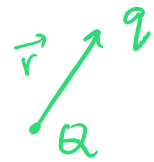
Jan 2, 2020 THURSDAY Lecture 1 # Lecture numbers are 1-indexed.

Grading:

Quizzes : 30% ($2 \times 15\%$ each)
Midsem : 30%
Endsem : 30%

$$\vec{F} = \frac{1}{4\pi\epsilon_0}\frac{Qq}{r^2}\hat{r}$$



$$U = -\int_{-\infty}^{r} \vec{F}\cdot d\vec{r} = \frac{Qq}{4\pi\epsilon_0 r}$$

Gauss law:

(i) $\nabla\cdot\vec{E} = \frac{\rho}{\epsilon_0}$ $\left(\frac{dE}{dx} = \frac{\rho}{\epsilon_0}\right)$

(ii) $E = -\nabla V$ $\left(E = -\frac{dV}{dx}\right)$

$V(x) = \int E\cdot dx$

(iii) $U(r) = qV(r)$

Jan 3, 2020 FRIDAY Lecture 2

- Heisenberg uncertainty Principle

$$\lambda = \frac{h}{p} \longrightarrow \Delta x\cdot\Delta p \geq \frac{\hbar}{2}$$

Car $\rightarrow$ $v = 20\ m/s$

$\Delta v = 0.2\ m/s$

$\Delta p = m\Delta v = 1000 \times 0.2$

$\Delta x \simeq 10^{-37}\ m$

Electron $\rightarrow$ max. velocity in solids $\sim 10^6\ m/s$

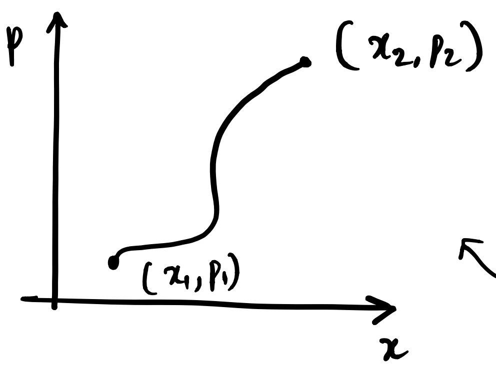
$v = 2\times10^5\ m/s$

$\Delta v = 1\%$ accuracy

$m = 9.1\times10^{-31}\ kg$

$\Delta p = m\Delta v = 9.1\times10^{-31}\ kg$

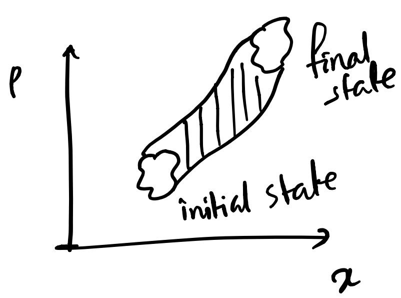
$\Delta x \approx 10\ nm$ $\leftarrow$ order of 10s of nanometers



Newton's law

$$\boxed{\vec{F} = \frac{d\vec{p}}{dt}}$$

can be applied



How to describe this?

$\rightarrow$ Described by wave-function $\psi(\vec{r}, t)$

$\psi(\vec{r}, t)$ lives in Hilbert Space.

- Schrodinger's Equation can describe the evolution of wave-function. (Time dependent Schrodinger eqn.)

Solve schrodinger Eqn. $\longrightarrow$ $\Psi(\vec{r},t)$ $\longrightarrow$ extract information.

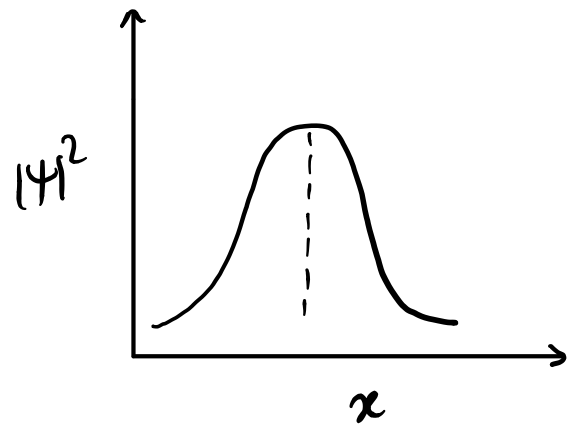
$\Psi(\vec{r},t)$ is a complex function.

$\Psi^*\Psi = |\Psi(\vec{x},t)|^2$ | $|\Psi|^2 dx$ is the Probability that the particle is between x and $x+dx$

- $\displaystyle\int_{-\infty}^{+\infty} |\Psi|^2 dx = 1$ $\leftarrow$ known as Normalization condition.

- Avg. position of particle

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^* x \Psi \, dx$$



- Average momentum of the particle

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^* \underbrace{\left(-i\hbar \frac{d}{dx}\right)}_{\text{Operator of } p} \Psi \, dx \qquad \text{— 1-D case}$$

<u>IN GENERAL</u>

$$\langle Q(x,p) \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi \, dx$$

$\hat{Q} \rightarrow$ Notation for operator of Q.

- KINETIC ENERGY —

Avg. kinetic Energy of the system

$T = \frac{1}{2} mv^2 = \frac{p^2}{2m}$ | $\displaystyle\langle T \rangle = \frac{1}{2m} \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)^2 \Psi \, dx$

$$\boxed{\langle v\rangle = \frac{d\langle x\rangle}{dt}, \quad \frac{d\langle p\rangle}{dt} = \left\langle -\frac{\partial V}{\partial x}\right\rangle}$$ ← These follow Newton's law.

- solving Schrödinger Equation —

$$\Psi(x,t) = \phi(x)\,\chi(t)$$

a constant, why?

$$-\frac{1}{\phi}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\phi] + V(x)\,\cancel{\phi}\,\cancel{\chi} = \frac{i\hbar\,\cancel{\phi}}{\chi}\frac{\partial}{\partial t}[\chi] = E$$

E is a constant because the equation's LHS is a function of x and RHS is a function of time. The only way LHS can be equal to RHS when they are varied is when they are constant.

$$\frac{\partial \chi}{\partial t} = \frac{-iE\chi}{\hbar} \quad \Big| \quad \chi(t) = e^{-iEt/\hbar}$$

$$H = \frac{p^2}{2m} + V(x) \longrightarrow \hat{H} \text{ (operator for total energy)}$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

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

$\boxed{\hat{H}\phi = E\phi}$ → solving this gives

eigenfunctions	eigenenergies
ϕ_1	E_1
ϕ_2	E_2
$\vdots$	$\vdots$

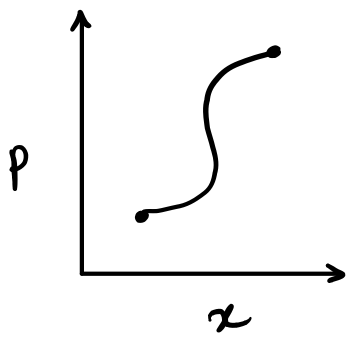
$$\Psi(x, t=0) = \sum_{n=1}^{\infty} a_n \phi_n(x)$$

Find $a_1, a_2, \ldots a_n$

$$\Psi(x,t) = \sum_{n=1}^{\infty} a_n \phi_n e^{-\frac{iE_n t}{\hbar}}$$

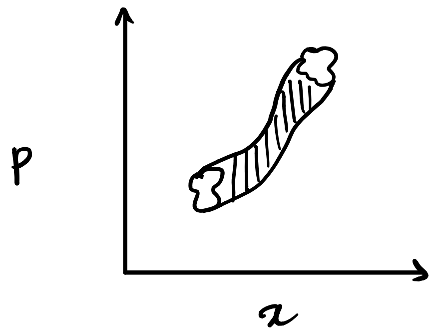
Jan 6, 2020 MONDAY Lecture 3

RECAP



$\vec{F} = \frac{d\vec{p}}{dt} \rightarrow$ TRUE for macroscopic objects

But we have dual nature of matter.



For dual nature described by $\psi(\vec{r}, t)$

$|\psi|^2$ tells us the probability density of the particle.

TDSE $\quad -\frac{\hbar^2}{2m} D^2 \psi + V\psi = i\hbar \frac{d\psi}{dt}$; $V(\vec{r}, t)$ in general

For the case of V:

TISE $\quad \hat{H}\psi = E\psi \rightarrow$ eigenvalue equation

$$\hat{H} = -\frac{\hbar^2}{2m} D^2 + V(x) \quad \therefore \quad \psi(x,t) = \psi(x) e^{-(iEt/\hbar)}$$

Example Free particle

Classical	Quantum Mechanics
$V(x) = 0 \rightarrow$ Time independent	TISE $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 0 = E\psi$
$T = \frac{p^2}{2m}$	$\frac{d^2\psi}{dx^2} = \frac{-2mE\psi}{\hbar^2}$
$E = \frac{p^2}{2m}$	Choose $k^2 = 2mE/\hbar^2$

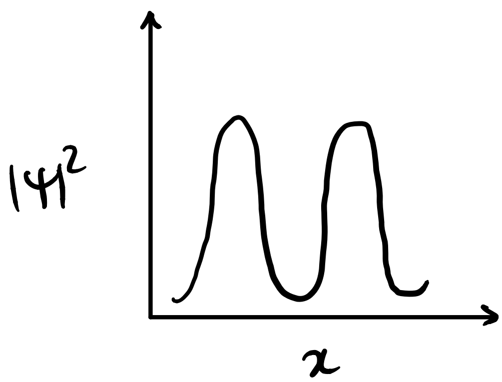
$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

Possible solutions

$\psi \propto \sin(kx),\ \cos(kx),\ e^{ikx},\ e^{-ikx}$

$|\psi|^2 \quad \sin^2(kx),\ \cos^2(kx),\ 1,\ 1$

$\sin(kx)$, $\cos(kx)$ are not realistic why?



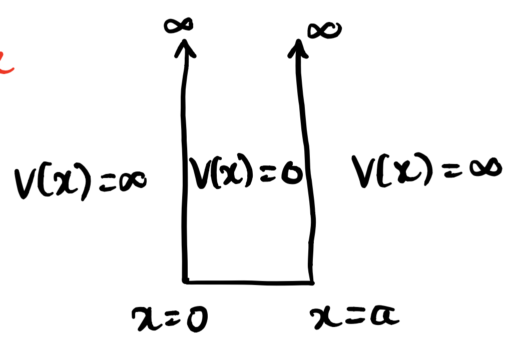
$\therefore\ \psi(x) \propto e^{ikx},\ e^{-ikx}$

$$\boxed{E = \frac{\hbar^2 k^2}{2m}}$$

$$\psi(x,t) \propto e^{ikx}\cdot e^{-iEt/\hbar}$$
$$\propto e^{i(kx-\omega t)}$$

$$p = \hbar k = \frac{\hbar\, 2\pi}{\lambda}\ ;\ \boxed{p = \frac{h}{\lambda}}$$

Example Particle in a 1D box



classical

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

Quantum mechanics

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + 0 = E\psi$$

$\psi(x) = 0 \quad \Big\}\ x \le 0;\ x \ge a$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

Let, $k^2 = \dfrac{2mE}{\hbar^2}$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad ; \quad \psi(x) = A\sin(kx) + B\cos(kx)$$

$\Rightarrow$ why not e^{ikx}, e^{-ikx} ?

put boundary conditions

$\psi(0) = 0 \quad ; \quad 0 = 0 + B \Rightarrow B = 0$

$\psi(a) = 0 \quad ; \quad 0 = A\sin(ka) \Rightarrow \sin(ka) = 0$

$ka = n\pi \quad ; \quad n = 1, 2, 3, \ldots$

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

$$\psi(x) = A\sin\left(\frac{n\pi}{a}x\right) \quad ; \quad n = 1, 2, 3, \ldots$$

Normalize $\psi(x)$ $\quad \int_{-\infty}^{\infty} |\psi|^2 dx = 1$

$$\int_0^a |\psi|^2 dx = 1 \quad [\text{since, a well}]$$

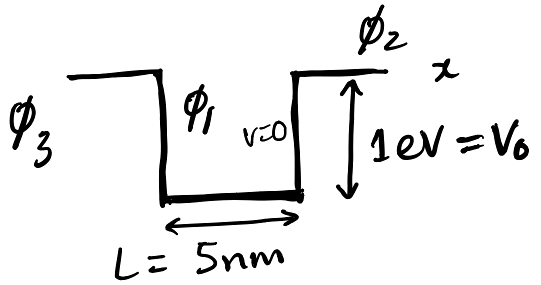
$$\rightarrow \quad A = \sqrt{\frac{2}{a}}$$

$$\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \quad ; \quad 0 \le x \le a$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \quad ; \quad n = 1, 2, 3, \ldots$$

HW: Particle in a 2D / 3D box

FINITE QUANTUM WELL   Lecture 4



$V=0 \rightarrow$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_1}{dx^2} + 0 = E\phi_1$$

$$\phi_1(x) = A\sin(kx) + B\cos(kx)$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_2}{dx^2} + V_0\phi_2 = E\phi_2$$

$$\frac{d^2\phi_2}{dx^2} = \frac{2m(V_0-E)}{\hbar^2}\phi_2$$

$E < V_0$

Let $\frac{2m(V_0-E)}{\hbar^2} = \alpha^2$

$$\frac{d^2\phi_2}{dx^2} = \alpha^2\phi_2$$

$$\phi_2(x) = Be^{\alpha x} + Ce^{-\alpha x}$$

$$\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

at $x=\infty$, $\phi_2(x) \rightarrow 0$

$$\phi_2(\infty) = \cancel{Be^{\alpha\cdot\infty}}^{\,0} + Ce^{-\alpha\cdot\infty}$$

not reasonable

$\phi_2(x) = Ce^{-\alpha x}$; $x > L$

Similarly

$\phi_3(x) = De^{\alpha x}$

$$\phi_1(0) = \phi_3(0)$$

$$\left.\frac{d\phi_1}{dx}\right|_{x=0} = \left.\frac{d\phi_3}{dx}\right|_{x=0}$$

$$\phi_1(L) = \phi_2(L)$$

$$\left.\frac{d\phi_1}{dx}\right|_{x=L} = \left.\frac{d\phi_2}{dx}\right|_{x=L}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$\alpha = k \tan\left(\frac{kL}{2}\right)$ | α is a function of E.

$\alpha = -k \cot\left(\frac{kL}{2}\right)$ | k is also a function of E.

Analytical solution is not possible. Hence, we resort to graphical or numerical solutions.

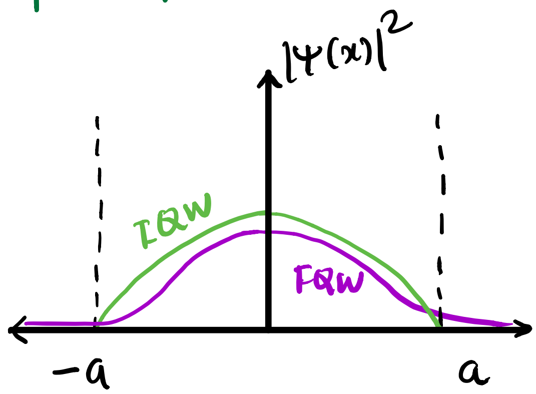
$$k = \frac{\sqrt{2mE}}{\hbar}, \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$\alpha^2 + k^2 = \frac{2mV_0}{\hbar^2} \quad \Big| \quad \alpha^2 = \frac{2mV_0}{\hbar^2} - k^2 \quad \Big| \quad \alpha = \sqrt{\frac{2mV_0}{\hbar^2} - k^2}$$

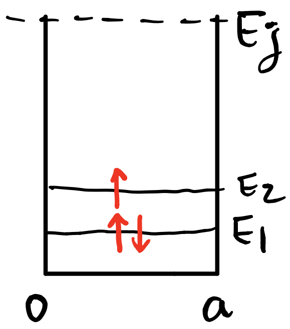
$$\alpha \cdot \frac{L}{2} = \sqrt{\frac{L^2 mV_0}{2\hbar^2} - \left(\frac{KL}{2}\right)^2}$$

	I/W (meV)	F/W (meV)
1	15	12.9
2	60.2	51.7
3	135.4	116
4	240.7	205.9
5	376	320.6
6	541.5	459.3
7	737	620.4
8	962.7	800.4
9		982.8

Δx for finite well is greater than that of infinite well.



Jan 9, 2020 THURSDAY Lecture 5



$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2, \quad n = 1, 2, 3, \ldots$$

Fermions – Spin half – Follows Pauli's exclusion principle

e.g. electrons

what?

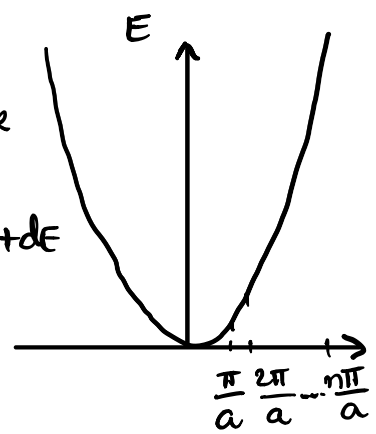
no two e^- can have the same set of all quantum numbers

Bosons – Integral

e.g. Photons

Fermi Energy – Energy of the top most filled state.

$$E_f = \frac{\hbar^2}{2m}\left[\frac{N}{2}\frac{\pi}{a}\right]^2 \leftarrow \text{Fermi Energy}$$



$D(k) = dN/dk \rightarrow$ States between $D(k)\,dk$ $k, k+dk$

$D(E) = dN/dE \rightarrow$ States between $D(E)\,dE$ $E, E+dE$

In k-space all the states are uniformly spaced.

$$\frac{dN}{dk} = 2 \times \frac{1}{(\pi/a)}$$ → Assuming dk is large enough so that we count at least one state.

$$\boxed{\frac{1}{a}\frac{dN}{dk} = \frac{2}{\pi}}$$ For 1-D system

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{1}{a}\frac{dN}{dE} = \frac{1}{a}\frac{dN}{dk} \times \frac{dk}{dE} \quad \Bigg| \quad \boxed{\frac{1}{a}\frac{dN}{dE} = \frac{2}{\pi} \times \sqrt{\frac{m}{2\hbar^2 E}} = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}}$$

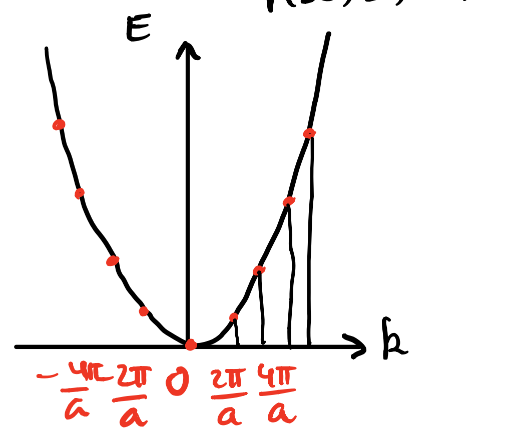
To find E_f $\int_0^{E_f} D(E)\, dE$

PERIODIC BOUNDARY CONDITIONS (PBC)

$\psi(x+a) = \psi(x)$ | $\psi(x) = Ae^{ikx}$

$$\cancel{A} e^{ik(x+a)} = \cancel{A} e^{ikx}$$

$$e^{ika} = 1, \quad k_n = \frac{2n\pi}{a}; \quad n = 0, \pm 1, \pm 2, \dots$$



HW:

Find D(E)

Jan 10, 2020 FRIDAY Lecture 6

1D

$$E = \frac{\hbar^2 k_n^2}{2m}, \quad k_n = \frac{n\pi}{a}; \quad n = 1, 2, 3, \dots$$

$$\boxed{\frac{1}{a} D(k) = \frac{2}{\pi}} \qquad \frac{1}{a} D(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}$$

$$\psi(x+a) = \psi(x)$$

$$A e^{ik(x+a)} = A e^{ikx}$$

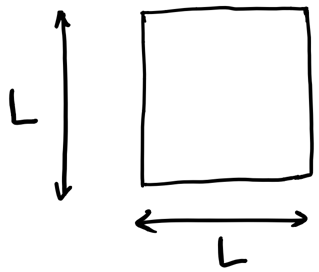
$$e^{ika} = 1 \rightarrow k_n = \frac{2n\pi}{a}; \quad n = 0, \pm 1, \pm 2, \dots$$

$$D(k) = 2 \times \frac{1}{(2\pi/a)} = \frac{a}{\pi}; \quad \boxed{\frac{1}{a} D(k) = \frac{1}{\pi}}$$

$$D(E) = \frac{dN}{dE} = 2\,\frac{dN}{dk} \times \frac{dk}{dE}$$

2: Spin degeneracy

2D



$$\psi(x,y) = B e^{i(k_x x + k_y y)}$$

$$\int_0^L \int_0^L dx\,dy\, \psi^* \psi = 1$$

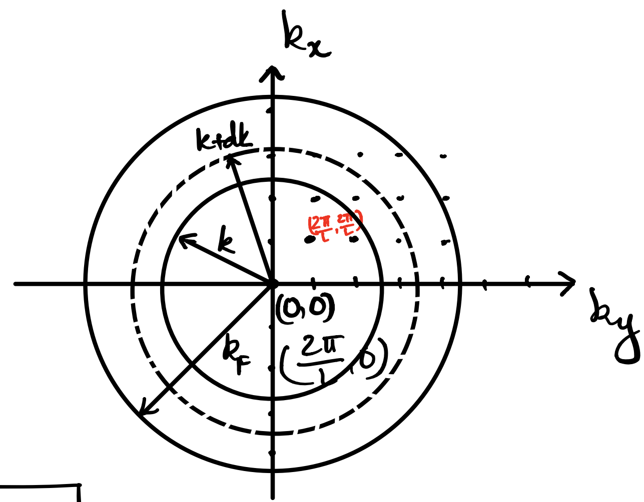
$$B^2 L^2 = 1, \quad B = \frac{1}{\sqrt{L^2}} = \frac{1}{\sqrt{A}}$$

$$\psi(x+L, y) = \psi(x,y) \quad \text{— (1)}$$

$$\psi(x, y+L) = \psi(x,y) \quad \text{— (2)}$$

$$k_x = \frac{2 n_x \pi}{L}, \quad k_y = \frac{2 n_y \pi}{L} \quad \Big|\; n_x, n_y = 0, \pm 1, \pm 2, \ldots$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m}$$



$$D(k) = \frac{dN}{dk} = 2 \times \frac{2\pi k\, dk}{\left(\frac{2\pi}{L}\right)^2 dk}$$

$$D(k) = L^2 \frac{k}{\pi}$$

$$\frac{1}{L^2} D(k) = \frac{k}{\pi} \quad \Big| \quad \boxed{\frac{1}{A} D(k) = \frac{k}{\pi}}$$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m}$$

$$D(E) = \frac{dN}{dE} = \frac{dN}{dk} \times \frac{dk}{dE}$$

$$\frac{1}{A} D(E) = \frac{k}{\pi} \times \frac{m}{\hbar^2 k} = \frac{m}{\pi \hbar^2}$$

Alternate:

$$N = 2 \times \frac{\pi k_F^2}{(2\pi/L)^2} \rightarrow E_F = \frac{\hbar^2 k_F^2}{2m}$$

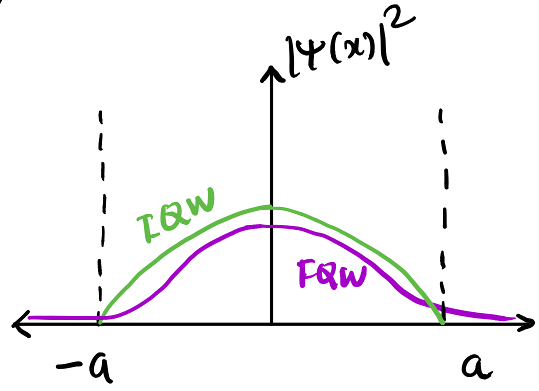
PBC is valid as long as we have a large enough system.

Jan 13, 2020 MONDAY Lecture 7

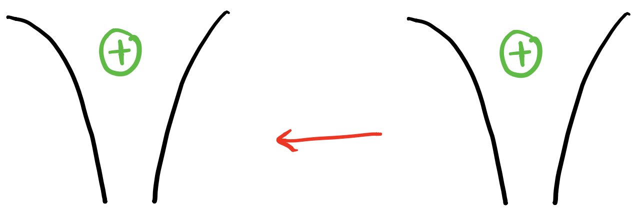
Atom vs. infinite quantum well → one can never make molecule if every atom was an infinite quantum well.

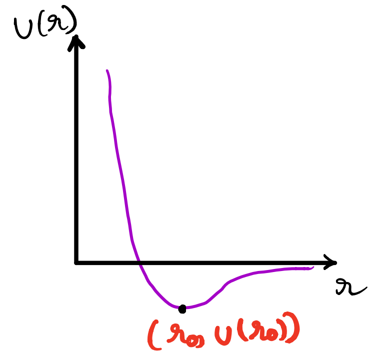
→ Atoms are finite quantum wells.

$\boxed{\text{Solve FQW, Griffiths}}$



FORMATION OF SOLIDS

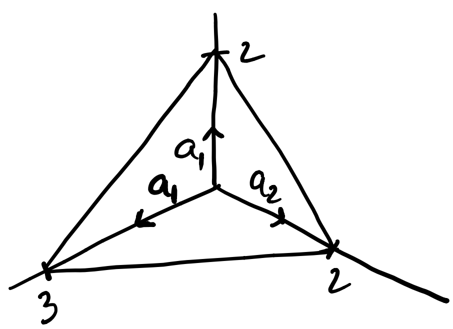




→ Primitive vs. non-primitive lattice | $\boxed{\text{Wigner – Seitz primitive cell}}$

DESCRIBING CRYSTAL PLANES

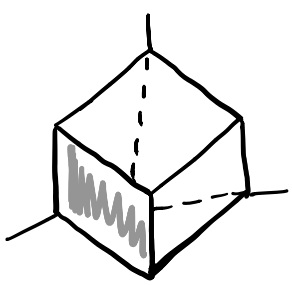
(2 3 3)



$322 \rightarrow \frac{1}{3}\ \frac{1}{2}\ \frac{1}{2} \rightarrow \frac{1}{3}\cdot 6\ \ \frac{1}{2}\cdot 6\ \ \frac{1}{2}\cdot 6$

$\rightarrow (2\ 3\ 3)$

(1 0 0)



quasi crystals, penrose tiles

Jan 16, 2020 THURSDAY Lecture 8

2D Bravais lattices : 5 in total

1. Oblique
2. Rectangular
3. Centered rectangular
4. Hexagonal
5. Square

3D Bravais lattices: 14 lattice types
7 Crystal systems

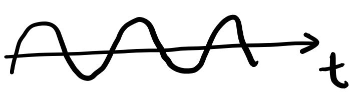
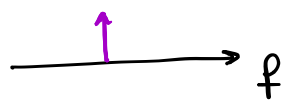
Si → FCC

Assignment discussion

Quiz 1: 30th Jan L18, 9–10 am

Jan 20, 2020 MONDAY lecture-9

Real and Reciprocal lattice

	Time domain	Frequency domain
Signal Representation	 [t]	 $[\frac{1}{t}]$
Crystal Representation	Real space $(\vec{r})$ [length]	Reciprocal space $(\vec{k})$ $[\frac{1}{\text{length}}]$

How to represent in $\vec{k}$ space?

lattice vectors : $\vec{a}_1, \vec{a}_2, \vec{a}_3$

lattice $R_{u_1,u_2,u_3} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$

Reciprocal lattice vectors : $\vec{b}_1, \vec{b}_2, \vec{b}_3$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$b_i \cdot a_j = 2\pi \delta_{ij}$; $\delta_{ij} = 1$; $i=j$
$\qquad\qquad\qquad\qquad = 0$; $i \neq j$ | $R = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$
$G = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{a}_3$ | $u_1, u_2, u_3, v_1, v_2, v_3 \in I$

Fourier Analysis of Crystal

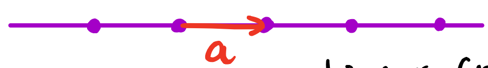
e^- density at two points should be same

$$n(r+R) = n(r) = \sum_G n_G \exp(iG\cdot r)$$

$$\sum n_G \exp(iG\cdot r)\exp(iG\cdot R) = \sum n_G \exp(iG\cdot r)$$

$$\exp(iG\cdot R) = 1$$

Linear Empty lattice : 1D

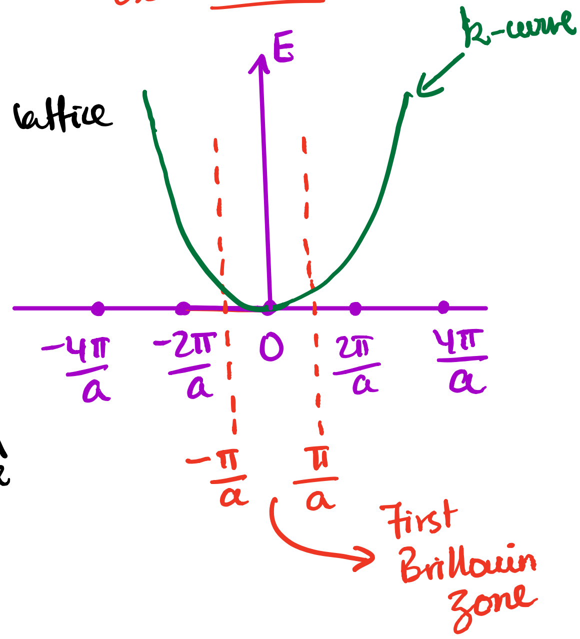


Linear crystal lattice

$$\left.\begin{array}{l}\vec{a}_1 = a\hat{x}\\ \vec{a}_2 = \hat{y}\\ \vec{a}_3 = \hat{z}\end{array}\right\} \rightarrow \vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$$

$$= \frac{2\pi}{a}\hat{x}$$ | $G = v_1\vec{b}$ $= \dfrac{2\pi v_1}{a}\hat{x}$

Extended zone

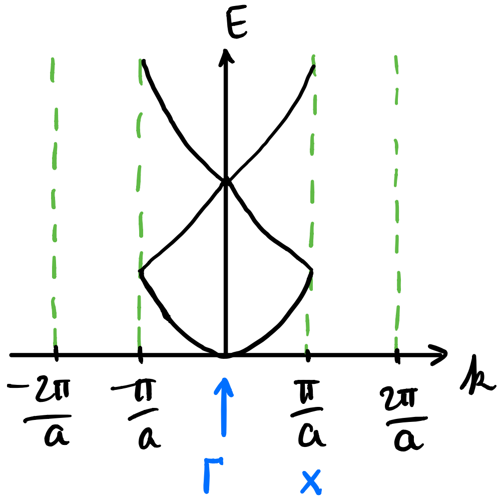


Electron wave function $\rightarrow \psi(x) = \dfrac{1}{\sqrt{L}}e^{ikx}$

$$k_u = \frac{2\pi u}{L} \; ; \; u = 0, \pm 1, \pm 2, \ldots$$

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

Reduced Zone



$$E = \frac{\hbar^2 (k' + G)^2}{2m}$$

k' in first BZ ; $-\frac{\pi}{a} \le k' \le \frac{\pi}{a}$

Γ : center of reciprocal lattice

X : Edge of BZ

Empty lattice case: $$E = \frac{\hbar^2}{2m}\left[k' + \frac{2\pi v_1}{a}\right]^2$$

$$\begin{bmatrix} n-2 & n-1 \\ 1 & 0 \end{bmatrix}^m \begin{matrix} 10 \\ 0 \end{matrix}$$

$v_1 = 0$, $$E = \frac{\hbar^2 k'^2}{2m}$$

$v_1 = 1$, $$E = \frac{\hbar^2}{2m}\left[k' + \frac{2\pi}{a}\right]^2$$

$$\begin{bmatrix} 1 & 2 \\ 1 & 0 \end{bmatrix}^4 \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Jan 23, 2020 THURSDAY

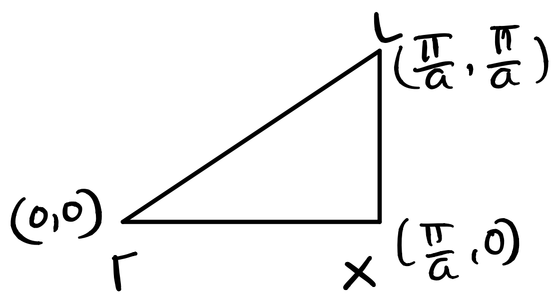
2D Empty Square lattice

$$\left.\begin{aligned} \vec{a}_1 &= a\hat{x} \\ \vec{a}_2 &= a\hat{y} \\ \vec{a}_3 &= \hat{z} \end{aligned}\right\} \rightarrow \begin{aligned} \vec{b}_1 &= \frac{2\pi}{a}\hat{x} \\ \vec{b}_2 &= \frac{2\pi}{a}\hat{y} \end{aligned}$$

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

$$\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2$$

$$\Psi \sim \frac{1}{\sqrt{L^2}} e^{i(k_x x + k_y y)}$$

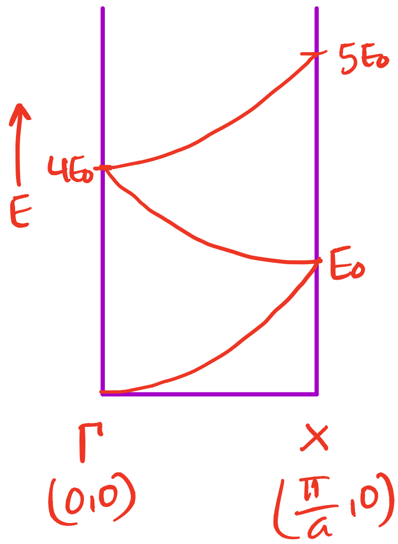


$$E = \frac{\hbar^2}{2m}(\vec{k}' + \vec{G})^2 \quad \Big| \quad E = \frac{\hbar^2}{2m}\left[\left(k_x' + \frac{2\pi}{a}v_1\right)^2 + \left(k_y' + \frac{2\pi}{a}v_2\right)^2\right]$$

Along $\Gamma \to X$

$$E = \frac{\hbar^2}{2m}\left[\left(k_x' + \frac{2\pi}{a}v_1\right)^2 + \left(\frac{2\pi v_2}{a}\right)^2\right]$$

$$E_0 = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$



v_1	v_2
0	0
0	-1
-1	0

Jan 27, 2020 MONDAY Lecture 12

Info from Bandstructure

Extra class on 1st Feb.
Quiz 1 on Thursday
Till today's lecture

① Metal vs. insulator

$\boxed{L = Na}$

even # of e^- in primitive unit cell → insulator
odd # of e^- " " " " → metal
exception : Mg 2 valence e^- → semi metal

② Band-gap

Direct vs indirect band gap

↓ Both min, max at the same K

↘ min, max are at different k values

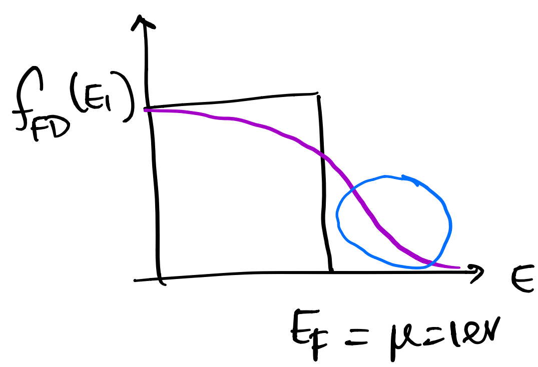
This affects optical properties.
direct band gap materials are important for optical devices.

③ Number of free carriers

Fermi-Dirac Distribution

$$f_{FD}(E) = \frac{1}{\exp\left[(E-\mu)/kT\right]+1}$$

↓
probability of occupation of states



$$n = \int_{E_{CB}}^{E_{CT}} dE\, f_{FD}(E)\, D(E)$$

E_{CB} → conduction band bottom
E_{CT} → conduction band top

Maxwell-Boltzman: If $E-\mu >> kT$

$$p = \int_{E_v} dE \left[1 - f_{FD}(E)\right] D(E)$$

$$E(\vec{k}) = E(\vec{k_0}) + \cancel{\frac{(\vec{k}-\vec{k_0})}{1!} \frac{dE}{dk}}^{\,0} + \frac{(\vec{k}-\vec{k_0})^2}{2!} \frac{d^2E}{dk^2} + \cdots$$

$$\approx E(\vec{k_0}) + \frac{(\vec{k}-\vec{k_0})^2}{2!} \frac{d^2E}{dk^2} \qquad [\text{For small } k]$$

$$\approx E(\vec{k_0}) + \frac{\hbar^2 (\vec{k}-\vec{k_0})^2}{2\left(\frac{\hbar^2}{\frac{d^2E}{dk^2}}\right)} \qquad m^* \to \text{effective mass}$$

Equations of motions in bands

$$\vec{v} = \frac{1}{\hbar} \nabla_k E(\vec{k}) = \frac{1}{\hbar}\left[\hat{x}\frac{\partial}{\partial k_x} + \hat{y}\frac{\partial}{\partial k_y} + \hat{z}\frac{\partial}{\partial k_z}\right] E(\vec{k})$$

$$E = \frac{\hbar^2 k^2}{2m} \longrightarrow v = \frac{1}{\hbar}\frac{\hbar^2 k}{m} = \frac{\hbar k}{m}$$

$$\boxed{\vec{F} = \hbar \frac{d\vec{k}}{dt}}$$

Toy models

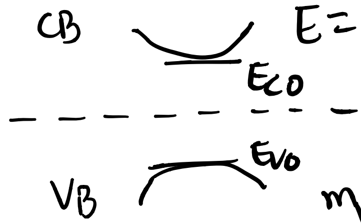
$$E = E_0 + 2 E_{ss} \cos(ka)$$

$$E = E_0 \pm \left(E_{ss}^2 + E_{ss}'^2 + 2 E_{ss} E_{ss}' \cos(ka)\right)^{1/2}$$

Jan 31, Friday — Lecture 13 — New-ish unit

- Number of mobile carriers at $T = 0K$ @ Equilibrium
  - Band structure
  - Fermi-level

$\boxed{\text{Extra class tomorrow! L8, 12-1:15}}$



$$E = \frac{\hbar^2}{2m}\overbrace{[k_x^2 + k_y^2 + k_z^2]}^{k^2}$$

m^*

$$n = \int_{E_{co}}^{E_{cT}} dE \, D(E) \, f_{FD}(E)$$

$E_{cT} \rightarrow$ Top of conduction band

$E_{co} \rightarrow$ bottom of conduction band

* when current flows, equilibrium is disturbed.

- At finite T:

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

Special case:

$E - E_F > 3k_BT$

$E_F - E_{vo} > 3k_BT$

Then $f_{FD}(E) \approx e^{-(E-E_F)/k_BT}$

3D case:

$$n = \int_0^\infty \frac{1}{2\pi^2}\left(\frac{2m_c^*}{\hbar}\right)^{3/2} E^{1/2} e^{-(E-E_F)/k_BT} \, dE$$

$$n = \frac{1}{2\pi^2}\left(\frac{2m_c^*}{\hbar}\right)^{3/2} e^{E_F/k_BT} \int_0^\infty E^{1/2} e^{-E/k_BT} \, dE$$

$$= \frac{(k_BT)^{3/2}}{2\pi^2}\left(\frac{2m_c^*}{\hbar}\right)^{3/2} e^{E_F/k_BT} \int_0^\infty \left(\frac{E}{k_BT}\right)^{1/2} e^{-E/k_BT}\, d\left(\frac{E}{k_BT}\right)$$

$$\boxed{\int_0^\infty x^{1/2} e^{ax} dx = \frac{\sqrt{\pi}}{2a\sqrt{a}}}$$

$$= \frac{(k_BT)^{3/2}}{2\pi^2}\left(\frac{2m_c^*}{\hbar}\right)^{3/2} e^{E_F/k_BT} \cdot \frac{\sqrt{\pi}}{2}$$

$$n = \underbrace{2\left(\frac{2\pi m_c^* k_B T}{h^2}\right)}_{N_C} e^{E_F/k_BT}$$

$\boxed{\text{assumed } E_{c0} = 0}$

if $E_{c0} \neq 0$: $\quad n_i = N_c\, e^{-(E_{c0}-E_F)/k_BT}$

N_c: effective density of states.

$$p = \int (1-f_{FD})\, D(E)\, dE$$

$$p_i = N_v\, e^{(E_{v0}-E_F)/k_BT}$$

Charge neutrality condition:

$$N_c\, e^{-(E_{c0}-E_F)/k_BT} = N_v\, e^{(E_{v0}-E_F)/k_BT}$$

$$\frac{N_c}{N_v} = e^{(E_{v0}-E_F+E_{c0}-E_F)/k_BT}$$

$$k_BT \ln\frac{N_c}{N_v} = E_{v0}+E_{c0}-2E_F \quad\Bigg|\quad E_F = \frac{E_{v0}+E_{c0}-k_BT\ln\left(\frac{N_c}{N_v}\right)}{2}$$

$$E_F = \frac{E_{v0}+E_{c0} - \ln\left(\frac{N_c}{N_v}\right)^{k_BT}}{2}$$

$$\boxed{E_F = \frac{E_{V0} + E_{C0}}{2} - \frac{3k_BT}{4} \ln\left(\frac{m_c^*}{m_v^*}\right)}$$

{ Probability of occupation
Density of states

Bandgap itself is also a function of temperature, duh!

$$n_i = \sqrt{N_c N_v}\, e^{-E_g/2k_BT} \quad \Big| \quad E_g = E_{C0} - E_{V0}$$

$$\boxed{E_F = \frac{E_g}{2} - \frac{3k_BT}{4} \ln\left(\frac{m_c^*}{m_v^*}\right)}$$

References matter

Feb 3, 2020 MONDAY

Substitutional doping → Replace host atom with a different one
→ can give e^- or holes

Activated dopants → substitute and accept / donate e^-

Amphoteric dopants → Si in GaAs. dopes as n-type or p-type

Activation energy of dopants

$$\left[\frac{-\hbar^2}{2m^*}\nabla^2 + V_{imp}(r)\right] f(r) = \left[E - E_c(r)\right] f(r)$$

— 3D effective mass eqn.

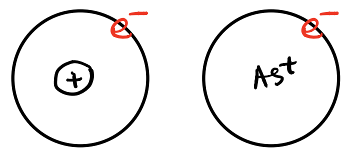
$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 - \frac{q^2}{4\pi\varepsilon r}\right] f(r) = \left[E - E_c(r)\right] f(r)$$

(Hydrogenic model of dopants)

$$E_n = \frac{1}{n^2}\left[\frac{m_0}{2\hbar^2}\left(\frac{q^2}{4\pi\epsilon_0}\right)^2\right] = \frac{-13.6\ eV}{n^2}$$

Typical numbers

$$\underbrace{E_c - E_d}_{\text{activation energy}} = \frac{13.6\ eV \times m^*}{(\mathcal{E}_r)^2} = \frac{13.6\ eV \times 0.1}{(10)^2} \approx 13.6\ meV$$



$$\underset{\text{Donor}}{N_D^+} = \frac{N_D}{1 + g_D\, e^{(E_f - E_D)/k_B T}} \quad ; \quad g_D = 2$$

↳ depends on spin up or spin down

$$\underset{\text{Acceptor}}{N_A^-} = \frac{N_A}{1 + g_A\, e^{(E_f - E_D)/k_B T}} \quad ; \quad g_A = 4$$

$$p + N_D^+ = n + N_A^-$$

$$\int \underbrace{[1 - f_{FD}(E)]\, D_v(E)\, dE}_{p_0 = N_v\, e^{(E_v - E_F)/k_B T}} + (\ ) = \int \underbrace{f_{FD}(E)\, D_c(E)}_{n_0 = N_c\, e^{(E_F - E_c)/k_B T}} + (\ )$$

$$n_0 p_0 = N_C N_V\, e^{-E_g/k_B T} = n_i^2$$

$$\boxed{n_0 p_0 = n_i^2} \rightarrow \text{law of mass action}$$

n-type: $N_A^- = 0$

$$\frac{n_i^2}{n_0} + N_D^+ = n_0$$

$$n_0^2 - N_D^+ n_0 - n_i^2 = 0$$

$$n_0 = \frac{N_D^+ + \sqrt{(N_D^+)^2 + 4n_i^2}}{2}$$

$N_D^+ \rightarrow N_D$

$$\rightarrow \quad n_0 = \frac{N_D + \sqrt{(N_D^+)^2 + 4n_i^2}}{2}$$

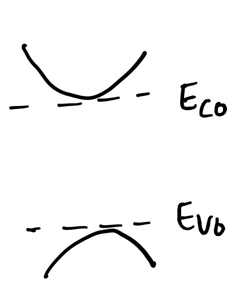
Feb 7, 2020 Friday

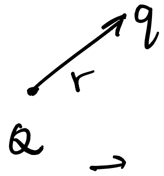
$$n = N_c \, e^{(E_{Fn} - E_c)/k_BT}$$

$$p = N_v \, e^{(E_v - E_{Fp})/k_BT}$$

$$np = \underbrace{N_c N_v \, e^{-E_g/k_BT}}_{n_i^2} \; e^{(E_{Fn} - E_{Fp})/k_BT}$$

Feb 10, 2020 Monday





$$\vec{F} = \frac{1}{4\pi\epsilon_0}\frac{Q}{r^2}\hat{r}$$

$$V(r) = \frac{1}{4\pi\epsilon_0}\frac{Q}{r}$$

$$E = qV(r)$$

electric field

$$F(x) = \frac{\partial V(x)}{\partial x}$$

$$\nabla\cdot\vec{F} = \rho/\epsilon$$

$$\downarrow$$

$$\frac{\partial}{\partial x}\left[\epsilon_s(x)\frac{\partial V(x)}{\partial x}\right] = -\rho(x)$$

$$\boxed{\frac{\partial^2 V(x)}{\partial x^2} = \frac{-\rho(x)}{\epsilon_s}}$$

each of these can be a f(x)

$$\rho(x) = q\left[\overbrace{p + N_D^+ - n - N_A^-}\right]$$

$$q \equiv e^- = 1.6\times10^{-19}\,C$$

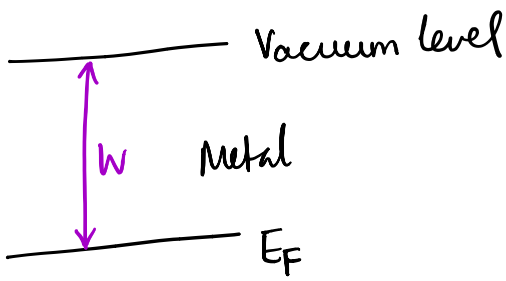
$$E_{C_0}(x) = -q\,V(x)$$

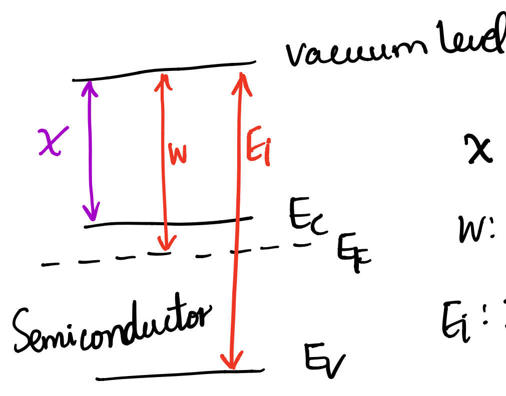
$$E_{V_0}(x) = E_{C_0}(x) - E_g$$

$$F(x) = +\frac{1}{q}\frac{dE_{C_0}(x)}{dx}$$

→ At equilibrium Fermi level is constant everywhere.

Relevant Energies





χ : Electron affinity

W: work function

E_i : Ionization energy

HW 3

Problem 2

$$n = \int_{E_{C_0}} D(E) f(E) \, dE$$

$$p = \int D(E) [1 - f(E)] \, dE$$

$\downarrow$

$$\left(\frac{m_v^*}{\pi \hbar^2} \right)$$

$$1 - \frac{1}{1 + e^{(E-E_F)/k_BT}}$$

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

$$n = \frac{m^*}{k_BT} \int_{E_{C_0}}^{\infty} e^{-(E-E_F)/k_BT} \, dE$$

$$= \frac{m^*}{k_BT} e^{E_F/k_BT} \, k_BT \int_{E_{C_0}}^{\infty} e^{-E/k_BT} \, d\left(\frac{E}{k_BT}\right)$$

$$n = N_c \ln \left[1 + e^{(E_F - E_{C_0})/k_BT} \right]$$

$\downarrow$

$$\frac{m_c^* k_BT}{\pi \hbar^2}$$