

The Hamiltonian

- Instead of Force, Hamiltonian describes system in terms of Energy

Hamiltonian of moving Particle

$$H(p, x) = \frac{p^2}{2m} + V(x)$$

Hamilton's Equations

1. $\frac{\partial H}{\partial p} = \frac{p}{m} = \frac{dx}{dt}$

2. $\frac{\partial H}{\partial x} = \frac{dV(x)}{dx} = -\frac{dp}{dt}$

Hamilton's Eqn. of Motion

$$\frac{\partial^2}{\partial x^2} = \frac{1}{m} * -\frac{dV(x)}{dx}$$

Math Review [8] Fourier operations

Euler Notation

$$e^{\pm i\theta} = \cos(\theta) \pm i\sin(\theta)$$

Trig Identities

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$$

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$$

Integration by Parts

$$\int M dv = uv - \int v du$$

Fourier Transform

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Used to transform a function from Periodic Space into Spatial space

Works best when periodic in one of these Domains

For Inverse Fourier Transform exponent becomes Positive

3.024 Exam #1

Fourier Series

Decompose Functions into

1. Even $\cos()$ terms

2. Odd $\sin()$ terms

$$a_0 = \frac{1}{L} \int_0^{2L} f(x') dx'$$

$$a_n = \frac{1}{L} \int_0^{2L} f(x') \cos\left[\frac{n\pi x}{L}\right] dx$$

$$b_n = \frac{1}{L} \int_0^{2L} f(x') \sin\left[\frac{n\pi x}{L}\right] dx$$

$f(x)$ Periodic on interval $[0, 2\pi]$

example: Hamiltonian of Single Spring

Hamiltonian: $\frac{p^2}{2m} + \frac{K(x-l)^2}{2}$

$$\frac{\partial H}{\partial p} = \frac{dx}{dt} = \frac{p}{m} \quad \left. \frac{d^2x}{dt^2} = \frac{1}{m} - K(x-l) \right.$$

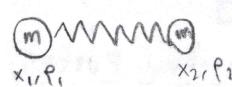
$$\frac{d^2x}{dt^2} + \frac{K}{m}(x-l) = 0 \quad \omega = \sqrt{\frac{K}{m}}$$

Solution Form:

$$Ae^{i\omega t} + Be^{-i\omega t} \Rightarrow \text{Solve using Initial conditions}$$

Example: Diatomic Molecule

System:



Hamiltonian:

$$H(x_1, x_2, p_1, p_2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{K}{2}(x_2 - x_1 - l)^2$$

Hamilton's eqns:

$$\frac{\partial H}{\partial p} = \frac{dx}{dt} \quad \frac{\partial H}{\partial x} = \frac{1}{2}K(x_2 - x_1 - l) = -\frac{dp}{dt}$$

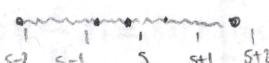
Eqns of Motion:

$$\frac{d^2x_{1/2}}{dt^2} = \pm \frac{K}{m}(x_2 - x_1 - l)$$

$$x_{1/2} = \mp \frac{l}{2} \left(1 - \cos\sqrt{\frac{2K}{m}} t \right)$$

Example: 1D lattice

System:



Hamiltonian: $H_S = \frac{p_S^2}{2m} + \frac{1}{2}K(h_{S+1} - h_S)^2 + \frac{1}{2}K(h_S - h_{S-1})^2$

Eqn of Motion:

$$\frac{d^2h_S}{dt^2} = \frac{K}{m}(h_{S+1} + h_{S-1} - 2h_S)$$

Known as a difference Eqn

has solution of Form $e^{ikx - i\omega t}$

Solving for Omega

$$\omega(k) = \sqrt{\frac{4K}{m}} \sin \frac{ka}{2}$$

The Dispersion Relation

$\omega(k)$ defines the dispersion relation of a system with a few properties

1. Crystal cannot transmit sound frequencies above $\sqrt{4K/m}$ $\omega_{max} = \sqrt{\frac{4K}{m}}$

2. The ratio of 2 adjacent Displacements:

$$\frac{h_{S+1}}{h_S} = e^{ikd}$$

3. Unique Solutions found only for k values in first Brillouin Zone

$$(-\frac{\pi}{a} \leq k \leq \frac{\pi}{a})$$

4. Phase Velocity: $c = \frac{\omega}{k}$

Group Velocity (v_g): $v_g = \frac{dw}{dk}$

5. Standing waves exist at edges of Brillouin where $v_g = 0$

6. As $k \ll 1$ (Long wavelength limit)

$$v_g = \frac{dw}{dk} = \sqrt{\frac{K}{m}} a$$

Elastic Theory: Young's Modulus

Potential Energy of Spring $V(u) = \frac{1}{2} Ku^2$

$$F = -\frac{dV(u)}{du} = -Ku$$

with N bonds and lattice parameters a

$$F = NKH$$

$$\sigma(\text{stress}) = \frac{F}{A} = \frac{NKH}{A}$$

$$\sigma = \frac{N}{Na^2} KH \rightarrow E = \frac{K}{a}$$

~~masses & spring constant~~

$$\text{Final Relation: } E = \rho v_g^2$$

Final Phonon Relation

2 masses connected by springs of 2 different spring constants

Hamiltonian

$$H_S = \frac{p_{1S}^2}{2m} + \frac{p_{2S}^2}{2m} + \frac{K}{2}(k_{1S}k_{1S})^2 + \frac{G}{2}(k_{1S} - k_{2S})^2 + \frac{G}{2}(k_1 - k_{2S})^2$$

Form of Solution:

$$u(x) = e^{ikx - i\omega t} \Rightarrow \text{Solve linear system for } u$$

Basics of QM

Energy of a Photon $E_{ph} = h\nu = \hbar\omega$

Momentum of Photon $p = \hbar k = \frac{\hbar(2\pi)}{\lambda}$

De-Broglie Conjecture All particles are waves & all waves are particles

All Particles are waves of Probability, essentially there is a probability of finding Each particle at a point in space & time

First Postulate of QM

Any Quantum Mechanical particle or system can be described by wave Function $\Psi(x, t)$

Properties of Wave Function:

- (a) Single Valued
- (b) Square Integrable
- (c) Nowhere infinity
- (d) continuous
- (e) Piecewise continuous 1st derivative

Wave Functions are Amplitude of Probability

Probability of finding Particle at r_0 at t_0

$$P(r_0, t_0) = |\Psi(r_0, t_0)|^2$$

Average Particle Position [8] Schrodinger

$$\begin{aligned} \text{Average Particle Position } \langle \vec{r} \rangle &= \int P(\vec{r}, t) \vec{r} d^3r \\ &= \int |\Psi(\vec{r}, t)|^2 \vec{r} d^3r \end{aligned}$$

Example: Plane Wave

wavefunction $\rightarrow e^{ikx - i\omega t}$

$$k = \frac{p}{\hbar}$$

B/c no external Forces,

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

How does wave move in time & space

$$\begin{array}{lll} \frac{\partial}{\partial x} e^{ikx - i\omega t} &= ik e^{ikx - i\omega t} & \frac{\partial}{\partial t} e^{ikx - i\omega t} = -i\omega e^{ikx - i\omega t} \\ \frac{\partial^2}{\partial x^2} e^{ikx - i\omega t} &= -k^2 e^{ikx - i\omega t} & \frac{\partial}{\partial t} e^{ikx - i\omega t} = -i\frac{E}{\hbar} e^{ikx - i\omega t} \\ \frac{\partial^2}{\partial x^2} e^{ikx - i\omega t} &= -\frac{p^2}{\hbar^2} e^{ikx - i\omega t} & \\ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} e^{ikx - i\omega t} &= E e^{ikx - i\omega t} & i\hbar \frac{\partial}{\partial t} e^{ikx - i\omega t} = E e^{ikx - i\omega t} \end{array}$$

- ↓
- ① Assuming 3-Dimensionality
 - ② Generic wavefunction $\Psi(\vec{r}, t)$
 - ③ Presence of Potential Force $V(x)$

Schrodinger's

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(x, t) \right] \Psi(x, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, t)$$

Sixth Postulate of QM

The time evolution of the wavefunction $\Psi(\vec{r}, t)$ is governed by the Schrodinger's Equation

Momentum & Position Operators

Recall

$$-i\hbar \frac{\partial}{\partial x} \Psi(x, t) = p \Psi(x, t)$$

similar to Eigen value problem $[Af = \lambda f]$

↳ where eigenvalue $(\lambda) = p$ (momentum)

↳ f (eigenfunction) = Ψ (wavefunction)

$$A(\text{operator}) = -i\hbar \frac{\partial}{\partial x}$$

$$\begin{array}{ll} \text{Momentum Operator} & \hat{p} = -i\hbar \frac{\partial}{\partial x} \\ \text{Position Operator} & \hat{x} = x \end{array}$$

Second Postulate of QM

Every Measurable Quantity a can be described by an operator \hat{A} . The operator is Hermitian and is called an observable

Properties of Hermitian operator

$$\text{① } \hat{A} = \hat{A}^\dagger, \int \Psi(\hat{A}\Psi) d^3r = \int \Psi(\hat{A}^\dagger\Psi) d^3r$$

↳ where * denotes complex conjugate

② Eigen values are Real

③ Eigen vectors are Orthogonal

** Eigen Functions can form a complete Basis

How to construct Observables

If a physical quantity f is a function of position & momentum Simply sub in $\hat{x} \rightarrow x$

$$\hat{p} \rightarrow p$$

$$f(r, p, t) \rightarrow \hat{f}(\vec{r}, \vec{p}, t)$$

ex

$$H = \frac{\hat{p}^2}{2m} + V(x, t) \quad \hat{A} = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(\vec{r})$$

30 # of Nodes vs. Energy of Eigenfunction (zeroes)

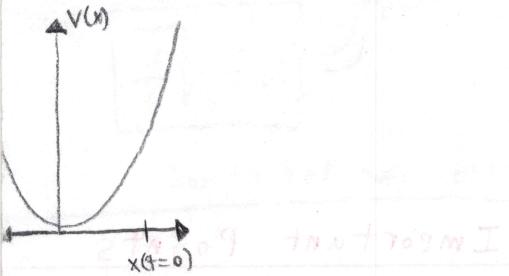
$H_n(x)$ has n-1 nodes between walls of well

4. Solutions are either even or odd

Harmonic Oscillator in Physics

↳ can be used to represent Potential energy $V(x)$ small distances from Resting Point

Quantum Mechanical Harmonic Oscillator



Classic Energy of system

$$E = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 = H(x, p), \text{ where } \omega = \sqrt{\frac{k}{m}}$$

General Form

$$H_n(x) = e^{-\frac{1}{2} \frac{m\omega^2}{\hbar^2} x^2} H_n(x)$$

↳ where H_n = Hermite Polynomial

Consequences:

1. Minimal Energy always greater than 0

2. Lowest Energy Eigenfunction always even

3. Energy is quantized

4. Spacing between energy levels is constant

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

Measuring Physical quantities in QM

* Recall any wavefunction can be represented by a linear superposition of eigenfunctions

↳ Therefore we use Eigenfunctions as "basis functions"

* We can express any state as a linear combo of eigenfunctions or Eigen vectors

Measuring Physical Quantities

* Consider a state characterized by wavefunction $\Psi(\vec{r}, t)$

↳ we want to predict physical quantity a associated with observable \hat{A}

↳ use a set of rules to predict probability of

$$\hat{A} H_n(x) = a_n H_n(x)$$

$$\Psi(x) = \sum_n C_n H_n(x)$$

$$C_n = \langle H_n | \Psi \rangle$$

* Basically seeing how much each eigenfunction affects the overall solution

* Greater C_n = Greater probability

Inner Product of 2 Functions

$$\langle H(x) | \Psi(x) \rangle = \int H(x)^* \Psi(x) dx$$

* denotes complex conjugate

$$\langle u_1 | \Psi \rangle = C_1$$

$$\langle u_2 | \Psi \rangle = C_2$$

4th Postulate of QM

* Probability of $P(a_n)$ obtained for eigenvalue a_n is

$$P(a_n) = |C_n|^2$$

$$\langle \hat{A} \rangle = \langle \Psi(x,t) | \hat{A} | \Psi(x,t) \rangle$$

Example: Particle in Free Space

consider a particle w/ wavefunction

$$\Psi(x,t) = \frac{1}{2} e^{ik_0 x - i\omega t} + \frac{1}{2} e^{-ik_0 x - i\omega t}$$

$$\langle \hat{p} \rangle = \langle \Psi(x,t) | \hat{p} | \Psi(x,t) \rangle$$

$$= \int_{-\infty}^{\infty} \left[\frac{1}{2} e^{-ik_0 x - i\omega t} + \frac{1}{2} e^{-ik_0 x + i\omega t} \right] \frac{1}{i} e^{ik_0 x + i\omega t} dx$$

$$= i \hbar \frac{\partial}{\partial x} \left[\frac{1}{2} e^{-ik_0 x - i\omega t} + \frac{1}{2} e^{-ik_0 x + i\omega t} \right]$$

$$= \frac{1}{4} \hbar k_0$$

5th Postulate of QM

* If a measurement on a system $\Psi(\vec{r}, t) = a_n$, then the state of the system is $H_n(x)$

* The state of a system right after a measurement is always an eigenvector of the eigenvalue measured

* the state of the system is disturbed when measured

Special Case: Time-Independent Hamiltonian

$$\hat{H}(\vec{r}, \vec{p}) = -\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(r) + \text{no time}$$

↳ Potential constant in time

Time-Independent Schrödinger's:

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \Psi(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t)$$

* we separate $\Psi(\vec{r}, t) = a(\vec{r}) b(t)$

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] a(\vec{r}) b(t) = i\hbar \frac{\partial}{\partial t} a(\vec{r}) b(t)$$

$$\frac{1}{a(\vec{r})} \left[\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] a(\vec{r}) \right] = \frac{1}{b(t)} i\hbar \frac{\partial}{\partial t} b(t)$$

Position Dependent | Time Dependent

Solving Time Dependent Partion

$$E = \frac{1}{b(t)} i\hbar \frac{\partial}{\partial t} b(t)$$

$$E b(t) = i\hbar \frac{\partial}{\partial t} b(t)$$

$$\downarrow \\ b(t) = e^{-iEt/\hbar}$$

Solving Position Dependent Partion

• Equation 2 is: $\hat{H} a(x) = E a(x)$

↳ Suppose this E is eigenvalue

Equation above has 2 Eigenvalues \boxed{E} and corresponding eigenfunctions $\boxed{a(x)}$

$$\Psi(\vec{r}, t) = a(x) e^{-iEt/\hbar}$$

↳ in general the solution will be a linear combination of different E terms of different Eigenfunctions

$$\Psi(\vec{r}, t) = \sum_E C_E a(\vec{r}) e^{-iEt/\hbar}$$

Example: Particle in a Potential well

System: Particle of Mass m in Potential well of infinite height

Hamiltonian:

$$H(x, p) = \frac{p^2}{2m} + V(x)$$

$$V(x) = \begin{cases} 0 & -\frac{d}{2} < x < \frac{d}{2} \\ \infty & x \leq -\frac{d}{2} \text{ or } x \geq \frac{d}{2} \end{cases}$$

Obtain \hat{H} :

$$\hat{H}(\vec{r}, \vec{p}) = \frac{\vec{p}^2}{2m} + V(\vec{r}) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right)$$

What are Eigenfunctions & eigenvalues of energy

$$\hat{H}(\vec{r}, \vec{p}) H(x) = E H(x)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} H(x) = E H(x)$$

$$-\frac{d^2 H(x)}{dx^2} - \frac{2E_m}{\hbar^2} H(x) = 0$$

$$H(x) = C_1 e^{ikx} + C_2 e^{-ikx} \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

* A diff. eq. will have a unique solution if we know boundary conditions

$$H(x = \pm \frac{d}{2}) = 0$$

$$H\left(\frac{d}{2}\right) = (a e^{ikd/2} + b e^{-ikd/2}) = 0$$

$$a \left[\cos\left(\frac{kd}{2}\right) + i \sin\left(\frac{kd}{2}\right) \right] + b \left[\cos\left(\frac{kd}{2}\right) - i \sin\left(\frac{kd}{2}\right) \right] = 0$$

$$(a+b) \cos\left(\frac{kd}{2}\right) + i(a-b) \sin\left(\frac{kd}{2}\right) = 0$$

if $a = b$

$$\frac{kd}{2} = n \frac{\pi}{2} \quad (n=1, 3, 5, \dots)$$

if $a = -b$

$$\frac{kd}{2} = n \frac{\pi}{2} \quad (n=2, 4, 6, \dots)$$

$$H_E(x) = H(x) = \begin{cases} \text{if } n \text{ odd} & C_n \cos\left(\frac{n\pi x}{d}\right) \\ \text{if } n \text{ even} & C_n \sin\left(\frac{n\pi x}{d}\right) \end{cases}$$

From this we get quantized energy levels too

How to find coefficients C_n & E_n

• Since the Probability of finding a particle in any state can't exceed 1, then Normalize all eigenfunctions

Remember

$$|\Psi(x)|^2 = \text{Probability}$$

$$\int_{-d/2}^{d/2} |\psi_n(x)|^2 \cos^2\left(\frac{2k-1}{d}x\right) dx = 1$$

$$|\psi_n(x)|^2 = \frac{1}{\pi} \int_{-d/2}^{d/2} \cos^2\left(\frac{2k-1}{d}z\right) dz = 1$$

* Do same for n is odd

Important Points

	Free Particle	Particle in a Box
Hamiltonian	$H(x) = \frac{i\hbar}{m} \vec{p}^2$	$H_n(x) = \frac{\hbar^2 k^2}{2m} \cos(kx)$
Eigenfunction	$\psi(x) = e^{ikx}$	$\psi_n(x) = \frac{1}{\sqrt{d}} \sin\left(\frac{n\pi x}{d}\right)$

IMPORTANT :

1. Unlike a free particle, which can have any energy value, Energy states in a well are Discrete

2. Dependence of Energy level separation on well size

$$\Delta E_n = E_{n+1} - E_n = \frac{\pi^2 \hbar^2}{2md^2} (2n+1)$$

* well & ΔE

Commutator Operator

- Commutator operator is

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

- Two Observables commute if

$$[\hat{A}, \hat{B}] = 0$$

* if 2 Observables commute they Share Eigenfunction solutions

Fundamental Theorem of Algebra

- If A and B commute, then one can construct an eigenfunction state space

Heisenberg's uncertainty principle

$$[\hat{x}, \hat{p}] \neq 0$$

\Downarrow so

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

Symmetries, ^{conserved} quantities of motion

- Symmetry implies a measurement taken at particular time or position is the same moving forward

EHRENFEST THEOREM

- ↳ describes Time-Evolution of Observable

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle + \frac{\partial \hat{A}}{\partial t}$$

- Operator constant in time if

$$1. \quad \frac{\partial \hat{A}}{\partial t} = 0$$

$$2. \quad [\hat{A}, \hat{H}] = 0$$

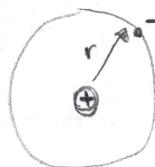
Conserved Quantities (Example)

↳ Particle in Free Space

$$[\hat{H} \psi(x), E \psi(x)] = E [\hat{H} \psi(x)] \quad H_E(x) = \frac{e^{i\sqrt{2mE}}}{x^2} x$$

Example 2: Angular Momentum & Spherical symmetry

- Consider a spherically symmetrical Hydrogen atom



$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

• Potential doesn't depend on position, only distance

Angular Momentum:

classically,

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \hat{i}_x & \hat{i}_y & \hat{i}_z \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

in Quantum Mechanics

$$\hat{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \text{Angular } T \\ \hat{i}_x & \hat{i}_y & \hat{i}_z \\ x & y & z \\ -i\hbar \frac{\partial}{\partial x} & -i\hbar \frac{\partial}{\partial y} & -i\hbar \frac{\partial}{\partial z} \end{vmatrix}$$

Now switch to spherical coordinates

$$\begin{cases} x = r \sin(\theta) \cos(\phi) \\ y = r \sin(\theta) \sin(\phi) \\ z = r \cos(\theta) \end{cases}$$

Two important Results:

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$

$$[\hat{L}_x, \hat{L}_z] \neq 0$$

↳ But

$$[\hat{L}_z, \hat{L}^2] = 0 \quad \left. \begin{array}{l} \text{meaning the} \\ \text{two share a} \\ \text{set of eigenfunctions} \end{array} \right\}$$

$$[\hat{L}_z Y_l^m] = m \hbar Y_l^m(\theta, \phi)$$

$$[\hat{L}^2 Y_l^m] = m \hbar Y_l^m(\theta, \phi)$$

The Hydrogen Atom

$$V(r) = -\frac{e^2}{r}$$

$$\text{Hamiltonian: } H(\vec{r}, \vec{p}) = \frac{\vec{p}^2}{2m} - \frac{e^2}{r}$$

↳ where $m = \frac{m_e p}{m_e + m_p}$ (reduced mass).

- Bohr originally assumed electron trajectory & Force Balance and arrived at correct result

QM approach to Hydrogen

- we split Hamiltonian to reflect energy of center of mass(translational) and relative (rotational motion)

$$\vec{R}_{cm} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$$

$$\vec{p}_{cm} = \vec{p}_1 + \vec{p}_2$$

$$\vec{p} = \frac{m_1 \vec{p}_1 + m_2 \vec{p}_2}{m_1 + m_2}$$

$$\hat{H} = \frac{\vec{p}_{cm}^2}{2M} + \frac{\vec{p}^2}{2m} + \hat{V}(\vec{r})$$

$$\hat{H}_{cm} \quad \hat{H}_{relative}$$

\hat{H}_{cm} & $\hat{H}_{relative}$ commute &

it splits into two problems

Deriving \hat{H} at cm Eigenstate

$$\hat{H}_r(\vec{r}, \vec{p}) = \frac{-\hbar^2}{2M} \frac{1}{r^2} \frac{\partial^2}{\partial r^2} + \frac{\vec{p}^2}{2Mr^2} - \frac{e^2}{r}$$

↳ because \hat{L}^2 commutes w/ \hat{H} that commutes w/ \hat{L}_z

$$u_{nlm} = R_{nl}(r) Y_l^m(\theta, \phi)$$

n - Number associated with eigenvalues of Energy operator (principal Quantum Number)

l - # associated Eigenvalues of \hat{L}^2 operator (orbital angular Quantum #)

m - Eigenvalues of \hat{L}_z operator (magnetic Quantum #)

Final facts about Hydrogen

$$H_{\text{H}}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

$$E_n = -\frac{E_1}{n^2} \quad E_1 \approx 13.6 \text{ eV} \quad a_0 = 0.529 \text{ Å}$$

Labelling of States

$n \geq 1$

$0 \leq l < n$ Rule: $n_{\min} = l + l_{\min}$

$-l \leq m \leq l$

conclusions:

* For each E_n there exist multiple values of l

↳ likewise a given l can exist, if measured, as part of an infinite number of energy levels

Multiple Eigenfunctions per Energy value

• Each l corresponds to $(2l+1)$ m values

• Angular component of Eigenfunctions determined by $Y_l^m(\theta, \phi)$

• $R_{nl}(r)$ is radial component

Periodic Potentials

• Periodic Potential inspired by a Crystal Lattice

↳ periodicity of Potential $V(x)$ defines electronic & optical properties of crystalline solid

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(\vec{r})$$

↳ where $V(\vec{r} + \vec{R}) = V(\vec{r})$

Translational Operator

$$\hat{T}_a \Psi = \Psi(x+a)$$

Eigenfunction

$$\hat{T}_a H(x) = \lambda H(x)$$

$$H(x) = e^{ikx} f(x)$$

Bloch's Theorem

$$H(\vec{R} + \vec{r}) = e^{i k \cdot \vec{R}} H(\vec{r})$$

↳ eigenfunction form

Direct & Reciprocal Lattice

• a 1D Bravais Lattice is a collection of vectors $\vec{R} = n \vec{a}$

• any point on x-axis

$$x' = x + n \vec{a}$$

• \vec{G} (Reciprocal Vectors)

$$\text{satisfy } e^{i G_n a} = 1 \rightarrow G = \frac{2\pi}{a}$$

• any point in reciprocal space

$$k' = k + \frac{2\pi}{a} \text{ where } (-\frac{\pi}{a} \leq k \leq \frac{\pi}{a})$$

Central Equation

$$\frac{\hbar^2}{2m} k^2 C_k + \sum_G V_G C_{k-G} = E C_k$$

• Recall Central Equation

Pretend

$$V(x) = 2V_0 \cos\left(\frac{2\pi}{a} x\right)$$

$$= V_0 e^{i \frac{2\pi}{a} x} + V_0 e^{-i \frac{2\pi}{a} x}$$

larger atoms

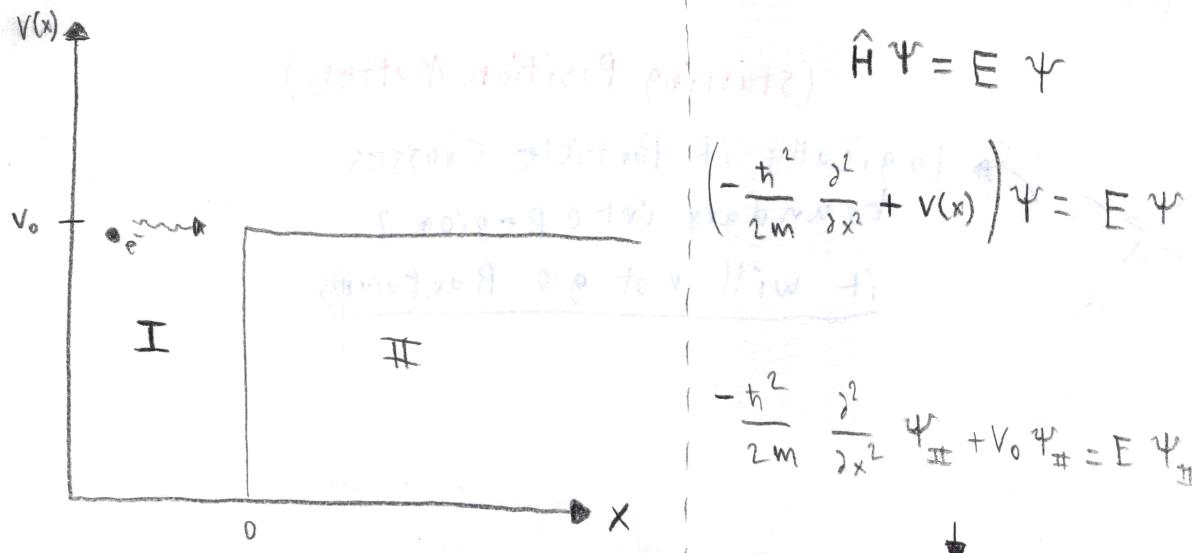


Smaller Potential



smaller Bandgap

3.024 Step - Potential Problem



Boundary Conditions

$$\textcircled{1} \quad \Psi_I(x=0) = \Psi_{II}(x=0)$$

$$\textcircled{2} \quad \frac{\partial \Psi_{II}}{\partial x}(x=0) = \frac{\partial \Psi_I}{\partial x}(x=0)$$

For Region 2

$$\frac{\partial^2 \Psi_{II}}{\partial x^2} + \rho^2 \Psi_{II} = 0$$

$$\text{, where } \rho = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

For Region I

$$\frac{\partial^2 \Psi_I}{\partial x^2} + k^2 \Psi_I = 0$$

$$\text{, where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Finding General solutions

Region 1: $A e^{ikx} + B e^{-ikx}$

(starting Position Matters)

Region 2: $D e^{ipx} + C e^{-ipx}$ ↗ logically if particle crosses boundary into Region 2 it will not go Backwards

Boundary condition 1:

$$A e^{ik(0)} + B e^{-ik(0)} = D e^{ik(0)} \rightarrow A + B = D$$

$$A = \frac{(\rho+1)D}{2}$$

$$B = \left(1 - \frac{(\rho+1)}{2}\right)D$$

Boundary condition 2:

$$iKA e^{ik(0)} - iKB e^{-ik(0)} = i\rho D e^{ik(0)}$$

$$A - B = \frac{\rho}{k} D$$

$$KA - KB = \rho D$$

Waves in Periodic Potential

- Periodicity of the potential defines the electronic & optical properties of crystalline solids

↳ Periodic Potential very important

$$\text{Hamiltonian: } \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad \text{where} \quad V(r+r) = V(r)$$

$$\text{Discrete Translational Operator: } \hat{T}_a \Psi(x) = \Psi(x+a)$$

$$\text{Eigenfunction: } H(x) = e^{ikx} f(x)$$

↳ $f(x)$ is function periodic in a (lattice period)

* \hat{T}_a commutes w/ Periodic \hat{H}

Bloch's Theorem

Eigenfunctions of one electron Hamiltonian obeys the following

$$* H(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} H(\vec{r})$$

Important Notes

[1] Eigenvalues depend only on K

[2] The only distinct eigenvalues are found in first BZ $K \in [-\frac{\pi}{a}, \frac{\pi}{a}]$

Direct & Reciprocal Lattice

• 1D Bravais Lattice = collection of vectors where $R = n\alpha$

↳ α is primitive vector

$$\rightarrow x' = x + n\alpha$$

• Suppose a set of vectors $\{G\}$ exist that satisfies $e^{iG \cdot R} = 1$

$$\text{so, } G = m \frac{2\pi}{a}$$

* So these characterize Reciprocal Vectors

↳ Larger the direct lattice spacing, smaller the inverse lattice spacing

$$b_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad b_2 = 2\pi \frac{(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_2 \cdot (\vec{a}_1 \times \vec{a}_3)} \quad b_3 = 2\pi \frac{(\vec{a}_1 \times \vec{a}_2)}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

3.024 Exam # 2

Properties of Crystal Momentum

- Since Function is periodic in a we can take a Fourier series of the potential

so if,

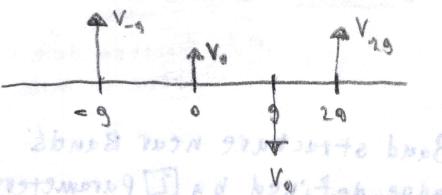
$$V(x) = \frac{V_0}{2} + \sum_{n=1}^{\infty} A_n \cos\left(\frac{2\pi n}{a} x\right) + B_n \sin\left(\frac{2\pi n}{a} x\right)$$

$$\text{so, } G = \frac{2\pi}{a} n = g \alpha$$

↓ complexity

$$V(x) = \sum_G V_G e^{iGx}$$

Graphical Representation of Fourier Co-efficients



Central Equation

New Form of Hamiltonian

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \sum_G V_G e^{iGx} \right) \Psi(x) = E \Psi(x)$$

• since we can't assume eigenfunction periodic with lattice period

$$\Psi(x) = \sum_K C_K e^{ikx}$$

Plugging into Hamiltonian

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \sum_G V_G e^{iGx} \right) \sum_K C_K e^{ikx} = E \sum_K C_K e^{ikx}$$

||

"central Equation"

$$\left(\frac{\hbar^2}{2m} k^2 - E \right) C_K + \sum_G V_G C_{K-G} = 0$$

* Solve this infinite systems of Equations

Find Energy Eigenvalues (E) and Eigenvectors \vec{C} of the form

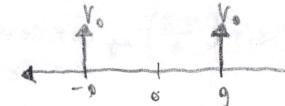
$$\Psi(x) = \sum_K C_K e^{ikx}$$

Cosine Potential & Central Matrix

Recall,

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$$

$$\bullet V(x) = 2V_0 \cos\left(\frac{2\pi}{a} x\right) \Rightarrow V_0 e^{i\frac{2\pi}{a} x} + V_0 e^{-i\frac{2\pi}{a} x}$$



Arrange System of Equations

$$\begin{pmatrix} \frac{\hbar^2}{2m}(k-2g)^2 & V & 0 & 0 & 0 \\ V & \frac{\hbar^2}{2m}(k-g)^2 & V & 0 & 0 \\ 0 & V & \frac{\hbar^2}{2m}k^2 & V & 0 \\ 0 & 0 & V & \frac{\hbar^2}{2m}(k+g)^2 & V \\ 0 & 0 & 0 & V & \frac{\hbar^2}{2m}(k+2g)^2 \end{pmatrix} \begin{pmatrix} C_{K-2g} \\ C_{K-g} \\ C_K \\ C_{K+g} \\ C_{K+2g} \end{pmatrix} = E_K \begin{pmatrix} C_{2K-g} \\ C_{K-g} \\ C_K \\ C_{K+g} \\ C_{2K+g} \end{pmatrix}$$

• since V are known, once k is specified you can set up system of equations

• NOTE: Matrix has been truncated

Discussion

[1] Eigenfunction has form

$$\Psi(x) = e^{ikx} \sum_G C_{K-G} e^{-iGx}$$

[2] 2 K values separated by reverse lattice vector G will yield identical solutions

* Implies Eigen vectors and Energy values periodic in G

[3] # of non-zero elements

determined by # of Fourier components that are needed to express the Potential Function

Band Gaps: Edges of BZ

• $K = \pm \frac{\pi}{a} = \pm \frac{g}{2}$ Assume Following Potential

$$V(x) = 2V_0 \cos(gx)$$

$$\begin{pmatrix} \frac{\hbar^2}{2m} k^2 - E & V \\ V & \frac{\hbar^2}{2m}(K+g)^2 - E \end{pmatrix} \begin{pmatrix} C_K \\ C_{K+g} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

* Only way homogenous system of equations has a non-zero soln is when $\det() = 0$

$$E_{\pm} = \frac{\hbar^2}{2m} \left(\frac{g}{2} \right)^2 \pm V$$

Notes :

ΔE between 2 Branches of Energy is the Bandgap

$$H_-(x) = 2 \cos\left(\frac{\pi x}{a}\right) \rightarrow \text{electrons concentrate at } x=0, a$$

$$H_+(x) = 2 \sin\left(\frac{\pi x}{a}\right) \rightarrow \text{concentrate at } x=\frac{a}{2}, \frac{3a}{2}$$

* Now Approximate Band shape at Brillouin edges as 2 Parabolas

1. Demonstrates allowed and forbidden Energies

2. Slope of Bands \rightarrow Group Velocity

3. Curvature of Band \rightarrow effective Mass

Conclusions

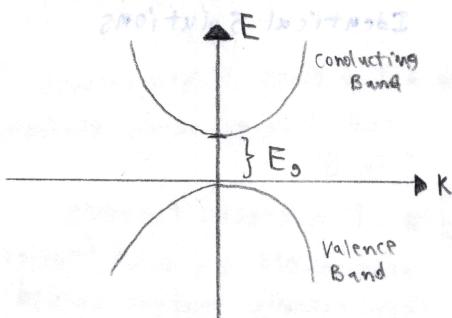
1. Larger Atoms = Smaller Bandgap

\hookrightarrow More Electron shielding

2. 0.08 - 5.4 eV

3. Wider the Gap \rightarrow Heavier the Electron

Information from Band Gap



1. Magnitude of Band Gaps

Larger Atoms \rightarrow smaller Potential \downarrow
smaller Bandgap

2. Group Velocity

$$\frac{(p_{n,k})}{m} = V_g = \frac{1}{\hbar} \frac{\partial E_n}{\partial k}$$

\hookrightarrow when group velocity is non-zero the eigenfunctions are translating with constant velocity

3. Effective mass

* take Taylor series expansion near where $K=0$

$$\text{Effective Mass} \quad m^* = \frac{1}{\hbar^2} \frac{\partial^2 E_{v,c}}{\partial k^2}$$

Charge carriers can have larger or smaller effective masses than actual electron mass depending on curvature of band

$$E_v(k) = -\frac{\hbar^2 k^2}{2m^*}$$

$$E_c(k) = E_g + \frac{\hbar^2 k^2}{2m^*}$$

\hookrightarrow where m^* = Electron effective mass
 m^* = Electron Hole effective mass

Band structure near Bands edge defined by 2 Parameters

1. Band Gap (E_g)

2. effective masses of holes & electrons

* However exact shape of curve needs to be calculated by solving Hamiltonian Eigenvalue Eqn.

Deriving Exact shape of Band edge

Recall

$$\frac{\hbar^2 k^2 - E}{2m} - V = 0 \quad \text{we shifted} \quad k' = k + \frac{q}{2}$$

\Downarrow Solving Quadratic Formula

$$E_{\pm} = \frac{\hbar^2}{2m} \left(1 \pm \sqrt{1 + \frac{4V}{\hbar^2 k^2}} \right)$$

\hookrightarrow where $\lambda = \frac{\hbar^2}{2m} \left(\frac{q}{2} \right)^2$
(λ = kinetic energy of electron having wavefunction at BZ edge)

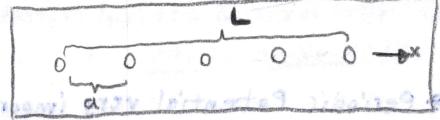
* We can now find effective mass of hole and electron

$$m_h^* = \frac{1}{m} = \frac{1}{m} \left(1 + \frac{2\lambda}{V} \right) \quad e^- \quad \text{* holes are heavier than electrons}$$

$$m_h^* = \frac{1}{m} = \frac{1}{m} \left(1 - \frac{2\lambda}{V} \right) \quad \text{holes}$$

Counting States of Periodic crystal

* Consider a 1D crystal



* Consider specific form of Bloch theorem

$$(H_k(x+L)) = H_k(x) \quad \Rightarrow e^{iKL} = 1$$

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

$$\# \text{ of states} = 2 \cdot \frac{2\pi/a}{2\pi/L} \rightarrow 2 \text{ comes from SPIN}$$

Spin

* Spin is a property of a particle that does not change can be represented by operator

$$\hat{S} = [\hat{S}_x, \hat{S}_y, \hat{S}_z]$$

* Properties of Spin operator similar to Angular Momentum

\hookrightarrow components don't commute

\hookrightarrow But Magnitude commutes w/ components

Eigensystems :

$$\hat{S}^2 |S_{ms}\rangle = \hbar^2 s(s+1) |S_{ms}\rangle$$

$$\hat{S}_z |S_{ms}\rangle = \hbar m_s |S_{ms}\rangle$$

* S is a characteristic value that can take values $0, \frac{1}{2}, 1, \dots$

* $m_s = -s, -s+1, \dots, s-1, s$

\hookrightarrow used to label states

Usefulness of spin in classifying system

1. Hydrogen Atom

$$|n, l, m_l, m_s\rangle (r, \theta, \phi)$$

2. Periodic Potential

* Two Particles Identical if their properties are the same and we can't experimentally distinguish them

Question: How do we construct multi-particle wave functions

Symmetrization

- Only certain wave vectors can be used to describe a physical system
- These vectors are either symmetric or anti-symmetric with respect to particle permutation
- Particles that result in symmetric wavefunctions are called **Bosons**
- Particles that result in anti-symmetric wavefunctions are called **Fermions**

Symmetry & Anti-Symmetry

Symmetry,

$$\text{Assume } \Psi_s(1,2) = \frac{1}{\sqrt{2}} (\varphi_{a1}(1)\varphi_{a2}(2) + \varphi_{a1}(2)\varphi_{a2}(1))$$

Swap 1 & 2 and you have same wavefunction

Anti-Symmetry

$$\Psi_a(1,2) = (\varphi_{a1}(1)\varphi_{a2}(2) - \varphi_{a1}(2)\varphi_{a2}(1))$$

Swap 1 & 2 and you have sign change

Notes:

- 2 Fermions cannot occupy same state
- How do electrons get distributed between bands?
- All crystalline Materials have Energy Bands & Band Gaps \rightarrow its the filling of bands that determines substance

Filling of Energy Bands

1. Density of States

How many states per energy can crystal provide?

2. Electron Distribution Function

How can we distribute electrons amongst available states

Free Electron Gas Density of States

- Metals can be approximated as a free space occupied by non-interacting electrons (a gas of sorts)

Gas of N free electrons in volume V

1. The system

N electrons in box where $L^3 = V$

2. Hamiltonian

$$\sum_i^N \frac{\hbar^2}{2m} \nabla_i^2$$

3. Eigenvalues & Eigenfunction

$$\hat{H}; H_k(x,y,z) = E_k H_k(x,y,z)$$

$$H_k(x,y,z) = h_k(\vec{r}) = \frac{1}{V^{1/2}} e^{ik\vec{r}}$$

$$E_k = \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m}$$

4. Born Von-Karman Boundaries

$$H_k(x+L, y, z) = H_k(x, y, z)$$

$$H_k(x, y+L, z) = H_k(x, y, z)$$

$$H_k(x, y, z+L) = H_k(x, y, z)$$

Application of Periodic Boundaries

$$e^{i k_x L} = e^{i k_y L} = e^{i k_z L} = 1$$

Quantizes \vec{k} vectors

$$K_{x,y,z} = \frac{2\pi n_{x,y,z}}{L}$$

$$E_k = \frac{\hbar^2 (2\pi)^2 (n_x^2 + n_y^2 + n_z^2)}{2m L^2}$$

Enumerating 2 states

$$1D: BZ \text{ length} = \frac{2\pi}{a}$$

$$k \text{ spacing} = \frac{2\pi}{L}$$

$$N = 2 \times \# \text{ of unit cells}$$

2D: (K_x - K_y) Plot

$$\# \text{ of Points} = \frac{\text{volume of k-space}}{V \text{ per point}}$$

$$N_{\text{sites}} = \frac{\Omega}{\left(\frac{2\pi}{L}\right)^2} = \left(\frac{L}{2\pi}\right)^2 \Omega$$

$$= DOS * Area$$

$$\Omega = \text{Volume}$$

Density of Levels

- A Density of State (DOS) Function tells us # of states that exist from $E \rightarrow E + dE$

First, ~~with better notes~~

call $E(\vec{r})$ = surface of constant energy in K-space

- Once we know surface shape we calculate **Volume** between E and $E + dE$

In the case of Free Electron

$$K = \sqrt{\frac{2mE}{\hbar^2}} \quad \begin{array}{l} \text{sphere of} \\ \text{radius } K \end{array}$$

- So we divide sphere of energy E by state volume $(2\pi/L)^3$

$$N = 2 \frac{4\pi K^3}{3} \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3} = \left(\frac{2mE}{\hbar^2}\right)^{3/2} \frac{V}{3\pi^2}$$

$$\text{Density of States} \quad \frac{dN}{dE} = \frac{m}{\hbar^2 \pi^2} \sqrt{\frac{2mE}{\hbar^2}}$$

- So if we introduce N electrons they will fill a sphere which separates filled states from unfilled Fermi Surface

Filling the States

• 2 Particles

1. Maxwell-Boltzmann Case (Distinguishable)

↳ 9 possible states

2. Bose-Einstein (Indistinguishable & Bosons)

↳ 6 Possible States

3. Fermi-Dirac Case (Indistinguishable & Fermions)

↳ 3 possible States

Tendency of Particles to bunch

$$E_{MB} = \frac{1}{2}, S = 1,$$

Notation + to discuss

- a_n = single electron Eigenstate
- E_s = single electron Eigenvalue
- n_s = occupation number
- S = eigenstate (also called Microstate) of entire electron gas region

E_s = energy of an Eigenstate for entire gas

	α_1	α_2	α_3
$S=1$	e^-	e^-	
$S=2$	e^-		e^-
$S=3$		e^-	e^-

Gas Properties:

$$E_s = \sum n_s E_s, N = \sum n_s$$

Probability of finding system in state S:

$$P(S) = \frac{e^{-\frac{E_S}{k_B T}}}{\sum_{\text{All } S} e^{-\frac{E_S}{k_B T}}}$$

Partition Function & Fermi-Dirac

• Denominator also called Z

↳ Thermo Dynamic Properties can be calculated from Z

$$\left. \begin{array}{l} \text{Helmoltz} \\ \text{Free} \\ \text{Energy} \end{array} \right\} F = -k_B T \ln Z$$

$$\left. \begin{array}{l} \text{chemical} \\ \text{potential} \end{array} \right\} F(N+1) - F(N) = \frac{\partial F}{\partial N}$$

Fermi-Dirac Distribution

• Range of allowable electron: $n_s = 0, 1$

* Mean Number of Particles in a single electron state is

$$\bar{n}_S = \left(\text{sum of Probabilities of obtaining gas states } S \text{ where } a_S \text{ is occupied} \right)$$

$$\left. \begin{array}{l} \bar{n}_S = \frac{1}{e^{\frac{(E_S - H)}{k_B T}} + 1} \end{array} \right\}$$

* This Relationship for Fermions is called Fermi-Dirac Function

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

Two important points:

$$f(E) \xrightarrow{E \rightarrow \infty} 0$$

$$f(E) \leq 1$$

- At 0 K all energy states less than H will be occupied. Any more than won't be

* chemical potential μ is an important intrinsic property called also the Fermi Level

Definitions:

Fermi Surface - surface in k -space that separates occupied and unoccupied states

Fermi Momentum - $\vec{p}_F = \hbar k_F$

Fermi Velocity - $\frac{\vec{p}_F}{m}$

Putting it all together

in 3D Metals

$$N_{\text{electrons}} = \frac{8 \pi k_F^3}{3} \cdot \frac{V}{(2\pi)^3} \quad n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

↳ all these depend on a single parameter density of free electrons

- Fermi Velocity $\sim 0.01 c$
- De Broglie wavelength in angstrom scale
- Fermi Energy $E_F = \frac{\hbar^2 k_F^2}{2m}$

$$\frac{E}{N} = \frac{3}{5} E_F$$

≈ compare to $E = \frac{3}{2} k_B T$

Fermi Temperature $T_F = \frac{E_F}{k_B}$

Heat capacity:

$$c_V = \frac{\pi^2}{2} \frac{k_B T}{E_F} n k_B$$

Intro to Semiconductors

what makes a semiconductor

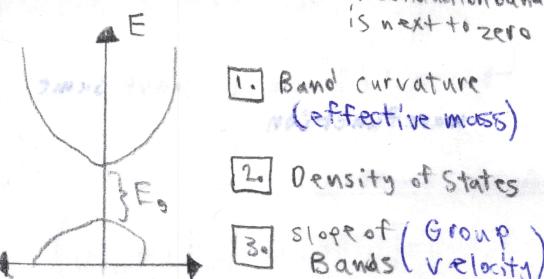
- Group 4 elements
 - Group 3 8 5 elements
 - Group 2 8 6 elements
- Classifications:
- Element vs. Compound
 - Direct vs. Indirect Bandgap
 - Intrinsic vs. Extrinsic

Review: Fermi Function & Band Structure

Fermi Function

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

When $E_c - H \gg k_B T$, $f(E) \approx 1$ if $E > E_c$ and $f(E) \approx 0$ if $E < E_c$. $| > 1$, number of electrons promoted to conduction band is next to zero



$$E_c = E_g + \frac{\hbar^2 k_c^2}{2m_c}$$

$$E_v = -\frac{\hbar^2 k_v^2}{2m_v}$$

Holes as charge carriers

- Holes are positively charged behaving voids where an electron is missing from

Distribution of holes:

$$1 - f(E)$$

Density of States in Semiconductors

$$\text{DOS for Conduction Band} \quad g_c(E) = \sqrt{2(E-E_c)} \frac{m_c^{3/2}}{\pi^2 h^3}$$

$$\text{DOS for Valence Band} \quad g_v(E) = \sqrt{2(E_v-E)} \frac{m_v^{3/2}}{\pi^2 h^3}$$

Density of carriers @ Equilibrium

$$n_c(T) = \int_{E_c}^{\infty} g_c(E) \frac{1}{e^{\frac{(E-H)}{k_B T}}} dE$$

$$p_v(T) = \int_{-\infty}^{E_v} g_v(E) (1 - f(E)) dE$$

Degenerate & non-degenerate semiconductors

- $E_c - E \gg k_B T$
- $H - E_v \gg k_B T$

Final Points on Intrinsic P-S-C

* When electron energy is far from Fermi Energy we can make this approximation for Fermi-Dirac

$$\frac{1}{e^{(E-E)/kT} + 1} \approx e^{-(E-E)/kT} \quad E > E_c$$

$$\frac{1}{e^{(H-E)/kT} + 1} \approx e^{-(H-E)/kT} \quad E < E_v$$

* We also get new expressions for

$$n_c(T) = N_c(T) e^{-(E_c - E)/kT}$$

$$P_v(T) = N_v(T) e^{-(H - E_v)/kT}$$

where

$$N_c(T) = \frac{1}{4} \left(\frac{2 m_e^* k T}{\pi \hbar^2} \right)^{3/2}$$

$$P_v(T) = \frac{1}{4} \left(\frac{2 m_v^* k T}{\pi \hbar^2} \right)^{3/2}$$

Law of Mass Action

* Not knowing Fermi Energy we still can say

$$n_c P_v = N_c P_v e^{(E_v - E_c)/kT} = N_c P_v e^{(-E_g/kT)}$$

* True for Both Intrinsic & Extrinsic
By adding a large # of other carriers you decrease the # of that carrier

Intrinsic vs. Extrinsic

Intrinsic:

- Pure crystal

↳ no doping with charged species

Properties:

$$n_c(T) = P_v(T) = n_i(T)$$

$$n_i(T) = \sqrt{N_c P_v} e^{-E_g/2kT}$$

$$n_c P_v = n_i^2 = N_c P_v e^{-E_g/kT}$$

$$H = E_v + \frac{1}{2} E_g + \frac{3}{4} kT \ln \left(\frac{m_v^*}{m_e^*} \right)$$

Engineering conductivity

• Electron Motion governed by Lorentz Force

$$\vec{F} = -e(\vec{E} + \frac{1}{c} \vec{v} \times \vec{B})$$

↳ \vec{E} is electric Field

↳ \vec{B} is magnetic Field

↳ \vec{v} is electron velocity

Recall: $\vec{F} = m \frac{d\vec{v}}{dt}$

$$\vec{F} = e \vec{E} \quad \vec{v}(t) = \frac{-eE t}{m}$$

Current Density

• # of charge carriers per unit Area per time

$$\vec{j} = n * v * \vec{v} = \frac{n e^2 t}{m} \vec{E} = \sigma \vec{E}$$

Now w/ Quantum

$$V_g = \frac{1}{m_e} \hbar \frac{dk}{dt} \quad V_g = \frac{e E T_e}{m_e^*}$$

$$\sigma = \frac{n e^2 T_e}{m_e^*}$$

* since conduction can occur through electrons or holes we need add a holes term

$$J_0 = n e \frac{n_c T_e}{m_e^*} + P_v e \frac{P_v T_e}{m_v^*}$$

$$n_e = \frac{n_c T_e}{m_e^*} \quad H_n$$

↳ H is mobility. Larger effective masses lead to lower mobilities

* as opposed to metals, semiconductors have greater conduction at high temp due to generation of additional charge carriers

Engineering conductivity through Doping

• Impurities that have electron energy levels close to conduction Band end up donating electrons to conduction band

↳ n-type

↳ increase conductivity

• Impurities w/ energy level close to Valence band extract electrons from Valence Band leading to holes

↳ p-type

↳ increase conductivity

• Impurities w/ Energy near Fermi level called Deep Traps

Semi-Conductor Carrier Engineering

• Adding very small amounts of impurities can make a big change in conductivity and define type

↳ called Extrinsic

Adding impurity to determine type:

• For Room temp Silicon

$$n_i^2 = N_e N_p e^{-E_g/kT} \Rightarrow 10^{10} \text{ cm}^{-3}$$

• By adding Phosphorus increases conductivity $\times 10^6$

$$so N_e = 10^{16} \text{ cm}^{-3} \quad N_h = 10^4 \text{ cm}^{-3}$$

↳ conductivity dominated by electrons

Electron + Hole Formulas for P-type semiconductors

N-Type

$$n_c \approx N_D$$

$$P_v \approx \frac{n_i^2}{N_D}$$

P-type

$$P_v \approx N_A$$

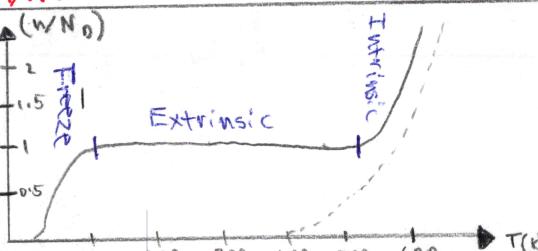
$$n_c \approx \frac{n_i^2}{N_A}$$

N_D = concentration of electrons from Donor

N_A = concentration of holes from Acceptor

Doped Semiconductors & Temperature

(W/N_D)



Calculating Fermi Level in Doped Semiconductor

• we can use condition of charge neutrality to find Fermi Level

↳ We need to balance

- 1. Donor impurity
- 2. Acceptor Impurities
- 3. Conduction Electrons
- 4. Valence Holes

$$P_V - n_c + N_D^+ - N_A^- = 0$$

↓

$$P_V e^{(E_V - E_F)/kT} - N_c e^{(E_F - E_c)/kT}$$

$$+ \frac{N_D}{1 + 2e^{(E_F - E_D)/kT}} + \frac{N_A}{1 + 2e^{(E_A - E_F)/kT}} = 0$$

• we can use this equation to find Fermi level (E_F)

n-type	8	p-type
--------	---	--------

$$n_c \approx N_D, P_V = \frac{n_i^2}{N_D}$$

↓

$$E_F = E_V + \frac{E_g}{2} + \frac{3}{4} kT \ln\left(\frac{m_c^*}{m_i^*}\right) + kT \ln\left(\frac{N_D}{n_i}\right)$$

$$E_F = E_V + \frac{E_g}{2} + \frac{3}{4} kT \ln\left(\frac{m_c^*}{m_i^*}\right) - kT \ln\left(\frac{N_A}{n_i}\right)$$

P-type & n-type: Summary

P-type & n-type

$P_V \approx N_A$ & $n_c \approx N_D$

$n_c \approx \frac{n_i^2}{N_A}$ & $P_V \approx \frac{n_i^2}{N_D}$

$H_p = H_i - kT \ln\left(\frac{N_A}{n_i}\right)$ & $H_n = H_i + kT \ln\left(\frac{N_D}{n_i}\right)$

$E_c, E_c, E_F, E_F, E_V, E_V$

E_F, E_F, E_V, E_V

E_F, E_F, E_V, E_V

E_F, E_F, E_V, E_V

E_F, E_F, E_V, E_V

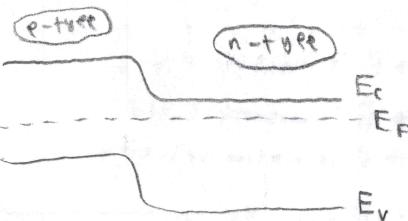
P-N Junction

• what happens when you join 2 n-type together?

* Carrier Flow driven by diffusion until Fermi Level Equilibrates

• Since E_F must be the same on Both sides Bands Bend

Result:



1. Electrons diffuse into p-type
2. Holes diffuse into n-type
3. Electric Field forms in Area of e-hole recombination

$$E = \frac{1}{a} \frac{d E_c}{d x}$$

↳ where $d E_c$ is change in energy of Conduction Band across Junction

* a steady state balance is achieved between diffusive flux & drift flux

• Loss of Charge Neutrality at Junction called V_{Bi}

Formulas governing P-N Junction

E-Field Strength $E = \int \frac{P(x)}{\epsilon_r \epsilon_0} dx$ $P(x)$ = space charge

$V_{Bi} = - \int E(x) dx$

Width of Depletion Region $W = \sqrt{\frac{2 \epsilon_r \epsilon_0 V_{Bi}}{q} \frac{N_A + N_D}{N_A N_D}}$

Width of Depleted n Region $X_n = \sqrt{\frac{2 \epsilon_r \epsilon_0 V_{Bi}}{q} \frac{N_A}{N_D (N_A + N_D)}}$

Width of Depleted p Region $X_p = \sqrt{\frac{2 \epsilon_r \epsilon_0 V_{Bi}}{q} \frac{N_D}{N_A (N_A + N_D)}}$

$$N_A X_p = N_D X_n$$

• Higher Doped Material will have a narrow depletion region and vice-versa

what is Built-in Voltage V_{Bi} :

• Simply the difference in Fermi levels before the 2 semiconductors joined

$$V_{Bi} = \frac{kT}{q} \ln\left(\frac{N_A N_D}{n_i^2}\right)$$

• Electrons that go from n → p or holes that go from p → n

↳ are called Minority Carriers

• αV_{Bi} becomes effective barrier to minority carrier mobility

$$P_n = P_p e^{-\alpha V_{Bi}/kT}$$

$$n_p = n_n e^{-\alpha V_{Bi}/kT}$$

Effect of Applied Voltage → Bias

• When we apply Positive Voltage to the p-side that's called Forward Bias

• When we apply Positive Voltage to the n-side that's called Reverse Bias

1. Lowers / Raises Potential Barrier to Diffusion

2. This is called a Minority Carrier Device

3. Forward Bias Decreases Depletion Region & Increases Diffusion Current Exponentially

4. Reverse Bias increases Depletion Region

$$J = J_s \left(e^{\frac{V_d}{kT}} - 1 \right)$$

External Quantum Efficiency

- Ratio of photons out to electrons in

$$EQE = \frac{\text{photons/s}}{\text{electrons/s}} = \frac{\phi}{I} \quad I = \text{current}$$

$\phi = \text{Flux}$

Note: However to find total Efficiency you need to integrate over all spectra

- Note: Device that makes good LED makes terrible solar cell & vice-versa

LED Electroluminescence Spectra

Spontaneous emission rate:

$$K_{sp}(w) = \frac{1}{\tau_r} g(w) f_e(\hbar w)$$

- Where $g(E)$ is a joint density of states & f_e is joint occupation probability

Finding Joint $g(B)$ & $f(E)$

Recall:

Parabolic Approximation

$$E_2 = \frac{\hbar^2 k^2}{2m_e} + E_g$$

$$E_1 = -\frac{\hbar^2 k^2}{2m_h}$$

Energy of Emitted Photon

$$E = \frac{\hbar^2 k^2}{2m_r} + E_g \quad m_r = \frac{m_e m_h}{m_e + m_h}$$

- B/c # of e-h pairs equals # of emitted photons in ideal case

$$\# \text{ of electrons} = \# \text{ of photons}$$

$$g_j(w) = \frac{(m_r)^{3/2}}{\pi^2 \hbar^2} \sqrt{2(\hbar w - E_g)}$$

- Emission condition expressed in terms of Fermi Distribution of electrons & holes

$$f_e(E) = f_c(E_2)(1 - f_v(E_1))$$

is there is there
electron a hole

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

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

Non-Equilibrium Fermi levels

- Quasi-Fermi levels emerge from carrier injection

Spontaneous Emission Rate

$$K_{sp}(w) = \frac{(\hbar w)^{3/2}}{\pi^2 \hbar^2 \tau_r} \frac{(E_{Fc} - E_{Fv} - E_g)/k_B T}{e^{-\hbar w - E_g/k_B T}}$$

or

Spontaneous Emission Rate

$$K_{sp} = D \sqrt{\hbar w - E_g} e^{-\hbar w - E_g/k_B T}$$

$$D = \frac{(\hbar m_r)^{3/2}}{2 \pi^2 \hbar^2 \tau_r} \frac{(E_{Fc} - E_{Fv} - E_g)/k_B T}{e^{-\hbar w - E_g/k_B T}}$$

- D increases exponentially in spacing between quasi-Fermi levels

- Photon Frequency is independent of injection amounts

Electro-luminescence Peak

- Found by taking derivative w/ respect to Photon Frequency of spontaneous Rate

Intro to wave optics

- Optical properties determined by electrons ability to interact w/ EM Field

↳ Most widely used metric is index of refraction

- when talking about optical properties we deal w/ light in infrared → UV spectra

- b/c these wavelengths are much larger than lattice constant, we treat EM Radiation as waves

Maxwell Equations

$$1. \vec{\nabla} \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0$$

$$2. \vec{\nabla} \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = 0$$

$$3. \vec{\nabla} \cdot \vec{B} = 0$$

$$4. \vec{\nabla} \cdot \vec{D} = \rho$$

- 2 Quantities used to describe EM Field

$$\vec{E} = (E_x, E_y, E_z)$$

$$\vec{H} = (H_x, H_y, H_z)$$

- 2 Quantities that describe effect of EM Field on Matter

$$\vec{D} = (D_x, D_y, D_z)$$

$$\vec{B} = (B_x, B_y, B_z)$$

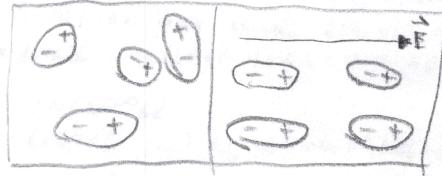
- We need additional relations to solve for unique solution

$$\vec{D} = \epsilon \vec{E} = \epsilon_0 \vec{E} + \vec{P}$$

$\vec{H} \rightarrow \text{permeability}$
 $\epsilon \rightarrow \text{electric permeability}$
 $\vec{B} = \mu \vec{H} = \mu_0 \vec{H} + \vec{M}$
 $\vec{P} = \text{electric polarization}$
 $\vec{M} = \text{magnetic polarization}$

Origins of Polarization

- ion electron dipoles always oscillating



- we describe distance bet ween ion & electron as d

$$\frac{d^2x}{dt^2} + \omega_0^2 x = 0 \quad \omega_0 \rightarrow \text{natural frequency}$$

Addition of External EM Field

- EM wave larger than lattice

↳ we approximate \vec{E} field as locally constant in space

$$\vec{E} = \vec{E}_0 e^{-i\omega t}$$

- Electrons would be pushed opposite of the direct ion of the applied field

$$\frac{d^2x}{dt^2} + \omega_0^2 x = \frac{\vec{F}}{m} \quad \vec{F} = \alpha \vec{E}_0 e^{-i\omega t}$$

- Polarization is the sum of all Dieole moments in a material

- Rewrite Equation of forced oscillator for polarization
- $$\frac{d^2 \vec{P}}{dt^2} + w_0^2 \vec{P} = \frac{N_a^2}{m \epsilon_0 w_0^2} \epsilon_0 w_0^2 \vec{E}$$

- Assume Dipoles at same frequency as \vec{E} field

$$\vec{P} = \vec{P}_0 e^{-i\omega t}$$

↓ solve for polarization using ERF

$$\vec{P} = \frac{w_0^2 \epsilon_0 X_0}{w_0^2 - \omega^2} \vec{E} \quad X_0 = \frac{N_a^2}{m \epsilon_0 w_0^2}$$

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = \epsilon_0 (1 + \chi) \vec{E} = \epsilon \vec{E}$$

$$X = X_0 \frac{w_0^2}{w_0^2 - \omega^2} \quad \vec{D} = \epsilon \vec{E} \quad \epsilon = \epsilon_0 (1 + \chi)$$

Absorbtion Materials

- When frequency approaches w_0 , $\chi(\omega)$ approaches ∞
- ↳ This doesn't make sense

- Their must be a damping force \Rightarrow ABSORBTION

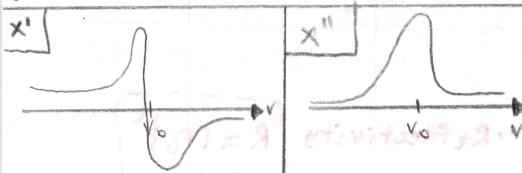
$$1. \frac{d^2 \vec{P}}{dt^2} + \sigma \frac{d \vec{P}}{dt} + w_0^2 \vec{P} = w_0^2 \epsilon_0 X_0 \vec{E}$$

$$2. \vec{P} = \frac{w_0^2 \epsilon_0 X_0}{w_0^2 - \omega^2 - i\sigma \omega} \vec{E}$$

$$3. \text{(Real Part)} X'(\omega) = X_0 \frac{w_0^2 (w_0^2 - \omega^2)}{(w_0^2 - \omega^2)^2 + (\sigma \omega)^2}$$

$$\text{(Imaginary Part)} X''(\omega) = X_0 \frac{i \omega^2 \sigma \omega}{(w_0^2 - \omega^2)^2 + (\sigma \omega)^2}$$

Graphical Analysis & Relations



Kramers-Kronig Relations between Real & Complex Parts

$$X'(w) = \frac{2}{\pi \tau_0} \int_0^\infty \frac{s X''(s)}{s^2 - w^2} ds$$

$$X''(w) = \frac{2}{\pi \tau_0} \int_0^\infty \frac{w X'(s)}{s^2 - w^2} ds$$

Dielectric Constant:

$$\epsilon = \epsilon_0 (1 + \chi) = \epsilon_0 (1 + \chi') + i \epsilon_0 \chi''$$

Refractive Index: (absent of magnetization)

$$n' = \sqrt{\frac{\epsilon}{\epsilon_0}} = \sqrt{1 + \chi' + \chi''} = n + ia$$

↳ n = index of refraction

↳ a = absorption coefficient

Effect of Material Structure on optic constants

- Crystal response to EM field will depend on Direction

- The Dielectric & Magnetic tensors are 2nd order Diagonal Matrices

$$\epsilon = \begin{bmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{bmatrix}, \quad H = \begin{bmatrix} H_1 & 0 & 0 \\ 0 & H_2 & 0 \\ 0 & 0 & H_3 \end{bmatrix}$$

$$\text{Cubic } \quad \epsilon_1 = \epsilon_2 = \epsilon_3$$

$$\text{Tetragonal } \quad \epsilon_1 \neq \epsilon_2 = \epsilon_3$$

Comments:

- ϵ & H not field dependent called **non-linear**

- we assume materials are isotropic

Wave Equations

$$\nabla^2 \vec{E} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

$$\nabla^2 \vec{H} - \frac{1}{c^2} \frac{\partial^2 \vec{H}}{\partial t^2} = 0$$

↳ we assume plane wave solutions

For EM Waves:

$$\omega = c |\vec{k}|$$

$$k = \frac{2\pi}{\lambda} = \frac{n}{c_0} \omega$$

Phase Velocity

- Plane wave $\vec{E}(x, y, z) = \vec{E}_0 e^{i\vec{k}\vec{r}-i\omega t}$ is a complex function with a phase $\phi = \vec{k} \cdot \vec{r} - \omega t$

- Surfaces of constant Phase (Fronts) move with velocity

$$V_{\text{phase}} = c \hat{k} \quad \begin{array}{l} \text{Phase Velocity,} \\ \text{usually lower inside} \\ \text{Materials} \end{array}$$

wave Packet & group velocity

- Monochromatic (single ω) waves don't exist

↳ we instead consider wave packets

$$E(r, t) = \int_0^\infty a_w(\vec{r}) e^{i k_r r - i \omega t} d\omega$$

↳ A superposition of mono chromatic waves

↳ a_w are Fourier coefficients of wave packet

- If refractive index **doesn't** depend on Frequency

$$V_{\text{phase}} = \frac{c_0}{n}$$

- if refractive index **does** depend on Frequency \rightarrow Dispersive

Energy Law of EM Fields

- EM theory says light intensity is Energy Flux of the Field

$$\text{Poynting Vector} \quad \vec{S} = \vec{E} \times \vec{H}$$

$$\vec{S} \parallel \vec{k}$$

Reflection & Refraction

- Boundary Conditions: continuity conditions for fields obeying

$$1. \hat{n} \cdot (\vec{B}_2 - \vec{B}_1) = 0$$

- component of Magnetic Induction Normal to the interface is continuous across interface

$$2. \hat{n} \cdot (\vec{D}_2 - \vec{D}_1) = 0$$

- The Normal component of electric Displacement changes by an amount equal to surface charge density

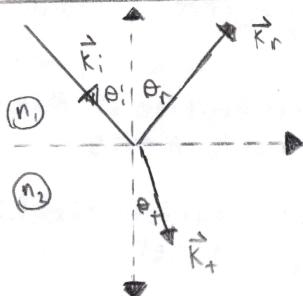
$$3. \hat{n} \times (\vec{E}_2 - \vec{E}_1) = 0$$

- component of electric field Parallel to interface in continu

$$4. \vec{n} \times (\vec{H}_2 - \vec{H}_1) = \vec{R}$$

In the presence of a surface current at the interface the magnetic induction will change equal to that amount.

Visualization



- Charge-Free, current-free incident wave from the top

$\vec{E}_i e^{i(\vec{k}_i \cdot \vec{r} - \omega t)}$	Incident wave
$\vec{E}_r e^{i(\vec{k}_r \cdot \vec{r} - \omega t)}$	Reflected wave
$\vec{E}_t e^{i(\vec{k}_t \cdot \vec{r} - \omega t)}$	Transmitted wave

Dispersion Relation:

$$|\vec{k}_i| = |\vec{k}_r| = \frac{\omega n_1}{c_0}$$

$$|\vec{k}_t| = \frac{\omega n_2}{c_0}$$

Implications of continuity

- Due to phase continuity phases of all 3 waves must be equal at interface ($x=0$)

$$(\vec{k}_i \cdot \vec{r}) = (\vec{k}_r \cdot \vec{r}) = (\vec{k}_t \cdot \vec{r})$$

$$(k_{iy} y + k_{iz} z) = k_{ry} y + k_{rz} z = k_{ty} y + k_{tz} z$$

2 consequences

- All three k 's lie in plane of incidence. Therefore we can say $\vec{E} = \vec{E}_0 e^{i(k_x x + k_z z - \omega t)}$

- Tangential wave vector components are equal no matter the medium

* Angle of Reflection is equal to angle of incidence

$$\text{Snell's Law: } n_1 \sin(\theta_i) = n_2 \sin(\theta_r)$$

Total Internal Reflection: Waveguides

$$\text{Recall } \sin(\theta_r) = \frac{n_1}{n_2} \sin(\theta_i)$$

- In the case of $n_1 > n_2$ there exists an incident angle that makes $\theta_r = 90^\circ$

means light can't escape through the interface

- effect is called total internal reflection where

$$\sin(\theta_c) = \frac{n_2}{n_1}$$

- called a cladding/core system where n_1 is much higher

Finding Maximum θ

- we find max angle at which we can still "couple" EM waves into the waveguide so we can take advantage of Total Internal Reflection

$$\begin{aligned} \sin(\theta_c) &= \frac{n_2}{n_1} \\ 1 \cdot \sin(\theta_{\max}) &= n_1 \sin\left(\frac{\pi}{2} - \theta_c\right) \end{aligned} \quad \left. \begin{array}{l} \text{use to} \\ \text{solve} \\ \text{for } \theta_{\max} \end{array} \right\}$$

$$\sin(\theta_{\max}) = n_1 \cos(\theta_c) = n_1 \sqrt{1 - \left(\frac{n_2}{n_1}\right)^2}$$

$$\text{Numerical} \quad 1 \cdot \sin(\theta_{\max}) = \sqrt{n_1^2 - n_2^2}$$

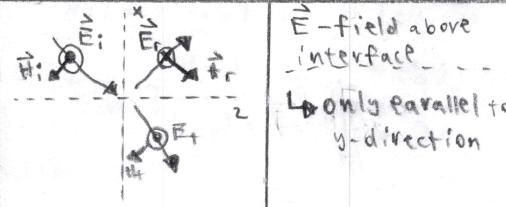
S-P polarization: transmission & reflection

$$\vec{E} = \begin{cases} (\vec{E}_i e^{i(\vec{k}_i \cdot \vec{r} - \omega t)} + \vec{E}_r e^{i(\vec{k}_r \cdot \vec{r} - \omega t)}) e^{-i\omega t}, & x < 0 \\ \vec{E}_t e^{i(\vec{k}_t \cdot \vec{r} - \omega t)}, & x > 0 \end{cases}$$

- Every wave can be represented by a superposition of 2 polarizations

- (P) \rightarrow in the plane of incidence
(S) \rightarrow perpendicular to plane of incidence

(S) Polarization



Boundary condition:

$$E_{iy} + E_{ry} = E_{ty}$$

Also

$$\vec{\nabla} \times \vec{E} + i\omega \mu \vec{H} = 0$$

$$\vec{\nabla} \times \vec{E} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ 0 & E_y & 0 \end{vmatrix}$$

- Since $\vec{E} \perp \vec{n}$, AND $\vec{E} \perp \text{Plane}$
 \vec{H} will lie in Plane

- In absence of currents

$$H_{iz} + H_{rz} = H_{tz}$$

$$H_{iz} = i k_{ix} \left(\frac{1}{i w \mu_0} \right) E_i e^{i(k_{ix} x + k_{iz} z)}$$

2 Equations

$$E_{iy} + E_{ry} = E_{ty}$$

$$n_1 \cos(\theta_i) E_{iy} - n_1 \cos(\theta_i) E_{ry} = \frac{n_1 \cos(\theta_i)}{n_2 \cos(\theta_r)} E_{ty}$$

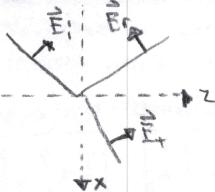
Reflection Coefficient

$$r_s = \left(\frac{E_{ry}}{E_{iy}} \right) = \frac{n_1 \cos(\theta_i) - n_2 \cos(\theta_r)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_r)}$$

$$r_s = \frac{2 n_1 \cos(\theta_i)}{n_1 \cos(\theta_i) + n_2 \cos(\theta_r)}$$

$$\text{Reflectivity } [R = |r_s|^2]$$

P-Polarization



E field in x & y directions

Boundary Conservations:

$$1. E_i E_{iz} + E_r E_{rz} = E_t E_{tz}$$

$$2. E_{ix} + E_{rx} = E_{tx}$$

||

$$n_1 E_i + n_2 E_r = n_2 E_t$$

$$\cos \theta_i (E_i - E_r) = \cos \theta_t E_t$$

Reflectance/Transmittance Co-eff

$$r_p: \frac{n_2 \cos(\theta_i) - n_1 \cos(\theta_t)}{n_2 \cos(\theta_i) + n_1 \cos(\theta_t)}$$

$$t_p: \frac{2 n_1 \cos(\theta_i)}{n_2 \cos(\theta_i) + n_1 \cos(\theta_t)}$$

Note For P-polarization
There exists an angle
known as Brewster angle
where reflection is 0

$$\sin^2(\theta_{\text{Brewster}}) = \frac{n_2^2}{n_1^2 + n_2^2}$$

Minimization of Reflection

Some applications require
maximum transmission into
a material

Laser Coatings

1. Anti-Reflective coating

$$n_{\text{coating}} = \sqrt{n_0 n_3}$$

2. Quarter Wave Approach

$$d = \frac{\lambda_0}{4 n_k}$$

Transfer Matrix Approach

A general treatment of
Multi-layered Optical Materials

$$n(x) = \begin{cases} n_1, x < 0 \\ n_2, 0 < x < d \\ n_3, d > x \end{cases}$$

↓x

As before, z-component of
wavevector ($k_z = \beta$) does not
change

↳ simple dependence on z
evolution

$$\vec{E} = \vec{E}(x) e^{i(wt - \beta z)}$$

* However x & y direction
are more complicated

Goal: Find a way to relate
Electric & Magnetic Field
Amplitudes in any layer
to one another

we break up into S & P
polarization

consideration of S-polarization

$$E(x) = \begin{cases} E_1 e^{ik_x x} + E_1' e^{-ik_x x}, x < 0 \\ E_2 e^{ik_x x} + E_2' e^{-ik_x x}, 0 < x < d \\ E_3 e^{ik_x(x-d)} + E_3' e^{-ik_x(x-d)}, x > d \end{cases}$$

Maxwell's Eqns
• E_1, E_2, E_3 are amplitudes of
forward propagating E-fields

• E_1', E_2', E_3' are amplitudes
of reverse reflected components

• Relating amplitudes in
layer 1 → 3 requires

- 2 interfaces

- 1 homogenous layer

• propagation through medium
of index n_2 and thickness d
captured by:

$$\text{Propagation Matrix } P_2 = \begin{pmatrix} e^{ik_x d} & 0 \\ 0 & e^{-ik_x d} \end{pmatrix}$$

Deriving Interface Matrices

Take Equations

$$1. E_{iy} + E_{1y} = E_{2y} + E_{1'y}$$

$$2. n_1 \cos \theta_i - n_2 \cos(\theta_2) E_{1y}' = n_2 \cos(\theta_2) E_2 - n_2 \cos \theta_2 E_{1'y}'$$

↓
Put into Matrix Form

$$\begin{pmatrix} 1 & 1 \\ n_1 \cos \theta_i - n_2 \cos(\theta_2) & n_2 \cos(\theta_2) - n_2 \cos \theta_2 \end{pmatrix} \begin{pmatrix} E_{iy} \\ E_{1'y}' \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ n_2 \cos(\theta_2) - n_2 \cos \theta_2 & n_2 \cos \theta_2 \end{pmatrix} \begin{pmatrix} E_{2y} \\ E_{1'y}' \end{pmatrix}$$

$$D_1 = \begin{pmatrix} 1 & 1 \\ n_1 \cos \theta_i - n_2 \cos(\theta_2) & n_2 \cos(\theta_2) - n_2 \cos \theta_2 \end{pmatrix}$$

$$D_{12} = D_2^{-1} D_1$$

So in order to find connection
between E-Field Amplitude in
layer 1 & layer 3 we need:

$$(P_{23} P_2 D_{12}) \begin{pmatrix} E_1 \\ E_1' \end{pmatrix} = \begin{pmatrix} E_3 \\ E_3' \end{pmatrix}$$

Periodic Medium

We saw before, Periodicity led to
Electronic Bandgaps. Now we consider
material periodic w/ respect to
light

$$a \left\{ \begin{array}{l} n_1, d_1 \\ n_2, d_2 \\ n_1, d_1 \\ n_2, d_2 \\ n_1, d_1 \\ n_2, d_2 \end{array} \right. \quad \begin{array}{l} x = (l-1)a \\ x = l a \end{array}$$

Index of Refraction:

$$n(x) = \begin{cases} n_2, (l-1)a < x < (l+1)a + d_2 \\ n_1, \text{ otherwise} \end{cases}$$

$$n(x+a) = n(x)$$

$$d_1 + d_2 = a$$

$$\text{General Solution Form } \left\{ \begin{array}{l} E = E(x) e^{i(wt - \beta z)} \\ E = E(x) e^{i(wt - \beta z)} \end{array} \right.$$

$$\text{Recall: } D_{ik} = D_k^{-1} D_i$$

$$= \begin{pmatrix} n_k \cos(\theta_k) + n_i \cos(\theta_i) & n_k \cos(\theta_k) - n_i \cos(\theta_i) \\ 2 n_k \cos(\theta_k) & 2 n_k \cos(\theta_k) \\ n_k \cos(\theta_k) - n_i \cos(\theta_i) & n_k \cos(\theta_k) + n_i \cos(\theta_i) \\ 2 n_k \cos(\theta_k) & 2 n_k \cos(\theta_k) \end{pmatrix}$$

$$P_1 = \begin{bmatrix} e^{-ik_1 x d_1} & 0 \\ 0 & e^{ik_1 x d_1} \end{bmatrix}$$

$$P_2 = \begin{bmatrix} e^{-ik_2 x d_2} & 0 \\ 0 & e^{ik_2 x d_2} \end{bmatrix}$$

Putting it together:

$$\begin{pmatrix} E_{11}(x-1) \\ E_{12}(x-1) \end{pmatrix} = P_1 D_1 P_2 D_2 P_1 D_1 P_1 \begin{pmatrix} E_{11} \\ E_{12} \end{pmatrix}$$

Application of Bloch Theorem

- Periodically constrained system has solution of

$$\begin{pmatrix} E_{11}(x-1) \\ E_{12}(x-1) \end{pmatrix} = e^{-ik_x} \begin{pmatrix} E_{11} \\ E_{12} \end{pmatrix}$$

- Eigenvalue-Eigenvector Problem

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = D_1^{-1} D_2 P_2 D_2^{-1} D_1 P_1$$

- $M_{11}, M_{12}, M_{21}, M_{22}$ in handout

$k_{1x} = k_1 \cos(\theta_1)$	$k_{1x} = k_2 \cos(\theta_2)$	$ k_1 \sin(\theta_1)$
		$ k_2 \sin(\theta_2)$
		β

Photonic Band Structure

- Matrix Equation becomes Eigenvalue Problem

$$e^{-ik_x} = \frac{1}{2} (M_{11} + M_{22}) + \sqrt{\frac{1}{4} (M_{11} + M_{22})^2 + M_{12} M_{21}}$$

* Reflection from a Dielectric mirror

- Consider N Periods are assembled into a stack arrangement

$$\begin{pmatrix} E_0 \\ E'_0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}^N \begin{pmatrix} E_N \\ E'_N \end{pmatrix}$$

$$\rightarrow R = |r_n|^2 = \frac{|M_{21}|^2}{|M_{21}|^2 + \left(\frac{\sin K_a}{\sin N K_a} \right)^2}$$

- This means we can achieve near perfect reflection with Large N

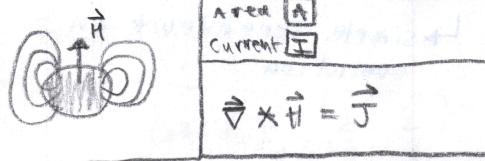
Origins of Magnetization

- We can describe a material as a collection of magnetic dipoles

Analogous Relationship:

$$\begin{aligned} \vec{P} &= N \vec{p} = \epsilon_0 \chi \vec{E} \\ \vec{D} &= \epsilon_0 \vec{E} + \vec{P} \end{aligned} \Rightarrow \begin{aligned} \vec{M} &= N \vec{m} = \mu_0 \chi m \vec{H} \\ \vec{B} &= \epsilon_0 \vec{H} + \vec{M} = \mu_0 (1+\chi) \vec{H} \end{aligned}$$

Hydrogen Atom



- We approximate a hydrogen atom w/ a current loop

$$8 \vec{H} = I \cdot \vec{A}$$

$$\bullet I = \frac{eV}{2\pi R} \Rightarrow \vec{H} = \frac{1}{2} eV R$$

- We relate to Angular Momentum

$$|\vec{H}| = \gamma |\vec{L}|, \gamma = \frac{e}{2me}$$

$$\text{Bohr Magneton} \quad \mu_B = \frac{e\hbar}{2me}$$

- The atom can be described by magnetic dipoles originating from both orbital & spin

Para Magnetism

- Approximate dipoles as independent & non interacting

- Magnetization (M) at room temp in absence of field is zero

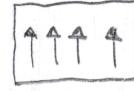
- When sufficiently large field is applied, magnetic dipoles orient in line w/ field

$$\rightarrow M = M_s \quad (\text{saturation point})$$

- However field strength needed for this to happen is way too high

Spontaneous orientation of Dipoles

- Magnetic Dipoles in Materials will interact to form arrangements Ferromagnetic Anti-Ferromagnetic Ferrimagnetic



origins :

- wavefunction for 2 Electron system

$$\Psi(1,2) = \underbrace{\psi(\vec{r}_1, \vec{r}_2)}_{\text{spatial}} \underbrace{\chi(1,2)}_{\text{spin}}$$

- Hamiltonian of 2-electron system

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{ex}}$$

$\hookrightarrow H_1, H_2$ are merely single electron Hamiltonians

$\hookrightarrow \hat{H}_{\text{ex}}$ is exchange interaction

$$\hat{H}_{\text{ex}} = -2J_{\text{ex}} \hat{S}_1 \cdot \hat{S}_2$$

Hamiltonian for system under Field

$$\hat{H} = \hat{H}_1 + \hat{H}_2 - J_{12} \hat{S}_1 \cdot \hat{S}_2 + \vec{B} \vec{n}_1 + \vec{B} \cdot \hat{H}_2$$

$$\hookrightarrow \text{where } \hat{H}_{1/2} = \frac{\mu_B}{\hbar} \hat{S}_{1/2}$$

Magnetic Hamiltonian:

$$-\sum_j J_{ij} \hat{S}_j \rightarrow \frac{\mu_B}{\hbar} \vec{B}_{\text{ext}}$$

$$\hat{H}_{\text{magnetic}} = \frac{\mu_B}{\hbar} \sum_i [\vec{B}_{\text{ext}} + \vec{B}_{\text{applied}}] \cdot \hat{S}_i$$

- This Mean Exchange Field is responsible for spontaneous ordering in absence of External

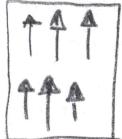
- At a certain temp T_c , thermal energy (kT) becomes greater than exchange Energy & becomes disordered

$T_c \rightarrow$ Ferromagnetic

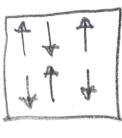
$T_H \rightarrow$ All others

Conclusions

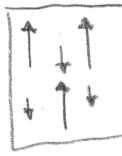
- Based on sign of Exchange Integral



- Jex > 0, Energy minimized when $\vec{M} \parallel \vec{H}$
- Large Magnetization $T < T_c$



- Jex < 0
- No M , but ordering at $T < T_n$



- Jex < 0
- Reduced Magnetization

* All Materials become paramagnetic above T_c or T_n

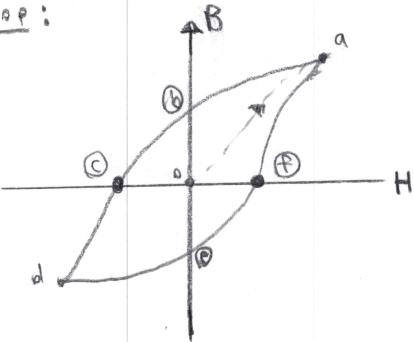
Hysteresis in Ferromagnetic Materials

- Now our focus turns to Ferromagnetic Material & Property

* Ferromagnetic Materials exhibit memory effects in their $M(H)$ dependence

Hysteresis Loop

Loop:



- If we apply sufficient magnetic field to produce complete saturation

↳ As Applied Field goes to zero "Remnant induction remains (b,e)"

- It will take the application of a coercive field (c,f) to completely de-Magnetize

* Materials that have large saturation magnetization



Have smaller coercive field

Magnetic Anisotropy

- Dependence of Magnetic Properties on Direction of Applied Field

↳ Depending on the orientation of the field more or less field strength is required to reach saturation magnetization

- Easy Axis → Direction along which the smallest field strength is needed for saturation

- Hard Axis → Direction along which the smallest field strength is needed for saturation

Examples + Formalization

- For BCC Fe $\langle 111 \rangle$ is hard axis & $\langle 100 \rangle$ is easy axis

- For FCC Ni the $\langle 111 \rangle$ is easy axis, $\langle 100 \rangle$ is hard axis

Energy of Magnetic Anisotropy:

$$E_a = K_{\text{an}} \sin^2 \theta$$

↳ K_{an} is Anisotropy constant

↳ θ is angle between magnetization & easy axis

For Cubic Materials (w/ 3 easy axes):

$$E_a = K_1 (a_1^2 a_2^2 + a_2^2 a_3^2 + a_3^2 a_1^2)$$

* Physical origin of anisotropy is interaction w/ mean exchange field & orbital angular momenta (spin-orbit coupling)

Deriving Hysteresis Loop

- Start w/ a single easy axis Ferro Magnet with a single Magnetic Domain

↳ assume angle θ between \vec{M} & easy axis



Anisotropy Energy

$$E_a \approx K_{\text{an}} \sin^2 \theta$$

- When External Field is applied we have

$$\text{Zeeman Energy} \quad E = HM_s \cos(\phi - \theta)$$

H = applied mag field
 M_s = saturated magnetization
 ϕ = angle between field & easy axis

Total Energy

$$K_{\text{an}} \sin^2(\theta) + HM_s \cos(\phi - \theta)$$

Hard axis Magnetization

$$\phi = \frac{\pi}{2} \quad E = K_{\text{an}} \sin^2(\theta) + HM_s \sin(\theta)$$

- Now let's find an angle θ that minimizes energy

$$\frac{dE}{d\theta} = 0 \Rightarrow \theta = \pm \frac{\pi}{2} + \pi n \left(\frac{M_s}{H} \right)$$

↳ conditions met when

$$H_a = \frac{2K_{\text{an}}}{M_s}$$

↳ H_a is anisotropy field where magnetization reaches saturation

In general (From 1st Order Energy Minimize)

$$(2K_{\text{an}} \sin \theta + HM_s) \cos \theta = 0$$

$$M = M_s \frac{H}{H_a}$$

* Hard Axis Magnetization changes linearly until saturation

Easy Axis Magnetization

$$\phi = 0 \quad E = K_{\text{an}} \sin^2 \theta + HM_s \cos \theta$$

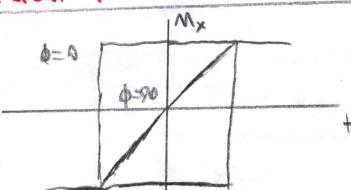
- Energy will be minimized for all H -field values

$$- \frac{2K_{\text{an}}}{M_s} < H < \frac{2K_{\text{an}}}{M_s}$$

$$H_c = \frac{2K_{\text{an}}}{M_s}$$

↳ All field values yield saturations

Ideal Hysteresis loop



$$H_c = 2K_{\text{an}} / M_s$$

Magnetic Domains

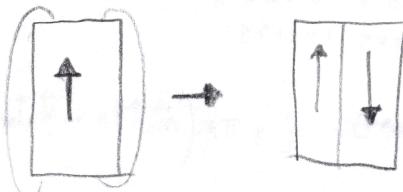
- If all ferromagnets consisted of magnetic dipoles magnetized to any one axis, any object would act as magnet.

↳ Not the case in real life

To minimize the Magnetostatic Energy

$$E_d = \vec{H}_d \cdot \vec{M}$$

- Material breaks into Domains
Note: Domains not defined by grain boundaries



Result: In absence of Applied Magnetic Field, Net Magnetization is zero

- Under influence of Applied Field
Domain walls change rather than there being magnetization rotation

Domain walls

- Boundaries between regions in which all spins are oriented in easy axis direction

↳ At Domain walls Dipoles must re-orient

Max Energy Exchange Penalty

$$E_{\max} = 2JS$$

* It's energetically cheaper to re-orient over multiple lattice spacings

- If we have N lattice spacings, angle between spins is

$$\theta = \frac{\pi}{N}$$

$$\text{Exchange} = JS^2 \frac{\pi^2}{N^2}$$

$$\text{Total Exchange} = JS^2 \frac{\pi^2}{N}$$

Exchange Energy / Penalty per Unit Area (For 180° Bloch Wall)

$$\sigma_{BW}^{ex} = JS^2 \frac{\pi^2}{a^2 N}$$

Wall Width

- It would seem as infinite layers $N \rightarrow \infty$ is energetically preferred
- ↳ This is not the case in Ferromagnets as Anisotropy Energy increases when dipoles not aligned

Domain Wall Width is Determined by a balance between exchange energy & Magnetic Anisotropy

$$E_a^{\text{Total}} = \frac{NK_u}{a}$$

$$\sigma_a^{\text{Total}} = \frac{NK_u a}{2}$$

Energy Density per Unit Area of Bloch Wall:

$$\sigma_{BW} = JS^2 \frac{\pi^2}{a^2 N} + \frac{NK_u a}{2}$$

Wall width

$$S = Na = \pi S \sqrt{\frac{2J}{K_u a}}$$

- Larger Exchange integral, wider walls
- Higher anisotropy, lower walls

giant magnetoresistance

giant magnetoresistance

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