

Physics of Semiconductor devices

Books

semiconductor physics and devices by D.A. Neaman

physics of semiconductor devices by S.M. Sze and K.K. Ng

inverter can be used to create all logical operations / gates

increase voltage → amplifier eg: op Amp

decrease voltage → rectifier

let the threshold current for 'on' state be 10mA.

even then, 9mA will be considered 'on' because there isn't sufficient difference and hence difficult to sense by hardware

$$V = IR \xrightarrow{\text{input output constant}} \text{consequence of the Ohm's Law}$$

$$\text{Ohm's Law} \rightarrow \bar{J} = \sigma \bar{E}$$

which leads to $V = IR$

Resistance is different for different metals because of mobility

Current : no. of electrons flowing per unit density area per length

$$\sigma \propto \frac{1}{R}$$

$$\sigma = \frac{\text{no. of electrons}}{\tau} \frac{q}{m_e} \mu_e$$

mobility
charge

generally, a system with high σ = metalSystems with lower σ = semiconductors

electrons are bound with the atom due to electrostatic forces

$$\bar{E} = -\frac{dV}{dx}$$

electric field goes from higher potential to lower potential

intel i7 processor has 7 bil transistors

processor has → contact pins

global interconnect } vias

local interconnect

(metals)

transistors

The vias enable us to access all billions of transistors using limited ~100 contact pins

imp question : Which material to be used

TRANSISTOR

Gate	metal
$\sim 2\text{nm}$	insulator
SiO ₂	semiconductor

silicon substrate

most probable

when electrons move between materials, they collide

these collision are inelastic

no conservation of energy/momentum

most probable

energy here is heat energy

This is the reason filament

bulbs glow

 x : real dimension K : momentum dimension

Passing marks:

25%

no N-1 policy

Assignment

2 × Assignment

4 × Quiz

Mid Sem

End Sem

15%

20%

30%

30%

Relative Grading

95% + 5% attendance

Deadline 15/02

8/04

Deadline 15/02

18/04

calculator allowed for quizzes

Attendance

>60% before & after mid sem

5%

>60% before only

2.5%

after only

2.5%

<60% 0%

0%

• LECTURE: 2

point contact transistor

↳ had germanium instead of silicon

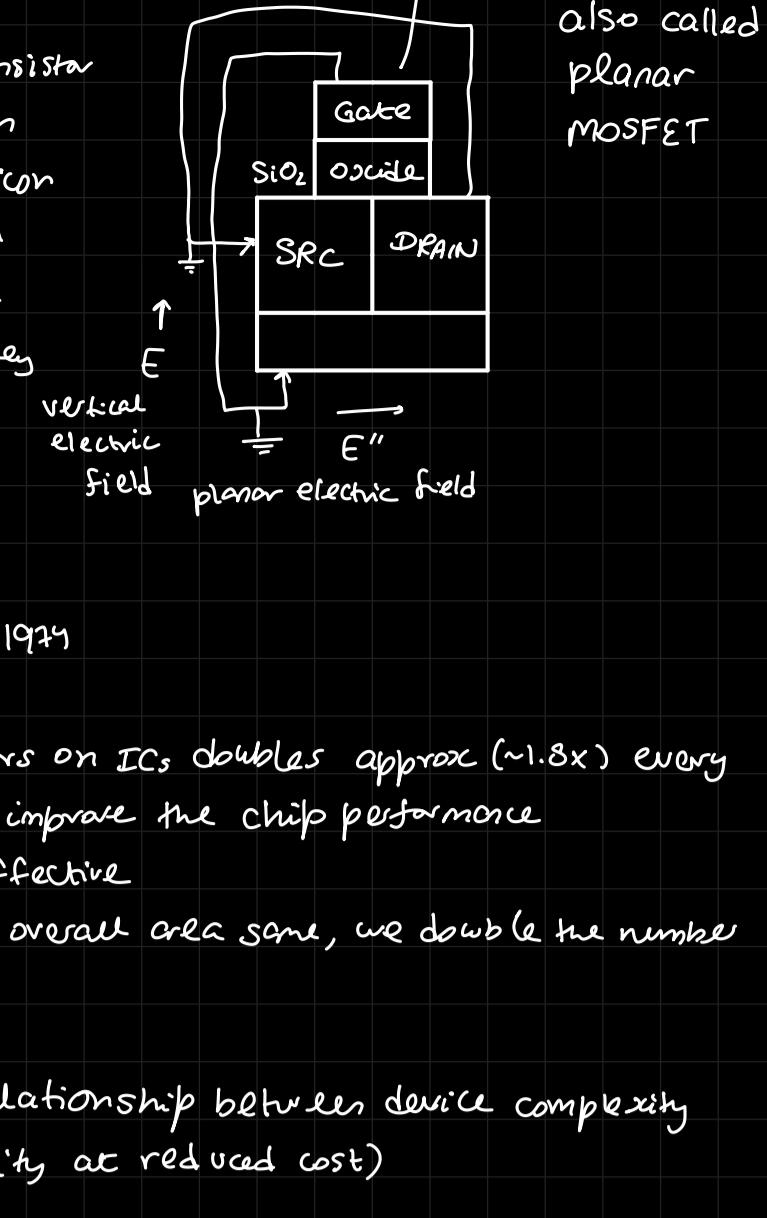
↳ Walter Brattain

↳ John Bardeen

↳ William Shockley

↳ Bell Labs

↳ 1947



* Moore's Law : 1971

num of transistors on ICs doubles approx (~1.8x) every two years to improve the chip performance

↳ also cost effective

↳ Keeping the overall area same, we double the number of transistors

Log-linear relationship between device complexity (higher clk-density at reduced cost)

Our regular computers deal with bits whereas quantum computers are based on q-bits

* Semiconductor wafer

↳ thin slice of semiconductor used for fabrication of ICs, solar cells etc.

↳ Semiconductor: crystalline silicon/germanium...

SiO_2 , glass/sand ↳ regular arrangement of atoms
↳ Silicon dioxide ↳ not amorphous

↳ covalent bonding ↳ irregularities present
↳ e⁻ are loosely bound in the outermost shell

↳ not ionic bonding where e⁻ are tightly packed

Poly-Crystalline also used for gate

↳ In between amorphous and crystalline

Transistors have PN junction

↳ has flow of holes and electrons

* CAPACITOR: two copper plates which have dielectric between them where electric field flows

if E is very high \rightarrow MV/cm

if E exceeds further than a set threshold

dielectric breakdown

↳ no longer acts as a capacitor

* CLASSICAL VS QUANTUM MECHANICS

↓ describe behaviour of macroscopic objects ↓ describe behaviour of systems of atomic level ↓ behaviour of physical objects when subjected to forces/displacement

observable by eyes ↓ changes with time

speed/position: dynamic variables/parameters of a system of a certain mass

↳ deterministic behaviour works in classical mechanics

↳ probabilistic/statistical behaviour works in quantum mechanics

for atomic level we use instruments to measure parameters and hence there will be some limit to precision

* Wave Particle DUALITY

wave-like behavior ↳ particle-like behavior

e.g. photoelectric effect ↳ e.g. Davisson-Germer experiment

State function of...

classical mech : $f(x, t)$

quantum mech : $\psi(x, t)$

can be represented as $Ae^{i\phi}$

$$p = mv \quad \text{planck constant}$$

$$\text{momentum of a photon: } p = \frac{h}{\lambda}$$

$$\text{wavelength of a particle: } \lambda = \frac{h}{p}$$

de Broglie wavelength

when can an object that appears as particle behave as wave?

↳ when the dimension(r) over which the change of potential energy V(r) of a particle becomes

smaller as compared to its wavelength, its wave nature reveals.

e.g.: $\lambda_{\text{baseball}} = 10^{-34} \text{ m} \rightarrow$ very small wavelength

→ cannot be visualized

→ doesn't behave as wave

$\lambda_{\text{electron}} = 10^{-10} \text{ m} \rightarrow$ ~ \AA atomic level

→ can be visualized

→ behaves as wave

* HEISENBERG'S UNCERTAINTY PRINCIPLE

conjugate variable : possible to move from one domain to another using Fourier Transform

$$\Delta p \Delta x \geq \hbar$$

$$\Delta E \Delta t \geq \hbar$$

if we want to precisely measure one var, the other in the conjugate pair cannot be precisely measured

Energy of a quantum system cannot be zero because of the uncertainty principle

The lowest Energy we can attain is Zero-Point Energy

$$E = KE + PE$$

if PE = 0,

KE cannot be zero

due to the uncertainty principle

$$KE \text{ should be atleast } \left(\frac{\hbar}{\Delta x} \right)^2$$

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

A continuous distribution of wavelengths can produce a localized wave packet.

• QUASI-PARTICLE

↳ In photoelectric effect

↳ not an actual particle

↳ e⁻: valence shell

• WAVE FUNCTION

$$\{\psi: \text{Psi}\}$$

describes the quantum state of an isolated system of one or more particles. There exists only one wave function

containing all info for an entire system.

Lecture 3

* **Wave Function** $\psi(x)$ = varies with time
(Born interpretation) or $\psi(r, t)$

for 1 particle system: $\psi = \psi(x, y, z, t)$

for 2 particle system: $\psi = \psi(x_1, y_1, z_1, x_2, y_2, z_2, t)$

wave function contains all info about the system

wave function \longleftrightarrow classical trajectory
(quantum mechanics) \longleftrightarrow (newtonian mechanics)

Probability density

$$\hookrightarrow P(r) = |\psi|^2 = \int \psi^* \psi \, d\tau \quad \text{--- (1)}$$

① COPENHAGEN/BORN'S INTERPRETATION

The probability that a particle can be found at a point x at time t is given by (1)

→ Psi can be represented as a linear combination of other Psis

② To every physical property, there corresponds a linear, Hermitian operator in quantum mechanics

	SYMBOL	OPERATOR
Position	x	\hat{x}
	y	\hat{y}
Momentum	p_x	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$
	p_z	$\hat{p} = -i\hbar \left(\frac{\partial}{\partial x} + \frac{j}{\partial y} + \frac{k}{\partial z} \right)$
KE	T_x	$\hat{T}_x = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
	T	$\hat{T} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) = -\frac{\hbar^2}{2m} \nabla^2$
P_E	$V(x)$ $V(x, y, z)$	$\hat{V}(x)$ $\hat{V}(x, y, z) \times V(x, y, z)$
Total energy	E $= E_k + P_E$	$\hat{H} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z) = -\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z)$

NOTE: Hermitian matrix:

$$\text{if } A = A^T$$

$$\hat{A}\psi = a\psi \quad \text{--- (2)}$$

In any measurement of the observable associated with operator \hat{A} , the only values that will be observed are the eigenvalues 'a' which satisfy: (2)

$$\hat{A}f(x) = kf(x)$$

$f(x)$: eigenfunction of A
with eigenvalue k

the eigenvalue gives the real observable

e.g.: e^{ikx} is an eigenfunction of the operator $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

if I operate \hat{p}_x on ψ , i.e. $(-i\hbar \frac{\partial}{\partial x})\psi$

and we get: # ψ

↳ some number

then # is eigenvalue

here $\psi = e^{ikx}$

$$-i\hbar \frac{\partial}{\partial x} e^{ikx} = -i\hbar k e^{ikx} = ik e^{ikx}$$

$$k = \text{wave number} : k = \frac{2\pi}{\lambda}$$

$$\lambda = \text{wave length}$$

$$P = \frac{h}{\lambda} = \frac{h}{2\pi k} = \frac{\hbar \cdot k}{\lambda} \quad \begin{matrix} \text{reduced plank constant} \\ \text{wave number} \end{matrix}$$

$$\hbar = \frac{h}{2\pi}$$

$$P = \hbar \cdot k$$

hence, momentum space is also called K-space and we can swap between the two using a real number k

$$\Psi = e^{ikx} \quad \text{time independent wave func}$$

$$\psi = e^{ikx - \omega t} \quad \text{time dependent wave func}$$

④ For a system in a state described by a normalized wave function ψ , the avg or expectation value of the observable corresponding to A is given by

$$\langle A \rangle = \int \psi A \psi^* dz$$

⑤ SCHRÖDINGER EQUATION

$$\text{if } \frac{\partial \psi}{\partial t} = \hat{H} \psi \quad \text{time dependent}$$

$$E = \hat{H}\psi$$

time independent

$$\hat{H} = \hat{T} + \hat{V} + V_{ext}$$

external potential energy

$$T_E = KE = p_E$$

$$\text{total energy}$$

$$V_{ext}$$

$$V$$

$$V + T$$

$$V_{ext}</math$$

• Lecture : 4

16/01/25

$$\hat{H} = \hat{T} + \hat{V}$$

↓
hamiltonian operator
associated the overall
energy of the system

$$\hat{H}\Psi = \hat{T}\Psi + \hat{V}\Psi = E\Psi$$

↓ ↓

$$\text{1d motion} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} \right) + V(x)\Psi = E\Psi$$

↓

Note: if there is Coulomb potential

btw the particle, the

$$\text{potential energy} \rightarrow V(x) \propto \frac{1}{x}$$

NOTE 3: Potential energy

~ stored energy

~ energy due to position

gravitational potential = mgh

NOTE 4: Elastic PE: $U = \frac{1}{2}kx^2$

k: spring constant : N/m

x: how much the spring

been stretched : m

① free particle: $V(x) = 0$ & x } $V(x)$ depends on
② harmonic oscillation: $V(x) = \frac{1}{2}kx^2$ } the physical state
of the particle

NOTE 2: Kinetic energy is

defined for individual
objects and anything
that moves has KE.

Any object at rest has

$$KE = 0$$

$$\text{Generally: } KE = \frac{1}{2}mv^2$$

NOTE 5: wave particle

duality principle:

momentum of photon →

$$\text{momentum } p = \frac{h}{\lambda} \begin{matrix} \text{plank's constant} \\ \text{de broglie's wavelength} \end{matrix}$$

→ When can an object that appears as particle behave as wave?

↳ when the dimension(r) over which the change of potential energy V(r) of a particle becomes smaller as compared to its wavelength, its wave nature reveals.

• Heisenberg's Uncertainty Principle

$$\Delta p \Delta x \geq \hbar$$

$$\# \text{ note: } \hbar = \frac{h}{2\pi}$$

both momentum and position cannot be precisely determined at the same time

$$\Delta E \Delta t \geq \hbar$$

energy of the particle

↳ the time instant the particle had

another form of

that Energy

the uncertainty principle

Using this version, Energy cannot be zero
minimum Energy \equiv ZPE \rightarrow Zero Point Energy $\neq 0$

• Wave Function Ψ

describes the quantum state of an isolated system of one or more particles.

There exists only one wave function containing info for an entire system

$$\Psi(x) / \Psi(r, t)$$

$$\text{Probability Density: } P(r) = |\Psi|^2 = \int \Psi^* \Psi d\tau$$

↓

probability that a particle can be found at a point x in time t

• POSTULATES OF QUANTUM MECHANICS

① The state of a quantum mechanical system is completely specified by a wave function $\Psi(\mathbf{r}, t)$ that depends on the particle's position \mathbf{r} and time t

$$\Psi(x_1, y_1, z_1, \dots, x_i, y_i, z_i, t)$$

$$P(\mathbf{r}) = |\Psi|^2 = \int \Psi^* \Psi d\mathbf{r}$$

the probability that the particle can be found at point \mathbf{r} at time t

$$\Rightarrow P(\mathbf{r}) \geq 0$$

$$\Rightarrow \int_{\text{all space}} \Psi^* \Psi d\mathbf{r} = 1$$

② To every physical property observable in classical mechanics, there corresponds a linear, hermitian operator in quantum mechanics

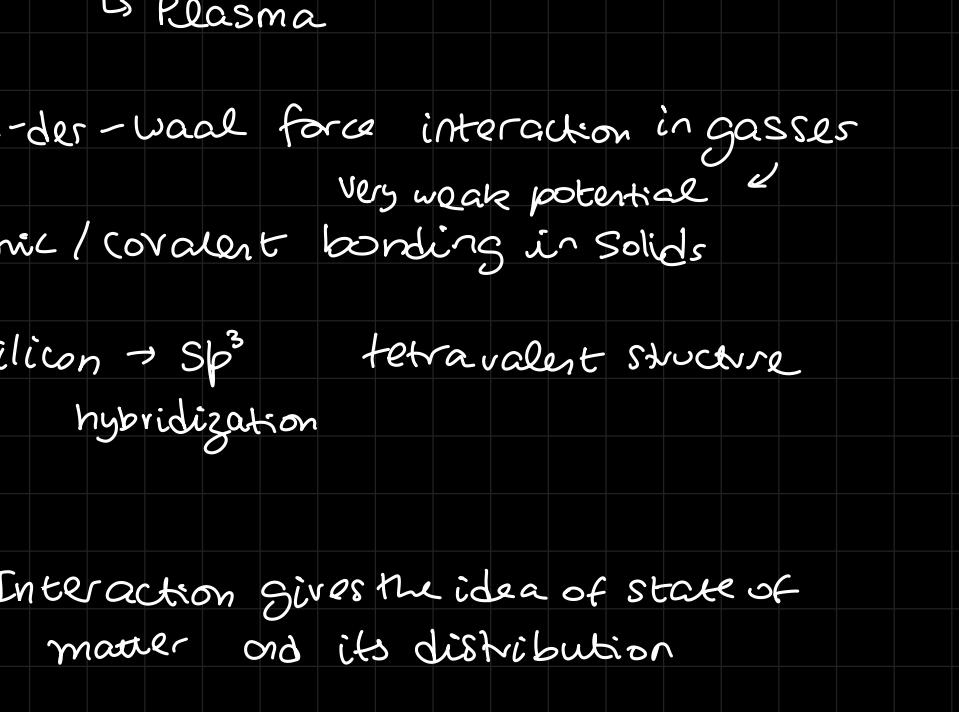
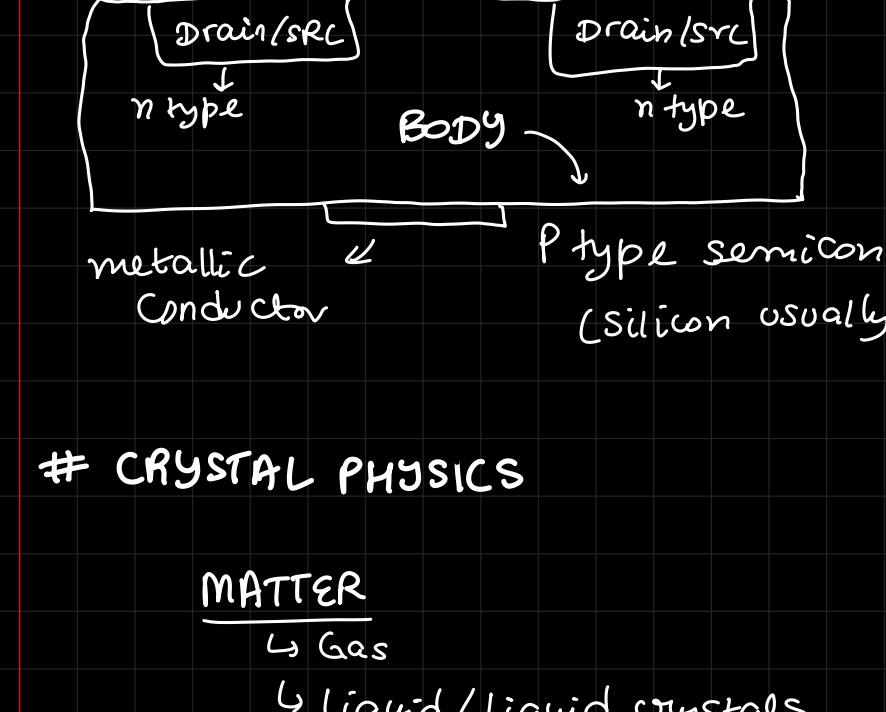
<u>OBSERVABLE</u>		<u>OPERATOR</u>	
Position	x	\hat{x}	multiply by x
	\mathbf{r}	$\hat{\mathbf{r}}$	multiply by \mathbf{r}
Momentum	p_x	\hat{p}_x	$-i\hbar \frac{\partial}{\partial x}$
	\mathbf{p}	$\hat{\mathbf{p}}$	$-i\hbar \left(i \frac{\partial}{\partial x} + j \frac{\partial}{\partial y} + k \frac{\partial}{\partial z} \right)$
Kinetic Energy	T_x	\hat{T}_x	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
	T	\hat{T}	$-\frac{\hbar^2}{2m} \underbrace{\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)}_{\nabla^2}$
Potential Energy	$V(x)$	$\hat{V}(\hat{x})$	multiply by $V(x)$
	$V(x, y, z)$	$\hat{V}(\hat{x}, \hat{y}, \hat{z})$	multiply by $V(x, y, z)$
Total Energy	E	\hat{H}	$-\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z)$
Angular Momentum	L_x	\hat{L}_x	$-i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$
	L_y	\hat{L}_y	$-i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$
	L_z	\hat{L}_z	$-i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$

③

Lecture: PSD 7

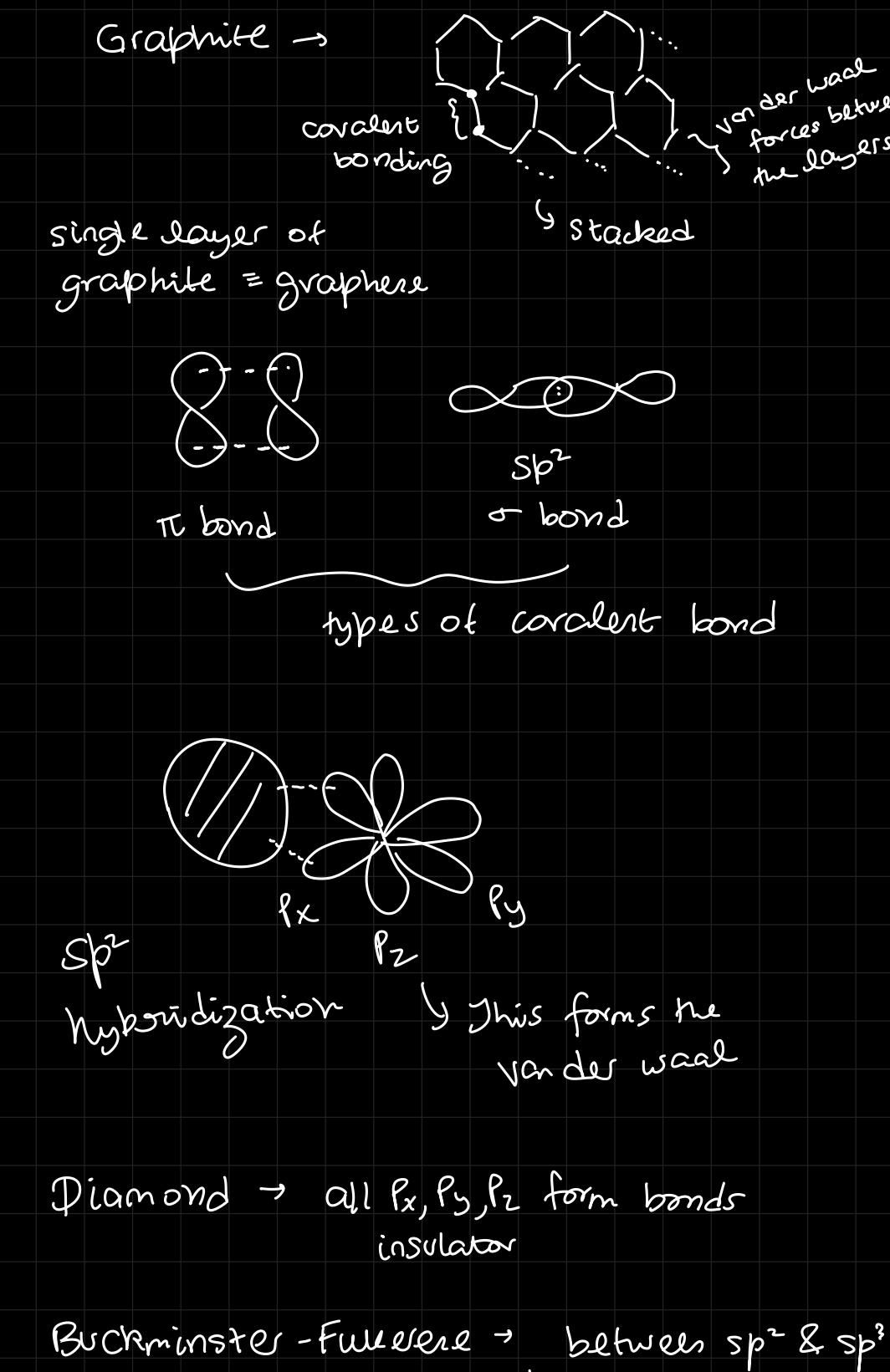
→ CRYSTAL STRUCTURE OF SOLIDS

PN junction acts as a diode when we provide a bias to the terminals using a "connection" / electrodes



MOS Transistor

↓
metal oxide semiconductor



CRYSTAL PHYSICS

MATTER

↳ Gas

↳ Liquid / Liquid crystals

↳ Solid

↳ Plasma

Van-der-Waal force interaction in gasses
Very weak potential ↲

Tonic / covalent bonding in solids

Silicon → sp^3 tetrahedral structure
hybridization

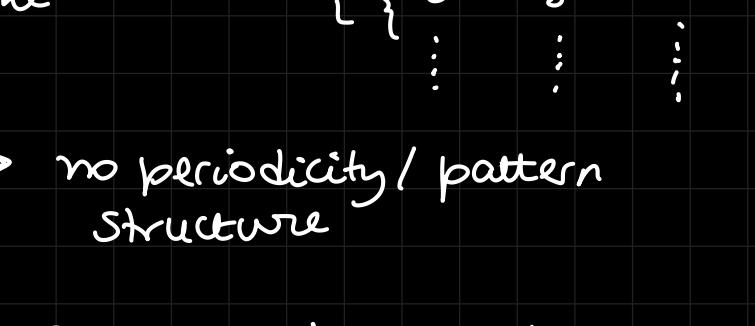
Interaction gives the idea of state of matter and its distribution

CARBON

sp^2 ↳ Graphite → metal
 sp^3 ↳ Diamond → insulator
↳ Buckminster-Fullerene → semiconductor

Some element but displays different properties because of different crystal structure

Graphite →



single layer of graphite = graphene

π bond σ bond

types of covalent bond

Diamond → all $\text{p}_x, \text{p}_y, \text{p}_z$ form bonds insulator

Buckminster-Fullerene → between sp^2 & sp^3 has hexagonal and pentagonal structure

Super conductor

↳ conducts electricity without any resistance

= zero resistance conduction

↳ electrical resistivity

↳ $T[\text{kelvin}]$

↳ is it possible that $2e^-$ form a pair ?

(usually) No, due to Coulomb force, like charged particles have this repulsive force

BUT at 0-50K temperature, the attractive force of e^- is massive as compared to repulsive forces and hence $2e^-$ form a Cooper pair

Vanadium Dioxide VO_2

Insulator ↳ Monoclinic VO_2 as we increase the temperature

metal Rutile VO_2 (cubic structure) ⇒ resistivity decreases

JUST changing the temperature, changes the nature and structure of the crystal

In insulators don't have as many free e^- as conductors

Conductors don't have band gap

↳ distance between conduction band and valence band

Mean Free Path : The distance an electron travels between two successive collisions dependent on temperature

include <stdio.h>

int main (int argc, char ** argv) {

 fork();

 printf ("Chemistry sux");

 return 0;

}

This code will print the stnt twice why?

because $\text{fork}()$ creates a parallel child process on another thread

SOLID MATERIALS

↳ CRYSTALLINE (single crystal) some particles kept at periodic distances

↳ POLYCRYSTALLINE ↳ periodic structure

↳ AMORPHOUS ↳ periodic structure

↳ single crystal ↳ from any point, it behaves the same

↳ POLYCRYSTALLINE ↳ contains differently oriented crystals called grains / domain

↳ AMORPHOUS ↳ usually 10nm - 100μm in diameter

↳ separated with each other by grain / domain boundaries

⇒ Polycrystals with grains that are < 10nm in diameter are called nanopoly-crystalline.

if we dope polycrystalline structure, it behaves as metal (conductor)

" " " amorphous structure, it behaves as oxide (insulator)

it behaves as metal (conductor)

Remember: for p type we have trivalent impurities for doping

wrt silicon eg: Boron

for n type, we have pentavalent impurities for doping wrt silicon.

eg: phosphorus

Does it change the structure?

↳ doping Silicon

→ GaN: gallium nitride

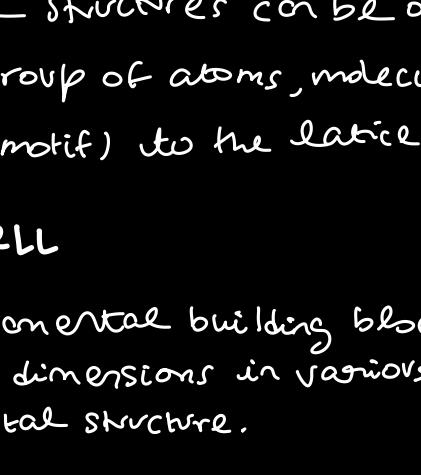
↳ only p type doping with magnesium

So, when we say doping, we define reference as well

Lecture: 8

→ CRYSTAL LATTICE

replacing each atom by a geometrical point because only their geometry is of use.



POLYCRYSTALLINE → finite array of points in space

Crystal structure = Crystal Lattice + Basis

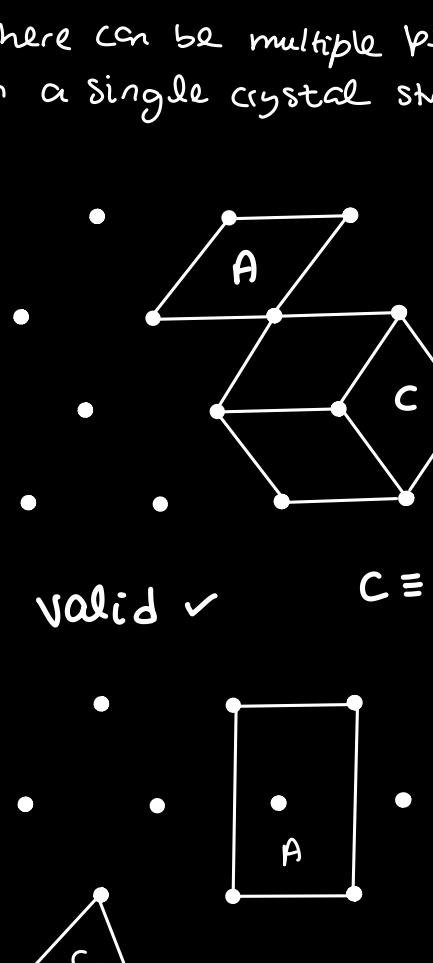
$$\begin{matrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{matrix} + \text{Atom} = \begin{matrix} \text{Atom} & \text{Atom} & \text{Atom} \\ \text{Atom} & \text{Atom} & \text{Atom} \end{matrix}$$

Crystal structures can be obtained by attaching atom, group of atoms, molecules which are called basis (motif) to the lattice sites of the lattice points.

UNIT CELL

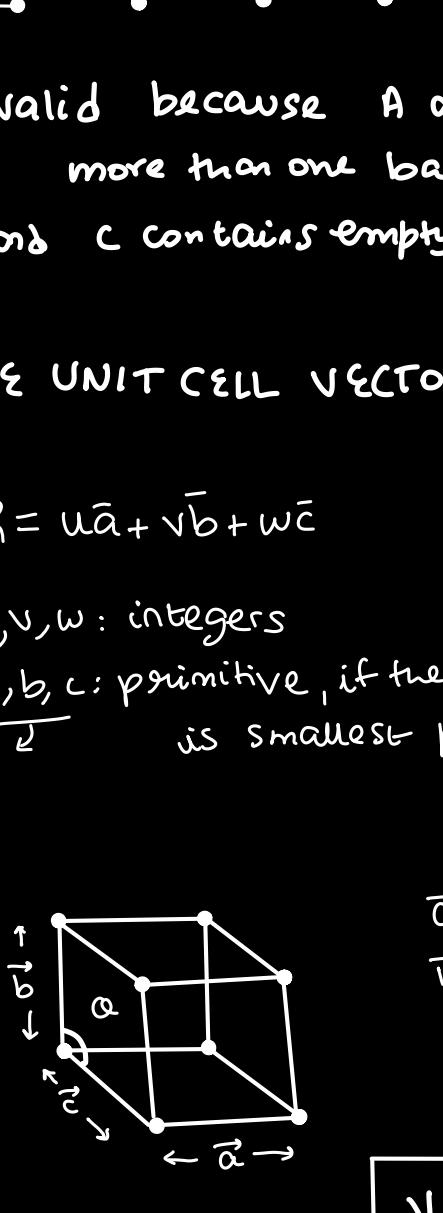
fundamental building block which repeats its own dimensions in various directions and gives crystal structure.

unit cell size should be constant throughout the crystal structure



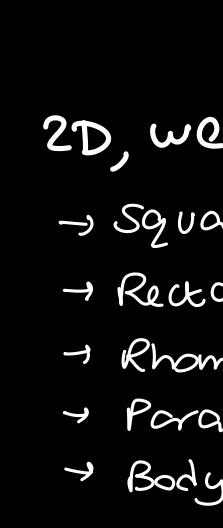
e.g.: 2-dimensional NaCl

e.g.:



→ empty space is not allowed
→ periodicity not maintained in context of translational and rotational symmetry.

e.g.:



is this fractal a valid crystal structure?

No, because even though we can find a repeating pattern, we cannot link up the unit cells.
i.e. there is no translational symmetry

No, because even though it maintains rotational symmetry but it does not maintain translational symmetry

QUASI CRYSTAL

aperiodic, yet exhibits orientational symmetry

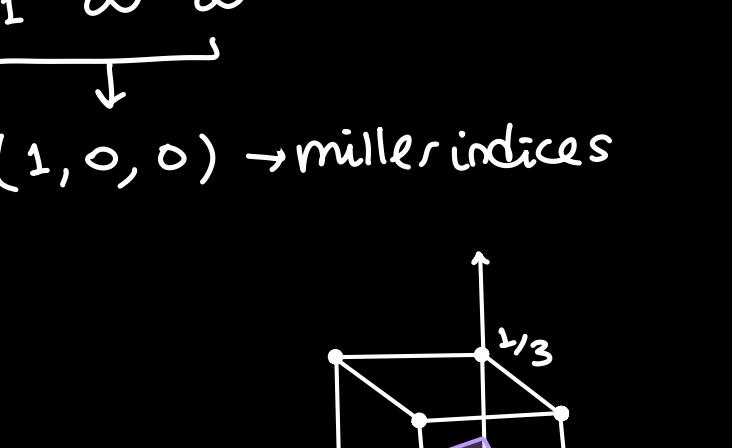
CONVENTIONAL/PRIMITIVE UNIT CELL

→ minimum volume unit cell.

→ always consists of only ONE basis.

→ There can be multiple primitive unit cells in a single crystal structure.

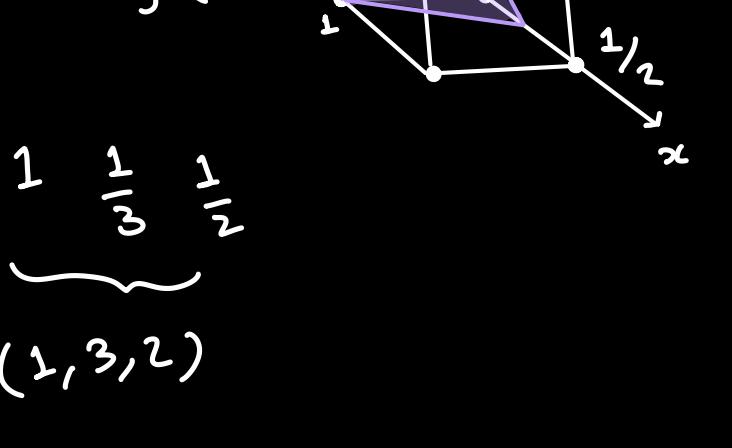
e.g.)



Valid ✓

C ≡ SUPERCELL / CONVENTIONAL CELL

e.g.:



invalid because A and B contain more than one basis

and C contains empty space

PRIMITIVE UNIT CELL VECTOR

$$\vec{R} = u\vec{a} + v\vec{b} + w\vec{c}$$

u, v, w: integers

$\vec{a}, \vec{b}, \vec{c}$: primitive, if the volume of cell is smallest possible

lattice constant

\vec{a} : along x axis
 \vec{b} : along y axis
 \vec{c} : along z axis

$$V_C = \vec{a} \cdot (\vec{b} \times \vec{c})$$

RULES

→ \vec{a} should be the shortest period of the lattice

→ \vec{b} to shortest period and non-parallel to \vec{a}

→ \vec{c} to shortest period and non-parallel to $(\vec{a} \times \vec{b})$

(= Periodicity implies translational symmetry)

e.g.)

Valid ✓

C ≡ SUPERCELL / CONVENTIONAL CELL

e.g.:

invalid because A and B contain more than one basis

and C contains empty space

BRAVAIS LATTICE

There are just 14 3d crystal lattices out of which 7 are main and other are subdivision of those main.

Seven main divisions:

Cubic, Tetragonal, Orthorhombic, Hexagonal, Trigonal, Monoclinic, Triclinic

Simple Cubic Body Centered Face Centered

In 1D, we have just one Bravais Lattice.

In 2D, we have 5 main divisions.

→ Square : $a=b$, $\theta=90^\circ$

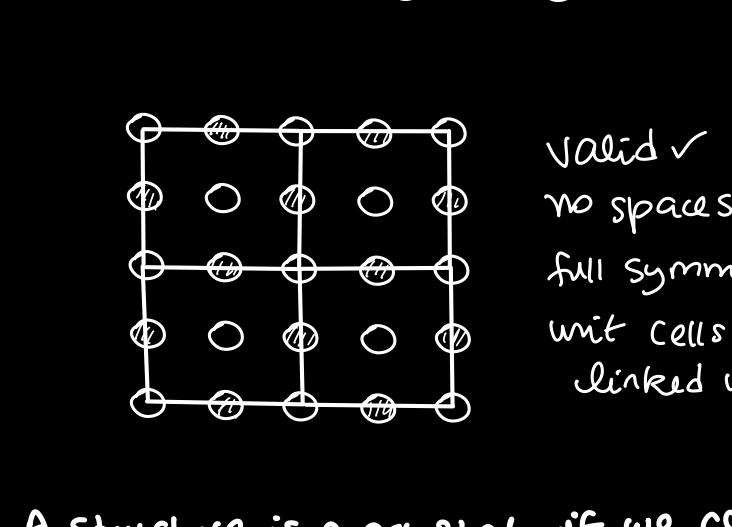
→ Rectangle : $a \neq b$, $\theta=90^\circ$

→ Rhombus : $a=b$, $\theta=60^\circ$

→ Parallelogram : $a \neq b$, $\theta=60^\circ$

→ Body centered cube

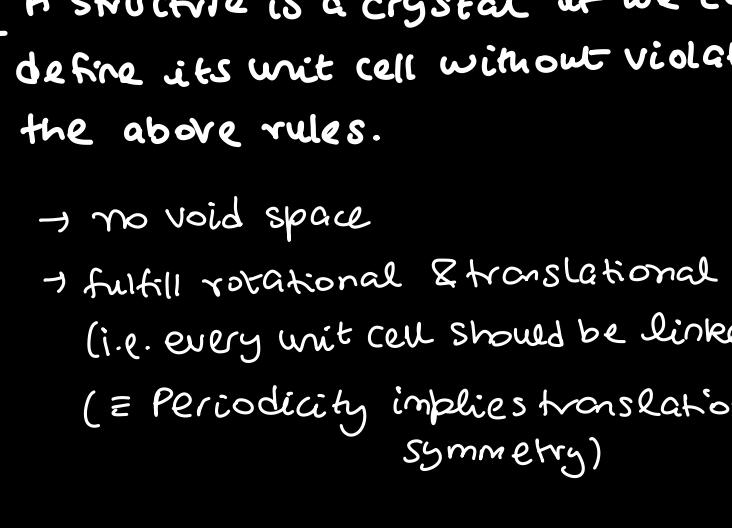
e.g.)



Valid ✓

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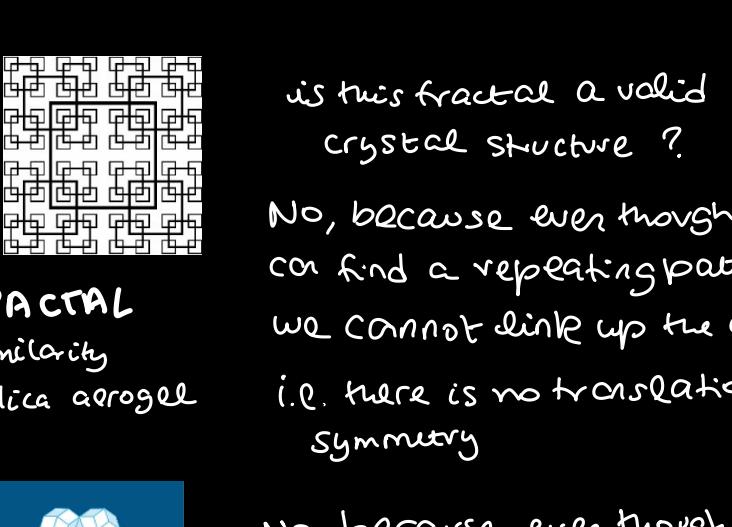
e.g.:



Valid ✓

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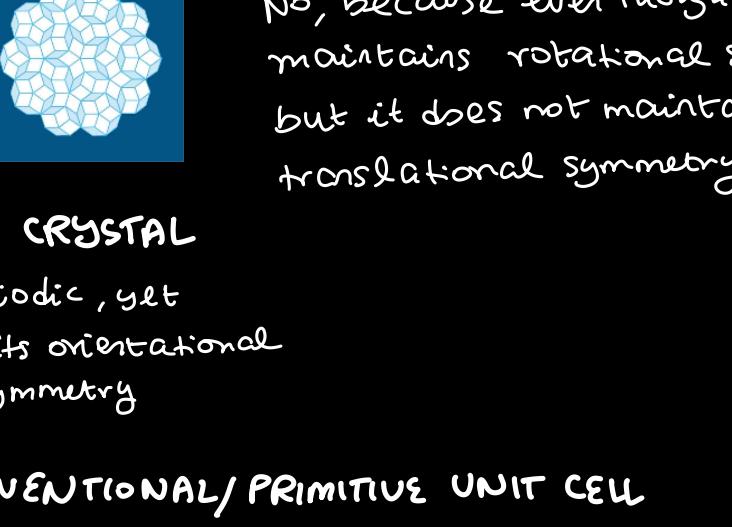
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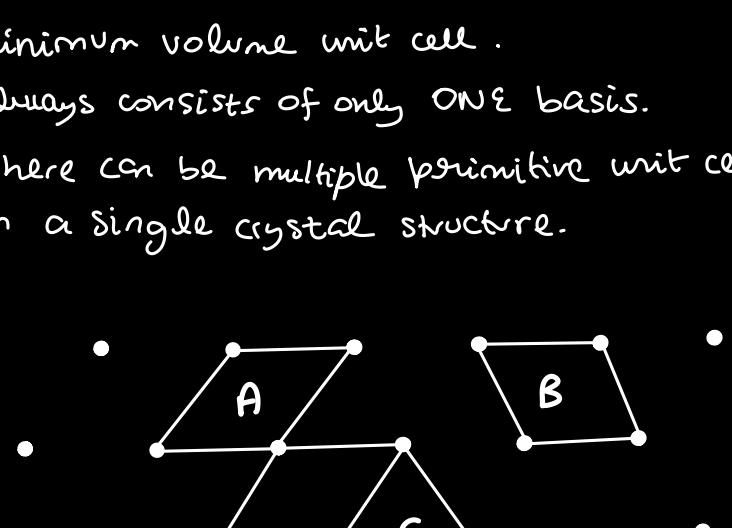
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Valid ✓

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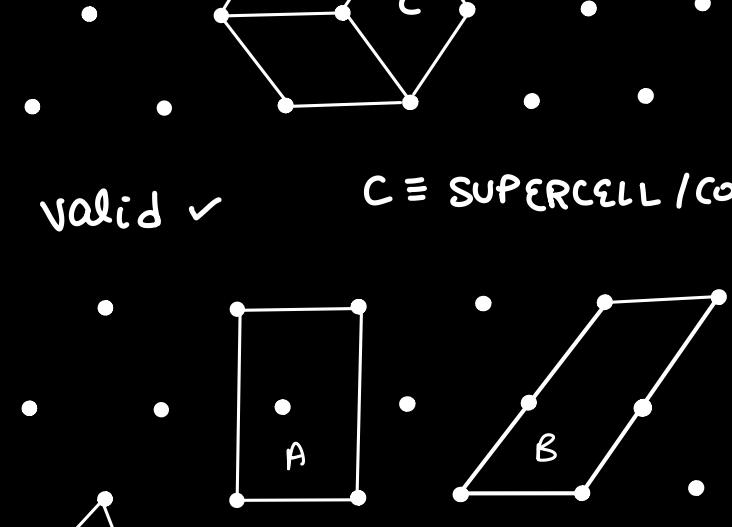
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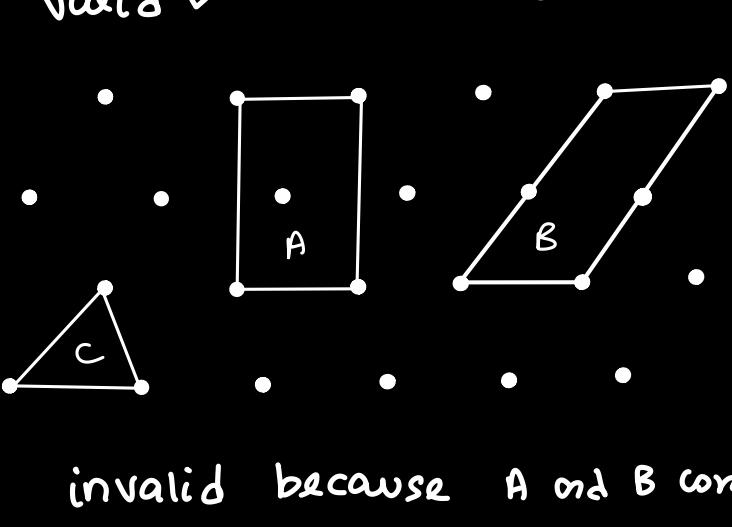
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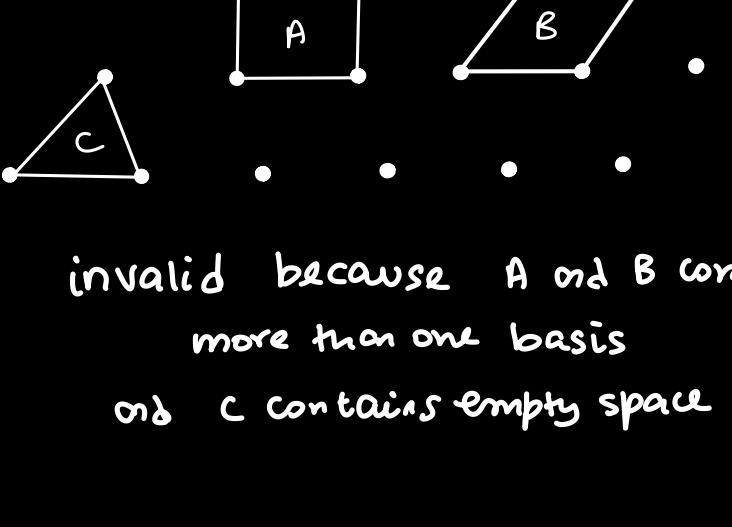
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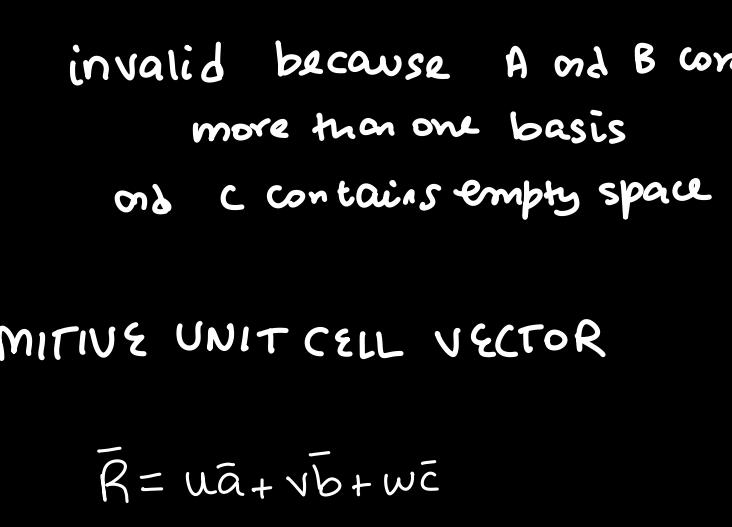
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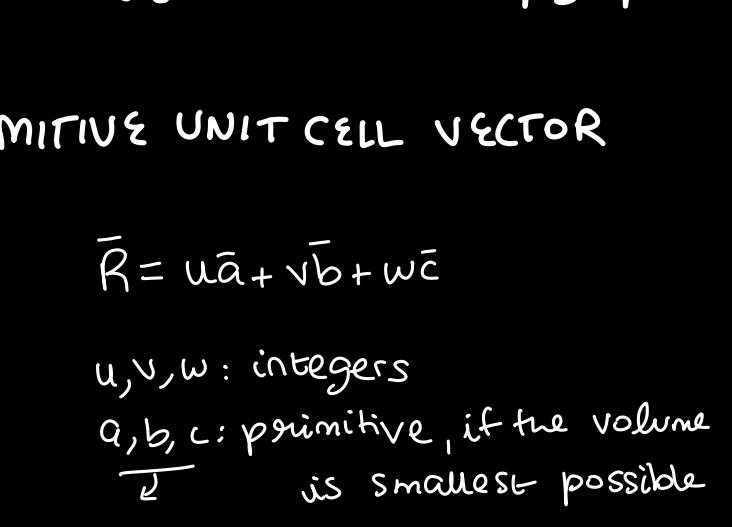
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Valid ✓

C ≡ SUPERCELL / CONVENTIONAL CELL

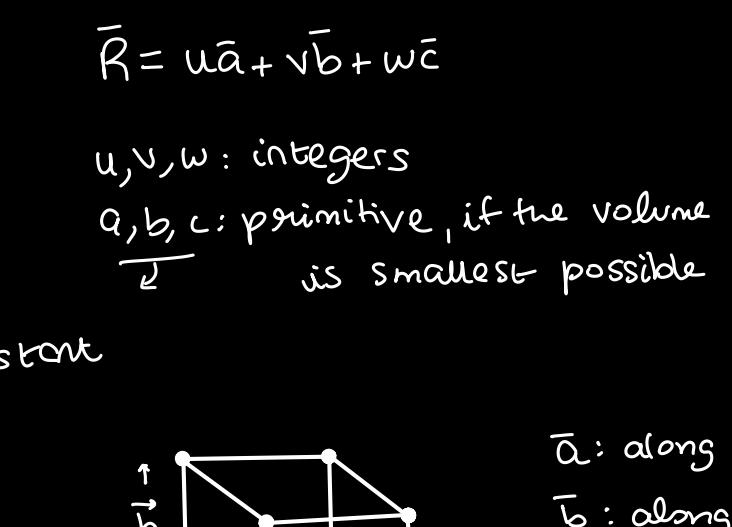
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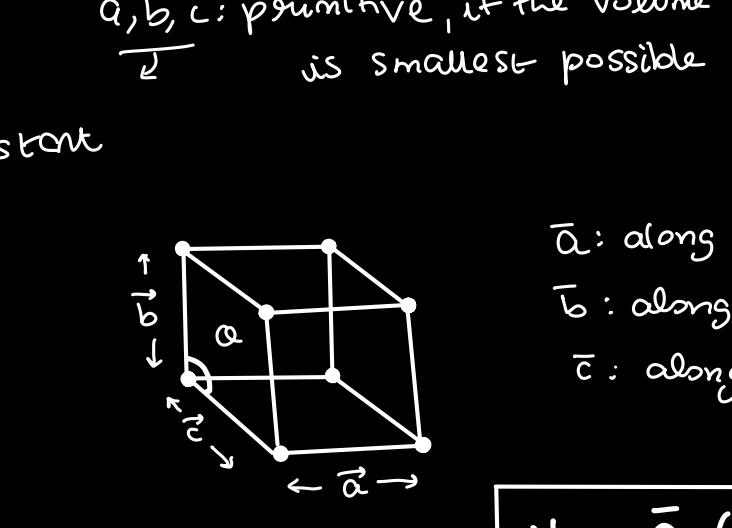
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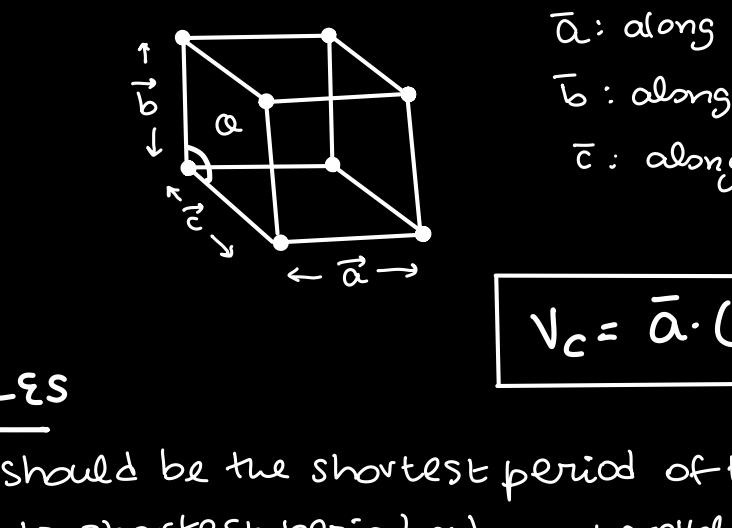
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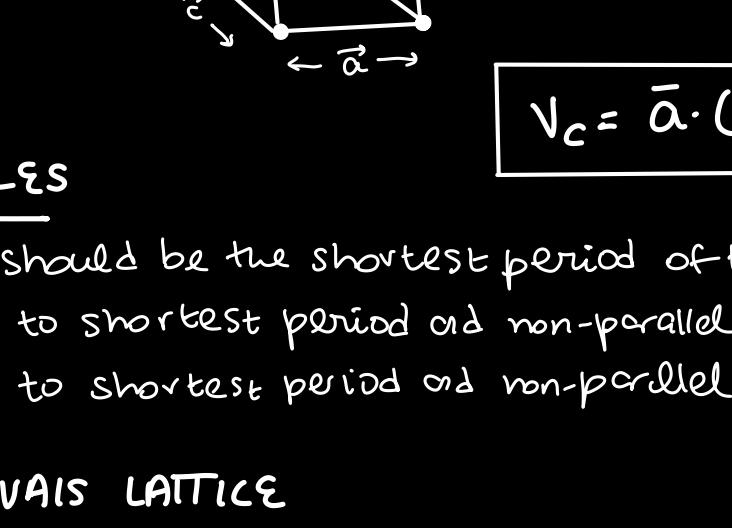
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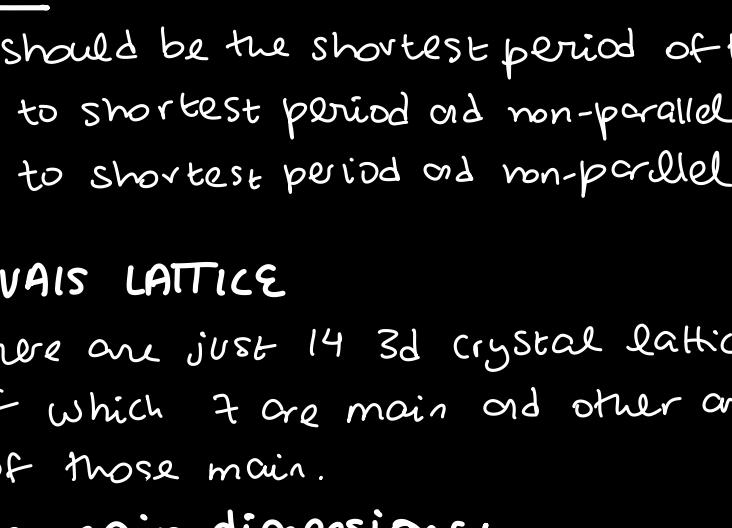
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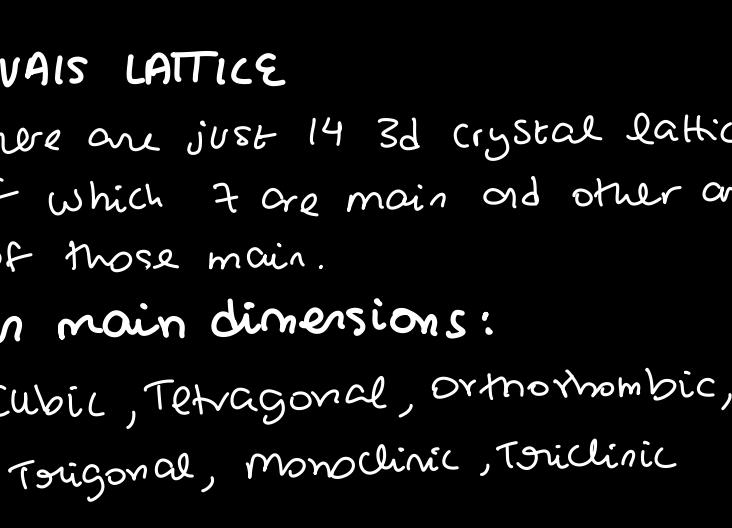
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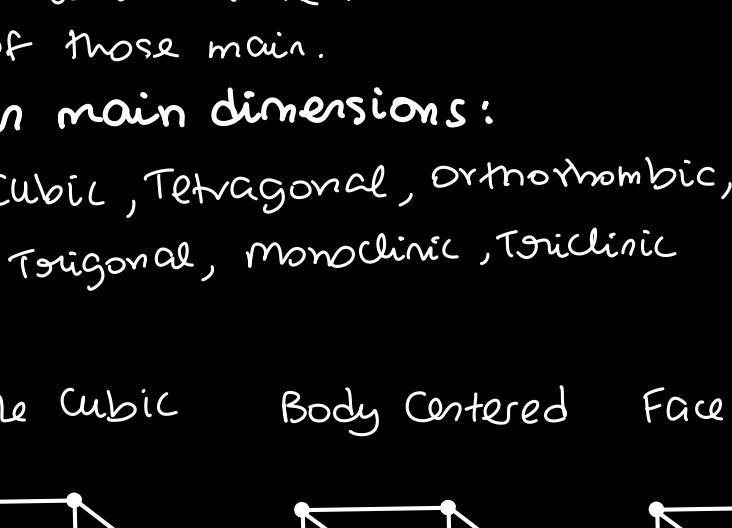
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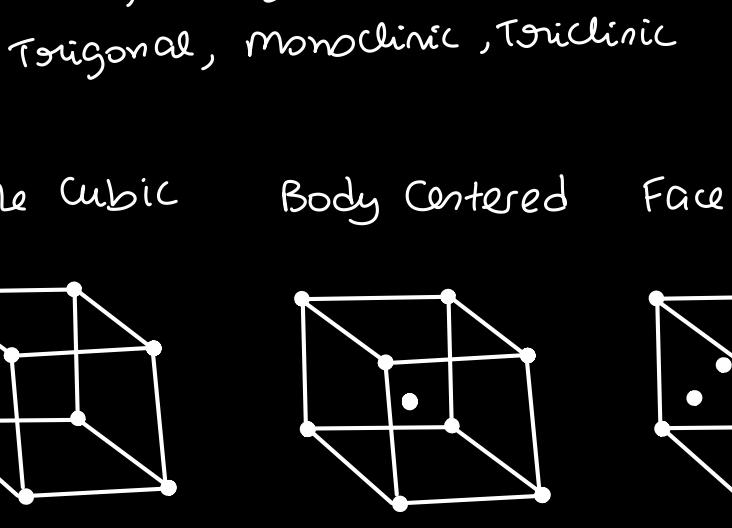
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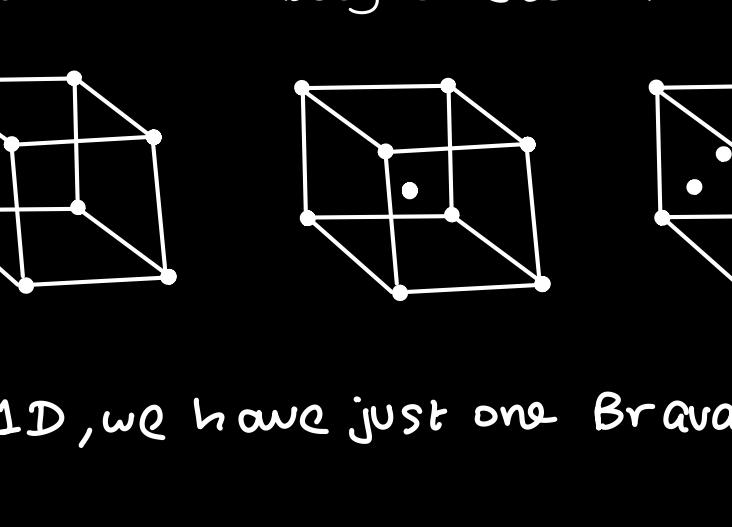
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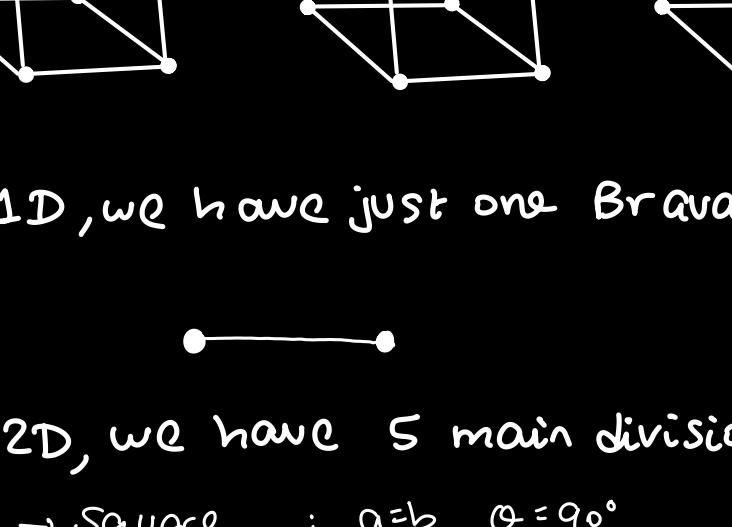
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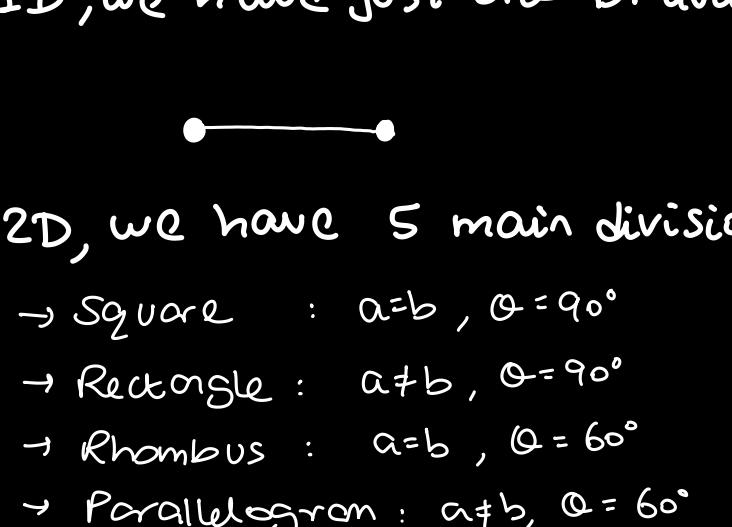
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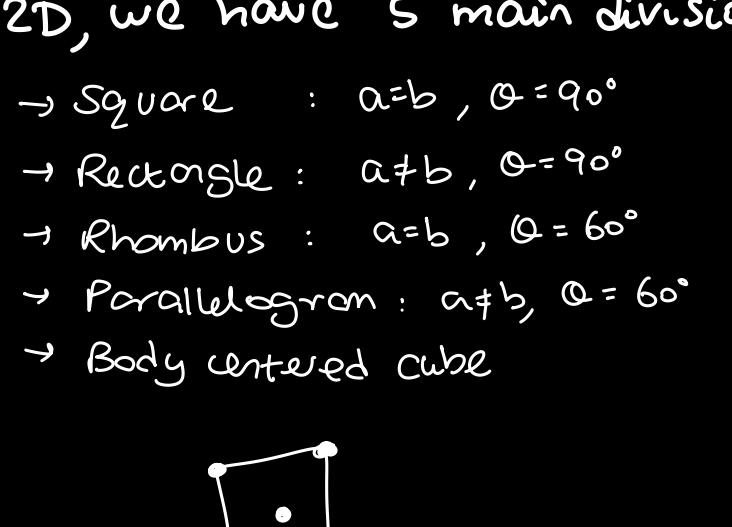
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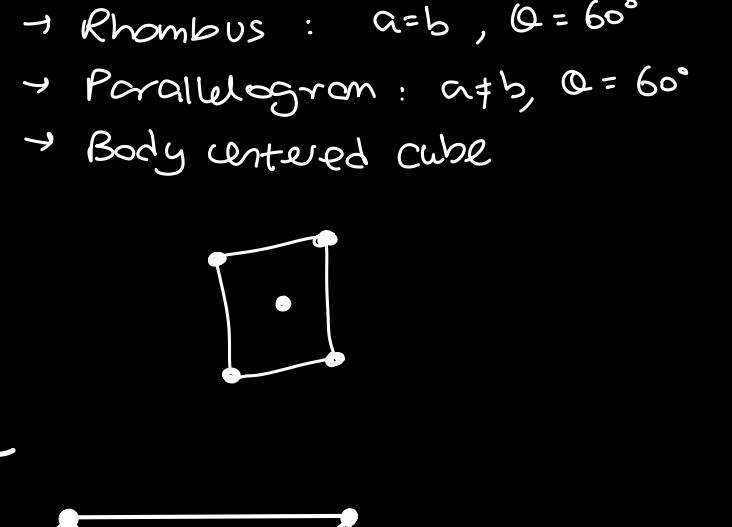
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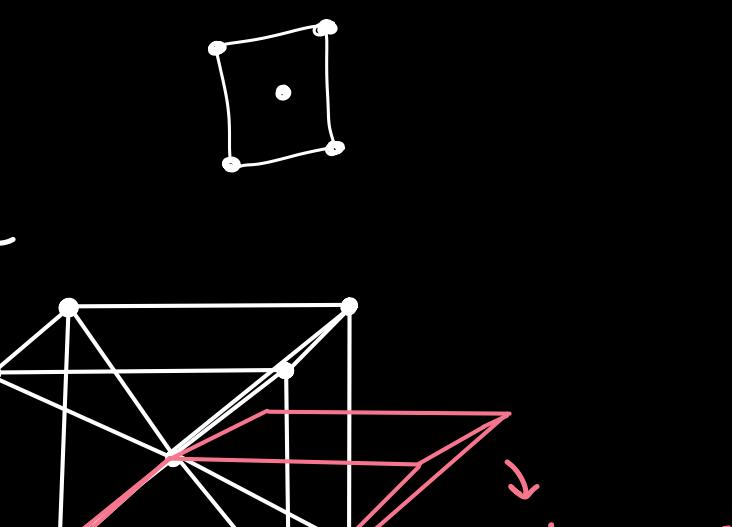
e.g.:



Valid ✓

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e.g.:



Valid ✓

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→ Schrodinger's wave equation

Total energy = Potential + Kinetic

$$\hat{H}\Psi = \hat{V}\Psi + \hat{E}\Psi \quad (\frac{P^2}{2m} - \frac{\hbar^2}{2m} \nabla^2\Psi)$$

$$E\Psi = V(x,y,z)\Psi - \frac{\hbar^2}{2m} \nabla^2\Psi$$

→ Particle moving in 1D

Side track → Ψ the solution of a differential eqn

$$\Psi = A\sin(kx) + B\cos(kx)$$

$$\frac{\partial\Psi}{\partial x} = k(A\cos(kx) - B\sin(kx))$$

$$\frac{\partial^2\Psi}{\partial x^2} = k^2(-A\sin(kx) - B\cos(kx))$$

$$\frac{\partial^2\Psi}{\partial x^2} = -k^2\Psi$$

① Free Particle : $V(x) = 0$

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

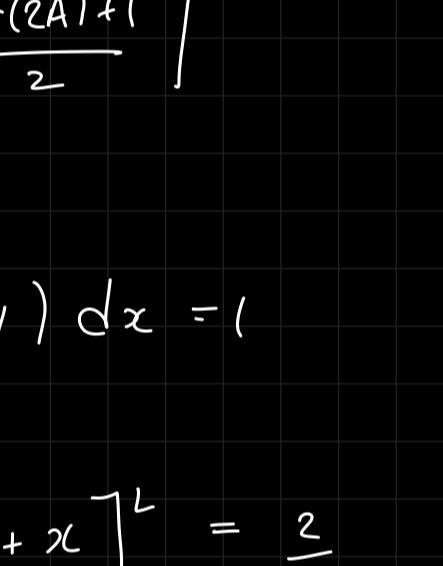
$$E = \frac{\hbar^2 k^2}{2m} \quad \text{---} \quad ①$$

Total Energy depends on wavenumber

POTENTIAL WELL

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

Schrodinger's time independent equation



Boundary conditions →

$$\text{R to I and III: } -\frac{\hbar^2}{2m} \frac{\partial^2\Psi}{\partial x^2} + \infty\Psi = E\Psi \quad \downarrow$$

ψ must be zero
in Regions I and III

$$\text{R to II: } -\frac{\hbar^2}{2m} \frac{\partial^2\Psi}{\partial x^2} + 0 = E\Psi$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2\Psi}{\partial x^2} = E\Psi$$

from ①, we know $k \propto E$

so, we can conclude that energy is discrete / quantized

And,

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

using probability density formula,

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$$

$$\int_0^L A^2 \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

$$\left\{ \begin{array}{l} \sin^2(x) = 1 - \cos^2(x) \\ \cos(A+B) = \cos A \cos B - \sin A \sin B \\ \cos(2A) = \cos^2 A - \sin^2 A \\ \cos(2A) = 2\cos^2 A - 1 \\ \cos^2(A) = \frac{\cos(2A) + 1}{2} \end{array} \right\}$$

$$\int_0^L \left(\cos\left(\frac{2n\pi}{L}x\right) + 1 \right) dx = 1$$

$$\left[\left(\sin\left(\frac{2n\pi}{L}x\right) \right) \frac{2n\pi}{L} + x \right]_0^L = \frac{2}{A^2}$$

$$\sin\left(2n\pi\right) \cdot \frac{2n\pi}{L} + L - 0 - 0 = \frac{2}{A^2}$$

$$A^2 = \frac{2}{L} \rightarrow A = \sqrt{\frac{2}{L}}$$

$$\Psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$\text{allowed energies} \rightarrow E_n = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$E \neq 0$ ever that would mean $\Psi = 0 \forall x$ (not allowed)

and $E_{\min} = ZPE$ lowest energy of the particle

$$E_n \propto \frac{n^2}{L^2}$$

$n \equiv \text{number of times curve cuts x-axis}$

Region I: the potential $V = 0$ hence Schrodinger's equation reduces to that of a free particle. Therefore, its wave function

$$\Psi_I = \Psi_{I,t}\Psi_{I,r} = Ae^{ikx} + Be^{-ikx} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Region II: finite potential barrier V

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

Therefore, its wave function is

$$\Psi_{II} = Ce^{-k'x} + De^{k'x} \quad \text{where } k' = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

Region III: the potential $V = 0$ and the transmitted particle is moving towards the right and has a positive momentum

$$\Psi_{III} = Fe^{ikx}$$

Classically forbidden region U_0

Incident Ae^{ikx} → Incoming particle wavefunction

Reflected $B'e^{-k'x}$ → particle wavefunction past the barrier

Within barrier

$Ce^{-\alpha x}$ → Transmitted

$D'e^{+\alpha x}$ → Transmitted

Tunneling probability:

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V^2 \sinh^2(k'L)}{4E(V-E)}}$$

Schrodinger's wave equation

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

⇒ Time Independent

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

$$\hat{H}\Psi(x,t) = i\hbar \frac{\partial\Psi(x,t)}{\partial t}$$

* BORN'S Interpretation (CRITERIAS)

Note

(a) Ψ must be continuous (no breaks)

(b) $\nabla\Psi = \frac{\partial\Psi}{\partial x}$ must be continuous (no kinks)

gradient of Psi we will have a divergence

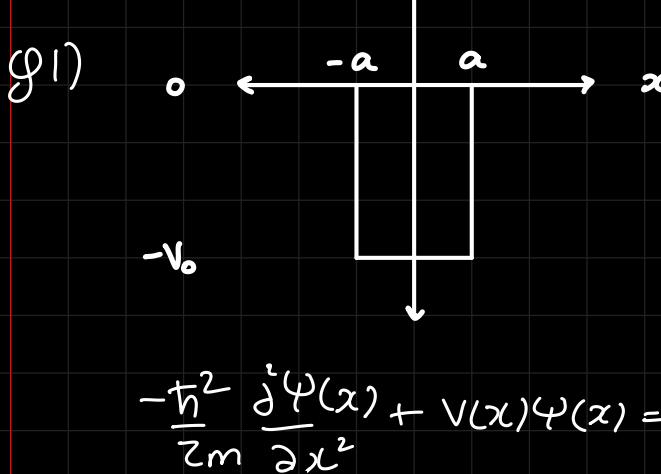
if gradient is discontinuous and so it will violate ∞

(c) Ψ must have a single value at any pt. in space

∴ Ψ must be finite everywhere

∴ Ψ cannot be zero everywhere

2024: Physics - I



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

at $x = |a|$: $V(x) = 0$

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

$$\frac{\partial^2 \psi}{\partial x^2} - \left(\frac{2m}{\hbar^2} \cdot E \right) \psi = 0$$

$$\text{Let } \psi(x) = A \sin(kx) + B \cos(kx)$$

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi$$

$$\text{So, } E = \frac{k^2 \hbar^2}{2m}$$

in the region II :

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} - V_0 \psi(x) = E \psi(x)$$

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + (V_0 + E) \psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (V_0 + E) \psi = 0$$

$$\text{let } \psi(x) = C e^{-kx} + D e^{kx}$$

for $x < -a \rightarrow \psi \neq \infty$

$$\text{so, } C = 0$$

for $x > a \rightarrow \psi \neq 0$

$$\text{so, } D = 0$$

$$\text{So, } \psi = \begin{cases} D e^{-kx} & : x < -a \\ A \sin(k'x) + B \cos(k'x) & : -a < x < a \\ C e^{-kx} & : x > a \end{cases}$$

at $x = -a \rightarrow \psi(x)$ and $\frac{\partial \psi(x)}{\partial x}$ must be continuous

$$-A \sin(k'a) + B \cos(k'a) = D e^{-ka} \quad \text{--- (2)}$$

$$+ k' A \cos(k'a) - k' B \sin(k'a) = k \cdot D e^{-ka} \quad \text{--- (3)}$$

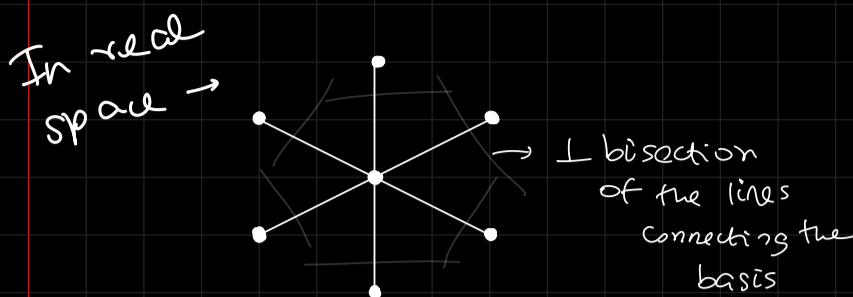
$$(2) + (3)$$

$$2B \cos(k'a) = (C + D) e^{-ka}$$

$$(2) - (3)$$

$$2A \sin(k'a) = (C - D) e^{-ka}$$

Wigner-Szilz cell → another primitive cell in the real space



draw the line between the nearest neighbour basis taking the least length and then take the perpendicular bisection of those lines and you will get the Wigner Szilz cell

Reciprocal Lattice

(= Fourier space / K space / momentum space)

Electronic number density $n(r)$ in the crystal is periodic

$$n(r) = n(r+R), \quad R: \text{primitive unit vector} \\ \equiv \text{period}$$

R equal to a direct lattice translational vector :

$$R = u\bar{a} + v\bar{b} + w\bar{c}$$

$u, v, w \rightarrow$ numbers (const)

$n(r)$ can be expressed as a Fourier series

$$n(r) = \sum_G n_G e^{ikr}$$

$$\text{where } n_G = \frac{1}{V_c} \int_0^a dV n(r) e^{-ikr}$$

where $\bar{k} =$ Reciprocal Lattice Vectors

reciprocal lattice represents the Fourier transform of another lattice like Bravais Lattice in real space

$$\boxed{\bar{k} \cdot \bar{R} = 2\pi \delta_{ij}} \quad \leftarrow e^{ikr} = 1$$

for unique \bar{R} , we have unique \bar{k}

We have 14 lattices for 3d
 " 5 lattices for 2d
 1 lattice for 1d

How about in reciprocal lattice?

What is the purpose of moving into the reciprocal lattice?

It decreases the complexity of theoretical & practical analysis

Electronic number density ($n(r)$) must be periodic $\rightarrow n(r) = n(r+R)$

$$\sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{R})\cdot\mathbf{r}} \quad \begin{matrix} \text{Fourier} \\ \text{transform} \end{matrix}$$

$$\sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{G}} n_{\mathbf{G}} e^{i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{R}\cdot\mathbf{r}}$$

So, $e^{i\mathbf{R}\cdot\mathbf{r}}$ must be equal to 1

$$R \cdot R = 2\pi \quad e^{i\mathbf{R}\cdot\mathbf{R}} = 1 \quad \begin{matrix} \# R \rightarrow \text{periodicity} \\ \# \mathbf{R} \rightarrow \text{Reciprocal lattice vector} \end{matrix}$$

$$\bar{R} \cdot \bar{R} = 2\pi \delta_{ij} \quad i, j = x, y, z \quad \delta_{ij} = 1 : i=j / 0 : \text{else}$$

When we move from real space to k /momentum space, our differential equations turn into quadratic eqn which is easier to solve

But,

$$\bar{R} = u\bar{a} + v\bar{b} + w\bar{c}$$

$$\text{and, } \bar{k} = h\bar{a}^* + k\bar{b}^* + l\bar{c}^*$$

where h, k, l are Miller indices

Reciprocal of the intersections

eg:

$$\begin{array}{ccccccc} \leftarrow & \rightarrow & \bullet & \bullet & \bullet & \bullet & \bullet \end{array}$$

[1d]

$$\text{then } \bar{a}\bar{a}^* = 2\pi$$

since they are in the same direction,

$$a\bar{a}^* = 2\pi$$

$$\boxed{\bar{a}^* = \frac{2\pi}{a}}$$

So, reciprocal lattice \rightarrow

$$\begin{array}{ccccccc} \vdots & \rightarrow & \bullet & \bullet & \bullet & \bullet & \bullet \end{array}$$

for [3d]

$$a\bar{a}^* = 2\pi$$

$$b\bar{b}^* = 2\pi$$

$$c\bar{c}^* = 2\pi$$

but $b\bar{a}^* = 0$

because of δ_{ij}

$$a^* = \frac{2\pi}{a} \frac{(b \times c)}{a \cdot (b \times c)}$$

$$b^* = \frac{2\pi}{b} \frac{(c \times a)}{b \cdot (c \times a)}$$

$$c^* = \frac{2\pi}{c} \frac{(a \times b)}{c \cdot (a \times b)}$$

Direct Lattice Vector:

$$\bar{R} = u\bar{a} + v\bar{b} + w\bar{c}$$

Reciprocal Lattice Vector:

$$\bar{k} = m\bar{a}^* + n\bar{b}^* + o\bar{c}^*$$

Reciprocal lattice is the Fourier transform of the real lattice

Note: Set of reciprocal lattice vectors \bar{k} is also known as lattice

since $b\bar{a}^* = 0$

and $c\bar{a}^* = 0$

so, a^* must be linear multiple of $(b \times c)$

i.e. \perp to both b and c

so, $a^* = 2\pi \frac{a}{(b \times c)}$

$$a^* = \frac{2\pi}{a} (b \times c)$$

$$b^* = \frac{2\pi}{b} (c \times a)$$

$$c^* = \frac{2\pi}{c} (a \times b)$$

We can compare here with the 3d also

$$\text{we had } a^* = \frac{2\pi (\bar{b} \times \bar{c})}{\bar{a} \cdot (\bar{b} \times \bar{c})}$$

$$\bar{a}^* = \frac{2\pi \bar{b}}{\bar{a} \cdot \bar{b}} \quad \text{because 2d}$$

but direction remains

$$\bar{a}^* = \frac{2\pi}{a} \hat{a}$$

$$\bar{b}^* = \frac{2\pi}{b} \hat{b}$$

$$\bar{c}^* = \frac{2\pi}{c} \hat{c}$$

let \rightarrow

$$\begin{array}{c} \hat{a} \\ \hat{b} \\ \hat{c} \end{array} \quad \begin{array}{c} \hat{a} \\ \hat{b} \\ \hat{c} \end{array}$$

a

$$b^* = \frac{2\pi}{b} \quad \text{and} \quad a^* = \frac{2\pi}{a}$$

$$\bar{b}^* = \frac{2\pi}{b} \frac{\hat{b}}{\hat{a}}$$

$$\bar{c}^* = \frac{2\pi}{c} \frac{\hat{c}}{\hat{a}}$$

Here b^* will be bigger than a^* as compared to b, c ratio

because we took the reciprocal in $\rightarrow b^* = \frac{2\pi}{b}$

coordinate transformation

[2d]

$$R = u\bar{a} + v\bar{b} \quad , \quad k = m\bar{a}^* + n\bar{b}^*$$

$$a^* = ?$$

$$R \cdot k_j = 2\pi \delta_{ij}$$

$$a\bar{a}^* = 2\pi$$

$$b\bar{b}^* = 2\pi$$

$$ab^* = 0$$

$$ba^* = 0 \rightarrow a^* \perp b$$

and since $a^* = 2\pi$,

a and a^* must be

parallel

$$a^* = \frac{2\pi}{a} \hat{a}$$

$$b^* = \frac{2\pi}{b} \hat{b}$$

$$c^* = \frac{2\pi}{c} \hat{c}$$

We can compare here with the 3d also

$$\text{we had } a^* = \frac{2\pi (\bar{b} \times \bar{c})}{\bar{a} \cdot (\bar{b} \times \bar{c})}$$

$$\bar{a}^* = \frac{2\pi \bar{b}}{\bar{a} \cdot \bar{b}}$$

$$\text{but direction remains}$$

$$\bar{a}^* = \frac{2\pi}{a} \hat{a}$$

$$\bar{b}^* = \frac{2\pi}{b} \hat{b}$$

$$\bar{c}^* = \frac{2\pi}{c} \hat{c}$$

here b^* will be bigger than a^* as compared to b, c ratio

because we took the reciprocal in $\rightarrow b^* = \frac{2\pi}{b}$

coordinate transformation

[BCC]

$$\bar{a} = \frac{a}{2} (i+j-k)$$

$$\bar{b} = \frac{a}{2} (j+k-i)$$

$$\bar{c} = \frac{a}{2} (k+i-j)$$

Remember last question of the quiz

↳ Work function

↳ if it is diff for a particular material, then the min energy must be too

$$\# E = \frac{2\pi k^2}{a^2} \quad \Rightarrow \quad \text{quantum mechanics}$$

$$-\frac{h^2}{8m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) = E \psi(x)$$

$$time \text{ independent Schrödinger's wave equation}$$

Let $\psi(x) = A \sin(kx) + B \cos(kx)$

then $\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x)$

$$- \frac{h^2}{8m} (-k^2) \psi(x) + V(x) \psi(x) = E \psi(x)$$

$$E = \frac{2\pi^2 m k^2}{a^2}$$

$$k = \frac{2\pi}{a}$$

$$E = \frac{2\pi^2 m}{a^2}$$

for the 2d potential well problem,

$$V(x) = 0$$

$$E = \frac{2\pi^2 m}{a^2}$$

we notice that the Reciprocal lattice of BCC is FCC and vice versa.

Face centered cube $\xrightarrow{\text{Fourier transform}}$ Body centered cube

Inverse Fourier transform

If we move into the Reciprocal space, the Weigner Seitz cell gives the first Brillouin zone.

Note: Weigner Seitz cell has square or hexagon structure

for FCC it is hexagon structure

$$\bar{a} = \frac{a}{2} (i+j)$$

$$\bar{b} = \frac{a}{2} (j+k)$$

$$\bar{c} = \frac{a}{2} (k+i)$$

In the Brillouin zone (FCC), we have a hexagon at [111]

Remember last question of the quiz

↳ Work function

↳ if it is diff for a particular material, then the min energy must be too

$$\# E = \frac{2\pi k^2}{a^2} \quad \Rightarrow \quad \text{quantum mechanics}$$

$$-\frac{h^2}{8m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) = E \psi(x)$$

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Let $\psi(x) = A \sin(kx) + B \cos(kx)$

then $\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x)$

$$- \frac{h^2}{8m} (-k^2) \psi(x) + V(x) \psi(x) = E \psi(x)$$

$$E = \frac{2\pi^2 m k^2}{a^2}$$

$$k = \frac{2\pi}{a}$$

for the 3d potential well problem,

$$V(x) = 0$$

$$E = \frac{2\pi^2 m}{a^2}$$

we notice that the Reciprocal lattice of BCC is FCC and vice versa.

Face centered cube $\xrightarrow{\text{Fourier transform}}$ Body centered cube

Inverse Fourier transform

* BAND THEORY OF SOLIDS {3rd Chp}

Bragg zone = Wigner-Seitz cell in the reciprocal space

→ FREE ELECTRON THEORY

↳ no potential energy

$$E\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad \text{from Schrodinger's wave eqn}$$

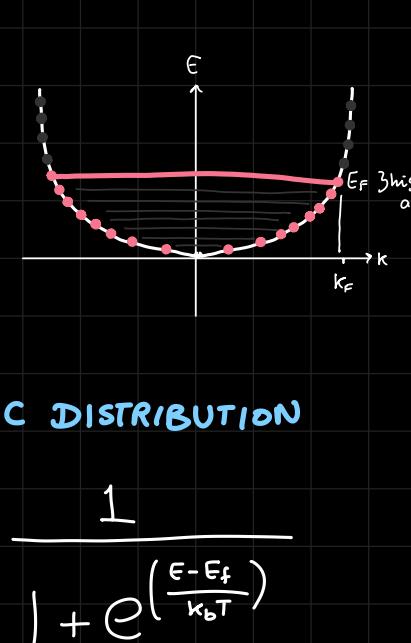
free e- are plane waves $\therefore \psi = A e^{\pm ikx}$

$$\rightarrow \text{momentum: } i\hbar \frac{\partial \psi}{\partial x} = \pm \hbar k \psi$$

$$\rightarrow \text{Energy: } -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \frac{\hbar^2 k^2}{2m} \psi$$

$$\rightarrow \text{Grp velocity: } \frac{\partial \omega}{\partial k} = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{\hbar k}{m}$$

Very closely packed energy bands if container of e- is very large, we can conclude that the energy band graph looks continuous.



wave packets: superposition of different waves of separate electrons

group velocity: velocity of a whole group e- / wave packets.

phase velocity: velocity of individual particles like e-

properties like conductivity, temperature etc. can be figured out using this free e-theory but this theory is incomplete on its own without the crystal nature.

→ FERMI-SURFACE

We have seen in the "particle in a box" problem, that energy levels are discretized. But as the width approaches $\rightarrow \infty$, the ΔE (energy band gap) tends to $\rightarrow 0$.

$$\frac{\hbar^2 k^2}{2m} = E_F \rightarrow \text{Fermi-level}$$



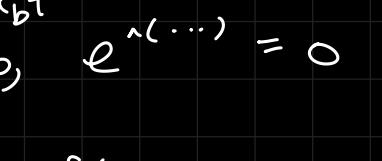
FERMI-DIRAC DISTRIBUTION

The probability that a particle has energy E is

$$f(E) = \frac{1}{1 + e^{\left(\frac{E-E_F}{k_b T}\right)}}$$

k_b : Boltzmann constant

T : temperature



At $T=0$, E_F is the highest energy where we can find a valence electron with energy $= E$

When we increase the temperature, the valence electrons move to higher energy levels

↳ valence e- \rightarrow conduction e-

LM : The e- occupy this space

LM : Holes occupy this space which was earlier occupied by electrons

In case of METAL, the gap between the new energy band (conduction) and E_F (Fermi level) is very small.

↳ # of free e- for metals is very high

In 12th, we were taught that there was an overlap between the conduction band and valence band but the idea was that they were indistinguishable

In case of SEMICONDUCTOR, the gap is high and hence conduction e- and valence e- can be distinguished easily.

Some case for insulators as well

FERMI LINE

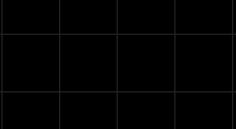
1d

FERMI SURFACE

2d

FERMI SPHERE

3d



$$\rightarrow k_F = \sqrt{\frac{2mE_F}{\hbar}}$$

k-space

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

so, $e^{(E-E_F)/k_b T} = 0$

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

at $T=0$ and for $E < E_F$,

$$E - E_F = -\infty$$

so, $e^{(E-E_F)/k_b T} = 0$

$$f(E) = 1$$

but at $E > E_F$,

$$E - E_F = \infty$$

so, $e^{(E-E_F)/k_b T} = \infty$

$$f(E) = 0$$

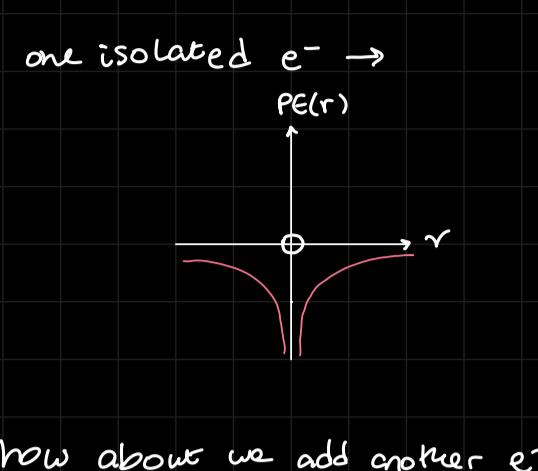
fermi energy = chemical potential

(E_F)

the probability that a particle has energy (E)

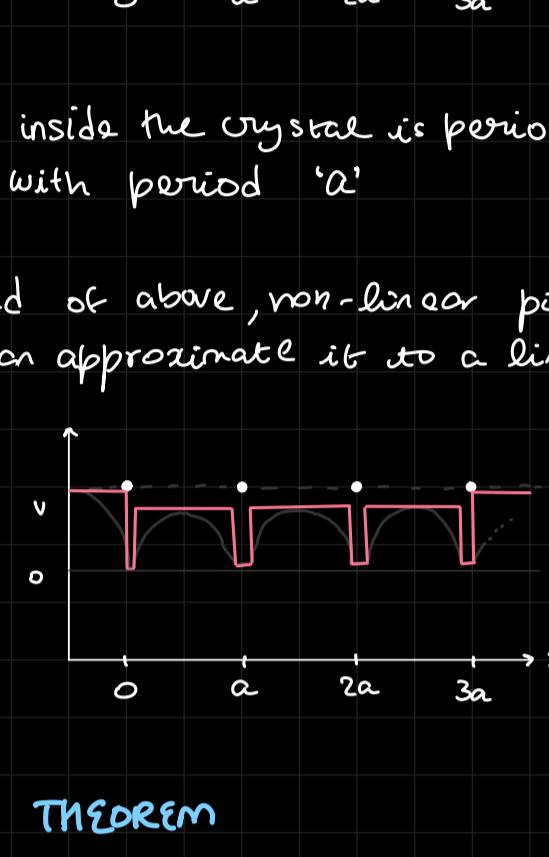
$$f(E) = \frac{1}{1 + e^{\left(\frac{E - E_F}{k_B T}\right)}}$$

PE of e^- in crystal

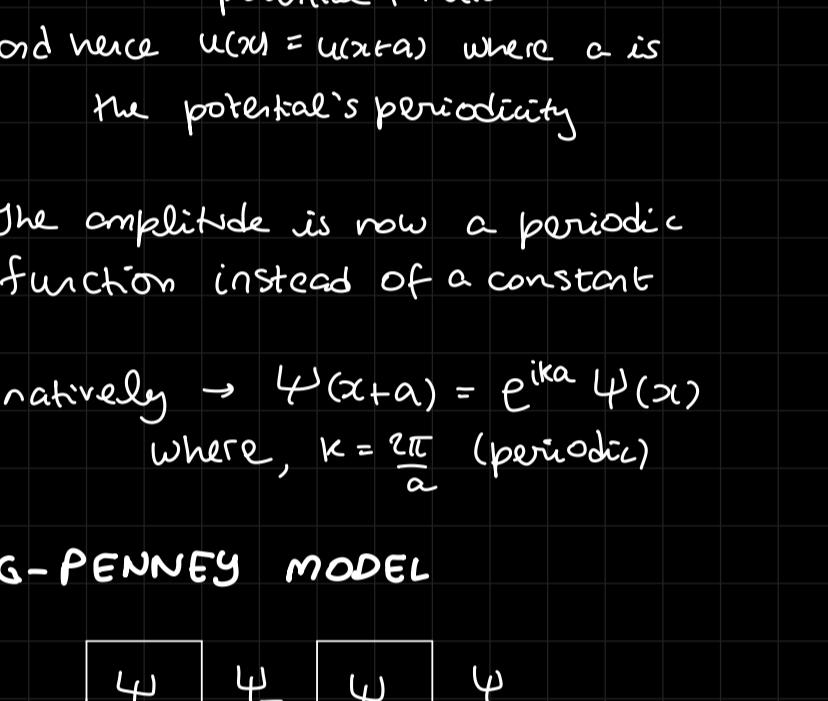


$$\text{for } 1d \rightarrow a\alpha^* = 2\pi \Rightarrow \alpha^* = \frac{2\pi}{a}$$

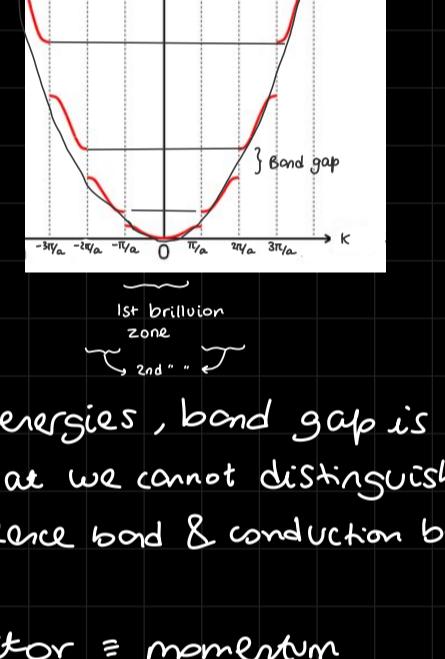
in k space \rightarrow we have Brillouin zone



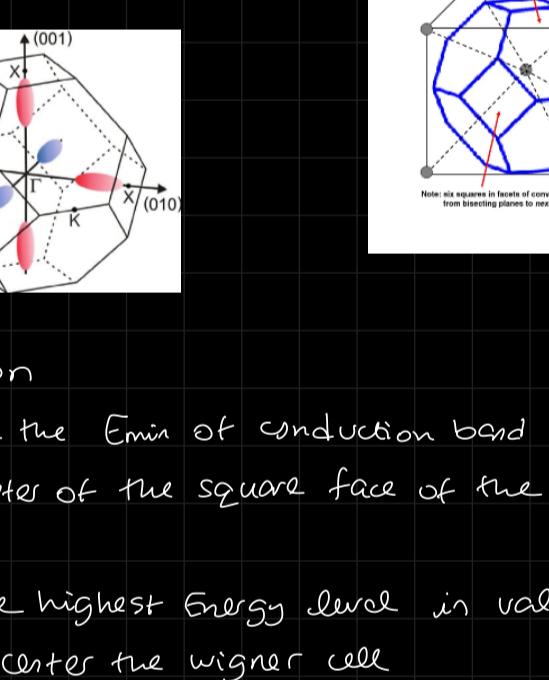
for one isolated $e^- \rightarrow$



how about we add another e^- ?

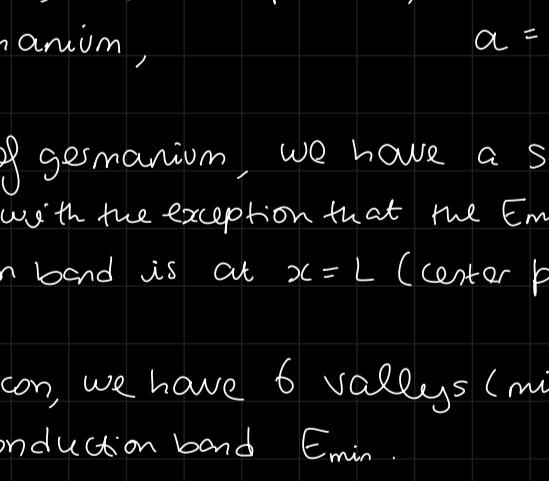


and we can have a long chain of particles as well



PE inside the crystal is periodic with period 'a'

instead of above, non-linear potential, we can approximate it to a linear potential.



BLOCH THEOREM

for a general crystal

$$\psi(x) = e^{ikx} u(x)$$

where $u(x)$ = periodic just like potential function

and hence $u(x) = u(x+a)$ where a is the potential's periodicity

note: The amplitude is now a periodic function instead of a constant

$$\text{alternatively} \rightarrow \psi(x+a) = e^{ika} \psi(x)$$

$$\text{where, } k = \frac{2\pi}{a} \text{ (periodicity)}$$

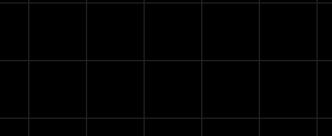
KRONIG-PENNEY MODEL



solution: D.A. Neeman pg 63-70

E-K relation \rightarrow

$$ka = \pm n\pi$$



initial assumption, continuous graph

as soon as we bring periodicity, we observe the band gap

at some energies, band gap is so less that we cannot distinguish between valence band & conduction band.

wave vector = momentum

In a Wigner-Seitz cell,

{ center point of the hexagonal face = L
center point of the square face = X
center point of the cell = r (gamma)

All these are wave vectors

for silicon, E_{min} at conduction band at $k=L$

i.e. the center of the square face of the Wigner Seitz cell

we achieve highest energy level in valence band at $k=r$, center the Wigner cell

and hence, band gap = $E(X) - E(r)$

for Si,

$$CB_{min} \rightarrow CB_{max}$$

$$VB_{max} \rightarrow VB_{min}$$

for Ge,

$$CB_{min} \rightarrow CB_{max}$$

$$VB_{max} \rightarrow VB_{min}$$

also called energy band valleys

energy band structure gives relation

between E and k (momentum space)

Energy band diagram gives relation between E and x (real dimension)

for silicon, (lattice parameter) $a = 5.45 \text{ \AA}$

for germanium, $a = 5.68 \text{ \AA}$

in case of germanium, we have a similar E-k relation with the exception that the E_{min} for the conduction band is at $x=L$ (center pt of hexagonal face)

for silicon, we have 6 valleys (minima condition).

for conduction band E_{min} .

CB_{min} at every center point of a square face of the Wigner cell

and 8 valleys for germanium

Since we have larger # of valleys, e^- will flow "more" in case of Ge and hence more current

Si and Ge are indirect band gap semiconductors

$\hookrightarrow CB_{min}$ and VB_{max} are not at the same momentum point

for Si, particle moves in momentum axis and then changes energy to move from $CB_{min} \rightarrow VB_{max}$

LEDs use direct band gap semiconductor

\hookrightarrow not losing energy when transitioning from $VB \rightarrow CB$. e.g? GaAs

DBGS very useful in optical electronic devices.

GaAs

$k: \text{const}$

Si

E_{min}

CB_{min}

VB_{max}

PHYSICS OF SEMICONDUCTOR DEVICES

ASSIGNMENT - 1

Aditya Gautam - 2023043

$$q1) \bar{A} = \left(\frac{a\sqrt{3}}{2} \hat{i} + \frac{a}{2} \hat{j} \right), \bar{B} = \left(-\frac{a\sqrt{3}}{2} \hat{i} + \frac{a}{2} \hat{j} \right), \bar{C} = c \hat{k}$$

We know that the volume of primitive unit cell with the primitive cell vector, $\bar{R} = u\bar{a} + v\bar{b} + w\bar{c}$ is $V_c = \bar{a} \cdot (\bar{b} \times \bar{c})$

$$\text{So, volume} = \bar{A} \cdot (\bar{B} \times \bar{C})$$

$$(\bar{B} \times \bar{C}) = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -\frac{a\sqrt{3}}{2} & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$= \hat{i} \left(\frac{ac}{2} - 0 \right) - \hat{j} \left(-\frac{ac\sqrt{3}}{2} - 0 \right) + \hat{k} (0 - 0)$$

$$= \left(\frac{ac}{2} \right) \hat{i} + \left(\frac{ac\sqrt{3}}{2} \right) \hat{j}$$

$$\begin{aligned} \text{now, } \bar{A} \cdot (\bar{B} \times \bar{C}) &= \left(\frac{a\sqrt{3}}{2} \cdot \frac{ac}{2} \right) + \left(ac\sqrt{3} \cdot \frac{a}{2} \right) \\ &= 2 \left(\frac{a^2 c \sqrt{3}}{4} \right) = \frac{\sqrt{3} a^2 c}{2} \end{aligned}$$

Hence, we conclude that the volume of the primitive unit cell is indeed $\rightarrow \frac{\sqrt{3}}{2} a^2 c$

Primitive Translational Vectors \rightarrow

for 3d crystal structure,

$$A^* = \frac{2\pi \cdot (B \times C)}{A \cdot (B \times C)}$$

$$= \frac{2\pi \left(\frac{ac}{2} \hat{i} + \frac{ac\sqrt{3}}{2} \hat{j} \right)}{\sqrt{3}/2 a^2 c}$$

$$= \frac{2\pi}{a} \left(\frac{1}{\sqrt{3}} \hat{j} + \hat{i} \right)$$

$$B^* = \frac{2\pi \cdot (C \times A)}{A \cdot (B \times C)}$$

$$(C \times A) = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & 0 & c \\ \frac{a\sqrt{3}}{2} & \frac{a}{2} & 0 \end{vmatrix}$$

$$\begin{aligned} &= \hat{i}(0 - \frac{ac}{2}) - \hat{j}(-\frac{ac\sqrt{3}}{2}) \\ &= \left(-\frac{ac}{2}\right)\hat{i} + \left(\frac{ac\sqrt{3}}{2}\right)\hat{j} \end{aligned}$$

$$B^* = \frac{-\pi ac \hat{i} + \pi ac\sqrt{3} \hat{j}}{\sqrt{3}/2 a^2 c}$$

$$\begin{aligned} &= \frac{-2\pi}{\sqrt{3}} \cdot \frac{1}{a} \hat{i} + \frac{2\pi}{a} \hat{j} \\ &= \frac{2\pi}{a} \left(\frac{-1}{\sqrt{3}} \hat{i} + \hat{j} \right) \end{aligned}$$

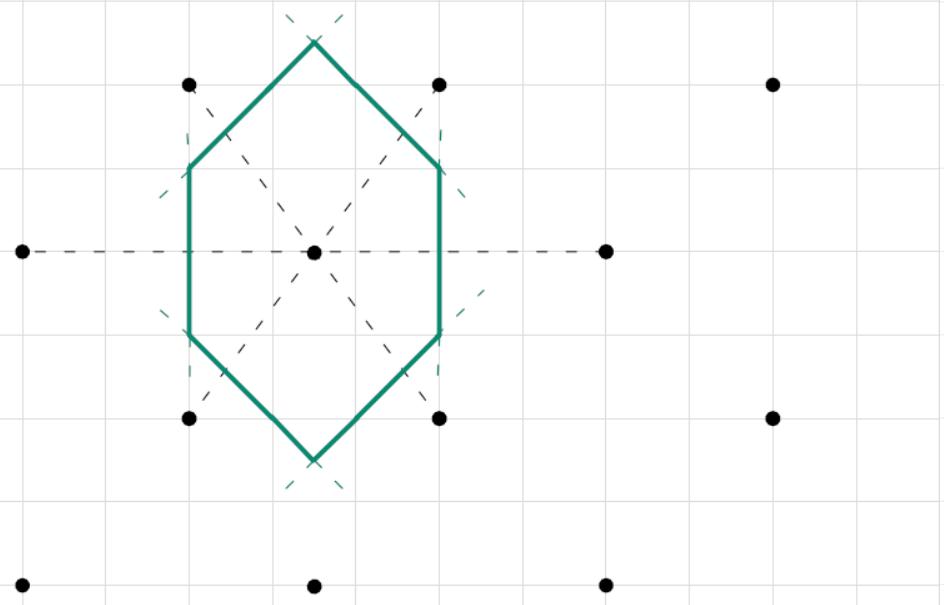
$$C^* = \frac{2\pi \cdot (A \times B)}{A \cdot (B \times C)}$$

$$A \times B = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{a\sqrt{3}}{2} & \frac{a}{2} & 0 \\ -\frac{a\sqrt{3}}{2} & \frac{a}{2} & 0 \end{vmatrix}$$

$$\begin{aligned}
 &= \hat{k} \left(\frac{\alpha^2 \sqrt{3}}{4} + \frac{\alpha^2 \sqrt{3}}{4} \right) \\
 &= \frac{\sqrt{3}}{2} \alpha^2 \hat{k}
 \end{aligned}$$

$$C^* = \frac{\pi \sqrt{3} \alpha^2 \hat{k}}{\sqrt{3}/2 \alpha^2 c} = \frac{2\pi}{c} \hat{k}$$

Brillouin zone of the hexagonal Space lattice



(Q2) Lattice constant = 4.3×10^{-10} m = a

for (321), miller indices are
 $h=3$; $k=2$; $l=1$

We know that the interplanar distance is,

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{4.3 \times 10^{-10}}{\sqrt{9+4+1}}$$
$$= \frac{4.3}{3.74} \text{ \AA} \approx 1.15 \text{ \AA}$$

We also know that constructive diffraction occurs only if $2ds\sin\theta = n\lambda$

for first order reflection, $n=1$

$$\begin{aligned} \text{So, } \lambda &= 2ds\sin\theta = 2 \times 1.15 \times 10^{-10} \times \sin(10^\circ) \\ &= 2.3 \times 0.1736 \times 10^{-10} \\ &\approx 0.4 \times 10^{-10} \text{ m} \end{aligned}$$

g3)

$$KE = 0.2 \text{ MeV}$$

$$V = 20 \text{ MeV}$$

note $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$

$$E = 3.2 \times 10^{-14} \text{ J}$$

$$V = 3.2 \times 10^{-12} \text{ J}$$

$$L = 2.97 \times 10^{-18} \text{ m}$$

$$\hbar = 1.054 \times 10^{-34} \text{ Js}$$

$$m = 6.68 \times 10^{-27} \text{ kg}$$

We know,

$$T = \frac{1}{1 + \frac{v^2 \sinh^2(k'L)}{4E(v-E)}}$$

where $k' = \sqrt{\frac{2m(v-E)}{\hbar^2}} = \sqrt{\frac{4.23 \times 10^{-38}}{1.11 \times 10^{-68}}}$

$$= \sqrt{3.81 \times 10^{30}} = 1.95 \times 10^{15}$$

$$k'L = 5.8 \times 10^{-3}$$

$$\sinh^2(k'L) = 3.36 \times 10^{-5}$$

$$T = \frac{1}{1 + \frac{3.44 \times 10^{-28}}{4.05 \times 10^{-21}}} = \frac{1}{1 + (0.85 \times 10^{-7})}$$

$= \boxed{0.99}$ This is incorrect since we cannot get ~ 1 tunnelling probability. Check last page ↓

(g4) $\Delta x = 4\text{\AA} = 4 \times 10^{-10}\text{m}$

(a) Heisenberg's uncertainty principle ↴

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

$$\Delta p \geq \frac{0.527 \times 10^{-34}}{4 \times 10^{-10}}$$

$$\Delta p \geq 0.13175 \times 10^{-24} \simeq 1.32 \times 10^{-25} \text{ kg m s}^{-1}$$

(b) $KE = \frac{p^2}{2m}$

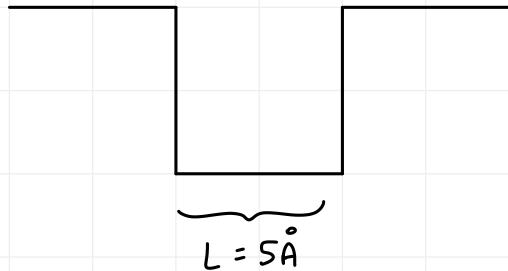
$$\frac{d(KE)}{dp} = \frac{1}{2m} \cdot 2p = \frac{p}{m} \rightarrow \Delta KE = \frac{p}{m} \Delta p$$

$$\Delta KE = \frac{2.4 \times 10^{-23}}{9.1 \times 10^{-31}} \times 1.32 \times 10^{-25}$$

$$= 0.26 \times 10^8 \times 1.32 \times 10^{-28}$$

$$= 3.432 \times 10^{-18} \text{ J}$$

(Q5)



(a) for ∞ potential well,

$$E_n = \frac{k^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$E_1 = \frac{\pi^2 \cdot (1.054 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times 25 \times 10^{-20}}$$

$$= \frac{\pi^2 \cdot (1.11) \times 10^{-68} \times 10^{51}}{455} = 2.4 \times 10^{-19} \text{ J}$$

$$E_2 = 4 \times 2.4 \times 10^{-19} = 9.6 \times 10^{-19} \text{ J}$$

$$E_3 = 9 \times 2.4 \times 10^{-19} = 21.6 \times 10^{-19} \text{ J}$$

$$(b) \quad \Delta E = E_3 - E_2 = \frac{hc}{\lambda}$$

$$\lambda = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{(21.6 - 9.6) 10^{-19}} = \frac{19.878 \times 10^{-26}}{12 \cdot 10^{-19}}$$

$$\lambda = \underline{1.656 \times 10^{-7} \text{ m}}$$

(Q3) note: $1\text{eV} = 1.602 \times 10^{-19} \text{J}$

$$E = 3.2 \times 10^{-14} \text{ J}$$

$$V = 3.2 \times 10^{-12} \text{ J}$$

$$L = 2.97 \times 10^{-18} \text{ m}$$

$$\hbar = 1.054 \times 10^{-34} \text{ Js}$$

$$m = 6.68 \times 10^{-27} \text{ kg}$$

Since $V \gg E \rightarrow$

$$T = 16 \left(\frac{E}{V} \right) \left(1 - \frac{E}{V} \right) e^{-2KL}$$

(according to
the book)

where $K = \sqrt{\frac{2m}{\hbar^2} (V - E)}$

$$K = 1.95 \times 10^{15}$$

$$T = 16 \left(\frac{1}{100} \right) \left(1 - \frac{1}{100} \right) e^{-2(1.95 \times 10^{15})(2.97 \times 10^{-18})}$$

$$T = (0.16)(0.99) e^{-11.583 \times 10^{-3}}$$

$$T = (0.16)(0.99)(0.988) = \underline{0.1565}$$

$n(r)$: electronic density

$$n(r) = n(r+R)$$

$$n(r) = \sum n_q e^{ikr}$$

$$n(r+R) = \sum n_q e^{ik(r+R)} = \sum n_q e^{ikr} e^{ikR}$$

and since $n(r) = n(r+R)$,

$$e^{ikR} = 1$$

$$\cos(kR) + j\sin(kR) = 1$$

$$\begin{matrix} \text{k-space} & \bar{k} \cdot \bar{R} = 2\pi \\ \text{vector} & \xrightarrow{\text{Real space}} \\ & \text{vector} \end{matrix} \quad \text{OR} \quad \bar{k}_i \bar{R}_j = 2\pi \delta_{ij}$$

$$1d: R = \bar{a}$$

$$k = \bar{a}^*$$

$$aa^* = 2\pi \rightarrow a^* = \frac{2\pi}{a}$$

$$2d: R = \bar{a} + \bar{b}$$

$$k = \bar{a}^* + \bar{b}^*$$

$$\begin{aligned} \bar{R} &= u\bar{a} + v\bar{b} + w\bar{c} \\ \bar{k} &= h\bar{a}^* + k\bar{b}^* + l\bar{c}^* \end{aligned}$$

3d

$$aa^* = 2\pi \quad bb^* = 2\pi \quad cc^* = 2\pi$$

$$\text{but } ba^* = 0 \text{ and so on...}$$

$$ca^* = 0$$

$$\text{So, } a^* = x(b \times c)$$

$$\text{i.e. } a^* \perp b \text{ and } c$$

$$aa^* = x a \cdot (b \times c) = 2\pi$$

$$x = \frac{2\pi}{a \cdot (b \times c)}$$

$$a^* = \frac{2\pi(b \times c)}{a \cdot (b \times c)}$$

2d

$$aa^* = 2\pi$$

$$ba^* = 0$$

$$bb^* = 2\pi$$

$$ab^* = 0$$

$$a^* \perp b$$

$$a \parallel a^*$$

$$a^* = \frac{2\pi}{a} \hat{a}$$

$$b^* = \frac{2\pi}{b} \hat{b}$$

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

$$= \frac{a}{\sqrt{b^2 + 36 + 9}} = \frac{a}{\sqrt{61}}$$

Effective mass :

$$\frac{1}{m_{ij}^*} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$$

Curvature of the band determines the effective mass

If $m^* = \infty$, we are referring to e^-
for -ve, we are referring to holes

for Ge, 8 valley degeneracy for e^-
1 " for holes

$\rightarrow E_0$ ($C_B \text{ min}$ is at $x = L$) so,
valley degeneracy = # of hexagon faces
in the Wigner cell

for Si, 6 $\rightarrow e^-$
1 \rightarrow hole

\rightarrow # of square faces in the Wigner Seitz cell
because $C_B \text{ min} \Rightarrow x = r$

for GaAs, 1 $\rightarrow e^-$ (Direct band gap)
1 \rightarrow hole semiconductor

\rightarrow # = 1 because $C_B \text{ min} \Rightarrow x = r$ and we are
at the center of the Wigner cell

\rightarrow for all 3 cases, $V_B \text{ max}$ is at $x = r$ i.e. the
center of the Wigner cell \rightarrow so, # valley
degeneracy for holes = 1

how to get more current?

↓

more charges

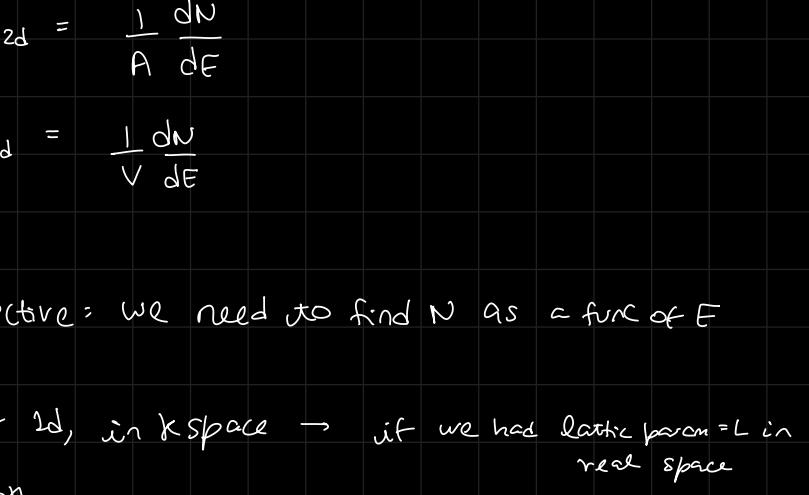
↓

more # of degenerate valleys

OR

wider curvature of
conduction band

narrow curvature \rightarrow low effective mass
wider curvature \rightarrow higher m^*



Curvature can also determine
the density of states

remember, for tunnelling prob \rightarrow

$$K = \sqrt{\frac{2m(v-E)}{\hbar}} \quad \text{for 1 particle}$$

$$= \sqrt{\frac{2m^*(v-E)}{\hbar}} \quad \text{generally}$$

Tunnelling prob $\propto \frac{1}{K} \propto \frac{1}{m^*}$

In case of Ge, we have an equienergy surface

\hookrightarrow isotropic effective mass

\hookrightarrow direction doesn't matter

$$m_e^* = 0.98 m_0 \quad m_t^* = 0.19 m_0$$

longitudinal

transverse

very high m^*

low m^*

slow mobility

higher mobility

band gap: Si \rightarrow 1.12 eV Ge \rightarrow 0.7 eV GaAs \rightarrow 1.45 eV

{ crystal structure is almost similar but the properties differ }

Ge \rightarrow very high off state current

GaAs \rightarrow very low off state current } only one valley
and some for on state current not so ideal

Si \rightarrow balance between Ge, GaAs



Density of States in 2d

$DOS(E) = \# \text{ of states per energy}$
per unit line / area / volume

of energy levels per unit energy
per unit $l/a/v$

$$\overbrace{n}^{\text{number of } e/\text{holes}} = \int DOS(E) \overbrace{f(E)}^{\text{fermi-dirac distribution}} dE$$

limit: $0 \rightarrow \infty$ for e^-

$\rightarrow \infty \rightarrow 0$ for holes

$$DOS_{1d} = \frac{1}{L} \frac{dN}{dE}$$

$$DOS_{2d} = \frac{1}{A} \frac{dN}{dE}$$

$$DOS_{3d} = \frac{1}{V} \frac{dN}{dE}$$

* Objective: we need to find N as a func of E

for 2d, in k-space \rightarrow if we had lattice parameter = L in real space

(1st Brillouin zone)

lowest length

in k-space

(1st Brillouin zone)

\rightarrow we just need the # of e^- in $[-\frac{\pi}{L}, \frac{\pi}{L}]$

for 2d \rightarrow circle and 3d \rightarrow sphere

as we move on the Brillouin zones

(1st \rightarrow 2nd $\rightarrow \dots$)

we are increasing the # of states as well

for 2d \rightarrow area in one quadrant $\rightarrow \pi L^2 \times \frac{1}{4}$

for 3d \rightarrow volume in 1 quad $\rightarrow \frac{4}{3} \pi L^3 \times \frac{1}{8}$

2e- in every state / cube

$$\text{for 3d} \rightarrow N = 2 \times \left(\frac{1}{8} \times \frac{4\pi}{3} L^3 \right)$$

{ lowest volume of each state}

$$DOS_{3d}(E) = \frac{\sqrt{2m}}{\pi^2 \hbar^2} \sqrt{E}$$

$$DOS_{3d} \propto m^{3/2} \text{ and also } \propto \sqrt{E}$$

$$DOS(E) \propto \sqrt{E}$$

$$f(E) \propto \sqrt{E}$$

we are multiplying f(E) and DOS(E)

and we set # e- / hole

density

$$DOS(E) \cdot f(E) dE$$

$$\int DOS(E) \cdot f(E) dE$$

$$n(E) = p(E) = n_i$$

{ intrinsic carrier concentration}

$$\int DOS(E) \cdot f(E) dE$$

$$n_i^2 = n_i^2$$

$$\int DOS(E) \cdot f(E) dE$$

$$n_i^2 = n_i^2$$

$$\int DOS(E) \cdot f(E) dE$$

$$n_i^2 = n_i^2$$