ACTIVE)

$\text{Y}_1$: $\text{O} \to \text{O} \to \text{O} \to \text{O}$

$\text{Y}_2$: $\text{O} \to \text{O} \to \text{O} \to \text{O}$

$\text{Y}_3$: NOT RAMAN ACTIVE

FOR MORE COMPLICATED ATOMS, MUST USE GROUP THEORY
HEAT CAPACITY:
DEF: HEAT CAPACITY \( C_V = \frac{\partial E}{\partial T} \) \nIN A GAS
\( E = 3NkT \) \( \Rightarrow C_V = 3Nk \)
PHONON AND ELECTRON CONTRIBUTION
WILL BE LOOKED AT.

WHAT IS \( \langle n_p(E) \rangle = \text{AVE. \# OF OSCILLATORS} \)
WITH ENERGY \( E \)

\( E = \text{FOR A HARMONIC OSCILLATOR} = (n + \frac{1}{2})\hbar \omega \)

USE BOLZMANN FACTOR:
\[
\frac{N_{n+1}}{N_n} = e^{-\frac{(E_{n+1} - E_n)}{kT}}
\]
FOR HARM OSC:
\[
N_{n+1} = e^{-\frac{\hbar \omega}{kT}}
\]

FRACTION OF FILLED STATES
AT ENERGY \( E_n = \frac{N_n}{\sum N_n} \)
\[
= e^{-\frac{E_n}{kT}}
\]
\[
= \frac{1}{\sum e^{-E_n/kT}}
\]

AVERAGE NUMBER OF QUANTA
IN A STATE \( \langle n \rangle = \langle n \rangle \)
\[
\langle n \rangle = \frac{\sum n e^{-n\hbar \omega/kT}}{\sum e^{-n\hbar \omega/kT}}
\]
Let $\frac{h\omega}{kT} = x$

$\Rightarrow \langle n \rangle = \sum_{n=1}^{\infty} \frac{n e^{-nx}}{e^{-nx}}$

Note: $n e^{-nx} = \frac{d}{dx} e^{-nx}$

\[
\sum_{n=0}^{\infty} e^{-nx} = \frac{1}{1-e^{-x}}
\]

Let $y = e^{-x} \Rightarrow \sum_{n=0}^{\infty} y^n = \frac{1}{1-y}$

$\Rightarrow S = \frac{1}{1-y} = \frac{1}{1-e^{-x}}$

\[
\langle n \rangle = \frac{\sum_{n=0}^{\infty} y^n}{1-y} = \frac{1}{1-e^{-h\omega/kT}}
\]

\[
\langle n \rangle = \frac{1}{e^{h\omega/kT} - 1}
\]

\[\text{OCCUPATION \# \ FOR} \ n^{th} \ \text{LEVEL} \]

\[\text{FOR BOSONS} \]

\[\text{RECALL FERMI - DIRAC DISTRIBUTION:} \]

\[
\frac{1}{e^{E/kT} + 1} \ \text{\ implies \ Pauli \ exclusion \ principle.}
\]

\[\text{FOR FERMIONS} \]

For small $\frac{h\omega}{kT}$

\[
\langle n \rangle \approx \frac{1}{1 + \frac{h\omega}{kT}} - 1 = \frac{kT}{h\omega}
\]

Then

\[
\langle E \rangle = \langle n \rangle \cdot h\omega = kT \ \text{\ classical \ result}
\]
\[
\langle E(w) \rangle = \frac{N_h \omega}{e^{\frac{\omega}{kT}} - 1}
\]

Then

\[
C_v = \frac{\delta \langle E \rangle}{\delta T} = N k \left( \frac{\omega}{kT} \right)^2 \frac{e^{\frac{\omega}{kT}}}{(e^{\frac{\omega}{kT}} - 1)^2}
\]

In 3D, we got three degrees of freedom \( \Rightarrow \) multiply \( C_v \) by 3

Homework: What is \( C_v \) for large temperature?

\[
E_{\text{total}} = \frac{1}{kT} \omega \langle n \rangle
= \int \left( \frac{\omega}{kT} \langle n \rangle \frac{dn}{dE} \right) dE
\]

Debye used density of states

\[
\frac{dn}{dE} = \frac{2 \pi^2 k}{V^3} \omega^2 ; \quad V = \text{velocity}
\]

\[
\omega = \frac{h}{k} \quad \text{Assumption of dispersion relation}
\]

\[
\omega_0 = \text{Debye frequency} = \text{maximum allowable freq.}
\]

\[
3N = \frac{h \omega_0}{2 \pi^2 k} V^3
\]

\[\Rightarrow \omega_0 = \frac{6 \pi^2 V^3 N}{(V \omega)}\]

Density of states

[Diagram of density of states with assumed real and imaginary parts]
\[ C_v = \frac{\partial \langle E \rangle}{\partial T} \nu = Nk \left( \frac{h^2 v}{2m} \right)^2 \left( e^{\frac{h^2 v}{2mkT}} - 1 \right)^2 \]

\[ E = \int_{\nu_{\text{min}}}^{\nu_{\text{max}}} \rho \omega \delta^2(\omega) n(\omega) d\omega \]

**KIND OF**

**DENSITY OF STATE IN A BOX**

\[ \frac{1}{V} \int \frac{dE}{d\omega} d\omega = \frac{\pi^2}{12} \frac{4\pi^2}{\nu_{\text{max}}^2} \]

GIVES

\[ d^2(\omega) d\omega = \frac{1}{12} \frac{d^2}{d\nu^2} d\omega \]

\[ \frac{\partial^2}{\partial \nu^2} d\omega \]

GIVES

\[ d^2(\omega) = (2\pi)^3 \int \frac{d\nu}{d\nu/dk} \]

**\( \frac{d\nu}{dk} = \text{WAVE PACKET GROUP VELOCITY} \)**

**EXAMPLE**: **ACOUSTIC PHONON**

\[ \omega = \omega_{\text{max}} \sim (\frac{k_0}{\nu_{\text{max}}}) \]

MAY FIND \( d(\omega) \)

**ONE CAN SHOW (EXTRA CREDIT)**

\[ d(\omega) = \frac{2L \delta_0}{k_0^2} \left( \omega_{\text{max}}^2 - \omega^2 \right)^{1/2} \]

**MODEL BREAKS DOWN AT** \( \omega_{\text{max}} \)

**\( L^2 d(\omega) \) CALCULATED**

**\( L^2 \) OBSERVED**
GoP: \[ \text{CALCIUM PREP} \quad \text{FID}\]

\[ F = 3.028 \text{eV} \]

\[ 0.203 \text{eV} \]

AT 5K, STRONG FLOURESCENCE

WHEN \( e^- \) IS IN CONDUCTION BAND

PHONON SIDERANKS NO PHONON

BACK TO \( C_v \)

RECALL: \[ E = \int_0^{\omega_d} \frac{\omega^2}{\omega^2 + \frac{\eta}{2} \sqrt{\omega^2 + \frac{\gamma}{2}} \left( \frac{t}{\omega} \right)} \text{d}\omega \]

DEBYE ASSUMED THAT: \( \omega = V \lambda k \)

\( (\lambda \text{ ACOUTIC PHONONS}), \)

GIVES: \( \omega_d = 6 \pi T^2 v^3 n / \text{VOLUME} \)

DEBYE APPROXIMATION

\[ E = \frac{3 V k^p T^4}{2 n^2 v^3 \lambda^3} \int_0^{\infty} x^3 \text{d}x / e^x - 1 \]

\[ x_o = \frac{\hbar \omega}{k T} \]

\[ x_o = \Theta_0 / T \]

\( \Theta_0 = \text{DEBYE TEMPERATURE} \)

THEN

\[ C_v = 3 n k \left( \frac{\Theta_0}{T} \right)^3 \int_0^{\infty} x \frac{x^4}{e^x - 1} \text{d}x \]

FOR SMALL \( T \)

\[ E_1 = \text{CONST} \int_0^{\infty} \frac{x^5}{e^x - 1} \text{d}x \]

(CONT)
RECALL: \( e^{x-1} = \frac{e^x}{e^1} \)

\[ E = \text{const} \int_0^{\infty} dx x^3 e^{-nx} \]

INTEGRATING TERMWISE

\[ E = \text{const} \times \int_0^{\infty} \frac{dx}{x^n} \]

\[ = \text{const} \times \frac{6 \pi^4}{15} \]

Thus, for \( T \) small

\[ C_V = \frac{dE}{dT} \approx \frac{12 \pi^4}{5} \text{NK} \left( \frac{T_0}{T} \right)^3 \]

**SIGNIFICANT RESULT**

**ELECTRON CONTRIBUTION TO SPECIFIC HEAT**

\[ E_{\text{electron}} \approx \frac{3}{2} kT n \]

\[ \Rightarrow C_V \approx \frac{3}{2} kT \]

DON'T WORK OUT EXACTLY MANUALLY

RECALL:

\[ E_F = \frac{1}{2} m \left( \frac{3 \pi^2}{2} n \right)^{2/3} \]

\[ \frac{dN}{dE} = \frac{V}{2} \left( \frac{2m}{\pi^2} \right)^{1/3} \sqrt{E} \]

THERMAL ENERGY \( \propto kT \)

\[ \text{LET } E_F \text{ BE } \text{FILLER} \]

\( k_T \text{ CAN'T DO THIS CAUSE OF PHYSICAL CONSTANT PROBLEM} \)

\( n \) AVAILABLE ROUGHLY \( \frac{1}{T} \) THERMODYNAMIC

(THIS AGREES WITH EXPERIMENT)
10-20-75 (Mon)

Cv assuming fermi-dirac:

\[ \Delta = \int_{-\infty}^{E_F} \frac{N(E) \, dE}{E - E_F} \]

Density of states subtracts \( E \) below \( E_F \)

This gives \( Cv = \frac{h^2}{8\pi^2} NkT/T^2 \)

Off an order of about 5.

Test questions:

\( e^- \) sharing.

Excited \( e^- \) in conduction band

\[ \Delta E = E_F + V_1q_1 + V_2q_2 \]

\[ + V_1q_1 + V_2q_{-1} \]

\( V_1, V_2 \) is a form of coupling.

Gives \( E = E_F + V_1q_1 k + 2 V_2 q_2 k^2 \)

\( V_1 \) and \( V_2 \) are measurable.

For quasi-free \( e^- \):

\( E \sim \frac{1}{2} k^2 / 2m^* \)

Tetrahedron: 4 triangles

\( \text{Si}, \, \text{Ge}, \ldots \)
SIMPLE HARMONIC OSCILLATOR
\[ V(x) = \frac{1}{2} m \omega^2 x^2 \quad \omega = \sqrt{\frac{k}{m}} \]

SCHRÖDINGER EQUATION
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{1}{2} m \omega^2 x^2 \psi = E \psi \]
\[ \Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \left( \frac{\hbar^2}{2m} \omega^2 - \frac{1}{2} \right) \psi = 0 \]

BRAKE FORCE SOLUTION
\[
\frac{\partial^2 \psi}{\partial \xi^2} + \left( E - \xi^2 \right) \psi = 0
\]

This is HERMITE DIFFERENTIAL EQUATION
\[ \psi = V(\xi) e^{-\frac{\xi^2}{2}} \]

GIVES
\[ \frac{\partial^2 V}{\partial \xi^2} - \xi \frac{\partial V}{\partial \xi} + (E - 1) V = 0 \]
\[ V(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \]

PLUG IN
\[ \frac{d}{d\xi} \frac{\partial V}{\partial \xi} = \sum_{n=0}^{\infty} n a_n \xi^{n-1} = \sum_{n=0}^{\infty} (n+1) a_{n+1} \xi^n \]
\[ \frac{1}{2} \frac{\partial^2 V}{\partial \xi^2} = \sum_{n=0}^{\infty} \frac{n(n-1)}{2} a_n \xi^{n-2} = \sum_{n=2}^{\infty} \frac{n(n-1)}{2} a_{n-2} \xi^n \]
\[ \Rightarrow \sum_{n=0}^{\infty} \left( (n+2)(n+1) a_{n+2} + \left[ (E - 1) - 2n \right] a_n \right) \xi^n = 0 \]
\[ \Rightarrow (n+2)(n+1) a_{n+2} + \left[ (E - 1) - 2n \right] a_n = 0 \]
\[ a_{n+2} = \frac{2n - (E - 1)}{(n+2)(n+1)} a_n \]

\[ \Rightarrow \text{TWO INDEPENDENT SOLUTIONS} \]

GOTTA KNOW \( a_0 \) AND \( a_1 \).

FIND BY NORMALIZATION.

TO KEEP THINGS \( \psi \) FROM BLOWING UP, WE MUST RESTRICT:
\[ E = 2n + 1 \]
\[ \frac{2E}{\hbar \omega} = \varepsilon = 2n + 1 \]

\[ \Rightarrow \varepsilon = \hbar \omega (n + \frac{1}{2}) \]

\[ 0 - 04 - 75 \text{ (F.R.I.)} \]

TEST: STANDARD DEVIATION = 10

AVG = 67 TO 72

FERMI ENERGY: \[ E_F = \frac{\varepsilon}{2} + \text{CURVATURE} \]

NOTES: HARMONIC OSCILLATOR

\[ V(x) = \frac{1}{2} m \omega^2 x^2 \]

\[ \psi = \sqrt{\frac{m \omega}{\pi}} e^{-\frac{x^2}{2\xi^2}} \quad \xi = \sqrt{\frac{m \omega}{\hbar}} x \]

\[ E_n = \hbar \omega (n + \frac{1}{2}) \]

SOLUTION WAS HERMITE POLYNOMIALS

\[ H = V(\xi) = \sum a_n \xi^n \]

\[ a_{n+2} = \frac{2n+1 - \xi_n}{(n+1)(n+2)} \quad \xi_n = \text{ENERGY} \]

\[ H_0(\xi) = 1 \]
\[ H_1(\xi) = 2 \xi \]
\[ H_2(\xi) = 4 \xi^2 - 2 \]
\[ H_3(\xi) = 8 \xi^3 - 12 \xi \]

ARE ORTHOGONAL: \[ \int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) d\xi = 0 \]

\[ H_n(\xi) = (-1)^n e^{-\xi^2} \frac{d^n}{d\xi^n} (e^{-\xi^2}) \text{ FOR } m \neq n \]

GENERATING FUNCTIONS

RECURSION:

\[ \frac{d}{d\xi} H_n(\xi) = 2n H_{n-1}(\xi) \]
\[ \psi_n = H_n e^{-\xi^2/2} \]

Normalization condition:
\[ \int_{-\infty}^{\infty} H_n^2(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} \frac{2^n}{n!} = 2n \int_{-\infty}^{\infty} H_{n+1}^2(\xi) e^{-\xi^2} d\xi \]

PROBLEM: SHOW THE ABOVE (DUE WEDNESDAY)

Oscillator Wave Functions:

\[ \psi_0 (0 \text{ nodes}) \]
\[ \psi_1 (1 \text{ node}) \]
\[ \psi_2 (2 \text{ nodes}) \]

\[ \sqrt{n+1} \psi_{n+1} - \sqrt{2} \xi \psi_n + \sqrt{n} \psi_{n-1} = 0 \]
\[ \xi \psi_n + \frac{d^2 \psi_n}{d\xi^2} = \sqrt{2n} \psi_{n-1} \]
\[ \xi \psi_n - \frac{d^2 \psi_n}{d\xi^2} = \sqrt{2(n+1)} \psi_{n+1} \]
**Matrix Elements**

\[ \langle \Psi_{f} | \text{PERT} | \Psi_{i} \rangle \]

\( \Psi_{i} \) = \( \phi_{i} \) (atom) \( \Delta \) (field)

\( \text{Norm} \quad \langle \Psi_{i} | \Psi_{i} \rangle = e^{x} \)

**Add Recurrence Relation**

\[ \frac{\Psi_{n+1}}{\sqrt{n+1}} = \Psi_{n}, \quad n = 0, 1, 2, \ldots \]

\[ \frac{\Psi_{n}}{\sqrt{n}} = \sqrt{2} \Psi_{n-1} \]

**Fermi's Golden Rule**

(Rate of Transition)

\[ E \rightarrow \sum (E + \Delta \rightarrow E) \]

**Cross-Section** \( \sigma \)

Recall:

\[ \Psi(x, t) = \sum_{n} a_{n} \phi_{n} e^{-i\omega_{n}t} \]

Solution of \( H \Psi = E \Psi \)

**Perturb:** \( V \)

Assume 0:

\[ a = a(t) \]

\[ \left\{ a(t) \right\} = \sum_{n} a_{n} V_{sn}(t) e^{-\frac{1}{\hbar} (E_{n} - E_{0})t} \]

Anyway, we get the following rate of change

\[ r(t) = \frac{2\pi}{\hbar} |V_{sn}|^{2} \delta (E_{n}) \]
Fermi's Golden Rule

\[ \gamma = \sum \lambda_n \phi_n(x) e^{-\frac{E_n - E}{h}} \]

Solution to \( H \psi = E \psi \)

Assume \( g = g(t) \)

Solve this pert. problem: \( (H + V) \psi = E \psi \)

Gives exactly:

\[ \frac{\phi_0}{E - E \phi_0} = -\frac{i}{\hbar} \sum \frac{\phi_n}{E - E \phi_n} \frac{1}{V_{sn} e^{\frac{E - E_n}{h}} + d \phi} \]

Then \( V_{sn} \neq V_{sn}(t) \)

Assuming \( V \) is not a function of time

Then

\[ \phi = \frac{e^{\frac{E - E_n}{h}}}{E - E_n} \]

Assume \( \phi_0(t) \) are small

Then \( g_n(t) \approx g_n(0) = g_n \)

Assuming system is initially in state \( n \):

\[ g_n(0) = 1 \approx g_n(t) \]

\[ g_n(t) = -\frac{1}{\hbar} \int_0^t V_{sn} e^{\frac{E - E_n}{h}} + d \phi \]

Then

\[ \phi_n(t) = \frac{e^{\frac{E - E_n}{h}} - 1}{E - E_n} \]

\[ P(\text{being in state } s) = P_s = |\phi_s(t)|^2 \]

\[ = \frac{1}{h} \left| V_{sn} \right|^2 \sin^2 \left[ \frac{t}{2h} \left( E_s - E_n \right) \right] \frac{(E_s - E_n)}{(E_s - E_n)^2} \]

\[ P(t) = \sum_s P_s(t) \]

\[ = \int \frac{1}{h} \left| V_{sn} \right|^2 \sin^2 \left[ \frac{t}{2h} (E_s - E_n) \right] \frac{(E_s - E_n)}{(E_s - E_n)^2} \]

\[ \rho(E_s - E_n) \, d(E_s - E_n) \]
$P(t) = \rho(E_n) \frac{2\pi}{\hbar} |V_{sa}|^2 \int_{-\infty}^{\infty} \frac{d(E_e - E_n)}{(E_e - E_n)^2}$

So, over region of interest

Let $\rho(E_e - E_n) = \text{Dens. of State} \ g(E_n)$

$P(t) = 4 |V_{sa}|^2 \rho(E_n) \int_{-\infty}^{\infty} \frac{d(E_e - E_n)}{(E_e - E_n)^2}$

\[\text{[Homework: Solve integral]}\]

Answer is

$P(t) = \rho(E_n) \frac{2\pi}{\hbar} |V_{sa}|^2 \int$

And rate of transition

$\frac{dP(t)}{dt} = \frac{2\pi}{\hbar} |V_{sa}|^2 \rho(E_n)$

Fermi's Golden Rule #2
EXAMPLE: RUTHERFORD SCATTERING

\[ \frac{1}{V\text{ol}} e^{-\frac{1}{2} \mathbf{p} \cdot \mathbf{x}} = \text{INITIAL STATE} \]

\[ V(x) \]

FROM CONS. OF ENERGY:
\[ |\mathbf{p}'| = |\mathbf{p}| \]

\[ V_{\text{sc}} = \frac{1}{V} \int V(x) e^{-\frac{1}{2} \mathbf{p}' \cdot \mathbf{p}' - \mathbf{p} \cdot \mathbf{x}} \, d\mathbf{x} \]

\[ \frac{1}{V} \mathcal{F}[V(x)] \Rightarrow \text{FOURIER TRANSFORM} \]

\[ \text{DENSITY OF STATES:} \]
\[ \frac{\hbar^2}{2m} \int \, d\mathbf{p} = \frac{1}{(2\pi \hbar)^3} \int dE \]

\[ \Delta \Omega \text{ INTEGRATED OUT BEFORE} \]

\[ \frac{d\Omega}{d\Omega} \]

\[ \text{RATE OF TRANSITION:} \]
\[ \frac{d\Omega}{d\Omega} = \frac{\frac{d\Omega}{d\Omega}}{d\Omega} \]

\[ d\Omega = \text{CROSS SECTION} \]
\[ d\Omega = \text{? going into } d\Omega \]

\[ \text{RATE OF TRANSITION:} \]
\[ \frac{d\Omega}{d\Omega} = \frac{2\pi^2}{\hbar^2} \left| \int V(x) \right|^2 \]

\[ \frac{V\mathbf{p}^2}{8\pi\hbar^2} \int \frac{\mathbf{p}^2}{V} \, d\Omega \]

\[ \text{GIVES} \]
\[ \frac{d\Omega}{d\Omega} = \frac{2\pi^2}{\hbar^2} \left( \frac{\mathbf{p}^2}{V} \right) \left| V_{\text{sc}} \right|^2 \]

\[ \frac{d\Omega}{d\Omega} \Rightarrow \text{NON-RELATIVISTICALLY} \]

\[ \frac{d\Omega}{d\Omega} = \frac{\mathbf{p}^2}{V} \]
FOR A COULOMB POTENTIAL:
\[ V(r) = \frac{Ze^2}{r} \quad \text{(Gaussian units)} \]

\[ V_{p,p'} = \frac{Z^2}{\pi \hbar^2} \int \frac{e^2}{(\mathbf{p} - \mathbf{p'})^2} \, d^3 x \]

This is solved in Jackson's text gives:
\[ V_{p,p'} = \frac{\pi \hbar^2 Z^2 e^2}{(4 \rho^2 \sin^2 \theta/2)} \]

which in turn gives:
\[ \frac{d\rho}{\rho} = \frac{Z^2 e^2}{4} \left( \frac{Me^2}{\rho^2} \right)^2 \frac{1}{\sin^4 \theta/2} \leq \frac{1}{4\theta^2} \leq \]  

same as Rutherford's solution.

HEAT DIFFUSION EQUATION:
\[ \nabla^2 T = \frac{\partial^2 T}{\partial t^2} \]

\[ K = \text{thermal conductivity} \]
\[ \rho = \text{density} \]
\[ C = \text{heat capacity} \]
10-29-75 (Wed)

Read Chap. 3.

Heat Diffusion Equation:

$$\nabla^2 T = \frac{\rho C}{k} \frac{dT}{dz}$$

$\rho$ = density

C = Specific heat

$k$ = Thermal conductivity

Assume beam is Gaussian:

$$I = I_0 e^{-\frac{x^2}{2 \sigma^2}}$$

$\sigma$ = Radial heat

2. Absorption

Energy (Heat) absorbed at surface, then transmitted.
 FOR CASE 1: (RADIAL)

USE CYLINDRICAL COORDINATES

\[ \frac{\partial T}{\partial z} = 0, \quad \frac{\partial T}{\partial \theta} = 0 \]

GIVES:

\[ \frac{pC}{k} \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \]

USE SEPARATION OF VARIABLES:

\[ T(r, t) = T_r(r) T_t(t) \]

\[ \frac{pC}{k} \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) \]

GIVES

\[ r \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) = -u^2 T_r \quad \text{(Bessel's Equ'n)} \]

\[ \frac{pC}{k} \frac{\partial T}{\partial t} = -u^2 T_t \]

GIVES

\[ T_r = A(u) J_0(\mu u) \]

\[ T_t = e^{-u^2 kt / \epsilon c} \]

\[ T = T_r T_t = A(u) J_0(\mu u) e^{-u^2 kt / \epsilon c} \]

APPLY BOUNDARY CONDITIONS:

\[ T(r, t = 0) = T_0 \ e^{-r^2/2 \sigma^2} \]

GIVES

\[ e^{-r^2/2 \sigma^2} = \int_0^\infty A(u) J_0(\mu u) \, du \]

\[ A(u) = \frac{1}{2\sigma} \ e^{-\sigma^2} J_0(\mu u) \]

\[ T(r, t) = \int_0^\infty A(u) e^{-u^2 kt / \epsilon c} J_0(\mu u) \, du \]
\[ T(r, t) = \int_0^\infty du \left( \int_0^\infty d\xi J_0(\xi u) e^{-\frac{x^2}{4D_t}} \right) \]
\[ \times e^{-\frac{1}{4D_c} \int_0^t \frac{r^2}{r_0^2} dr} J_0(\alpha r) \]

For solution, see Watson (13.3) gives
\[ T(r, t) = r^2 \int_0^\infty du \ J_0(\alpha r) e^{-\left(1 - \frac{2KT}{\alpha} \right) \frac{r^2}{r_0^2}} \]
\[ = T_0 \left(1 + \frac{2KT}{\alpha} \right) \frac{1}{r_0^2} \alpha \frac{r^2}{r_0^2} \]
\[ \frac{T(\infty)}{T(0)} = \frac{1}{2} \]
\[ \alpha = \left(1 + \frac{2KT}{E} \right) \]

\[ \text{Homework: Suppose } r_0 = 10 \mu m, 100 \mu m. \]
(1) Solve for a semiconductor at \( T = 4^\circ K, 300^\circ K \)
(2) Solve for water @ 300^\circ K

\[ \text{Si} \quad C_p |_{4^\circ K} = 1.68 \times 10^{-6} \text{ Joulle/degree m}^{-2} \text{ Kg}^{-1} \]
\[ C_p |_{100^\circ K} = 0.259 \]

Gr
\[ C_p |_{4^\circ K} = 1.44 \times 10^{-5} \text{ Joulle/degree m}^{-2} \text{ Kg}^{-1} \]
\[ C_p |_{100^\circ K} = 0.191 \]
\( \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial z^2} \)  \( T(z_t) \Rightarrow U^2 = \frac{\rho c \frac{\partial T}{\partial t}}{\kappa} \)

\[
T(z, t) = A(z) \cos(z) e^{-\frac{u^2 \kappa t}{\epsilon c}}
\]

\[
T(z_t) = T_0 e^{\mu(z_0 - z)}
\]

\[
T(z, t) = \int_0^\infty A(u) \cos(u z) e^{-\frac{u^2 \kappa t}{\epsilon c}}
\]

\[
\Rightarrow A(u) = \frac{1}{\pi} \int_0^\infty T(z, 0) \cos(u z) dz
\]

\[
T(z, t) = \int_0^\infty A(u) \cos(u z) e^{-\frac{u^2 \kappa t}{\epsilon c}}
\]

\[
= \frac{T_0}{2 \sqrt{\pi \kappa \epsilon c}} \int_0^\infty e^{-\frac{t}{x^2} + \frac{z^2}{4 \kappa t}} + \frac{\epsilon c}{(x - \frac{z}{2})^3} \frac{e^{-\frac{z^2}{4 \kappa t}}}{\sqrt{\kappa t}}
\]

\[
T(z, t) = \frac{2 T_0}{\sqrt{\pi \kappa \epsilon c}} \int_0^\infty e^{-\frac{z^2}{4 \kappa t}} \frac{e^{-\frac{z^2}{4 \kappa t}}}{\sqrt{\kappa t}}
\]

\[
t_\frac{1}{2} = Z_0 \frac{\epsilon c}{\kappa}
\]
10-31-75 (FRI) 2 STATE QUANTUM SYSTEM

\[ H = H_0 + V \]

**KNOWN SOLUTION EXTRACTED FOR LIGHT FIELD**

**ONE ASSUMES THAT:**

\[ H_0 \text{ gives } \psi = a \phi_a e^{-i \omega_0 t} + b \phi_b e^{-i \omega t} \]

\[ \phi_a \implies |a\rangle \]
\[ \phi_b \implies |b\rangle \]

\[ \langle a | b \rangle_\text{KET} = \delta_{ab} \]

\[ \psi = a |a\rangle e^{-i \omega_0 t} + b |b\rangle e^{-i \omega t} \]

**ASSUME \( a \neq b \) ARE FUNCTIONS OF TIME**

\[ a = a(t) \quad b = b(t) \]

**WANNA FIND \( \psi \) FOR \( H_0 + V \)**

\[ E_0 = \langle 0 | H_0 | 0 \rangle \]

**WANNA FIND:**

\[ \langle a | H_0 + V | \psi \rangle \]
Using \( \langle a | b \rangle = 0 \)
\( \langle a | a \rangle = 1 \)

Gives
\[
\langle a | H_0 + V | b \rangle = \langle a | H_0 | a \rangle e^{-i\omega t} + \langle a | V | b \rangle e^{-i\omega t}
\]
\[\langle a | H_0 | b \rangle = \langle a | E_b | b \rangle = 0\]

Since
\[H \psi = \frac{-i}{\hbar} \frac{\partial \psi}{\partial t}\]

\[
\langle a | H_0 | a \rangle e^{-i\omega t} + \langle a | V | b \rangle b e^{-i\omega t} = i\hbar \left[ a e^{-i\omega t} - i\omega a e^{-i\omega t} \right]
\]

Define:
\( V_{ab} = \langle a | V | b \rangle \)

Assume
\( V_{aa} = V_{bb} = 0 \quad \Rightarrow \quad V_{ab} = V_{ba} \)

\[
\begin{align*}
    H_w & = w_e - w_q \\
    V_{ab} b e^{-i\omega t} & = \frac{i}{\hbar} a e^{-i\omega t} \\
    V_{ba} a e^{-i\omega t} & = \frac{i}{\hbar} b e^{-i\omega t}
\end{align*}
\]

Equivalently:
\[
\begin{align*}
    a & = \frac{-i}{\hbar} V_{ab} b e^{-i\omega t} \quad \text{WANNA SOLVE} \\
    b & = \frac{-i}{\hbar} V_{ba} a e^{i\omega t}
\end{align*}
\]
\[ V = E_0 x_b \cos \omega t \leq \text{APPLIED \ E \ FIELD} \]
\[ e^{\langle a \mid x \mid b \rangle} = \langle x \rangle = \text{POLAR} \]

\[ a = \frac{n}{2} \frac{\mu_0}{2} E_{ab} \left[ e^{i (\omega t - \omega_0 t)} + e^{-i (\omega t + \omega_0 t)} \right] \]

\[ b = \frac{n}{2} \frac{\mu_0}{2} E_{ab} \left[ e^{i (\omega t - \omega_0 t)} + e^{-i (\omega t + \omega_0 t)} \right] \]

\text{Assume damping:}
\[ a = -\frac{\delta}{2} a, \quad b = -\frac{\delta}{2} b \]

\[ a = \frac{i \omega_0 \mu_0 E_{ab}}{2} e^{i \omega t} - \frac{i n}{2} a \]

\[ b = -\frac{i \omega_0 \mu_0 E_{ab}}{2} e^{-i \omega t} - \frac{i n}{2} b \]

\[ \delta = \omega - \omega_0 \]

\[ \delta = \frac{V_{ab}}{V_{ba}} \]
\[ \alpha = \alpha e^{-i(\omega t + \frac{\alpha}{2})} \]
\[ \beta = \beta e^{-i(\omega t + \frac{\beta}{2})} \]

**INITIAL CONDITIONS**

1. \( \alpha = 1, \beta = 0 \) at \( t = t_0 \)
2. \( \beta = 1, \alpha = 0 \) at \( t = t_0 \)

\[
\begin{align*}
\alpha &= \frac{-i\omega E_0}{\hbar} e^{i(\omega t - \frac{\alpha}{2})} e^{-i(\omega t + \frac{\alpha}{2})} e^{i\omega t} \\
\beta &= \frac{i\omega E_0}{\hbar} e^{i(\omega t - \frac{\beta}{2})} e^{-i(\omega t + \frac{\beta}{2})} e^{i\omega t}
\end{align*}
\]

**TO FIRST ORDER IN E FIELD**

\[
\beta(t) = \int_{t_0}^{t} e^{-i\omega t} \, dt
\]

\[
= \frac{i\omega E_0}{\hbar} e^{-i\omega t} e^{-i(\omega t - \frac{\alpha}{2})} e^{i\omega t} e^{i(\omega t - \frac{\beta}{2})} e^{-i\omega t}
\]

\[
= \frac{i\omega E_0}{\hbar} \left[ e^{i(\omega t - \frac{\alpha}{2})} e^{i(\omega t - \frac{\beta}{2})} - 1 \right]
\]

\[
P = \text{POLARIZATION} = \langle \gamma / \mu \rangle
\]

\[
P = \mu \left[ \alpha^* \beta e^{-i\omega t} + ab^* e^{i\omega t} \right]
\]

\[
= \mu \left[ \alpha^* \beta e^{-i\omega t} + ab^* e^{i\omega t} \right]
\]

\[
P = \mu \left( \frac{\alpha^* \beta}{\hbar} \right) \left[ e^{i\omega t + \frac{\alpha}{2}} e^{-i\omega t - \frac{\beta}{2}} \right]
\]

\[
= \frac{\alpha^* \beta}{\hbar} \left( e^{i\omega t + \frac{\alpha}{2}} - e^{-i\omega t - \frac{\beta}{2}} \right)
\]

\[
= \frac{\alpha^* \beta}{\hbar} \left( e^{i\omega t + \frac{\alpha}{2}} - e^{-i\omega t - \frac{\beta}{2}} \right)
\]
Assume $R_a(t) = \text{constant}$.

(Which atoms are excited into state $a$)

Anyway, the answer is:

$$P = \frac{n_2 E_0}{2 \hbar} \left( \frac{R_b R_a}{\delta_a} - \frac{R_b R_a}{\delta_b} \right)$$

$$\times \frac{1}{(\omega - \omega_0)^2 + \delta_b^2} \left[ (\omega - \omega_0) \text{constant} - \text{decay} \right]$$

= Steady State Polarization

11-3-75 (Mon)

E Field on 2 State System

$R_a$, $R_b$ = Humans

$\delta_a$, $\delta_b$ = Decay

We get:

$$P = \frac{n_2 E_0}{2 \hbar} \left( \frac{R_b R_a}{\delta_b} - \frac{R_b R_a}{\delta_a} \right) \left[ \frac{e^{i \omega t} - e^{-i \omega t}}{2 - i \delta_b} - \frac{e^{i \omega t} - e^{-i \omega t}}{2 + i \delta_b} \right]$$

$$= \frac{n_2 E_0}{\hbar} \left( \frac{R_b R_a}{\delta_b} - \frac{R_b R_a}{\delta_a} \right) \left[ (\omega - \omega_0) \text{constant} - \text{decay} \right]$$
\[ \langle i | v | b \rangle \]

\[ \text{PROB } i \rightarrow b \sim \langle i | v | b \rangle^2 \]

\[ \begin{align*}
&\{ \text{FOR A COLLISION} \\
&\quad \langle \text{OUTGOING} \mid v \mid \text{INCOMING} \rangle \\
&\quad \langle e^{-i K \cdot x} \mid v(x) \rangle
\end{align*} \]

\[ = \mathcal{E}_1 \langle v(x) \rangle \]

\[ \text{ANYWAY, ASSUMING INDEPENDENCE} \]

\[ p_t = \text{PROB. OF TRANSITION} = \sum_i \langle i | v_0 | b \rangle^2 \]

\[ = \sum_i \langle i | v_0 | b \rangle^2 \]

\[ \text{DECAY } \frac{d n_b}{dt} = p_t n_b \]

\[ \Rightarrow n_b = n_{b_0} e^{-t \delta_b} \Rightarrow \delta_b = \frac{1}{p_t} \]

\[ \Rightarrow y_b = \sum_i \langle i_e | v | b \rangle^2 \]
BOLTZMANN TRANSPORT EQN.

\[ f(\mathbf{v}, x, t) = \frac{6}{5} \mathbf{v} \cdot \mathbf{a} + \frac{6}{5} \nabla \cdot \mathbf{v} + \frac{\mathbf{v} \cdot \mathbf{v}}{5} = 0 \]

\[ \frac{df}{dt} = \frac{6}{5} \frac{\mathbf{v}}{\mathbf{a}} + \frac{3}{5} \frac{\mathbf{a}}{\mathbf{a}} + \frac{\mathbf{v} \cdot \mathbf{v}}{5} + \frac{\mathbf{v}}{5} \]

= 0 IN AN EQUILIBRIUM

\[ \frac{dv}{dx} = a = \frac{F}{m^2} \]

\[ \frac{dx}{dt} = v \]

\[ \frac{d}{dt} = -\frac{v}{\tau} \]

\[ \frac{d}{dt} = -\frac{f}{\tau} \]

IN EQUILIBRIUM:

\[ \frac{v}{t} = v \cdot \nabla f + a \cdot \nabla f \]

NOW \( \beta = \frac{v}{k} \)

IN QM:

\[ \frac{f_0 - f}{\tau} = \frac{\hbar}{m^2} \cdot \nabla f + \frac{\hbar}{v} \cdot \nabla f \]
TEST # 2 NEXT WEDNESDAY
MATERIAL IN TEXT: CHART 4

\[
\frac{\mathbf{f}_0 - \mathbf{f}}{\gamma} = \mathbf{V} \cdot \nabla \mathbf{f} + \frac{1}{\rho} \cdot \nabla \mathbf{f}
\]

APPROXIMATION:

\[
\frac{\delta^2 \mathbf{f}}{\delta x \delta y} = \frac{\delta^2 \rho_0}{\delta x \delta y}
\]

**METAL**

\[
f_0 = n \left( \frac{m}{2 \pi kT} \right)^{3/2} e^{-\frac{mV^2}{2kT}} \text{ MAXWELL BOLTZMANN DISTRIBUTION}
\]

WILL CALCULATE

① ELECTRON CURRENT DENSITY

② HEAT CURRENT DENSITY

WORK INVOLVES SOLUTION OF:

\[
I_n = \int_{-\infty}^{\infty} e^{-ax^2} dV = \frac{\sqrt{\pi} a^{3/2}}{2} e^{a/V^2}
\]

\[
\rho_n = \int_{-\infty}^{\infty} e^{-ax^2} x^n dx
\]

① \( I_n = \int_{-\infty}^{\infty} e^{-ax^2} dV = \frac{1}{2} \sqrt{\frac{\pi}{a}} \)

② \( \rho_n = \frac{1}{2} \sqrt{\frac{\pi}{a}} \)

\[
(\rho_n) = \int_{-\infty}^{\infty} e^{-ax^2} x^n dx
\]

\[
(\rho_n) = \frac{1}{2} \sqrt{\frac{\pi}{a}} \]

\[
\rho_n = -\frac{5}{8a} \left[ \int_{-\infty}^{\infty} e^{-ax^2} x^{n-2} dx \right]
\]

\[
\rho_n = -\frac{5}{8a} \rho_{n-2}
\]
\[ \mathcal{O}_3' = -\frac{3}{2} \mathcal{O}_2 \mathcal{O}_2' = \frac{4}{9} \mathcal{O}_2 \mathcal{E}^{-3/2} \]

Etc.,

\[ \mathcal{O}_3' = \frac{1}{2} \mathcal{O}_3 \]

\[ \mathcal{O}_2' = \mathcal{O}_2 \mathcal{E}^{-3/2} \]

\[ \mathcal{O}_3' = \frac{1}{2} \mathcal{O}_3 \]

\[ \mathcal{O}_n' = \frac{1}{2} \Bigl( \frac{n+1}{2} \Bigr) \mathcal{O}_2 \]

Rewriting Boltzmann Eqn.: (1-0)

\[
\mathcal{T} = \mathcal{T}_0 - \gamma \left( v_x \frac{\partial f}{\partial v_x} + a_x \frac{\partial f}{\partial v} \right)
\]

Define current density:

\[
\mathcal{J}_x = -e \sum \mathcal{E} \mathcal{V}_x
\]

\[
= -e \int_{-\infty}^{\infty} \mathcal{V}_x \mathcal{F} d\mathcal{V}_x
\]

\[
= \int_{-\infty}^{\infty} \gamma \left( \mathcal{V}_x \frac{\partial f}{\partial \mathcal{V}_x} + a_x \frac{\partial f}{\partial \mathcal{V}^2} \right)
\]

Thermal current density:

\[
\mathcal{C}_x = \int_{-\infty}^{\infty} \mathcal{F} \mathcal{V}_x \mathcal{E} d\mathcal{V}
\]

Now

\[
\frac{\partial f}{\partial \mathcal{V}_x} = \left( \frac{\mathcal{M} v^2}{2 \mathcal{K} T} - \frac{1}{2} \right) \frac{f_0}{\mathcal{E}_x}
\]

\[
\frac{\partial f}{\partial \mathcal{V}_x} \frac{\partial \mathcal{V}_x}{\partial \mathcal{E}_x} \Rightarrow \frac{\partial \mathcal{V}_x}{\partial \mathcal{E}_x} = \frac{e \mathcal{E}_x}{m^2}
\]

\[
\Rightarrow \frac{\partial f}{\partial \mathcal{V}_x} \frac{\partial \mathcal{V}_x}{\partial \mathcal{E}_x} = \frac{e \mathcal{E}_x}{m^2} \mathcal{V}_x + f_0
\]

Gives

\[
\mathcal{J}_x = \frac{n e \mathcal{K} T}{\mathcal{E}_x} \mathcal{S} \mathcal{T} + \frac{n e \mathcal{K} T}{\mathcal{E}_x} \mathcal{E}_x
\]

\[
\mathcal{C}_x = \frac{-5 n k^2 T \mathcal{E}_x}{\mathcal{S} \mathcal{T}} - \frac{5 n e \mathcal{K} T \mathcal{E}_x}{2 m}
\]
\[ I = 0 \quad \text{at} \quad T = 0 \quad \text{gives} \quad \alpha = ne^2 / y m \]

**Thermal Conductivity**

\[ K = \frac{C_y}{S} \frac{1}{8x} \]

**For \( E_x = 0 \) \Rightarrow K = \frac{-5nK^2T^2}{m}**

**Wiedemann-Franz Ratio**

\[ \frac{K}{\sigma T} = \frac{\pi^2}{3} \left( \frac{k_e}{e} \right)^2 \leq \text{Material Independent} \]

\[ \approx 2.5 \times 10^{-8} \]

To get, use Fermi-Dirac

\[ f_0 = \frac{1}{1 + e^{-(E-E_F) / kT}} \]

And \( \sigma \) (see book)

\[ \int_{-\infty}^{\infty} \frac{x^2 e^x}{(1 + e^x)^2} \, dx = \frac{\pi^2}{2} \]

End of material covered on test #2
9-10-75 (Mon) (Guest Lecture)

Crystal Structure

Single crystal - same crystal structure throughout

Poly-crystalline - many crystal structures

Amorphous - changing crystalline structure

Liquid crystal - two dimensional crystal structure

\[ \bar{c} = \bar{c} + a_1 \bar{a} + a_2 \bar{b} \]

In 3-D, simplest is a cube

Face centered cube

[Diagram of a face-centered cubic unit cell]
BODY CENTERED CUBIC

Each atom shared with 8 others (sharing)

Atoms per unit cell

\[ \begin{array}{cccc}
\text{Simple} & a^3 & 1 & 6 & \frac{\sqrt{3}a}{2} \\
\text{Body Center} & a^3 & 2 & 8 & \frac{\sqrt{3}a}{2} \\
\text{Space Center} & a^3 & 4 & 12 & \frac{\sqrt{3}a}{2} \\
\end{array} \]

Parallelepiped

BRAVAIS LATTICE - PERIODIC STRUCTURE

Def: \( \# \) pts, in space with the property that the arrangement of points around a given pt. is identical with that about any other point.

Get 7 classes:

1. Cubic: \( a = b = c, \alpha = \beta = \gamma = \frac{\pi}{2} \)

2. Triclinic: \( a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq \frac{\pi}{2} \)

3. Monoclinic: \( a = \beta = \frac{\pi}{2}, \alpha \neq \beta \neq \gamma \)

4. Rhombohedral:
   \( a = b = c, \alpha = \beta = \gamma = \frac{\pi}{3} \)

5. Tetragonal:
   \( a = b > c, \alpha = \beta = \gamma = \frac{\pi}{2} \)

6. Orthorhombic:
   \( a \neq b \neq c, \alpha = \beta = \gamma = \frac{\pi}{2} \)

7. Hexagonal:
   \( a = b < c, \gamma = 120^\circ, \alpha = 60^\circ \)
EACH OF THESE CAN BE PRIMITIVE, BCC, FCC, OR CUBIC CENTERED

0 FOLD ROTATION: MAY ROTATE \( \frac{360^\circ}{n} \) AND GET THE SAME THING.

11-14-75 (FRI) (GUEST LECTURE)

MILLER INDICES

DEFINED SPACE LATTICE VIA TRANSLATION

\[ \mathbf{R} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c} \]

WISH TO FIND INTEGERS \( h, k, l \)

SUCH THAT

\[ h, k, l = \frac{p}{g}, \frac{q}{g}, \frac{r}{g} \]

EX: \( p = 2, q = 3, r = 1 \)

\[ \Rightarrow (h, k, l) = (3, 2, 6) \]

FOR NEGATIVE INTERCEPTS, USE \( -1 \)

IF NO INTERCEPT, USE \( 0 = \frac{1}{\mathbf{c}} \)

L FROM PLANE TO ORIGIN:

\[ \mathbf{d} = \frac{n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}}{g} \]

\[ = \frac{h}{a}, \frac{k}{b}, \frac{l}{c} \]

\[ d = \left( \frac{\mathbf{a} \cdot \mathbf{c}}{\mathbf{a} \cdot \mathbf{c}} \right) \cos \alpha \]

\[ = \frac{2}{d} \cos 2\alpha \]
\[ \cos^2 \alpha = \frac{d^2 h^2}{a^2} \]
\[ \cos^2 \beta = \frac{d^2 k^2}{a^2} \]
\[ \cos^2 \gamma = \frac{d^2 l^2}{a^2} \]
\[ \sum \cos^2 = 1 \]

\[ \Rightarrow \frac{d^2}{a^2} (h^2 + k^2 + l^2) = 1 \]

\[ \Rightarrow d = \sqrt{h^2 + k^2 + l^2} \]

**EXPERIMENTAL DETERMINATION**

**X-RAY DIFFRACTION**

1. **BRAGG**

2. **VAN LAUE**

\[ \bar{a} (s_1 - s_0) = h \lambda \]
\[ \bar{b} (s_2 - s_0) = k \lambda \]
\[ \bar{c} (s_3 - s_0) = l \lambda \]
RECIPIRAL LATTICE

\[ \mathbf{a}^* = \mathbf{a} \times \mathbf{b} / (\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}) \]
\[ \mathbf{b}^* = (\mathbf{c} \times \mathbf{a}) / (\mathbf{b} \cdot \mathbf{c} \times \mathbf{a}) \]
\[ \mathbf{c}^* = \mathbf{a} \times \mathbf{b} / (\mathbf{c} \cdot \mathbf{a} \times \mathbf{b}) \]

PROPERTIES

1. VOL UNIT CELL = \( \frac{1}{\mathbf{V}_{UNIT\ CELL}} \)
2. \( \mathbf{a}^* \cdot \mathbf{a} = 1 \)
3. \( \mathbf{a} \cdot \mathbf{b}^* = 1 \)
4. \( \mathbf{b} \cdot \mathbf{b}^* = 1 \)
5. \( \mathbf{a} \cdot \mathbf{b} = 0 \)

OTHER PROPERTIES

1. \( \mathbf{r}^* = (h, k, l) \) is \( (h, k, l) \) LATTICE PLANE
2. \( |\mathbf{r}^*(h, k, l)| = \frac{1}{d(h, k, l)} \)
3. RECIPROCAL OF F.C.C. IS B.C.C.

11.7.25 (MON) WAVE FUNCTION FOR ELECTRON

\[ \psi(x) = e^{ik \cdot x} \]
\[ U_k(x) \subseteq PERIODIC\ LATTICE \]
\[ U_k(x) IS\ PERIODIC = BLOCK\ FUNCTIONS \]

\[ \psi(x) \]
\[ U_k(x) \]
\[ \psi(x) \]  

1. USE PERIODIC PROPERTY
\[ |\psi(x)| = |\psi(x+a)|^2 \]
\[ \psi(x+a) = e^{i \times (x, a)} \psi(x) \]

KINEMATICAL CONSIDERATIONS:

1. TRANSLATION
\[ \psi(x_0 + x) = \psi(x_0) + \frac{\partial \psi(x_0)}{\partial x} \left|_{x_0} \right. + \frac{\hbar^2}{2m} \left. \frac{\partial^2 \psi(x_0)}{\partial x^2} \right|_{x_0} \]
\[ y(x + x_0) = y(x_0) + \frac{1}{2!} \frac{\delta^2 y(x_0)}{\delta x^2} (x - x_0)^2 \]

\[ \Rightarrow y(x + x_0) = y(x_0) e^{x_0^2/k} \]

\[ \frac{\delta}{\delta x} \Rightarrow \frac{\partial}{\partial p} \Rightarrow \frac{\partial}{\partial k} \]

\[ \Rightarrow y(x + x_0) = y(x_0) e^{x_0^2/k} \]

Thus, \( f(k, a) = k \cdot \bar{a} \)

\[ \text{In } k = 0: \]

\[ y_{1/2}(x) = \psi(x) e^{i \cdot k \cdot x} \]

\[ \text{ABELIAN GROUPS (COMMUTE)} \]

\[ AB = BA \]

\[ \exists N \Rightarrow A^N = A \quad (A^{N-1} = 1) \]

\[ \text{ONE DIMENSIONAL IRREDUCIBLE REPRESENTATION} \]

\[ \Rightarrow A = e^{i \cdot k \cdot x} \]
K - P Method

For behavior of electrons (holes) for small \( k \),

For an electron:

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi_{K,P}(\mathbf{r}) = E(\mathbf{r}) \Psi_{K,P}(\mathbf{r})
\]

Cropping through:

\[
\left( \frac{\hbar^2}{2m} \nabla^2 + \frac{\hbar^2 k^2}{2m} + V \right) \Psi_{K,P}(\mathbf{r}) = E(\mathbf{r}) \Psi_{K,P}(\mathbf{r})
\]

For direct gap material (small \( k \)),

Conduction band (in Co, spreading of 5 state)

\( \Psi_K = \frac{1}{d} \phi_U + \frac{1}{d} \phi_U \phi_U \phi_U \)

Valence band (in Co, from a P state)

S wave function

P state functions

3 states (Co w/ spin)
\[ U_{z} = \frac{4}{\pi} \sum_{k=1}^{N} q_k \cdot U_k \]

Assume \( k \) is small

\[ \int U_{x}^* U_{y}(r) \, dr = \delta_{ij} \quad \text{ORTHONORMAL} \]

Then

\[ E_{C} U_{C} + \frac{k}{m} \left[ k_{x} \int P_{x} U_{C}^{2}(r) \, dr + k_{y} \int P_{y} U_{C}^{2}(r) \, dr \right] \]

\[ -k_{z} \int \overline{P} U_{C}^{2}(r) \, dr - E(k) U_{C} = 0 \]

Multiply by \( dr^2 \) and \( \int \) gives

\[ \int U_{C}^* (r) E_{C} U_{C} (r) \, dr^2 + \frac{k}{m} \left[ k_{x} \int U_{C}^* \overline{P}_{x} U_{C} \, dr \, dr + k_{y} \int U_{C}^* \overline{P}_{y} U_{C} \, dr \, dr \right] \]

\[ -k_{z} \int \overline{P} U_{C}^{2}(r) \, dr + k_{z} \int U_{C}^* \overline{P} U_{C} \, dr \]

\[ = E_{C} - E(k) - \frac{k}{m} \left[ k_{x} \int U_{C}^* \overline{P}_{x} U_{C} \, dr \, dr + k_{y} \int U_{C}^* \overline{P}_{y} U_{C} \, dr \right. \]

\[ \left. + k_{z} \int \overline{P} U_{C}^{2}(r) \, dr \right] \]

Due to symmetry

\[ = -E(k) + E_{C} \]
11-19-75 (Wed)

**K·P APPROXIMATION**

\[ \sum_{c} C_{k}^{c} \left( \mathbf{r} \right) U_{c}^{c} \left( \mathbf{r} \right) \Rightarrow \text{IN CONDUCTION BAND} \]

\[ \sum_{v} C_{k}^{v} \left( \mathbf{r} \right) U_{v}^{v} \left( \mathbf{r} \right) \Rightarrow \text{IN VALENCE BAND} \]

GAVE

\[ 0 = \sum_{i} \left( E_{x}^{i} - \frac{1}{m} \mathbf{K} \cdot \mathbf{P} - E^{i} \left( \mathbf{r} \right) \right) C_{k}^{i} V_{k}^{i} \left( \mathbf{r} \right) \]

USING ORTHOGONALITY OF \( U_{c}^{c} \)'S AND \( U_{v}^{v} \)'S GIVES FOUR EQUATIONS.

\[ E - E^{i} \left( \mathbf{r} \right) \]

\[ = \sum_{c} E_{c} U_{c}^{c} + \frac{1}{m} \sum_{x} \left( k_{x} \sum_{c} U_{c}^{c} p_{x} U_{c}^{c} + k_{y} \sum_{y} + k_{z} \sum_{z} - \int U_{c}^{c} E^{i} \left( \mathbf{r} \right) U_{c}^{c} d\mathbf{r} \right) \]

\[ \int U_{c}^{c} E_{x} U_{x} d\mathbf{r} + \frac{1}{m} \sum_{x} \left( k_{x} \sum_{c} U_{c}^{c} p_{x} U_{c}^{c} \right) \]

\[ + k_{y} \sum_{y} U_{c}^{c} U_{x} d\mathbf{r} + k_{z} \sum_{z} U_{c}^{c} U_{x} d\mathbf{r} \]

\[ = \frac{1}{m} k_{x} \sum_{c} U_{c}^{c} p_{x} U_{c}^{c} \]

NOTE:

\[ \int U_{c}^{c} p_{x} U_{x} d\mathbf{r} = \int U_{c}^{c} p_{y} U_{y} d\mathbf{r} \]

DENOTE:

\[ \frac{1}{m} \int U_{c}^{c} p_{i} U_{i} = P_{c}^{i} \text{ MATRIX ELEMENT} \]

**IN SUMMARY, DETERMINE COEFFICIENTS**

\[ \begin{vmatrix}
E_{c} - E^{i} \\
K_{x} p \\
K_{y} p \\
K_{z} p
\end{vmatrix}
\]

\[ K_{x} p \quad K_{y} p \quad K_{z} p \quad K_{x} p \quad K_{y} p \quad K_{z} p \]

\[ = 0 \]

\[ E_{c} - E^{i} \]

\[ K_{x} p \quad E_{x} - E^{i} \quad K_{y} p \quad E_{y} - E^{i} \quad K_{z} p \quad E_{z} - E^{i} \]

\[ 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \]
PLUGGING ON GIVES:

\[ 0 = \left[ E_0 - E(K^2) \right] \left[ E_V - E(K^2) \right] - 1 \alpha x^2 \beta^2 (E_V - E(K^2))^2 - k_\perp^2 \beta^2 (E_V - E(K^2))^2 - k_\perp^2 \beta^2 (E_V - E(K^2))^2 \]

SIMPLIFYING:

\[ 0 = \left[ E_V - E(K^2) \right]^2 \left[ \left[ E_0 - E(K^2) \right] \left[ E_V - E(K^2) \right] - k_\perp^2 \beta^2 \right] \]

FOUR SOLUTIONS ARE

\[ E(K^2) = \begin{cases} \frac{E_V}{2} + \sqrt{\frac{E_0 + E_V}{2} + \frac{(E_0 - E_V)^2 - k_\perp^2 \beta^2}{4}} \frac{1}{2} \\ \frac{E_0 + E_V}{2} - \sqrt{\frac{(E_0 - E_V)^2 + k_\perp^2 \beta^2}{4}} \frac{1}{2} \end{cases} \]

FOR SMALL \( k_\perp \), ONE MAY APPROXIMATE:

\[ E(K^2) \approx E_0 \pm \frac{2k_\perp^2 \beta^2}{E_0 - E_V} \leftrightarrow \text{PARABOLIC BAND} \]

"FREE LIKE" FOR SMALL \( k_\perp \)

\[ \text{TWO FOLD DEGENERATE} \]

OBSERVED IN GERMANIUM
BAND STRUCTURE CALCULATION

HARTREE METHOD

1. N electrons, 1 in outer shell
   \[ V(x) \Rightarrow N - 1 \text{ inner electrons} \]
2. Assumed spherical symmetry
3. Required self consistency

Charge density: \[ \rho = e \sum_{i=1}^{N-1} \phi_i^* \phi_i \]

Cave potential \[ V(r) \]

Assume two electrons, \( \phi_1(x_1), \phi_2(x_2) \)

to include exclusion principle

Use wave function
\[
\frac{1}{\sqrt{N!}} \begin{vmatrix}
\phi_1(x_1) & \phi_2(x_2) \\
\phi_1(x_2) & \phi_2(x_1)
\end{vmatrix}
\]

= \frac{1}{2} \begin{vmatrix}
\phi_1(x_1) & \phi_2(x_2) \\
\phi_1(x_2) & \phi_2(x_1)
\end{vmatrix}

Exchange term

In general

\[
\frac{1}{\sqrt{N!}} \begin{vmatrix}
\phi_1(x_1) & \phi_2(x_1) & \ldots & \phi_n(x_1) \\
\phi_1(x_2) & \phi_2(x_2) & \ldots & \phi_n(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_1(x_N) & \phi_2(x_N) & \ldots & \phi_n(x_N)
\end{vmatrix}
\]

\[ \Rightarrow \text{anti-symmetrize} \]

Called Slater determinant
Hartree - Fock Approach to Calculating Band Structure

\[ H = - \sum_i \frac{\hbar^2}{2m} \nabla_i^2 - \sum_j \frac{\hbar^2}{2m} \nabla_j^2 + \frac{i e^2}{\hbar} \sum \frac{1}{|R_i - R_j|} \]

Nucleus - electrons Elec/Elec Term

\[ + \frac{1}{2} \sum_k \sum_l \frac{e^2}{|R_k - R_l|} - \frac{1}{2} \sum_k \frac{e^2}{|R_k - R_l|} \]

Nucleus - Nucleus Nucleus/Electron

Too hairy to solve.

Born - Oppenheimer Approximation

Separate Electronic & Vibrational Motion

\[ \psi_n \]

Nucleus

Assume \( \psi = \psi_e \psi_n \) (neglect H\text{\textsubscript{no}})

Gives

\( (H_e + H_n) \psi_e \psi_n = E \psi_e \psi_n \)

References:
1. Slater, Quantum Theory of Molecules and Solids (I)
2. Slater - Quantum Theory of Matter
3. Eminan - Electrons and Phonons in Solids
Using 2nd, 3rd, & 5th terms

Assume

\[ E_e = \sum \psi_e \phi_e \psi_e \]

\[ \psi_e = \phi_1 \phi_2 ... \phi_N \text{ each indiv. } e^- \]

Include Slater determinant

\[ \psi_e = \prod \phi_i \]

The

\[ E_e = \sum E_j + \frac{1}{2} \sum \sum \phi_i^* \phi_j^* V_{ij} \phi_i \phi_j \]

where

\[ V_{ij} = \frac{e^2}{|r_i - r_j|} \]

Hartree Eqn. is

\[ \hat{H} \psi_e + \frac{1}{2} \sum \sum \phi_i^* \phi_j^* V_{ij} \phi_i \phi_j \psi_e = E_e \psi_e \]

It's a one-electron Eqn.
HARTREE-FOCH SUMMARY

WAYS TO DETERMINE ENERGY LEVELS

ASSUME: \[ \Psi = \phi_1(x_1) \phi_2(x_2) \]

\[ \phi_n = \text{WAVE FNC. OF N^{th} ELEC.} \]

YOU GET \[ H \Psi = E \Psi \]

WANNA MINIMIZE USING VARIATION PRINCIPLE

HARTREE-FOCH INCLUDED EXCHANGE TERMS

\[ \sqrt{N!} \begin{bmatrix} \phi_1(x_1) \\ \phi_2(x_2) \\ \vdots \\ \phi_N(x_N) \end{bmatrix} \]

FOR TWO ELECTRONS

\[ \Psi = \frac{1}{2} \begin{bmatrix} \phi_1(x_1) & \phi_2(x_2) \\ -\phi_2(x_2) & \phi_1(x_1) \end{bmatrix} \]

EACH GOT TWO PARTS

\[ \phi_1(x_1) = \phi_1\text{SPACE} (x_1) \phi_1\text{SPIN} (m_1 = \frac{1}{2}) \]

WISH TO DESYMPLIFIZE WAVE FNC.

FOR AN ELECTRON

\[ \Psi = \phi_1\text{SPACE} (x_1) \phi_1\text{SPACE} (x_2) \phi_1\text{SPIN} (1) \phi_1\text{SPIN} (2) \]

RESULTING ENERGY IS

\[ E = \sum \int \phi_i^* \left( -\frac{\hbar^2}{2m} \nabla_i^2 \right) \phi_i \\
+ \sum_{i,j} \int \phi_i^* (x_1) \phi_j^* (x_2) \left[ \frac{e^2}{4\pi \epsilon_0 |x_1 - x_2|} \right] \]

\[ \times \left[ \phi_i^*(x_1) \phi_j^*(x_2) - \delta_{m_{SPIN_i} m_{SPIN_j}} \phi_j(x_2) \phi_i(x_1) \right] d^2x_1 d^2x_2 \]
HOMEWORK PROBLEM: DESCRIBE IN ONE OR TWO PAGES A METHOD OF ENERGY BAND STRUCTURE CALCULATION.

1. LCAO = LINEAR COMBINATION OF ATOMIC ORBITALS
2. ORTHOG. PLANE WAVE (OPW)
3. W-S CELLULAR (WIGNER-SEITZ)
4. X-Ω METHOD
5. TIGHT BINDING APPROXIMATION

POINT OUT
A. APPLICABILITY AND WHY & WHAT
B. OPTIONAL PROBLEM: WHAT IS THE PHYSICAL SIGNIFICANCE OF THE EXCHANGE TERM? (HINT: PAULI EXCLUSION PRINCIPLE) LOOK AT TWO ELECTRON WAVE FUNCTION.

ABSORPTION OF LIGHT IN SOLID
MAXWELL'S EQN.'S
\[ \mu = \text{PERMITTIVITY} = 1 \]
\[ \epsilon = \text{DIELECTRIC CONST.} \]
\[ \frac{\mu}{\sqrt{\epsilon}} - \frac{\epsilon}{\mu} \]

GIVES
\[ \frac{\mu^2 \epsilon}{\epsilon^2} - \frac{\epsilon}{\mu} \frac{\mu^2 \epsilon}{\epsilon^2} = \frac{4\pi\epsilon_0}{\mu} \frac{\mu^2 \epsilon}{\epsilon^2} \]

(OPTIONAL HOMEWORK \Rightarrow DERIVE IT)

ASSUME \[ \epsilon = \epsilon_0 (\kappa \kappa' - \omega^2) \]

YOU GET
\[ \frac{\mu^2}{\omega^2} = \frac{\epsilon_0}{\epsilon^2} + \frac{4\pi\epsilon_0}{\omega^2} = \frac{1}{\gamma^2} \]

REFRACTIVE INDEX (\gamma \rightarrow 0); \gamma = \sqrt{\epsilon}

IMAGINARY TERM DESCRIBES
ABSORPTION
\[ \gamma = \frac{\mu^2}{\sqrt{\epsilon}} \]

(COMPLEX DIELECTRIC CONST ?)

\[ = \left[ \epsilon + \frac{4\pi\epsilon_0}{\omega} \right]^{1/2} \]

\[ = \gamma (1 + i\Delta) \]

INDEX OF REFRACTION
\[ E = A e^{-\frac{y}{r_2}} e^{i (kx - \omega t)} \]

\[ r = \sqrt{\frac{1}{r} \left[ \frac{1}{\varepsilon} \right] \left[ \frac{1}{\varepsilon} \right] \left[ \frac{1}{\varepsilon} \right]} \]

\[ \lambda = \frac{c}{\omega} \]

**Homework:** What is \( \sigma \) for \( |r_2^*| \) to vary from \( r \) by \( > 10^7 \)? Give answer in \( \Omega - \text{cm}^{-1} \) with \( \lambda = 5000 \) Å. Answer is \( 4000 / \Omega \text{cm} \)

\[ dI = -\alpha (1 - R) I dx \approx \text{Assume} \]

\[ \alpha = \frac{2\sigma}{c} = \text{Absorption} = \gamma \]

\[ \frac{r_1^*}{r_2^*} \]

**Maxwell's Eqn's give**

\[ E_y = A e^{i \omega (r_1^* \frac{r_2^*}{c} - t)} \]

\[ H_z = A r_1 e^{i \omega (r_1^* \frac{r_2^*}{c} - t)} \]

Reflected light = 

Assume transmitted light

\[ E_y = A'' e^{i \omega (r_2^* \frac{r_2^*}{c} - t)} \]

\[ H_z = A'' r_2 e^{i \omega (r_2^* \frac{r_2^*}{c} - t)} \]

Show \( R = \text{Reflection Coefficient} = \frac{A' A'^*}{A A'^*} = \frac{(r_2 - r_1)^2 + (r_2 \delta_2 - r_1 \delta_1)^2}{(r_2 + r_1)^2 + (r_2 \delta_2 + r_1 \delta_1)^2} \)
\[ \frac{A'}{A} = \frac{r_2 - r_1}{r_2 + r_1} \tan \theta \cos \theta \]

**Special Cases:**
1. \( \theta = 0^\circ \), \( r = 2.15 \) \((n_1, n_2)\)
2. *Vacuum Metal Interface*

**Calculate Reflection Coeff.**

*For Metal, \( R = 1 - \frac{1}{\sqrt{n_1 n_2}} \)*
11-26-75 (WEO)

**ELECTRON GAS W/ E.M. FIELD FREQ. OF \( \omega \)**

\[
\frac{\text{d} \mathbf{v}}{\text{d} \tau} = -e \mathbf{E} - \frac{e}{m^*} \mathbf{v}
\]

**SOLVING**

\[
\mathbf{v} = \frac{e}{m^*} \left( \mathbf{E} - \frac{\mathbf{E}}{1 - i \omega \tau} \right)
\]

\( \tau = \text{TIME} \)

**CURRENT DENSITY:**

\[
\mathbf{J} = n e \mathbf{v}
\]

\( n = \# \text{ OF ELECTRONS/CM}^3 \)

**GIVES:**

\[
\sigma^* = \frac{n e^2}{m^*} \left( \frac{\gamma}{1 + \omega^2 \gamma^2} + i \frac{\omega \gamma^2}{1 + \omega^2 \gamma^2} \right)
\]

\[
= \sigma = -\frac{\omega}{4\pi} \varepsilon_e
\]

\( \varepsilon_e \Rightarrow \text{ELECTRONIC CONTRIBUTION} \)

\[
\sigma^* = -\frac{i \omega}{4\pi} \varepsilon_e^*
\]

\( \varepsilon_e \Rightarrow \text{LATTICE} \)

\[
\varepsilon = \varepsilon_L - \frac{4\pi n e^2}{m^*} \left( \frac{\gamma^2}{1 + \omega^2 \gamma^2} \right)
\]

\( \langle \cdot \rangle \Rightarrow \text{AVERAGING OVER ENERGY} \)

\[
\sigma(\omega = 0) = \frac{n e^2 \gamma}{m^*}
\]

\( \alpha = \frac{2\pi}{c} \sigma \Rightarrow \text{ABSORPTION} \)

\[
\sigma = \left[ \frac{n e^3 \lambda^2}{16 \pi m^* r c^3} \right] \langle \gamma \rangle^2
\]

\[
\gamma = \left( \frac{e}{m^*} \right) \frac{\hbar}{\omega^2} \langle \gamma \rangle^2
\]
SECOND TEST AVERAGED IN THE 50's

REFLECTIVITY OF A METAL

\[ R = 1 - \sqrt{\frac{2 \mu}{\mu_0}} \] FOR HI W

\[ \sigma = \frac{n e^2}{m^*} \langle \gamma^* \gamma \rangle e^{-2} \text{ AVERAGING OVER ENERGY} \]

\[ \sigma(\omega \to 0) = \frac{n e^2}{m^*} \]

\[ m^* = \text{EFFECTIVE MASS OF ELECTRON} \]

\[ \alpha = \text{ABSORPTION COEFFICIENT (-BEER'S LAW)} \]

\[ = \sqrt{\frac{2\mu}{\mu_0}} (\sigma, \omega) \frac{1}{2} \]

\[ \omega T \ll 1 \text{ FOR A METAL (LOTS OF FREE ELECTRONS)} \]

\[ \omega T \gg 1, \quad \sigma = \frac{n e^2}{m^*} \left( \frac{1}{T} \right) \text{ (SEMI-CONDUCTOR)} \]

\[ m^* c^2 \langle \gamma^* \gamma \rangle \]

\[ \alpha = \frac{n e^2}{m^*} \frac{c^2}{T} \langle \gamma^* \gamma \rangle \]

\[ \Gamma = \text{REAL PART OF ATTENUATION INDEX} \]

BAND TO BAND TRANSITION

ASSUME NON-DEGENERACY OF VALENCE BAND

\[ E_v(k') = -E_g - \frac{\hbar^2}{2m^*} k'^2 \]

\[ E_c(k'') = \frac{\hbar^2}{2m^*} \frac{k''^2}{2} \]

FROM ENERGY CONSERVATION:

\[ \hbar \omega = E_c(k'') - E_v(k') \]

TRANSITION PROBABILITY:

MATRIX ELEMENTS:

\[ \langle \alpha | \cos \omega t \rangle = \frac{\pi}{2} \langle \alpha | h_0 \rangle \left[ e^{i \omega t} + e^{-i \omega t} \right] \]
Matrix Element
\[ \sum_{\text{unit cell}} \psi_m^* H_0(r) \psi_0 \]
\[ \psi_0 = \text{valence band wave function} \]
\[ \psi_m = \text{conduction band wave function} \]
\[ \psi_0 \propto \frac{1}{\sqrt{N_1}} U_0(r, k') e^{-i k \cdot r} \]
\[ \psi_m \propto \frac{1}{\sqrt{N_1}} U_c(r, k'') e^{-i k'' \cdot r} \]

BLOCH FUNCTIONS

Momentum Operator: \( \vec{p} \leftrightarrow i \hbar \vec{\nabla} \)

\[ \nabla \times A = \overrightarrow{\nabla} \times \vec{A} = 0 \]
\[ \overrightarrow{\nabla} \cdot \vec{A} = 0 \]
\[ \vec{A} = \text{magnetic potential} \]
\[ \vec{p} = i \hbar \vec{\nabla} + \frac{e \vec{A}}{c} \]

\[ \frac{\hbar^2}{2m^*} \nabla^2 + \frac{i e \hbar}{m^*} \vec{A} \cdot \vec{\nabla} + \frac{e^2}{2m^*} \vec{A}^2 \]

Perturbation
\[ H'(r) = \frac{i e \hbar}{m^*} \vec{A} \cdot \vec{\nabla} \]

Good if \( \vec{A} \cdot \vec{\nabla} \gg |\vec{A}|^2 \)

Now \( \vec{A} = \frac{\hbar}{m^* c} \vec{A}_c \cos \left( \frac{\hbar}{m^* c} \vec{r} - \omega t \right) \)
\[ = \frac{i e \hbar}{m^* c} \vec{A}_c \left[ e^{i (\vec{r} \cdot \vec{A} - \omega t)} + e^{-i (\vec{r} \cdot \vec{A} - \omega t)} \right] \]

Usually \( \frac{1}{\hbar^2} = \frac{\omega}{c} \Rightarrow r = R \left( \frac{\hbar}{\omega} \right) \)

\[ H'(r) = \text{Fermi Potential} \]
\[ = \frac{i e \hbar}{2m^* c} \vec{A} \cdot \left[ e^{i (\vec{r} \cdot \vec{A} - \omega t)} \vec{A}_c + e^{-i (\vec{r} \cdot \vec{A} - \omega t)} \vec{A}_c \right] \]
RATE OF TRANSITION
\[ P = \frac{4 \pi^2 k''_{\text{t}}}{(E_{k''} - E_{k'} - \hbar \omega)^2} \]

MATRIX ELEMENT
\[ H_{k'' k'} = \frac{i e^{2 \pi A}}{2 N mc} \int \frac{U_c(r, k'')}{\text{all states}} \left( e^{-i k'' \cdot r} \right) \times \left[ e^{i(\mathbf{q} \cdot \mathbf{r})} U_v^*(r, k') e^{-i k' \cdot r} \right] d^3 r \]
\[ H_{k'' k'} = \frac{i e^{2 \pi A}}{2 N mc} \int U_c(r, k'') \left[ e^{i(\mathbf{q} \cdot \mathbf{r})} U_v^*(r, k') \right] e^{i(\mathbf{k}'' + \mathbf{k} - \mathbf{k'}) \cdot \mathbf{r}} d^3 r \]

NOW \( U_c(r, k) \approx U_v(r, k) \)
\[ \frac{2 \pi A}{k'' - k'} \text{ IS SMALL} \]
\[ \Rightarrow \int U_c U_v^* d^3 r = 0 \]
\[ \int U_c U_v^* e^{i \mathbf{q} \cdot \mathbf{r}} d^3 r = 0 \]

CHANGE INTEGRAL OVER JUST UNIT CELL, THEN SUM UP OVER CRYSTALS, GET
\[ H_{k'' k'} = \frac{N}{2} \sum_{j = 1}^{2} e^{i (k'' + \mathbf{q} - \mathbf{k}) \cdot \mathbf{r}_j} \int_{\text{UNIT CELL}} \left[ \int d^3 r \right] \]
NON-ZERO ONLY FOR \( \mathbf{q} + \mathbf{k}_\text{CELL} = \mathbf{k}'' \)
THEN \[ H_{k'' k'} = N \int_{\text{UNIT CELL}} \left[ \int d^3 r \right] \]
TRANSITION PROB. IN SEMICONDUCTOR

\[ H_{k''} \rightarrow k' = \frac{\epsilon_{k''}}{2m} \int \nabla U_{\text{eff}}(\vec{r}, k'') \cdot \nabla U_{\text{eff}}(\vec{r}, k') d^3r \]

\[ \text{ALLOWED} \quad \Rightarrow \quad \int \nabla U \cdot \nabla U \text{ is small} \]

\[ \text{FORBIDDEN TRANSITION} \]

\[ H_{k''} \rightarrow k' = -\frac{\hbar^2}{2m} \nabla^2 \]

\[ \vec{P}_{k''} \rightarrow k' = -i\hbar \int \nabla U_{\text{eff}}(\vec{r}, k'') \cdot \nabla U_{\text{eff}}(\vec{r}, k') d^3r \]

(MOST USE DENSITY OF STATES NOW)

RECALL \( \vec{P} = -i\hbar \nabla \)

ASSUME MONOCHROMATIC INCIDENCE

USE DENSITY OF STATES INTEGRATE OVER \( k \)

TRANSITION PROBABILITY \( P(E) t = \frac{e^2 A^2}{4\pi^2 \hbar^3 m^2 c^2} \frac{E_{k''} - E_{k'} - \hbar \omega \delta}{(E_{k''} - E_{k'} - \hbar \omega)^2} \frac{d^3 k''}{d^3 k'} \)

IN SPHERICAL COORDINATES

\[ \frac{1}{k'' k'} \int \frac{d^3 k''}{d^3 k'} \]

\[ \frac{e^2 A^2}{(4\pi mc^2)^2} \frac{1}{k'' k'} \frac{E_{k''} - E_{k'} - \hbar \omega}{(E_{k''} - E_{k'} - \hbar \omega)^2} \]

\[ P(E) t = \frac{e^2 A^2}{(4\pi mc^2)^2} \int \frac{d^3 k''}{d^3 k'} \frac{1}{k'' k'} \frac{E_{k''} - E_{k'} - \hbar \omega}{(E_{k''} - E_{k'} - \hbar \omega)^2} \]
\[ P_{k',k} \]

So to good approximation, may take \( P_{k',k} \) term outside integral.

Define \( m^* = \frac{m_e m_h}{m_e + m_h} \)

\[ k_0 = \hbar \omega = E_g + \frac{\hbar^2 k_0^2}{2m^*_h} \]

\[ \Rightarrow k_0 = \sqrt{\frac{2m^*_h}{\hbar}} \sqrt{\hbar \omega - E_g} \]

Put into integral subject to earlier restrictions. (Similar to previous homework)

\[ P(\omega) = \frac{e^2 A^2 \sqrt{2m^*_h}}{4 \pi m^*_h c^2 \hbar^4} \frac{1}{k_0 k' \sqrt{\hbar \omega - E_g}} \]

Must relate this probability to an absorption coefficient

\[ \text{# of incident photons} = \frac{1}{h \omega} \]

\[ \vec{S} = \text{pointing vector} \]

\[ \text{Number of absorbed photons} = e^{-\alpha d} \times \# \text{ of inc. photons} \]

\[ d = \text{thickness of material} \]
For $\alpha d \ll 1$

$$P(E) \propto \frac{1}{E^{3/2}} = \alpha$$

Now $S = \frac{\hbar}{4\pi} \vec{E} \times \vec{H}$ (from field theory)

$$= A^2 k \omega / 8\pi \Rightarrow k = k_{\text{photon}}$$

$$\nabla \times \vec{A} = \vec{H}$$

$$\beta_{k''} = \text{oscillator strength}$$

$$= \frac{2 \left| P_{k''} \right|^2}{\mathcal{M}}$$

Then

$$\alpha \text{ allowed direct absorption}$$

(in units of $1 / \text{length}$)

$$\alpha \text{ allowed direct absorption}$$

(Approximation in semiconductor is)

$$\frac{1}{\text{Semiconductor}} \sim \frac{1}{\text{Conduction band}}$$


For forbidden

$$\beta' = \int_{\text{unit cell}} U_c(\vec{r}, k'') U_v(\vec{r}, k'') d^3 r$$

$$P(E) = \frac{e^2 A^2}{12\pi m^2 \hbar^4} \left( \frac{2m^*}{m} \right)^{5/2} \left( \frac{\hbar \omega - E_g}{\hbar} \right)^{3/2}$$

$$\alpha \text{ forbidden} = 1.8 \times 10^5 \left( \frac{2m^*}{m} \right)^{5/2} \frac{A^4}{(\hbar \omega - E_g)^{3/2}}$$
For allowed 
\[ m' \approx \frac{m}{\hbar}, \quad r = 4, \quad \ell = 1, \quad \hbar \omega - E_g = 0.01 eV \]

\[ \Rightarrow \delta \text{allowed} = 7 \times 10^{-3} \text{cm} \]

Same values with
\[ \ell' = 0.1, \quad \hbar \omega = 1 \text{eV} \]

\[ \Rightarrow \delta \text{forbidden} = 5 \text{cm} \]

In solving

\[ U_v(r, k) = U_v(\frac{r}{k}) + k \cdot \nabla_k U_v(\frac{r}{k}) + \frac{k^2}{2} \nabla^2 \left( \frac{\delta}{k} \right) + \ldots \]

12-5-75 (Fri)

Homework (Due Friday):

1. Derive the Ebers-Moll equation for current flow in a transistor.

2. Explain the derivation in physical terms.

3. Why doesn’t current leave (enter) at the base?
**Absorption Coefficients**

**Direct Allowed Transition**

\[ \alpha \sim \sqrt{\hbar \omega - E_g} \]

**Direct Forbidden Transition**

\[ \frac{1}{\hbar \omega (\hbar \omega - E_g)^{3/2}} \]

**Indirect Transitions**

*Allowed:*

\[ \left( \frac{\hbar \omega + \hbar \omega_{\text{phonon}} - E_g}{e^{\frac{\hbar \omega_{\text{phonon}}}{kT}} + 1} \right)^{3/2} \]

*Forbidden:*

\[ \left( \frac{\hbar \omega + \hbar \omega_{\text{phonon}} - E_g}{e^{\frac{\hbar \omega_{\text{phonon}}}{kT}} - 1} \right)^{3/2} \]

\[ k_{\text{val}} = k_{\text{phonon}} + k_{\text{cond}} \]

**Indirect Transition**

Optional problem: Find argument for absorption relation w/o hairy Q.M. (density of states and occupancy)
(Good qualitative questions to follow)

1. P-N Junction

\[ \text{CHARGE NEUTRALITY IN BOTH JUNCTIONS WHEN THEY BECOME TOGETHER:} \]

\[ J = 0 = ( ) \bigtriangleup n(x) + ( ) E \]

\[ E = f \left( N^+, N^- \right) = f \left( \text{IONIZED DONORS} \right) \]

\[ E = V_B - V_F = \Delta V_I \]
\[ n_p = n_n e^{-\frac{e(V_i + V)}{kT}} \]

For bias
\[ n_p = n_n e^{-\frac{e(V_i + V)}{kT}} \]

Similarly
\[ p_n = p_p e^{-\frac{e(V_x + V)}{kT}} \]

\[ J = (\text{const}) \left[ (n_p + p_n) + \left( n_n + p_p \right) e^{-\frac{eV}{kT}} - \frac{e^2}{kT} \right] \]

\[ = J_{so} \left[ e^{\frac{eV}{kT}} - 1 \right] \]

\[ \text{AT ROOM TEMP:} \]
\[ \frac{I}{kT} \approx 0.02 \text{ VOLTS} \]

Reverse Breakdown

\( \text{(Not included in our model)} \)
MODELING IN A LINEAR REGION

\[ J = J_0 \left[ 1 + \frac{q}{kT} \ln \left( \frac{N_a N_d}{n_i^2} \right) \right] \]

\[ \text{Assume } \frac{q}{kT} \ll 1 \]

\[ J = \frac{q U J_0}{kT} \]

COMPUTATION OF JUNCTION VOLTAGE

\[ N_{a}^{+} = \text{IONIZED DONOR ATOMS} \]

\[ N_{a}^{-} = \text{IONIZED ACCEPTOR} \]

USE GAUSS'S LAW: \( \vec{\nabla} \cdot \vec{D} = \rho \)

\[ \omega = x_d + x_a = \sqrt{\frac{2 e^2 k T}{\varepsilon^2} \ln \left( \frac{N_a N_d}{n_i^2} \right) \left( \frac{1}{N_a} + \frac{1}{N_d} \right)} \]

\[ V_d = \frac{kT}{\varepsilon} \ln \left( \frac{N_a N_d}{n_i^2} \right) \]

\[ W = \left[ \frac{2 e V_d}{\varepsilon} \left( \frac{N_a + N_d}{N_d} \right) \right] V_2 \approx \sqrt{V_d} \]

\[ W(V) = \text{Const} \sqrt{V} \]
\[ w(V) = \sqrt{V} \]

**Operating Principle of FET Transistor Devices Look More Like (in equilibrium)**

12-8-75 (Wed)

**Transistor Common Base Configuration**

Input Impedance, \( R_{in} \), is small compared with \( R_{load} \)

\[ I_E \approx I_C \]

Power Gain \( \approx \left( \frac{I_E}{I_C} \right) R_{load} \)
COMMON BASE
α = CURRENT GAIN
  = FRACTION OF COLLECTOR CURRENT
  MOVING ACROSS EMITTER JUNCTION

\[ \text{Inc} \ll \text{Ipe} \quad \text{Inc} \ll \text{Ipc} \]
\[ \text{Inc, Inc small w.r.t. Ipc} \]

MODEL:

\[ J = q \left[ \frac{D_p P_{nc}}{L_p} + \frac{D_n}{2ln N_{pc}} \right] \left[ e^{\frac{qV}{2kT}} - 1 \right] \]

WHERE
\[ D_n = \text{DIFFUSION CONSTANT FOR ELECTRONS} \]
\[ D_p = 11 \quad (\text{HOLES}) \]
\[ L_n = \text{MEAN FREE PATH FOR ELECTRONS} \]
\[ L_p = \text{DIFFUSION LENGTH} \]
\[ L_p = \text{FOR HOLES} \]
\[ P_{nc} = \text{EQUILIBRIUM CONCENTRATION} \]
\[ N_{pc} = \text{FOR HOLES ON N SIDE} \]
\[ N_{pe} = \text{FOR ELECTRONS ON P SIDE} \]

P.N. JUNCTION:
\[ P = P_n e^{-\frac{qV}{kT}} \]  
\text{BOLTZMAN APPROX.}

**ASSUMPTIONS:**

1. "ABRupt" DEPLETION LAYER
   ASSUMPTION

\[ P \rightarrow 0 \]

ALLOWS BOLTZMAN FACTOR USE

SUDDEN
\[ P \rightarrow 0 \] CHANGE

2. BOLTZMAN APPROXIMATION
3. CONSTANT \( e \) \& \( h \) CURRENT THRU DEPLETION LAYER
   (THRU JUNCTION)
4. LOW LEVEL INJECTION

ELECTRON HOLE DENSITY

\[ I = I_n + I_p \]
\[ V = V_d - V_j \]

\[ V_d = \text{APPLIED BIAS VOLTAGE} \]

\[ V_j = \text{BUILT IN JUNCTION BIAS} \]

\[ n_p = n_n e^{(q/V_d)(V_a - V_j)} \]

\[ = n_n e^{(eV_a)/kT} \]

\[ E = E_c - E_0 \]

\[ \# \text{IN COND. BAND} = N_p e^{-E/kT} \]

\[ n_n^2 = n_p \leftrightarrow \text{MASS ACTION LAW} \]

\[ n_p = \# \text{OF } e^- \text{ ON } p \text{ SIDE WHEN} \]

\[ V_a \text{ IS APPLIED} \]

\[ n_n = \text{CONCENTRATION OF } e^- \text{ ON} \]

\[ n \text{ SIDE} \]

\[ p_n = p_n e^{(qV_a)/kT} \]

**I. CONTINUITY Eq. (OF CHARGE)**

\[ \frac{dn}{dt} = G - \frac{n - n_n}{n_n} + \frac{1}{q} \nabla \cdot J_n \]

\[ G = \text{RATE OF GENERATION OF } e^- \text{ PAIRS} \]

\[ n - n_n = \text{EXCESS CARRIER DENSITY} \]

**HOLE CURRENT**

\[ \frac{dp}{dt} = G - \frac{p - p_n}{p_n} - \frac{1}{q} \nabla \cdot J_p \]
II) CURRENT EQUATION
(FROM BOLTZMANN XPORT EQU.)

\[ J_n = q \mu_n n \mathbf{E} + \mathbf{q} \mathbf{D}_n \nabla n \]

\[ J_p = q \mu_p n \mathbf{E} - \mathbf{q} \mathbf{D}_p \nabla p \]

\[ \mu = \frac{q}{m} \langle \frac{v^2}{2} \rangle \langle v \rangle \]

\[ D = \langle \frac{v^2}{2} \rangle \]

\[ D_n = \frac{kT}{q} \mu_n \]

COMBINING I & II:

III) \[ D_n \frac{\partial^2 n}{\partial x^2} + \mu_n [E \frac{\partial n}{\partial x} + \frac{\partial E}{\partial x}] - \frac{n - n_0}{n_0} = 0 \]

\[ D_p \frac{\partial^2 p}{\partial x^2} - \mu_p [E \frac{\partial p}{\partial x} + \frac{\partial E}{\partial x}] - \frac{p - p_0}{p_0} = 0 \]

NEGLECT \[ \frac{dv}{dt} \]

ASSUME: \[ \frac{n - n_0}{n_0} = \frac{p - p_0}{p_0} \rightarrow \text{NEUTRALITY} \]

IV) COMBINING, YOU GET: (ADJOINING)

\[ \frac{p \frac{\partial^2 n}{\partial x^2} + n \frac{\partial^2 p}{\partial x^2}}{p + n} + \mu E \frac{\partial n}{\partial x} - \frac{n \frac{\partial p}{\partial x} - p \frac{\partial n}{\partial x}}{p - n} = 0 \]

\[ \mu = \text{MODIFIED MOBILITY} = \frac{n - p}{\mu_p + \mu_n} \]

\[ D = \frac{n + p}{\mu_p + \mu_n} \]

USED BY EBER'S MOLL
LOW LEVEL INJECTION:
\[ P_n \text{ on n side } \ll 1 \]
\[ (\text{controlled by minority}) \]

HIGH LEVEL INJ.
\[ P = N \]
REDUCES TO DIFFUSION EQ.
SINCE FIELD TERM BECOMES NEGLIGIBLE.

\[ P_n \]
FOR AN ABRupt JUNCTION

\[ J_p (\text{on n side}) = -q D_p \frac{dp}{dx} \]

ANSWER IS

\[ P - P_{in} = P_{no} e^{-x/L_D} \left( e^{\frac{q V_a}{k T}} - 1 \right) \]

ti = 15 IS 15 ELM

\[ \frac{d^2 p}{dx^2} = \ldots \]
12-10-75 (WEO)

REVIEW

"ABRUPT"

\[ n_p = n_{p_0} \exp \left( \frac{-qV_o}{kT} \right) \]

ASSUMPTION

\[ n_p = n_{p_0} \exp \left( -\frac{qV_o}{kT} \right) \]

CONSERVATION OF CHARGE

(CONtinuity EQUATION)

FOR ELECTRONS:

\[ \frac{dn}{dx} = \sigma - \frac{n-n_{p_0}}{\tau} + \frac{q}{\hbar} \mathbf{J} \]

CURRENT DUE TO ELECTRONS

\[ \mathbf{J}_n = \frac{q}{\hbar} \mathbf{E} \nu_n + q \mathbf{D}_n \nu_n \]

MOBILITY

III. FOR P-N JUNCTION

\[ \mathbf{J}_p = -q \mathbf{D}_p \frac{\partial n}{\partial x} \]

\[ \frac{\partial n}{\partial x} = \frac{\partial p}{\partial x} \]

\[ P(x=0) = P_{n_0} \exp \left( \frac{-qV_o}{kT} \right) \]

\[ P(x=\infty) = P_{n_0} \]

BOUNDARY CONDITIONS

IV. ASSUMING LOW LEVEL INJECTION:

\[ \frac{\partial^2 p}{\partial x^2} - \frac{P - P_{n_0}}{P_{n_0}} = 0 \]

DEFINING \( L_P = \sqrt{\frac{P}{P_{n_0}}} \)

SOLN. IS

\[ P - P_{n_0} = P_{n_0} e^{-x/L_P} \left( e^{\frac{qV_o}{kT}} - 1 \right) \]

\[ \Rightarrow J_p = \frac{q \mathbf{D}_P P_{n_0}}{L_P} \left( e^{\frac{qV_o}{kT}} - 1 \right) \]

HOLE CURRENT DENSITY FOR A P-N JUNCTION
ELECTRICAL CURRENT DENSITY FOR P-0 Junction:
\[ J_n = \frac{q N_{PC} D_n}{L_n} \left( \frac{q V_B}{kT} - 1 \right) \]

\( \therefore J_{so} = \frac{q N_{PC} D_n}{L_n} + \frac{q P_{NO} D_P}{L_P} \)

\( \leftarrow \text{IDEAL} \)

\( \leftarrow \text{REAL} \)

ON TO PNP X-SISTOR

\( \begin{array}{c}
\begin{array}{c}
\text{P} \\
\text{N} \\
\text{P}
\end{array}
\end{array} \)

\( W_B = \text{WIDTH OF BASE} \)

\( V_E = \frac{q V_B}{kT} \)

\( p(x=0) = \frac{P_{NE} E}{kT} \)

USE AS B.C. FOR EQ IV

\( p(x) = p(x=0) \sinh \left( \frac{w_B - x}{L_P} \right) \sinh \left( \frac{w_B}{L_P} \right) \)

\( J_P = -q P_{NO} \frac{dP}{dx} \)

\( J_P |_{\text{EMITTER}} = q P(x=0) \frac{D_P}{L_P} \cosh \left( \frac{w_B}{L_P} \right) \)

\( J_P |_{\text{COLLECTOR}} = q P(x=0) \frac{D_P}{L_P} \sinh \left( \frac{w_B}{L_P} \right) \)

\( J_P |_{\text{EMIT}} \sim J_P |_{\text{COL}} \)

CRITICAL \[ \Rightarrow \frac{w_B}{L_P} \text{ MUST BE A SMALL } \]
TOTAL CURRENT IN $E$

\[ I_E = \left( \frac{q \cdot D_n \cdot N_n}{L_n} \right) \left( e^{\frac{qV_E}{kT}} - 1 \right) \]

\[ + \frac{qP_n(x=0) \cdot L_p}{kT} \cosh \left( \frac{W_B}{L_p} \right) \]

HOLE CURRENT

TOTAL CURRENT IN $C$

\[ I_C = \frac{9D_n \cdot D_p}{L_n} + qP_n(x=0) \cdot e^{\frac{qV_E}{kT}} \frac{D_p}{L_p} \sinh \left( \frac{W_B}{L_p} \right) \]

ELECTRON COLLECTOR CURRENT

DEFINE $\alpha = \frac{N_{PC}}{N_{EC}} = 1$ (WANT $\alpha = 1$)

$\gamma = \frac{SI_{E}(\text{HOLE})}{SI_{E}(\text{TOTAL})}$

\[ \gamma = 1 + \frac{\ln L_p \cdot \ln e}{D_n L_p ^2} \cosh \left( \frac{W_B}{L_p} \right) \]

EMISSION EFFICIENCY OF FRACTION OF Emitted CURRENT THAT IS HOLES.

\[ \beta = \frac{dI_E(\text{HOLES})}{dI_E(\text{TOTAL})} \]

\[ \beta = \cosh \left( \frac{W_B}{L_p} \right) \]

BASE TRANSPORT FACTOR (FRACTION OF Emitted HOLES THAT MAKE IT TO THE COLLECTOR)
\[ \alpha^* = \text{ratio of collector current to incident hole current} \]

\[ \alpha^* = 1 \]

Assume \( \alpha^* = 1 \) (minority)

Actually: \( \alpha^* = \sigma (\text{majority}) + 1 \)

\( \sigma = \text{conductivity} \)

Make \( \varepsilon = 1 \): \( p \approx n_A (e) > n_0 (B) \)

Junction FET

JFET: want conductivity

\[ \text{Gate} \]

\[ \frac{dv}{dr} = I_d \, \frac{dR}{dr} \]

\[ R \propto \frac{dy}{dA} \]

Conductivity a function of this width

\[ y = \sqrt{\frac{2e}{9N_0}} (V(x) + V_0 - V_{GS}) \]

Assuming \( n_0 << n_A \)

\[ V_{GS} = \frac{qA}{W} \]

\[ W = \text{width with no potential} \]

\[ x \left[ 1 - \frac{(V_{GS} - V_{BS})V_0}{\text{const}} \right] \]
12-12-75 (Fri)

Final: 9 a.m., Tues.

(how many e^- in cono band?)

- little two state
- no heat diffusion in insulators

Impurity scattering in semi-conductor

Scattering cross section:

\[ \sigma = \frac{2\pi b d b}{2\pi m b d b} \]

\( b = \) impact parameter
\( a = 2\pi b d b \)

\( S = \) scattering cross section

Assume

1. \( k = \vec{k} \)

2. scattering angle small

3. Assume velocity initial = \( v \)

\[ \Delta t = \frac{2e}{b v} \]

\[ \text{Then:} \quad \frac{\Delta p}{b v} = \frac{2e^2}{b v} \]
FOR SMALL ANGLE: \( \Theta = 1 \) \( \frac{\Delta P}{P} = \Theta \)

\[
\Theta = \frac{\Delta P}{P} = \frac{2Ze^2}{bmv^2}
\]

\( \Delta E = \text{LOSS IN ENERGY} \)

\[
= \frac{(\Delta P)^2}{zm} = \frac{2Ze^4}{mb^2v^2}
\]

REAL ANSWER IS

\[
\tan \frac{\Theta}{2} = \frac{2Ze^2}{bmv^2}
\]

GIVES

\[
S = \left( \frac{Ze^2}{2Ze^2} \right) \frac{1}{\sin^2 \left( \frac{\Theta}{2} \right)}
\]

IN A SOLID \( \Rightarrow \) LET \( mv^2 \approx kT \)
TEST #1 (STUDY SHEET)

1. CANTON EFFECT
2. THE GOHR ATOM
3. \( E \) AND \( V \) IN CM\(^{-1}\)
4. IDE SCHROD'S EQU.
5. FREE PARTICLE JOIN
6. INFINITE WELL JOIN
7. ENERGY LEVELS IN A SOLID
8. HARMONIC OSC
9. PHASE AND GROUP VELOCITIES
10. PAULI EXCLUSION PRINCIPLE
11. PERTURBED HARMONIC OSCILLATOR
12. BRILLOUIN ZONES
13. DISPERION CURVES
14. BRILLOUIN ZONE FOR TWO MASSES
15. ATTENUATION (EVANESSENCE)
16. TRANSMISSION LINE EQUIVALENTS
17. DISPERION CURVE IN 1D LATTICE
18. INTERPRETATION
19. A PERTURBATION
20. ELECTRONS IN A SOLID
21. IN THE OPTICAL MODE
22. MILLER INDICES
23. E-HOLE INTERACTION
24. EFFECTIVE MASS
25. MEASURING EFFECTIVE MASS
26. ABSORPTION MEASUREMENT
15. Fermi-Dirac Distribution Definition
15. Boltzmann Factor
16. C.D.D. Derivation
16. D(E)
17. Effective Density of States
17. Mass-Action Law
18. F.D.D. Graphs
18. Density of States Graphs
19. Impurity Distribution Function
20. Effects of Doping on Fermi Level
\[ \omega_2 - \omega_1 = \frac{1}{m} [1 - \cos \gamma] \]

**Description:** A photon having energy \( E = h\nu \) "collides" with an electron. Part of the energy is lost to the now "moving" electron. The photon now has energy \( E_2 = h\nu_2 \leq E_1 \). Here, \( \omega = 2\pi \nu \).

**The Bohr Atom**

Bohr made a model of the hydrogen atom to explain observed quantum effects. His assumptions were:

\[
E = Ke^2 / r^2 + \frac{1}{2}mv^2 + \frac{Ze^2}{4\pi\varepsilon_0 r} = \text{conservation of energy} \]

\[
\frac{mv^2}{r} + \frac{Ze^2}{4\pi\varepsilon_0 r^2} = 0 \quad \Rightarrow \quad \text{Equation for force} \]

\[
L = nh \quad \Rightarrow \quad \text{Angular momentum assumption} \]

\[
E_2 - E_1 = h\nu \quad \Rightarrow \quad \text{Quantized energy assumption} \]

These assumptions are for an electron in a circular orbit.

\[
E = e^2 / 2m \quad \frac{1}{h} \quad \text{Planck's constant} \]

\[
E = \# \text{energy} / \# \text{electrons} \]

Putting together: \( E_n = 2\pi \hbar \gamma \epsilon_{n\gamma} \leftrightarrow \text{original energies} \)

Or, equivalently:

\[
E_n - E_m = h\nu_{nm} = \frac{m^2 \gamma^2 \epsilon_{n\gamma}^2}{32\pi^2 \hbar^2} \left( \frac{1}{1} - \frac{1}{n^2} \right) \]

Ionization energy is gotten by:

Setting \( m = \infty, n = 1 \) \( \Rightarrow E = R_H = \frac{m^2 \gamma^2 \epsilon_{1\gamma}^2}{32\pi^2 \hbar^2} = 13.6 \) eV

\( R_H \) is the Rydberg energy observed experimentally prior to Bohr's model.
MEASURING $E$ AND $\nu$ IN CM$^{-1}$

\[ E = h\nu = h\frac{c}{\lambda} \]

SINCE $E = h\nu = h\frac{c}{\lambda}$, A PHOTON'S ENERGY OR FREQUENCY IS MANY TIMES GIVEN AS WAVELENGTH $\lambda$, IN INVERSE CENTIMETERS.

SCHRÖDINGER'S EQUATION IN ONE DIMENSION

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + (V - E)\psi = 0 \]

IT'S SOMETHING LIKE A CONSERVATION OF ENERGY: $KE + PE = E$, $\psi$ IS THE WAVE FUNCTION.

I. SOLUTION FOR FREE PARTICLE ($V = 0$)

\[ \frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \Rightarrow \quad k^2 = \frac{-2mE}{\hbar^2} \]

\[ \psi = Ae^{\pm ikx} + Be^{\pm ikx} = \tilde{A}e^{ikx} + \tilde{B}e^{-ikx} \]

$|\psi|^2$ IS A PROBABILITY DENSITY FUNCTION.

FOR A FREE PARTICLE, WE DON'T KNOW AT ALL WHERE IT IS.

II. SOLUTION IN AN INFINITE WELL

\[ \begin{array}{c|c|c}
0 & \psi & \psi \\
\hline
V = 0 & V = 0 & V = 0 \\
\end{array} \]

Boundary conditions dictate $\psi(0) = \psi(1) = 0$.

Applying to the solution of free particle, $B = 0$ and $k = \frac{\pi}{a}$.

Since $k^2 = \frac{-2mE}{\hbar^2}$, we have

$E_n = \frac{n^2\hbar^2}{2ma^2}$

To find $A$, use the fact that

\[ \int_0^1 |\psi|^2 dx = A^2 \int_0^1 e^{\pm ikx} dx \]

Gives $A = \sqrt{\frac{1}{k}}$.

$E = \nu$ IN CM$^{-1}$/$\nu$ SCHRÖD. EQ (INF. WELL)
**Energy Levels in a Solid**

A. **Metal** has a few electrons in the **conduction band** to play with.

B. **Insulator** has no electrons in the **conduction band**.

C. ** Semiconductor** conduction band not fully not empty.

D. **Doped Semiconductor**
   - Conduction band
   - Exiton
   - Donor impurity
   - Acceptor impurity
   - Valence band

Another band occurs from an **exiton** (bound electron hole) pair. Absorption spectra for doped semiconductor has bumps.

Absorption due to impurities:

\[ y = \frac{E_g}{h} \]

**Energy Levels in a Solid**
• Schrödinger equation: Harmonic Oscillator

\[ V = \frac{1}{2} m \omega^2 x^2 \text{ like potential of a spring} \]

In one dimension:

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} y + \frac{1}{2} m \omega^2 x^2 = E y \]

The harmonic oscillator is, for example, an approximation to an atom which has a potential something like:

\[ V(r) \] repulsive by valence electrons

A Taylor series expansion about \( r_0 \) would give, to second order, a parabola. Anyway, solution in one dimension gives "Hermite polynomials" and eigen frequencies \( E_n = (n + \frac{1}{2}) \hbar \omega \)

• Velocities

\[ \text{Phase velocity} = \frac{\hbar}{k} = \nu \]

\[ \text{Group velocity} = \frac{d\nu}{dk} \]

• Pauli exclusion principle: No two electrons can occupy a state with the same quantum numbers

• Perturbed Harmonic Oscillator

\[ V = \frac{1}{2} \psi x^2 + \cos \psi x^3 \] \( (\psi = m \omega^2) \) is a third order Taylor expansion of \( V(r) \) above. Eigen energies are slightly increased
For waves in a "one-dimensional" solid, the displacement of an atom, either transverse or longitudinal, is given by

\[ y_0 = A \cos (\omega t - k_0 d) \]

Note that substitution of \( k \) by \( k + \frac{2\pi}{d} \) would give the same exact solution, that is, there are a number of sinusoids that pass through the displacements.

The frequency \( \nu \) of the wave is thus periodic with respect to the wave number \( k \). The lowest order of this periodicity is termed the Brillouin zone,

\[ \nu = \sin \left( \frac{2\pi}{d} \right) = A \sin \left( \frac{2K}{d} \right) \]

\[ y = \sin \left( \frac{2\pi}{d} x \right) \]

\[ \text{First Brillouin Zone} \]

\[ \frac{1}{d}, \frac{1}{d} \]
DISPERSION CURVES

The relationship between $v$ and $\frac{1}{\lambda}$, or equivalently $\omega$ and $k$, is a dispersion curve. The Brillouin zone is a dispersion curve.

BRILLOUIN ZONE FOR UNEQUAL MASSES

Modeled as:

\[ \frac{1}{\lambda} \rightarrow \frac{1}{\lambda_{\text{max}}} \]

produces a Brillouin zone:

\[ \lambda_{\text{optical mode}} \]

\[ \lambda_{\text{longitudinal mode}} \]

\[ \lambda_{\text{transverse mode}} \]

The optical mode vibrates like this:

\[ \uparrow \quad \downarrow \quad \uparrow \quad \downarrow \quad \uparrow \quad \downarrow \]

It produces a dipole moment.

ATTENUATION (EVAANESCENCE)

If a crystal is excited at a frequency not allowed for on the dispersion curve, it is attenuated (or in the evanescent mode).
**TRANSMISSION LINE EQUIVALENTS**

**ONE DIMENSIONAL CRYSTALS ARE MATHEMATICALLY AKIN TO TRANSMISSION LINES, THAT IS, YOU GET DISPERSION CURVES FOR BOTH. FOR THE TWO-MASS CASE, THE TRANSMISSION LINE EQUIVALENT IS**

\[
\begin{align*}
\text{Using Kirchhoff's laws: } & L_2 \frac{d^2 \phi_2}{dx^2} - L_1 \frac{d^2 \phi_1}{dx^2} = \frac{d^2 \phi_0}{dx^2} \\
\text{Also: } & L_1 \frac{d^2 \phi_1}{dx^2} = \frac{d^2 \phi_0}{dx^2} - \frac{d^2 \phi_2}{dx^2} \\
\text{Using } & \phi_0 = A_0 e^{i(\omega t - \omega x)}, \\
\text{gives: } & \left[ -\frac{1}{L_1} \omega^2 + \frac{1}{C_1} + \frac{1}{C_2} \right] A_1 - \left[ \frac{1}{C_0} + \frac{1}{C_2} \right] A_2 = 0 \\
& \left[ \frac{1}{L_2} \omega^2 + \frac{1}{C_1} + \frac{1}{C_2} \right] A_2 = \left[ \frac{1}{C_0} + \frac{1}{C_2} \right] A_1 = 0 \\
\text{Setting } & 2 \omega \left( \frac{1}{L_1} \omega^2 + \frac{1}{C_1} + \frac{1}{C_2} \right) A_1 - \frac{1}{C_2} A_2 = 0 \\
\omega &= \frac{1}{2} \left( \frac{1}{L_1} \omega^2 + \frac{1}{C_1} + \frac{1}{C_2} \right) \frac{1}{C_2} A_2 \\
& = \frac{1}{2} \left( \frac{1}{L_1} \omega^2 + \frac{1}{C_1} + \frac{1}{C_2} \right) \left( \frac{1}{C_0} + \frac{1}{C_2} \right) - \frac{1}{2C_2} \omega^2 \frac{1}{C_2}
**Dispersion Curve for 1D Lattice**

\[
\begin{align*}
X_{n+m} & \quad d \quad X_n \\
U[|x_{n+m} - x_n|] & \quad \text{Potential between } n \text{ and } n+m \text{ mass} \\
= U(x) + (y_{n+m} - y_n) U'(x) + \frac{1}{2} (y_{n+m} - y_n)^2 U''(x) \\
= & \sum_{m \geq 0} U(x_m) + (y_{n+m} - y_n) U'(x_m) + \frac{1}{2} (y_{n+m} - y_n)^2 U''(x_m) \\
F = \text{Force on } n \text{ mass} \\
= -\frac{5U}{6} + \frac{1}{2} \sum_{m \geq 0} (y_{n+m} - y_n) U'(x_m) + \frac{1}{2} (y_{n+m} - y_n)^2 U''(x_m) \\
& \sum_{m \geq 0} U''(x_m) [y_{n+m} + y_{n+m+1} - 2y_n] \\
\text{Ignoring higher ordered terms:} \\
F_{2n} = U''(y_{n+1} + y_{n+2} - 2y_n) = M_2 \frac{d^2 y_{n+1}}{dt^2} \\
F_{2n+1} = U''(y_{n} + y_{n+2} - 2y_{n+1}) = M_1 \frac{d^2 y_{n+1}}{dt^2} \\
\text{Assume solutions:} \\
y_{2n} = A_2 e^{i(wt - nkd)} \\
y_{2n+1} = A_1 e^{i(wt - (n+1)kd)} \\
\text{Gives:} \\
A_2 (M_2 w^2 - 2U''') + 2A_1 U'' \cos \frac{kd}{2} = 0 \\
A_1 (M_1 w^2 - 2U''') + 2A_2 U'' \cos \frac{kd}{2} = 0 \\
\det | \begin{pmatrix} w^2 & U'' \end{pmatrix} | \begin{pmatrix} M_2 & U'' \end{pmatrix} \begin{pmatrix} M_1 & U'' \end{pmatrix} = 0 \\
\omega = U'' \left[ \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \pm \sqrt{\left( \frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4A_2 M_1 \cos \frac{kd}{2}}{M_2}} \right] \\
1 \text{- D Lattice Disp. Curve}
Interpretation of 1-D Lattice Dispersion Curve

The dispersion curve relationship may be rewritten as:

\[ \omega^2 = \frac{v''}{M_1 M_2} \left[ M_1 + M_2 \mp \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos^2 \frac{k d}{2}} \right] \]

WLOG, assume that \( M_1 > M_2 \)

For long wavelengths \( \lambda >> d \) and \( k << \frac{1}{d} \)

\[ \Rightarrow \cos \frac{k d}{2} \approx 1 - \frac{k^2 d^2}{2} \]

\[ \Rightarrow \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos^2 \frac{k d}{2}} \approx M_1 M_2 \left[ 1 - \frac{k^2 d^2}{2M_2 M_1} \right] \]

\[ \omega^2 = k d \sqrt{\frac{v''}{M_1 + M_2}} \frac{1 - \frac{k^2 d^2}{2M_2 M_1}}{M_1 + M_2} \]

\[ \omega^1 = \sqrt{2} v'' \left( \frac{1}{M_1} + \frac{1}{M_2} \right) - \frac{k^2 d^2}{2M_2 M_1} \]

\[ \omega^- = \sqrt{2} v'' \left( \frac{1}{M_1} + \frac{1}{M_2} \right) + \frac{k^2 d^2}{2M_2 M_1} \]

At the forbidden zones

\[ \sin \frac{k d}{2} > 1 \]

\[ k d = \alpha + i \beta \]

\[ \sin \frac{k d}{2} = \sin \frac{\beta}{2} \cosh \frac{\alpha}{2} + i \cos \frac{\beta}{2} \sinh \frac{\alpha}{2} \]

\[ \alpha = 0 \Rightarrow k = \pm \frac{2 \beta}{d} \]
A PERTURBATION

SCHRÖDINGER'S EQN IS:

\[ i \hbar \frac{\partial}{\partial t} \psi = H \psi \]

ADD A PERTURBATION V:

\[ \frac{\partial}{\partial t} \psi_{h+V} = (E_n + E_\nu) \psi_{h+V} \]

WITHOUT PERTURBATION:

\[ \psi = \sum \phi_n \psi_n(x) e^{-i E_n t/\hbar} \]

ASSUME WITH PERTURBATION, \( \psi_n = \phi_n (x) \) IN EQ. RECOGNIZING

ORTHOGONALITY OF \( \phi_n \), THIS GIVES

\[ \frac{\partial}{\partial t} \phi_n = \frac{\hbar}{i} \sum \phi_n \psi_n - \frac{\hbar}{i} (E_n - E \nu) \phi_n \]

\[ V_{\nu n} = \int \phi_n^* \phi_{\nu} dx = \text{MATRIX ELEMENT} \]

RECALL

\[ \int \phi_n^* \phi_\nu dx = E \nu \delta_{\nu n} \]

THE MATRIX ELEMENT, \( V_{\nu n} \), IS A COUPLING TYPE NUMBER, AND CAN BE MEASURED EXPERIMENTALLY.

FOR THE SPECIAL CASE WHERE \( E \nu = E_n \)

\[ \frac{\partial}{\partial t} \phi_n = - \frac{\hbar}{i} \phi_n V_{\nu n} \]
ELECTRONS IN A SOLID

\[ E_0 = V_0 \Rightarrow \text{Assume } E_0 = E_0 s + V_0 s, \quad V_0 s = \sum_n \alpha_n s \]

\[ \text{Assume } \beta \text{ jump only to adjacent atoms.} \]

\[ E_0 s = V_0 s, \quad \alpha_n s = \alpha_n s_n \]

\[ (E - E_0) s_n = -V (\alpha_n s_{n+1}, \alpha_n s_{n-1}) \]

\[ \text{Let } s_{n+1} = e^{i k n d}, \quad s_{n-1} = e^{-i k n d} \]

\[ \Rightarrow E = E_0 - 2V \cos k d \]

\[ \text{At } k \text{ near } 0, \quad \cos k d \approx 1 - \frac{k^2 d^2}{2} \]

\[ \Rightarrow E = E_0 - 2V + V d^2 k^2 \leq \text{Parabola (Harmonic Osc.)} \]

RECALL THAT FOR AN ELECTRON IN FREE SPACE:

\[ E = \frac{\hbar^2 k^2}{2m} \Rightarrow m = \text{Effective mass} = \frac{\hbar^2}{2V d^2} \]
ELECTRONS IN A SOLID: OPTICAL MODE

The last effort was an approximation to
\[ i \hbar \frac{\partial}{\partial t} = E_{0} + \sum V_{k} \cos(k \cdot r) \]

If you assume electrons can jump diagonally,

\[ d \rightarrow c \]

You get
\[ E = E_{0} - 2V \cos(kd/\sqrt{2}) \]

MILLER INDICES

To specify directions in a crystal, you use Miller indices. If you go \( d \) in the \( x \) direction, \( b \) in the \( y \), and \( c \) in the \( z \), and the crystal starts its period over, then the Miller index is \( (\frac{d}{a}, \frac{b}{b}, \frac{c}{c}) \).
**ELECTRON-HELL INTERACTION**

An electron in the conduction band and a hole in the valence band may combine to give off a photon with energy proportional to the energy gap plus an exciton phonon:

\[ E_{\text{photon}} = E_{\text{gap}} + E_{\text{phonon}} \]

Momentum must be conserved:

\[ \mathbf{k} + \mathbf{q} = \mathbf{0} \]

**EFFECTIVE MASS**

\[ V_0 = \frac{d^2 E}{d \mathbf{k}^2} = \frac{-\hbar^2}{m^*} \Rightarrow m^* = \frac{-\hbar^2}{\frac{d^2 E}{d \mathbf{k}^2}} \]

\[ \mathbf{E} = \phi \Rightarrow V_0 = \frac{\hbar^2}{m^*} \frac{\partial^2 \phi}{\partial \mathbf{x}^2} \]

\[ \Rightarrow \frac{d^2 \phi}{d \mathbf{k}^2} = \frac{\hbar^2}{m^*} \phi \Rightarrow m^* = \frac{-\hbar^2}{\frac{d^2 \phi}{d \mathbf{k}^2}} \]

**MEASURING EFFECTIVE MASS**

Put a magnetic field \( B \) on a particle of charge \( q \):

\[ E_x = q \vec{V} \times \vec{B} = q \mathbf{v} \times \mathbf{B} = q \mathbf{v} \times (\mathbf{m}^* \mathbf{k}) \]

\[ E_x = -q \mathbf{v} \mathbf{B} = -q \mathbf{v} \mathbf{m}^* \mathbf{k} \]

Assuming \( m \mathbf{v} = m^* \mathbf{v} \) (not always true):

\[ m (x + y) = q B (x - y) \]

Assuming \( x = \text{max} \), \( y = \text{max} \):

\[ \mathbf{x} = \frac{q B \text{max}}{m} \]

\[ \mathbf{y} = \frac{-q B \text{max}}{m} \]

\[ m = \frac{q B \text{max}^2}{\mathbf{x}^2 + \mathbf{y}^2} \]
**Absorption Measurement**

To find the absorption spectra at low T, the sample is placed in a "Dewar."
THE FERMI-DIRAC DISTRIBUTION DEFINITION

\( \eta = \# \text{ELECTRONS IN CONDUCTION BAND} \)
\( p = \# \text{HOLES IN VALENCE BAND} \)

\( n(e) = \int f(e) e(e) \Rightarrow f(e) = \frac{n(e)}{e(e)} \)
\( \hat{f}(e) = \text{FERMI-DIRAC DISTRIBUTION} \)
\( = p \left[ e^{-\frac{e}{kT}} \text{HASS ENERGY } e \right] \)
\( c(e) = \# \text{OF QUANTUM STATES AS A FUNC. OF } e \)
\( n(e) = \# \text{OF ELECTRONS WITH ENERGY } e \)
\( \eta = \int n(e) de = \int \hat{f}(e) e(e) de \)

ASSUMPTIONS:
1. THERMAL EQUILIBRIUM
2. PAULI'S EXCLUSION PRINCIPLE

BOLTZMANN FACTOR

\[ n_i = \text{NUMBER OF } e^-'s \text{ WITH ENERGY } E_i \]
\[ \frac{n_i}{n_0} = e^{-\frac{E_i}{kT}} = \text{BOLTZMANN FACTOR} \]
FERMI - DIRAC DISTRIBUTION DERIVATION

\[ P_{\text{output}} = f(E) P[E \rightarrow E + \Delta E] \left[ 1 - f(E + \Delta) \right] \]

\[ P_{\text{output}} = f(E + \Delta) P[E + \Delta \rightarrow E] \left[ 1 - f(E) \right] \]

EQUATING GIVES
\[ \frac{P[E \rightarrow E + \Delta E]}{P[E + \Delta \rightarrow E]} = \frac{f(E + \Delta)}{f(E)} \left[ \frac{1 - f(E + \Delta)}{1 - f(E)} \right] \]
\[ = e^{-\Delta E/kT} = BOLTZMANN FACTOR \]

SOLVING FOR \( f(E) \) GIVES
\[ f(E) = \frac{e^{E/kT} + 1}{e^{E/kT} - 1} \]

\( n(E) = \) # ELECTRONS WITH ENERGY \( E \)
\[ = P[E \text{ CAN HAVE ENERGY } E] \, dN \]
\[ dN = \text{NUMBER OF BOXES TO PUT } E \text{ INTO} \]
\[ n(E) = f(E) \, dN \]

RECALL THAT FOR AN INFINITE WELL
\[ E_n = n^2 \left( \frac{\pi^2 m E}{2} \right) \Rightarrow n = \frac{\sqrt{m \pi^2 E}}{\hbar} \]

THEREFORE:
\[ dN = \frac{1}{2} \left( \frac{2m \pi^2 \hbar^2}{E} \right)^{1/2} E^{-1/2} \quad \text{ONE DIMENSION} \]

FOR THREE DIMENSIONS,
\[ dN^3 = \frac{4}{3} (4\pi m^2 \hbar^2)^{1/2} E^{-3/2} \quad \text{SURFACE AREA OF A SPHERE} \]

THE \( \frac{1}{2} \) IS PUT IN TO SINGLE OUT THE FIRST OCTANT ANYWAY, THIS GIVES
\[ dN^3 = (\ ) E^{-1/2} \, dE \Rightarrow (\ ) \text{ IS CONSTANT} \]
\[ n(E) = f(E) \, dN^3 = \text{CONST} \, \sqrt{E} \left( \frac{E - E_F}{1} \right) \]
**Effective Density of States**

\[ n = \int_{E_0}^{\infty} dE = \text{Electrons in Cond. Band} \]

\[ = \text{const} \int_{E_0}^{\infty} \frac{1}{1 + e^{(E - E_F)/kT}} dE \]

\[ \approx \text{const} \int_{E_0}^{\infty} e^{- (E - E_F)/kT} dE \]

This approximation is good at room temperature since \( kT \) is so small.

\[ \langle \frac{e^{(E - E_F)/kT}}{kT} \rangle \gg 1 \]

\[ n = 2 \left( \frac{2\pi m^*}{k^2} \right) e^{(E - E_F)/kT} \]

\[ = N_c e^{- (E - E_F)/kT} = \text{Effective Densities of State} \]

\( p = \# \text{holes in valence band} \)

\[ = 2 \left( \frac{2\pi m^*}{k^2} \right) e^{-(E_F - E)/kT} \]

\[ = N_v e^{-(E_F - E)/kT} \]

**Mass Action Law**

\[ \Delta P = \frac{N_c N_v e^{-(E_F - E)/kT}}{kT} \]

\[ = \frac{N_c N_v e^{-E_F/kT}}{kT} \]

\[ E_g = \text{Energy Gap} = E_F - E_v \]
FERMI-DISTRIBUTION GRAPHS

\[ f(E) \]

ELECTRONS

\[ E_V \quad E_F \quad E_C \quad E \]

(ACCEPTOR LEVEL) (DONOR LEVEL)

\[ 1 - f(E) \]

HOLEs

\[ 1 \]

DENSITY OF STATE GRAPHS

\[ n(E) \]

ELECTRONS

\[ E_V \quad E_A \quad E_F \quad E_D \quad E_Y \]

HOLEs

\[ E_C \quad E_G \]

FOR HOLEs: \[ n(E) = (1 - f(E)) \]

\[ p(E) \]

FOR ELECTRONS: \[ n(E) = \rho(E) f(E) \]
IMPUURITY DISTRIBUTION FUNCTION

FOR DONORS

ASSUME 1 ELECTRON ON DONOR

\[ f_0 = \text{IMPUURITY DISTRIBUTION FUNCTION} \]

\[ = f \left[ \text{\textit{e}^- IS IN STATE } \ell \text{ IN DONOR COMPLEX} \right] \]

\[ = \left[ \text{\textit{e}^- IS ON DONOR} \right] P \left( \text{\textit{e}^- has energy } E_0 \right) \]

\[ \text{EXCITED STATES} \]

\[ E_0 \rightarrow E_F \]

\[ E_F \rightarrow E_F \]

\[ f_0 = \left[ 1 + \frac{e^{-\frac{E_0}{kT}}}{1 + e^{-\frac{E_0 - E_F}{kT}}} \right] \]

\[ F^+ = P \left( \text{DONOR HAS NO ELECTRON} \right) \]

\[ f_0 = e^{-\frac{E_0}{kT}} \text{ and } \frac{1}{n_0} = \frac{n_e}{N_0} \]

\[ n_0 = \# \text{ \textit{e}^- IN COND. BAND FROM DONORS} \]

\[ N_0 = \# \text{ DONOR ATOMS} \]

Allowing for degeneracy

\[ F^+ \propto 1 + \frac{1}{e^{-\frac{E_0 - E_F}{kT}}} = 1 + \frac{1}{e^{-\frac{E_0 - E_F}{kT}}} \]

\[ \sigma = E_0 - E_F \]

\[ \sigma_0 = \text{DEGENERACY OF GROUND STATE} \]
EFFECTS OF DOPING ON FERMI LEVEL

\[ N^D = N_e^D \text{ IN CONDUCTION BAND FROM DONORS} = N_0 e^{-(E_c - E_F)/kT} \]

\[ N_0 = \text{NUMBER OF DONORS} \]
\[ N_0^D = \text{NUMBER OF NEUTRAL DONORS} \]
\[ N^D = N_0 - N_0^D \]

AT HIGH TEMP: \[ E_F = E_0 - kT \ln \frac{N_0}{N_0^D} \]

AT LOW TEMP: \[ E_F = E_0 + \frac{kT}{2} \ln \frac{N_0^D}{N_0} \]

\( \gamma = \text{DEGENERACY} \)
TEST #2 (STUDY SHEET)

1. SPECIFIC HEAT (HARMONIC OSCILLATOR)
2. DEBYE'S MODEL
3. ELECTRON CONTRIBUTION TO SPECIFIC HEAT
4. HARMONIC OSCILLATOR (RIGOROUS SOLN.)
5. MATRIX ELEMENTS
6. FERMI'S GOLDEN RULE
7. RUTHERFORD SCATTERING
8. HEAT DIFFUSION (RADIAL)
9. " " (TRANSVERSE)
10. TWO STATE QUANTUM SYSTEM
11. BOLTZMANN TRANSPORT EQUATION
**Specific Heat**

\[ C_V = \frac{\partial E}{\partial T} \bigg|_V \]

**Classically, in a gas,** \( E = 3NkT \Rightarrow C_V = 3nk \)

**For a Harmonic Oscillator**

\[ E_n = \left(n + \frac{1}{2}\right)\hbar \omega \Leftrightarrow \text{SOLN. of Schröd's Eqn.} \]

\[ \frac{N_{n+1}}{N_n} = e^{-\left(E_{n+1} - E_n\right)/kT} \Leftrightarrow \text{Boltzmann Factor} \]

\[ e^{-\hbar \omega / kT} \Leftrightarrow \text{FOR HARMONIC OSCILLATOR} \]

\[ \langle n \rangle = \text{AVG \# OF QUANTA IN A STATE \( n \)} \]

\[ = \sum_{n=0}^{\infty} n e^{-\hbar \omega / kT} / \sum_{n=0}^{\infty} e^{-n\hbar \omega / kT} \]

\[ = \frac{\frac{\hbar \omega}{kT} \sum_{n=0}^{\infty} e^{-n\hbar \omega / kT}}{\sum_{n=0}^{\infty} e^{-n\hbar \omega / kT}} \]

\[ \sum_{n=0}^{\infty} e^{-n\hbar \omega / kT} = 1 - e^{-\hbar \omega / kT} \Leftrightarrow \text{FROM S. OF GEOMETRIC SERIES} \]

Gives \( \langle n \rangle = \frac{1}{e^{\hbar \omega / kT} - 1} \Leftrightarrow \text{FOR BOSONS} \)

(\text{FERMI'S OBEY PAULI EXCLUSION PRINCIPLE,})

\( \text{(BOSONS DON'T. \ FOR \ FERMIONS, \ FROM \ THE)} \)

\( \text{(FERMI-DIRAC DISTRIBUTION,} \langle n \rangle = \frac{1}{e^{\hbar \omega / kT} + 1} \)

\( \text{NOTE, \ FOR \ SMALL \( T, \) \} \langle n \rangle \approx \frac{kT}{\hbar \omega} \)

\[ \langle E \rangle = \langle n \rangle \hbar \omega = kT \Leftrightarrow \text{CLASSICAL RESULT} \]

**Generally:** \( \langle E(\omega) \rangle = \frac{\hbar \omega}{k} \frac{1}{e^{\hbar \omega / kT} - 1} \)

\[ \Rightarrow C_V = \frac{\partial \langle E \rangle}{\partial T} \bigg|_V = nk \left( \frac{\hbar \omega}{kT} \right)^2 \frac{e^{\hbar \omega / kT}}{(e^{\hbar \omega / kT} - 1)^2} \]
DEBYE'S MODEL

\[ \langle E \rangle = \frac{1}{3} \omega \langle n \rangle \Rightarrow E_{\text{total}} = \int \frac{1}{3} \omega \langle n \rangle \left( \frac{d \rho}{dE} \right) dE \]

\[ \frac{d \rho}{dE} = \text{DENSITY OF STATES} \]

DEBYE ASSUMED

1. \[ \frac{d \rho}{dE} = \frac{V^3}{2\pi^2 V^3} \] , \( V = \text{VELOCITY} \) , \( V = \text{VOLUME} \)

2. \( \omega = \nu k \) \( \Rightarrow \) \( \text{LINEAR DISPERSION CURVE} \)

3. \( \omega_0 = \text{MAXIMUM FREQUENCY} = \text{DEBYE FREQUENCY} \)

\[ E = \int_0^{\omega_0} \frac{\omega^2}{2m^2 V^3} \left( \frac{k_B T}{e^{\omega/k_B T} - 1} \right) d\omega \]

\[ = \frac{3\pi^4 k_B^4 T^4}{2m^2 V^3 k_B^2} \int_0^{\frac{\omega_0}{k_B T}} \frac{x^3}{e^x - 1} dx \]

\[ \Theta_0 = \text{DEBYE TEMPERATURE} = \frac{\hbar \omega_0}{k_B} \]

\[ C_V = 3 N k_\text{B} \left( \frac{T}{\Theta_0} \right)^3 \int_0^{\Theta_0/k_B T} \frac{x^4 e^x}{e^x - 1} dx \]

\[ = \frac{12}{5} \pi^4 N k_\text{B} \left( \frac{T}{\Theta_0} \right)^3 \text{ FOR SMALL } T \]

DEBYE'S MODEL
Electron Contribution to Specific Heat

Classically: \( E = \frac{3}{2} kT N \Rightarrow C_V = \frac{3}{2} kT \)

This doesn't work out to well due to Pauli's Exclusion Principle:

\( E = \text{Fermi-Dirac distribution} \)

Recall: \( E = \frac{3}{2} kT \left( \frac{2\pi^2 \hbar^2}{m k} \right)^{3/2} \)

\( \frac{dE}{d\epsilon} = \frac{3\pi^2 \hbar^2}{2m \sqrt{kT}} \left( \frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\epsilon} \)

\( \Delta E = \text{allowed states} = \int_{E_F}^{E_F + \Delta E} E F_E(E) \frac{dE}{d\epsilon} \ d\epsilon \)

\(- \frac{1}{4\pi^2} \frac{3\pi^2 \hbar^2}{2m \sqrt{kT}} \left( \frac{2m}{\hbar^2} \right)^{3/2} \)

where \( T_F = \frac{E_F}{k} \)

\( \Rightarrow C_V = \frac{d\Delta E}{dT} = \frac{3\pi^2 \hbar^2}{2m \sqrt{kT}} \left( \frac{2m}{\hbar^2} \right)^{3/2} \)
**RISCOURS SOLUTION TO SIMPLE HARMONIC OSC.**

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + (E - V) \psi = 0 \]

\[ V(x) = \frac{1}{2} m \omega^2 x^2 \] \[ \text{HARMONIC OSCILLATOR POTENTIAL} \]

Let \( \xi = \sqrt{\frac{m \omega}{\hbar}} x \); \( \xi = \frac{\hbar}{m \omega} \) gives:

\[ \frac{\hbar^2}{8 \xi^2} + (E - \xi^2) \psi = 0 \]

Substituting \( \psi = \text{ve}^{-\xi^2/2} \) gives HERMITE'S DIFF. EQU.:

\[ \frac{\hbar^2}{8 \xi^2} - 2 \xi \frac{d}{d\xi} + (E - 1) \psi = 0 \]

In order for things not to blow up, it turns out:

\[ E = (n + \frac{1}{2}) \hbar \omega \]

**SOLN': THEN HERMITE POLYNOMIALS:**

\[ V = H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2} \]

**THE WAVE FUNCTION IS:**

\[ \psi_n = H_n e^{-\xi^2/2} \]

**HERMITE POLYNOMIALS AND WAVE FUNCTION**

\[ H_0(\xi) = 1 \]

\[ H_1(\xi) = 2 \xi - 2 \]

\[ dH_n(\xi) = 2n \xi H_{n-1}(\xi) \]

\[ \psi_n = H_n e^{-\xi^2/2} \]

\[ \int_{-\infty}^{\infty} H_n^2 e^{-\xi^2/2} d\xi = \int_{-\infty}^{\infty} |\psi_n|^2 d\xi = \sqrt{\pi} 2^n n! \]

\[ = 2\pi \int_{-\infty}^{\infty} H_{n-1}^2 e^{-\xi^2} d\xi = 2\pi \int_{-\infty}^{\infty} |\psi_{n-1}|^2 d\xi \]

\[ \left\{ \begin{array}{l}
\frac{\delta}{\delta \xi} \psi_n = \sqrt{2n+1} \psi_{n-1} \\
\frac{\delta}{\delta \xi} \psi_{n+1} = \sqrt{2(n+1)} \psi_n
\end{array} \right. \]
\textbf{MATRIX ELEMENT}
\[ \langle n' | V | m \rangle = \int_{-\infty}^{+\infty} \psi^*_n(x) V \psi_m(x) \, dx \]
\text{V = PERTURBATION}

\textbf{FERMI'S GOLDEN RULE}

Schrödinger's equation (time dependent) \[ \dot{\psi} = \frac{i}{\hbar} \frac{\partial}{\partial t} \psi \]

\text{PERTURBED WITH A POTENTIAL V}
\[ \psi = \sum_n \phi_n(t) e^{-iE_n / \hbar} \]
\text{\( \phi_n \) = UNPERTURBED WAVE FUNCTION}

\[ \frac{\Delta \psi}{\Delta t} = \sum_n \phi_n(t) \sum_n V_{SN} e^{i(E_n - E_n) / \hbar} \]
\text{WHERE}
\[ V_{SN} = \langle S | V | N \rangle \]

\text{ASSUMPTIONS:}
\begin{enumerate}
  \item \( \Delta q_S(t) = 0 \Rightarrow q_n(t) = \frac{1}{\hbar} \sum_n q_n V_{SN} e^{i(E_n - E_n) / \hbar} \]
  \item \( V \) IS TIME INDEPENDENT
  \item \( q_S(t) \) IS IN STATE \( \langle S | q_n \rangle = 1 \)
\end{enumerate}

\[ q_S(t) = \frac{1}{\hbar} \sum_n q_n(t) \]

\[ q_S(t) \cdot q_S(t) = \frac{1}{\hbar} \sum_n q_n(t) \sum_n q_n(t) \]

\[ p_S(t) = \frac{\hbar}{\pi} \sum_n q_n(t) \sum_n q_n(t) \]

\[ p(t) = \frac{\hbar}{\pi} \sum_n q_n(t) \sum_n q_n(t) \]

\text{OVER REGION OF INTEREST, IF \( \langle E_n - E_n \rangle \)}

\[ \text{DENSITY OF STATES} \rightarrow \rho(E_n) \]

\[ \frac{d\rho(t)}{dt} = \frac{2\pi}{\hbar} |V_{SN}|^2 \rho(E_n) \]

\( \rightarrow \) FERMI'S GOLDEN RULE #2

\textbf{FERMI'S GOLDEN RULE}

\[ \frac{d\rho(t)}{dt} = \frac{2\pi}{\hbar} |V_{SN}|^2 \rho(E_n) \]
Rutherford Scattering

\[ \sqrt{\frac{\hbar^2}{m^2}} \frac{e}{\hbar} P \cdot x = \gamma \]

Due to energy conservation, \( |p| = |p'| \)

\[ V_{SR} = \frac{1}{2} \int V(x) \cdot \frac{1}{\sqrt{2\pi}} \delta(x - P - P') \cdot x \, dx \]

\[ = \frac{1}{2} \int \mathcal{F}[V(x)] \cdot \mathcal{F}^{-1}[\delta(P - P')] \, dx \]

\( \mathcal{F}[E_n] = \left( \frac{2\pi \hbar^2}{m} \right)^{3/2} \oint \frac{dp_1 dp_2 dp_3}{p^2} \)

\[ \frac{d\sigma}{d\Omega} = \text{solid angle cross-section} \]

\[ d\sigma = \text{fraction of particles going into } d\Omega \]

\[ \Rightarrow \frac{d\sigma}{d\Omega} = \frac{1}{2\pi} \left| \mathcal{F}[V(r)] \right|^2 \]

Gives

\[ \frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2 \hbar^2} \frac{\partial^2}{\partial \phi^2} \left| \mathcal{F}[V_{SR}(r)] \right|^2 \]

For a Coulomb potential

\[ V(r) = -\frac{e^2}{r} \]

\[ V_{SR} = -\frac{e^2}{r} \int \frac{e^{i \mathbf{r} \cdot \mathbf{P}}}{\mathbf{r}} \, d^3x \]

\[ = \frac{\pi e^2}{4 \rho^2 \Delta \theta} \]

Which gives

\[ \frac{d\sigma}{d\Omega} = \frac{\pi e^2}{4} \left( \frac{m e^2}{\hbar^2} \right)^2 \frac{1}{\sin^2 \theta/2} \]

Same as Rutherford Scattering

RHR - 9/2
HEAT DIFFUSION EQUATION

\[ \nabla^2 T = \frac{\rho C}{\kappa} \frac{\partial T}{\partial t} \]

\( \rho \) = density, \( C \) = specific heat, \( k \) = thermal conduct.

**Gaussian Beam:** \( I = I_0 e^{-r^2/2r_0^2} \)

1. **Radial Diffusion**

Use cylindrical coord: \( \rho \rightarrow r \)

\[ \frac{\partial T}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial T}{\partial \rho} \right) = 0 \]

Leaves \( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial T}{\partial \rho} \right) = \frac{\partial T}{\partial t} \)

Using \textit{separation of variables}: \( T(\rho, t) = T_\rho T_t \)

\[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial T_\rho}{\partial \rho} \right) = -\frac{v^2}{c^2} T_t \]  

\( \text{Bessel's Eqn.} \)

Gives \( T_\rho = C e^{-v^2 \kappa t/c^2} \)

\( T_t = A(v) J_0(v \rho) \)

or \( T = T_\rho T_t = A(v) J_0(v \rho) e^{-v^2 \kappa t/c^2} \)

**Boundary Conditions:** \( T(\rho, 0) = T_0 e^{-r^2/2r_0^2} \)

\[ e^{-v^2 \kappa t/c^2} = \int_0^\infty A(v) J_0(v \rho) dv \]

\( A(v) = \int_0^\infty r \rho \ \rho \ e^{-r^2/2r_0^2} J_0(v \rho) \)

**T(\rho, t) = \int_0^\infty \rho u \ \rho \ x \ dx \ J_0(v \rho) \ e^{-v^2 \kappa t/c^2} \ dx \]

\[ T_0 \alpha \ e^{-v^2 \kappa t/c^2} \]

\( \alpha = (1 + \frac{2 \kappa T}{r_0^2 \rho C})^{-1} \)

**Note:** \( r = 0 \rightarrow \rho^2 \frac{\partial T}{\partial \rho} = 1 \) => \( \frac{z}{k T} = \frac{r_0^2}{\rho C} \)
DIFFUSION IN Z DIRECTION

\[ \frac{\partial T}{\partial t} = 0, \quad \frac{\partial^2 T}{\partial z^2} = 0 \]

USING SEPARATION OF VARIABLES

\[ \frac{1}{z^2} \frac{\partial^2 T}{\partial z^2} = -u^2 = \frac{1}{k} \frac{\partial^2 T}{\partial z^2} \]

GIVES:

\[ T(z, t) = A(u) \cos(uz) e^{-u^2 t/k} \]

\[ \mu(z - z_0) \quad \text{BOUNDARY CONDITION} \]

\[ T(0, t) = T_0 \mu(z - z_0) \]

\[ T(z, t) = \int_0^\infty A(u) \cos(uz) e^{-u^2 t/k} du = \text{FOURIER XFORM} \]

\[ \Rightarrow A(u) = \frac{1}{\pi} \int_0^\infty T(z, t) \cos(uz) du \]

AND

\[ T(z, t) = \int_0^\infty A(u) \cos(uz) e^{-u^2 t/k} du \]

\[ = \frac{1}{k} \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} e^{-x^2} \cos(xz) dx \]

\[ T(z, 0) = \frac{1}{\sqrt{4\pi k}} \int_{-\infty}^{\infty} e^{-u^2} du = To \text{ erf}(z / \sqrt{4kT}) \]
TWO STATE QUANTUM SYSTEM

\[ H = H_0 + V \]  
\( H_0 = \text{HAMILTONIAN} \)

\( \omega_0 = \omega_a - \omega_b \)

ASSUMPTIONS:
1. \( a = a(t), b = b(t) \)
2. \( <a|H_0|b> = <a|E_0|b> = E_0 \delta_{ab} \)
3. \( V_{ab} = V_{ba} = 0 \)

WE THEN HAVE:

\[ <a|H_0 + V|\psi> = <a|H_0|a>e^{-i\omega_0 t}a + <a|V|b>e^{-i\omega_0 t}b \]

USING \( H\psi = \frac{-i}{\hbar}\frac{d\psi}{dt} \) GIVES \( (\omega_0 = \omega_b - \omega_a) \):

\[ \begin{align*}
\dot{a} &= -\frac{i}{\hbar}\frac{V_{ab}}{2}\sqrt{\frac{\omega_0}{2}}a e^{-i\omega_0 t} \\
\dot{b} &= \frac{i}{\hbar}\frac{V_{ab}}{2}\sqrt{\frac{\omega_0}{2}}b e^{-i\omega_0 t}
\end{align*} \]

APPLIED FIELD \( \Rightarrow V = eE_0 X_{ab} \cos \omega t \)

\[ <a|V|b> = V_{ab} = e <a|X|b> = \mu_{ab} \leftrightarrow \text{DIPOLE} \]

THEN

\[ \begin{align*}
\dot{a} &= -\frac{i}{\hbar}\frac{V_{ab}}{2}\sqrt{\frac{\omega_0}{2}}b e^{-i\omega_0 t} + \frac{\gamma_0}{2}a \\
\dot{b} &= \frac{i}{\hbar}\frac{V_{ab}}{2}\sqrt{\frac{\omega_0}{2}}a e^{-i\omega_0 t} - \frac{\gamma_0}{2}b
\end{align*} \]

DAMPING ASSUMED:

\[ \begin{align*}
\dot{a} &= -\frac{i}{\hbar}\frac{V_{ab}}{2}\sqrt{\frac{\omega_0}{2}}b e^{-i\omega_0 t} \\
\dot{b} &= \frac{i}{\hbar}\frac{V_{ab}}{2}\sqrt{\frac{\omega_0}{2}}a e^{-i\omega_0 t}
\end{align*} \]

SOLUTION:

\[ a = a(t) e^{-\frac{\gamma_0}{2}(t-t_0)} \quad b = b(t) e^{-\frac{\gamma_0}{2}(t-t_0)} \]

INITIAL CONDITIONS:

\[ t = t_0, \quad a = 1, \quad b = 0 \]

POLARIZATION: (STEADY STATE)

\[ P_x = \frac{\langle \psi | \mu | \psi \rangle}{\hbar} = \frac{\mu_{ab}}{2\hbar} \left[ \frac{R_{ab}}{\delta_a} - \frac{R_{ba}}{\delta_b} \right] (\omega_0)^2 + \delta_a (\omega - \omega_0) \delta_{ab} \]

\( \eta_d \equiv \text{N_{ATOMS}} \), \( \eta_p \equiv \text{PUMPING CONSTANT} \), \( \delta_a \equiv \text{DEcay CONSTANT} \)

\( \eta_{bc} \equiv \text{PROBABILITY OF TRANSITION} = \sum_d \rho_d = \sum_d |<d|V|b>|^2 \)

DECAY:

\[ \frac{d \rho_b}{dt} = \rho_T \rho_b \]

\[ \rho_b = n_b e^{-t\rho_b} \Rightarrow \rho_b = \frac{n_b}{t} \]
**Boltzmann Transport Equation**

*Six-Dimensional $(\vec{x}, \vec{v})$ or $(\vec{r}, \vec{p})$ Probability Distribution Varying in Time*

\[
\nabla \cdot \vec{V} + \vec{a} \cdot \nabla f = \frac{f - f_0}{\gamma} \]

or

\[
\frac{1}{\hbar} \left( \nabla_k \vec{E} \right) \cdot \left( \nabla \vec{p} \right) + \frac{1}{\hbar^2} \cdot \vec{p} \cdot \nabla f = \frac{1}{\gamma} (\vec{f} - \vec{f_0})
\]

\[
\vec{E} = \hbar^2 k^2 / 2m^* \quad \vec{V} = \hbar k / m^*
\]

[Time Dependent]

\[
\frac{\delta f}{\delta t} = -\frac{\vec{J} \cdot \nabla f}{\gamma} - \vec{a} \cdot \nabla f - \vec{V} \cdot \nabla \vec{f}
\]

\[
\gamma = \text{Time Constant}
\]

\[
f_0 = \text{Known Distribution}
\]

1-D D.C. Disturbance

\[
f = f_0 - \gamma \left( V_x \frac{\delta f}{\delta x} + a_x \frac{\delta f}{\delta V_x} \right)
\]

**Current Density:**

\[
J_x = -e \frac{\partial}{\partial V_x} \int f \, V_x \, dV = \int f \, \frac{V_x}{m_e} \, dV
\]

All known \( f_0 \) are even w.r.t. \( V \) \( \Rightarrow \int f_0 \, dV = 0 \)

\[
J_x = -e \int f \, \gamma \left( V_x \frac{\delta f}{\delta x} + a_x \frac{\delta f}{\delta V_x} \right) V_x \, dV
\]

**Thermal Current Density:**

\[
C_x \frac{\text{Watt}}{m^2} \text{per free} \epsilon s
\]

\[
C_x = \int \int f \, V_x \, dV \, dV_x \, dV_y \, dV_z
\]

\[
= -e \gamma \int \int \left( V_x \frac{\delta f}{\delta x} + a_x \frac{\delta f}{\delta V_x} \right) V_x \, dV_x \, dV_y \, dV_z
\]

**For Maxwell-Boltzmann Distribution**

\[
f_0 = n \left( \frac{m}{2\pi kT} \right)^{3/2} e^{-mV^2 / 2kT}
\]

Assume \( \frac{\delta f}{\delta x} = -\left( \frac{mV_x^2}{2kT} - \frac{3}{2} \right) \frac{\delta f}{\delta x} \text{ const.} \int \epsilon_x \text{ for } \epsilon_x \text{ at 0}
\]

\[
C_x = -\frac{5n(2kT)^2}{2m} \frac{\epsilon_x(2kT)}{2m} - \frac{5n(2kT)^2}{m} \frac{\epsilon_x(2kT)^2}{2m}
\]

\[
\gamma \text{ assumed constant}
\]

Boltzmann Transport Theory
**Conductivity**

\[ \frac{J_x}{E_x} = \sigma = \text{Conductivity} = \frac{n e^2 v}{m} = \sigma \mu \]

From \( \frac{\partial T}{\partial x} = 0 \)

\[ K = \frac{C_v}{\partial T/\partial x} \bigg|_{T=0} = \frac{5 n^2 k^2 T}{\pi^2 m} \]

Thermal Conductivity

\[ \frac{1}{\sigma T} = 5 k^2 / 2 e^2 \]

**Thermal Electric \( \rightarrow J_x \) flows, \( \text{no } E \) due to \( T \) difference**

**Fermi (Degenerate Gasses) (Metal)**

\[ \frac{f(E)}{1 + e^{(E-E_F)/kT}} \]

\[ E = \frac{1}{2} k^2 \]

gives \( \sigma = \frac{e^2}{2}\pi m^2 \gamma(E_F) \)

\[ K = \frac{5}{3} \frac{e^2}{m^2} n \gamma(E_F) \]

\[ \frac{1}{\sigma T} = \frac{5}{3} \left( \frac{k^2}{e^2} \right)^2 \text{ WEISSELMANN-FRANZ RATIO} \]
TEST # 3, FINAL STUDY SHEET

1. BAND STRUCTURE CALCULATION
   BORN-OFFENHEIMER | HARTREE-FOCK | LDA

2. BLOCH FUNCTIONS

3. K.P. APPROXIMATION

4. BAND TO BAND TRANSITION

4. LIGHT ABSORPTION (REFER. INDEX

5. ABSORPTION COEFFICIENTS

5. P-N JUNCTION

6. NPN. BJT

7. NPN BJT (CONT.)

7. JFET

8. IMPURITY SCATTERING
**BAND-STRUCTURE CALCULATION**

**ACTUAL HAMILTONIAN**

\[ H = -\sum_{\text{nucleus}} \frac{\hbar^2}{2m} (a_n^2 + b_n^2) + \sum_{\text{elec}} \frac{\hbar^2}{2m} (a_e^2 + b_e^2) + \frac{e^2}{\epsilon} \frac{1}{r_{ne}} + \frac{e^2}{\epsilon} \frac{1}{r_{nm}} - \frac{1}{2} \sum_{\text{elec/elec}} \frac{e^2}{4\pi\epsilon_0 r_{de}} \]

**BORN-OPPENHEIMER APPROXIMATION**

**SEPARATE ELECTRONIC & VIBRATIONAL MOTION**

\[ \psi = \psi_e \psi_n \]

**ELECTRONIC TERM**

\[ E_e = \sum \psi_e^* H \psi_e = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial x_e^2} \phi_e + \frac{e^2}{\epsilon} \sum \frac{1}{r_{ne}} \phi_e^* \phi_n \]

\[ V_{ee} = \frac{1}{2} \sum \frac{\partial}{\partial x_e} \left( \frac{e^2}{\epsilon} \frac{1}{r_{me}} \right) + \frac{1}{2} \sum \frac{\partial}{\partial x_e} \left( \frac{e^2}{\epsilon} \frac{1}{r_{me}} \right) \]

\[ \Rightarrow E_e = \sum \left( E_{e0} + \frac{1}{2} \sum \frac{e^2}{\epsilon} \frac{1}{r_{ne}} \phi_e^* \phi_e \right) \phi_e = E_{e0} \phi_e \]

**GOOD FOR ONLY ONE ELECTRON:**

**HARTREE-FOCH APPROX. (SLATER DETERMINANT)**

**ASSUME:** 1 ON ELEC, 1 IN OUTER SHELL, SPHER. SYM., SELF CONSISTENCY

**HARTREE ASSUMPTION:**

\[ \psi = \phi_1 \phi_2 \ldots \phi_n = \psi_n^{\text{n-th}} \] **WAVE FUNCTION**

**HARTREE-FOCH INCLUDED EXCHANGE TERMS:**

\[ \psi(x) = \frac{1}{N!} \left[ \phi_e(x_1) \phi_e(x_2) \ldots \right] \phi_n(x) = \text{SLATER DETERMINANT} \]

\[ \phi_e(x_i) = \phi_1(\text{SPACE}) \phi_1(\text{SPIN}) (m = \pm \frac{1}{2}) \]

**WISH TO DESYMMETRIZE WAVE FUNCTION**

\[ \psi = \left[ \phi_1(x_1) \phi_2(x_2) - \phi_2(x_1) \phi_1(x_2) \right] \left[ \phi_1(1) \phi_1(2) - \phi_1(2) \phi_1(1) \right] \]

**RESULTING ENERGY IS:**

\[ E = \sum \phi_e^* \left( \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_e^2} \phi_e \right) + \sum \left[ \phi_e^* \phi_e \right] \left[ \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial x_e^2} \phi_e \right] + \frac{e^2}{\epsilon} \sum \frac{1}{r_{ne}} \phi_e^* \phi_n \phi_e \phi_n \]

\[ = \sum \left[ \phi_e^* \phi_e \right] \left[ \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial x_e^2} \phi_e \right] + \sum \frac{e^2}{4\pi\epsilon_0 r_{de}} \phi_e^* \phi_n \]

**LINEAR COMBINATION OF ORBITALS**

\[ \psi \rightarrow \sum \phi_e \rightarrow \psi \rightarrow \text{BAND-STRUCTURE, BORN-OPPENHEIMER, HARTREE-FOCH, SLATER} \]
BLOCK FUNCTIONS (ELECTRON IN A CRYSTAL)

\[ \psi(x) = e^{-\frac{x^2}{a^2}} \]

PERIODIC PROPERTY: \[ \psi(x+q)^2 = \psi(x)^2 \]

TAYLOR SERIES: \[ \psi(x+q) = \psi(x) + \frac{\partial \psi}{\partial x} q + \frac{1}{2!} \frac{\partial^2 \psi}{\partial x^2} q^2 + \ldots \]

RECALL \[ \hbar^2 \frac{\partial^2}{\partial x^2} \psi(x) \]

\[ \Rightarrow \psi(x+q) = \psi(x) e^{i \frac{\hbar^2}{2m} q^2} \]

\[ \psi(x+q) \in \mathbb{C} \]

K-P APPROXIMATION (USING BLOCK FUNCTIONS)

\[ \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) U_K(x) = E(k) U_K(x) \]

APPLICATION TO GERMANIUM (DIRECT GAP, SMALL k)

CONDUCTION BAND

(SPREAD S STATE)

VALENCE BAND

(P STATE: 3 STATES)

(4 STATES W/ SPIN)

OLD FUNCTION, TWO FUNCTIONS

GIVES \[ 0 = \sum_{\alpha, \beta} \left( E_\alpha + \frac{\hbar^2}{2m} K \cdot P - E(k) \right) \langle \alpha | U_K | \beta \rangle \equiv K \cdot P \]

FOR SMALL \( K \)

GIVES \[ E_\alpha - E(k) \]

FOR SMALL \( K \)

\[ E(k) \approx E_0 + \frac{1}{2} \frac{\hbar^2 K^2}{m} \]

FREE LIKE \( e^- \)
Band to Band Transition (Non-Degenerate)

\[ E_{\text{V}}(k) = -\frac{\hbar^2 k^2}{2m^*} \]

\[ E_{\text{c}}(k) = \left( \frac{\hbar^2 k^2}{2m^*} \right) \]

\[ \psi_0 = \text{val. band} = \frac{1}{\sqrt{V}} \psi_0(\mathbf{r}, k) \in k \]

\[ \psi_m = \text{cond. band} = \frac{1}{\sqrt{V}} \psi_m(\mathbf{r}, k) \in k \]

Applied Field: \[ \nabla \times A = \frac{\mathbf{E}}{c}, \nabla \cdot A = 0, A = \text{magnetic potential} \]

\[ \mathbf{p} = m \mathbf{v} + \frac{\mathbf{e} A}{c} \Rightarrow \frac{\mathbf{p}_x^2}{2m} = \frac{\hbar^2}{2m} \mathbf{v}_x^2 + \frac{e^2 A_x}{2mc^2} + \frac{e^2 A_y}{2mc^2} \Rightarrow \text{small} \]

\[ A = \mathbf{B} \cdot \mathbf{r} - \frac{1}{c} \frac{d\mathbf{E}}{dt} \]

Fermi Potential: \[ H'(\mathbf{r}) = \frac{1}{2m} \mathbf{p}^2 + \frac{\mathbf{B} \cdot \mathbf{r}}{c} + \mathbf{c.c.} \]

Rate of Transition: \[ \rho = \frac{\rho_{\text{transmission}}}{\text{allowed}} \]

Matrix Element:

\[ H_{kk''} = \frac{i e^2 A}{2mc} \int \psi_0^*(\mathbf{r}, k) \left[ \frac{1}{\sqrt{V}} \nabla \psi_0(\mathbf{r}, k) + \frac{i}{\sqrt{V}} \left( \frac{\mathbf{B} \cdot \mathbf{r}}{c} + \mathbf{c.c.} \right) \right] \psi_m(\mathbf{r}, k) e^{-i \mathbf{k} \cdot \mathbf{r}} \]

\[ H_{kk''} = \frac{i e^2 A}{2mc} \int \psi_0^*(\mathbf{r}, k) \left[ \frac{1}{\sqrt{V}} \nabla \psi_0(\mathbf{r}, k) + \frac{i}{\sqrt{V}} \left( \frac{\mathbf{B} \cdot \mathbf{r}}{c} + \mathbf{c.c.} \right) \right] \psi_m(\mathbf{r}, k) d^3r \]

\[ \text{Allowed Transition} \]

\[ \rho = \frac{\rho_{\text{transmission}}}{\text{allowed}} \]

\[ \rho(\mathbf{E}) \cdot \rho(\mathbf{E}) = \frac{e^2 A}{2mc} \int \psi_0^*(\mathbf{r}, k) \left[ \frac{1}{\sqrt{V}} \nabla \psi_0(\mathbf{r}, k) + \frac{i}{\sqrt{V}} \left( \frac{\mathbf{B} \cdot \mathbf{r}}{c} + \mathbf{c.c.} \right) \right] \psi_m(\mathbf{r}, k) d^3r \]

\[ \rho(\mathbf{E}) = \frac{e^2 A}{2mc} \int \psi_0^*(\mathbf{r}, k) \left[ \frac{1}{\sqrt{V}} \nabla \psi_0(\mathbf{r}, k) + \frac{i}{\sqrt{V}} \left( \frac{\mathbf{B} \cdot \mathbf{r}}{c} + \mathbf{c.c.} \right) \right] \psi_m(\mathbf{r}, k) d^3r \]

Absorbed Photons \(=\) Incident Photons \(\times \rho(\mathbf{E}) \cdot \rho(\mathbf{E}) \]

\[ \alpha = \frac{\rho(\mathbf{E}) \cdot \rho(\mathbf{E})}{\rho_{\text{transmission}}} \]

Oscillator Strength:

\[ \frac{\alpha_{kk''}}{\alpha_{kk' = k'k''}} = \frac{\rho(\mathbf{E}) \cdot \rho(\mathbf{E})}{\rho_{\text{transmission}}} \]

\[ \rho_{\text{transmission}} = \frac{\alpha_{kk''}}{\alpha_{kk' = k'k''}} \int \rho(\mathbf{E}) \cdot \rho(\mathbf{E}) \]
LIGHT ABSORPTION IN A SOLID (REFR. INDEX)

From Maxwell:

\[ \epsilon = \mu = \text{dielectric constant; } c = \frac{1}{\mu} \epsilon = \frac{4\pi\epsilon_0}{c^2} \]

\[ \epsilon = \epsilon_{0}\frac{4\pi}{c^2} \]

REFRACTIVE INDEX:

\[ \gamma^* = \frac{\epsilon - \mu}{\sqrt{\epsilon + \mu}} \]

\[ \gamma = \frac{\epsilon - 1}{\sqrt{\epsilon + 1}} \]

BEER ABSORPTION:

\[ dI = -\alpha (1 - \rho) Idx \]

\[ \alpha = \frac{2\pi}{\lambda} \gamma \]

\[ \alpha = \text{absorption coeff} \]

\[ E_\perp \rightarrow E_\perp \]

\[ \rho = \text{Polarized} \]

\[ \rho = \text{Polarized} \]

\[ E_\parallel = E_{\perp} \]

\[ E_\perp = E_{\parallel} \]

\[ H_\parallel = H_{\perp} \]

\[ H_{\perp} = -H_{\parallel} \]

BOUNDARY CONDITIONS:

\[ E_{\perp} = E_{\parallel} + c \]

\[ H_{\parallel} = c H_{\perp} \]

GIVES:

\[ \frac{E_{\perp}}{E_{\parallel}} = \frac{c^{*} - \gamma}{c^{*} + \gamma} \]

R = REFLECTION COEFFICIENT:

\[ R = \left| \frac{E_{\perp}}{E_{\parallel}} \right|^2 \frac{(\rho - \gamma)^2 + (\rho + \gamma)^2}{(\rho - \gamma)^2 + (\rho + \gamma)^2} \]

FOR A METAL (w > o):

\[ \sigma = \frac{n e^2 \hbar}{M_e} \left( \frac{1}{1 + w^2 \gamma^2} \right) \]

\[ \alpha = \frac{\sqrt{\epsilon \gamma}}{\sigma_o (\gamma^2 + 1)} \]

\[ \alpha = \text{absorption coeff} \]

FOR A METAL: w \gamma << 1 (LOTS A FREE e^*)

FOR AN INS (SEMICOND): w \gamma >> 1

\[ \alpha = \frac{n e^2 \hbar}{M_e \omega} \left( \frac{1}{1 + \gamma^2} \right) \]

\[ \alpha = \frac{n e^2 \hbar}{M_e \omega} \left( \frac{1}{1 + \gamma^2} \right) \]

\[ \alpha = \frac{n e^2 \hbar}{M_e \omega} \left( \frac{1}{1 + \gamma^2} \right) \]
ABSORPTION COEFFICIENTS

DIRECT ALLOWED XSITION: $\alpha = \sqrt{\frac{\hbar \omega - E_0}{\hbar \omega}}$

DIRECT FORBIDDEN XSITION: $\alpha = \frac{1}{\hbar \omega} \left( \frac{\hbar \omega - E_0}{\hbar \omega} \right)^{3/2}$

INDIRECT TRANSITIONS:

ALLOWED: $\alpha = \frac{1}{\hbar \omega} \left( \frac{\hbar \omega - E_{\text{Fermi}}}{\hbar \omega} \right)^{3/2} \left[ e^{-\frac{E_{\text{Fermi}}}{kT}} - 1 \right]$

FORBIDDEN: $\alpha = e^{-\frac{\hbar \omega - E_0}{kT}}$

$K_{\text{ind}} = \frac{1}{2} \left( \frac{\hbar \omega - E_0}{kT} \right)^{3/2}$

P-N JUNCTION

$E_x = E_g - \frac{qV}{kT}$

$W = \frac{x_d + x_b}{2} = \frac{\sqrt{2eN_x}}{\sqrt{n_x} + \sqrt{p_x}}$

$V_b = \frac{kT}{q} \ln \frac{n_x}{p_x}$

$N_p = n_0 e^{-q(V_b + V)/kT}$

$P_n = P_0 e^{-q(V_b + V)/kT}$

$J = \text{const} \left[ (n_x + p_n) + (n_0 + p_0) \right] = J_{so} \left[ e^{qW/kT} - 1 \right]$

LINEARIZING:

$J = J_{so} \left[ 1 + \frac{qV}{kT} + \ldots \right]$

$J = \frac{qVJ_{so}}{kT}$ FOR $kT << 1$
\[ J = q \left( \frac{D_n D_n^{eq}}{L_n} + \frac{D_p D_p^{eq}}{L_p} \right) \left[ e^{\frac{qV}{kT}} - 1 \right] \]

\[ D_n = \text{DIFF. CONST. FOR \( n \)} \]
\[ D_p = \text{HOLE S} \]
\[ L_n = \text{MEAN FREE \( n \) PATH} \]
\[ L_p = \text{MEAN FREE \( p \) PATH} \]
\[ \nu_n = \text{EQ. \( n \) CONC.} \]
\[ \nu_p = \text{EQ. \( p \) CONC.} \]
\[ \nu_n = \nu_p = \frac{e^qV_0}{kT} \]

Assumptions:

1. 

2. Boltzmann Approx

3. Const. \( e \neq h \) CURRENT

4. Low Level Injection

5. 

6. Continuity: \( \frac{\partial N}{\partial t} = G - \frac{n_n - n_p}{\tau_n} + \frac{1}{q} \frac{\partial}{\partial x} J \leq \text{CURRENT} \)

7. Rate of Excess

8. Current Eq. from Boltzmann Export Eq.

9. Assume LL Injection \( \Rightarrow \frac{qD_n^{eq}}{L_n} = 0 \)

10. \( L_p = \frac{e^qV_0}{kT} \Rightarrow p - p_{\text{eq}} = p_{\text{eq}} e^{-x/L_p} \left[ e^{\frac{qV_0}{kT}} - 1 \right] \)

11. \( J = J_n \left[ e^{\frac{qV_0}{kT}} - 1 \right] \Rightarrow J_n = \frac{qD_n^{eq} D_n^{eq}}{L_n} \left[ e^{\frac{qV_0}{kT}} - 1 \right] \)
\[ x = 0 \]

**B.C.:** \[ P(x = 0) = P_0 \ e^{- \frac{q V_{bc}}{kT}} \]

\[ V_c = \text{Emit/Base} \]

\[ \text{INTO} \ \Rightarrow \ P(x) = P(x = 0) \ \text{inh} \left( \frac{x_1 - x}{L_p} \right) \]

\[ \begin{align*}
  J_P & = -q \ \frac{\partial P}{\partial x}, \quad J_P|_{x = 0} = q \ P(x = 0) \ \frac{L_p}{L_p} \ \text{inh} \left( \frac{x_1}{L_p} \right) \\
  J_P|_{\text{coll}} & = q \ P(x = 0) \ \frac{L_p}{L_p} \ \text{inh} \left( \frac{x_1}{L_p} \right)
\end{align*} \]

**CRITICAL:** \[ \frac{L_p}{L} \text{ MUST BE SMALL} \]

- **IN E:** \[ I_{E} = \frac{q \ \text{D}_{\text{H}}(x) (e^{\frac{q V_{bc}}{kT}} - 1)}{L_p} \ 	ext{EL} \text{ cu} \text{r} \text{e} \text{n} \text{t} \]
  \[ + \ q \ P_n(x = 0) \ \frac{L_p}{L_p} \ \text{inh} \left( \frac{x_1}{L_p} \right) \]

- **IN C:** \[ I_{C} = \frac{q \ \text{D}_{\text{H}}(x) + q \ P_n(x = 0)}{L_p} \ \text{inh} \left( \frac{x_1}{L_p} \right) \]

- **Nc equals equilibrium value of in. coll.**

\[ \frac{d}{dx} \alpha \] = \[ \frac{\text{EMISSION EFF. OF FRAC OF EMITTED HOLE CURR}}{\text{BASE \ \text{XPORT \ \text{FACTOR, FRAC EMITTED \ \text{HOLE \ \CURR}}}} \]

\[ \beta = \frac{\text{CURR. \ \text{OF \ \text{HOLE \ \CURR. \ \\text{IN}} \ \text{COLLECTOR}}}{\text{CURR. \ \text{OF \ \text{HOLE \ \CURR. \ \text{IN}} \ \text{BASE}}}} \]

- **JFET:** \[ Z \] is function of width \( y \)

\[ y = \sqrt{\frac{2 \ \frac{E_s}{q N_p}}{V(x) + V_0 - V_{ce}}} \]
Impurity Scattering in Semiconductor

\[ b = \text{impact parameter} \]

\[ s = \text{scattering cross section} = \frac{2\pi b t db}{2\pi} \]

Assume: \[ f = \frac{Ze^2}{\varepsilon_r^2} \]

1. Small scatter angle

2. Initial velocity: \( v \)

\[ \Rightarrow \Delta p = \frac{Ze^2}{\varepsilon_r^2} v \]

Small angle: \[ \frac{\Delta p}{p} = \theta = \frac{Ze^2}{\varepsilon_r^2} \]

Gives: \( \Delta E = \text{loss in energy} = \frac{(\Delta p)^2}{2m} = \frac{Ze^2e^4}{m^3c^2} \)

Real answer is: \( \frac{cm^2}{\varepsilon_r^2} = \frac{Ze^2}{\varepsilon_r^2} \)

\( S = \frac{1}{\sin^2(\theta/2)} \)