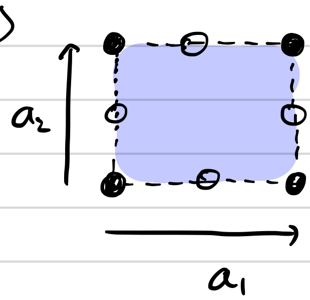
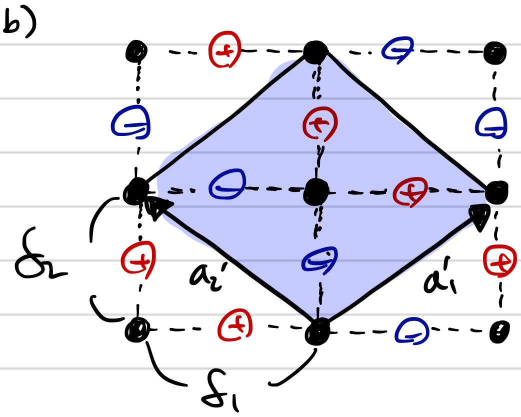
1. (a)



basis : $d_1 = 0$,
$d_2 = \frac{1}{2} a_1$
$d_3 = \frac{1}{2} a_2$

(b)



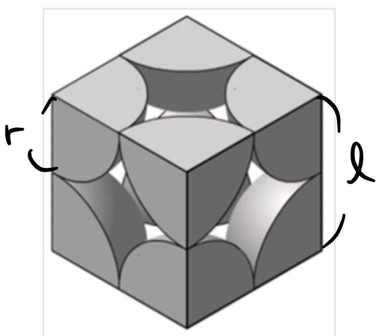
let ● form rectangular lattice with spacing (δ_1, δ_2). Then

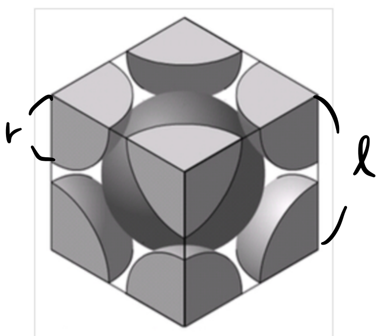
$a_1' = (\delta_1, \delta_2)$ → $b_1' = \frac{1}{\alpha}(\delta_2, \delta_1)$

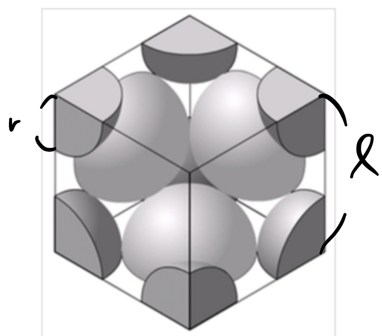
$a_2' = (-\delta_1, \delta_2)$ $b_2' = \frac{1}{\alpha}(-\delta_2, \delta_1)$

$$\underline{\alpha^{-1} = \pi / \delta_1 \delta_2}$$ "

2. ① Simple Cubic ② Body-Centred Cubic ③ Face-Centred Cubic







① SC : $l = 2r$ → ratio $= \frac{4}{3}\pi r^3 / l^3 = \frac{\pi}{6}$

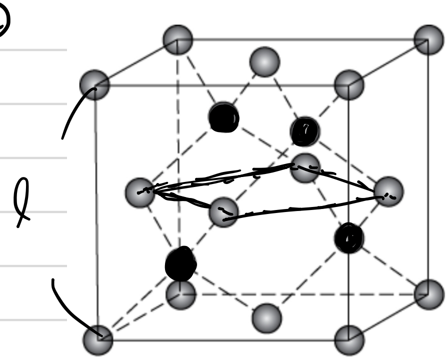
② BCC : diagonal of the cube $= \sqrt{3} l = 4r$ ~> ratio $= \frac{2 \cdot \frac{4}{3}\pi r^3}{l^3} = \frac{\frac{8}{3}\pi}{\frac{64\sqrt{3}}{9}}$

$\therefore l = \frac{4\sqrt{3}}{3} r$ $l^3 = \frac{64 \cdot 3\sqrt{3}}{27} r^3$ $= \frac{\sqrt{3}\pi}{8}$

③ FCC : $4r = \sqrt{2} l$ ~> ratio $= \frac{4 \frac{4}{3}\pi r^3}{l^3} = \frac{\frac{16\pi}{3}}{16\sqrt{2}} = \frac{\sqrt{2}\pi}{6}$

$l = 2\sqrt{2} r$

④



closest interatomic distance in this structure

$$2r = \frac{\sqrt{3}}{4} l \rightarrow l = \frac{8\sqrt{3}r}{3}$$

$$\text{ratio} = \frac{(4+3+1) \times \frac{4}{3}\pi r^3}{l^3} = \frac{\frac{32}{3}\pi r^3}{8 \cdot \frac{64}{27} 3\sqrt{3} r^3}$$

$$= \frac{\pi}{8 \cdot \frac{2}{8}\sqrt{3}} = \frac{3\pi}{16\sqrt{3}} = \frac{\sqrt{3}}{16}\pi$$

3. Use the identity $A \times B \times C \times D$ (vector quadruple product)

$$= [A, B, D]\, C - [A, B, C]\, D$$

$$[A, B, C] := A \cdot (B \times C)$$

(a) $V \equiv a_1 \cdot (a_2 \times a_3)$

$$b_2 \times b_3 = \left(\frac{2\pi}{V}\right)^2 (a_3 \times a_1) \times (a_1 \times a_2) = \left(\frac{2\pi}{V}\right)^2 [a_3, a_1, a_2]\, a_1$$

$$= \left(\frac{2\pi}{V}\right)^2 \cdot V \cdot \vec{a_1}$$

$$\Rightarrow b_1 \cdot (b_2 \times b_3) = \left(\frac{2\pi}{V}\right)^3 \cdot V \cdot a_1 \cdot (a_2 \times a_3) = \frac{(2\pi)^3}{V}$$

(b) WLOG, let's show this for a_1'

$$a_1' = 2\pi \frac{b_2 \times b_3}{b_1 \cdot (b_2 \times b_3)} = 2\pi \frac{V}{(2\pi)^3} \left(\frac{2\pi}{V}\right)^2 \cdot V \cdot a_1 = a_1$$

(c) See any calculus I textbook.

4. $H\psi = E\psi \qquad V(x) = \sum_n aV_0\,\delta(x-na)$

(a) $\left(\frac{\hat{p}^2}{2m} + V(x)\right)\psi(x) = E\psi(x)$

$$\hat{p} = -i\hbar\partial_x \rightsquigarrow \left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\psi(x) = E\psi(x) \quad \text{— (1)}$$

- For an open interval $(0,a) \equiv I_1$, we see that

$$\psi'' = -\frac{2mE}{\hbar^2}\psi \rightarrow \psi_1(x) = A\,e^{iKx} + Be^{-iKx}$$

- Bloch's theorem tells $\psi(x) = e^{ikx}\,u(x)$ for some k and a periodic function $u(x+a) = u(x) \rightsquigarrow \psi(x+a) = e^{ika}\,\psi(x)$

- For an open interval $(-a,0) \equiv I_2$, we see that

$$\underset{\substack{\uparrow\\ I_2}}{\psi_2(x)} = e^{-ika}\,\underset{\substack{\uparrow\\ I_1}}{\psi_1(x+a)} = e^{-ika}\left(A\,e^{iK(x+a)} + Be^{-iK(x+a)}\right)$$

- 1) Continuity of $\psi(x) \Rightarrow \psi_1(0) = \psi_2(0)$

$$\rightsquigarrow A+B = e^{-ika}\left(Ae^{iKa} + Be^{-iKa}\right)$$

$$\left(1 - e^{-ia(k-K)}\right)A + \left(1 - e^{-ia(k+K)}\right)B = 0$$

2) Schrodinger Eqn $\Rightarrow$ Integrating (1) on $\left(-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right)$

$$\Rightarrow \left[\frac{d\psi}{dx}\right]_{-\frac{\varepsilon}{2}}^{\frac{\varepsilon}{2}} = +\overbrace{\frac{2maV_0}{\hbar^2}}^{\equiv\eta}\psi(0) = +\eta(A+B)$$

$$\Downarrow$$

$$(iKA - iKB) - \left(iKAe^{-i(k-K)a} - iKBe^{-i(k+K)a}\right) = +\eta(A+B)$$

$$\rightsquigarrow A\left(1 - e^{-i(k-K)a} - \frac{\eta}{iK}\right) - B\left(1 - e^{-i(k+K)a} + \frac{\eta}{iK}\right) = 0.$$

$$\frac{A}{B} = \frac{-\left(1 - e^{-ia(k+K)}\right)}{1 - e^{-ia(k-K)}} = \frac{1 - e^{-i(k+K)a} + \frac{\eta}{iK}}{1 - e^{-i(k-K)a} - \frac{\eta}{iK}}$$

$$\frac{A}{B} = \frac{-(1-e^{-ia(k+K)})}{1-e^{-ia(k-K)}} = \frac{1-e^{-i(k+K)a} + \frac{\eta}{iK}}{1-e^{-i(k-K)a} - \frac{\eta}{iK}}$$

$$\Rightarrow \quad 1 - e^{-ia(k-K)} - e^{-ia(k+K)a} + e^{-2iak} - \frac{\eta}{iK} e^{-ia(k-K)} + \frac{\eta}{iK}$$

$$= -\left(1 - e^{-ia(k+K)} - e^{-ia(k-K)} + e^{-2iak} + \frac{\eta}{iK} e^{-ia(k+K)} - \frac{\eta}{iK}\right)$$

$$\rightarrow \quad 2(e^{ika} + e^{-ika}) - e^{iaK} - e^{-iaK} - \frac{\eta}{iK} e^{iaK} + \cancel{\frac{\eta}{iK}} e^{+ika}$$

$$- e^{-iKa} - e^{iKa} + \frac{\eta}{iK} e^{-iKa} - \cancel{\frac{\eta}{iK}} e^{ika} = 0$$

$$\rightarrow \quad 4\cos ka - 4\cos Ka - \frac{\eta}{K} 2\sin Ka = 0$$

$$\cos ka = \cos Ka + \frac{\eta}{2K}\sin Ka$$

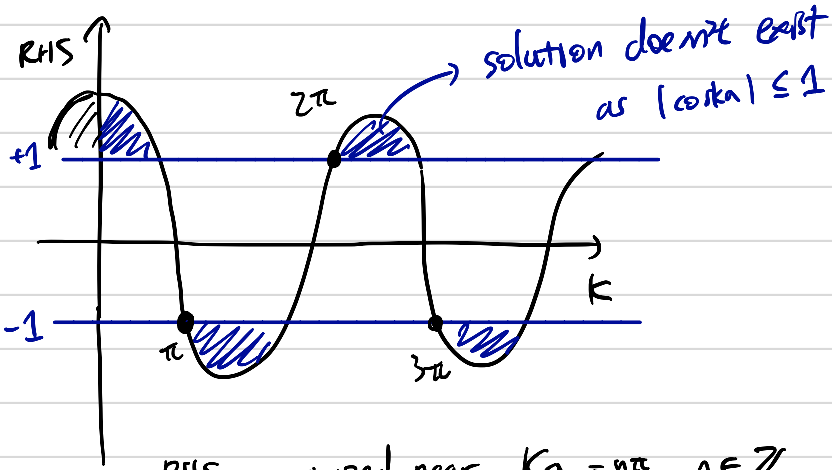
$$= \cos Ka + \frac{maV_0}{\hbar^2 K}\sin Ka$$

$$\parallel$$

$$\frac{aV_0}{K} \Rightarrow \boxed{\alpha = \frac{ma}{\hbar^2}}$$

(b) $\overbrace{\cos ka}^{LHS} = \overbrace{\frac{H}{k}\sin ka + \cos ka}^{RHS}$

if $V_0 \ll \frac{\hbar^2}{ma^2}$ $\quad k = \frac{\sqrt{2mE}}{\hbar}$ $\quad H = \frac{ma}{\hbar^2}V_0$



RHS maximized near $ka = n\pi$ $\quad n \in \mathbb{Z}$

⇒ Expand RHS around $ka = n\pi$

$$\frac{H}{k}\sin ka = \frac{H}{k}\sin[(ka-n\pi)+n\pi]$$

$$= \frac{H}{k}(-1)^n(ka-n\pi)$$

$$\cos ka = \cos[(ka-n\pi)+n\pi]$$

$$= (-1)^n\left(1-\frac{1}{2}(ka-n\pi)^2\right)$$

let $ka - n\pi \equiv \delta$

⇒ $\cos ka = (-1)^n\left[\frac{H}{k}\delta + 1 - \frac{1}{2}\delta^2\right]$

$\parallel$

$1 + \frac{Ha}{\delta+n\pi}\delta - \frac{1}{2}\delta^2 = 1$

⇒ $\frac{Ha}{\delta+n\pi} = \frac{1}{2}\delta$ ⇒ $2Ha = \delta^2 + \delta n\pi$

⇒ $\delta^2 + n\pi\delta - 2Ha = 0$

→ $\delta \approx \frac{2Ha}{n\pi}$ (and 0)

$\delta = 0$ is also solution. (obviously).

⇒ since $E = \frac{\hbar^2k^2}{2m}$

$$\Delta E = \frac{\hbar^2}{2ma^2}\left((n\pi+\delta)^2 - (n\pi)^2\right)$$

$$= \frac{\hbar^2}{2ma^2}2n\pi\delta$$

$$= \frac{2n\pi\hbar^2}{ma^2}\frac{Ha}{n\pi} = \frac{2Ha\hbar^2}{m} = 2V_0$$

Other Method.

$$\sum_{n\in\mathbb{Z}} V_0 a\,\delta(x-na)$$

$$= \sum_n V_0 e^{i\frac{2\pi n}{a}x}$$

"Dirac Comb"

for any n: V_0 connects k, $k+\frac{2\pi n}{a}$

V_0 〃 k, $k-\frac{2\pi n}{a}$

$$\begin{pmatrix} E^0_{\frac{n\pi}{a}} & V_0 \\ V_0 & E^0_{-\frac{n\pi}{a}} \end{pmatrix}\begin{pmatrix} \psi_{\frac{n\pi}{a}} \\ \psi_{-\frac{n\pi}{a}} \end{pmatrix} = E\left(\;\;\right)$$

$E_{\frac{n\pi}{a}} = E_{-\frac{n\pi}{a}}$

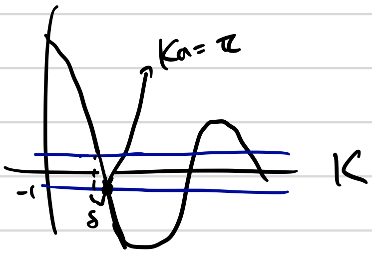
$$E_{\frac{n\pi}{a}} = E^{(0)}_{\frac{n\pi}{a}} \pm V_0$$

Naively stating result from class is totally wrong

(c) When $U_0 \gg \frac{\hbar^2}{ma^2}$

$\cos ka$ contribution ignorable for first band.

$\rightsquigarrow \quad \cos ka = \frac{H}{K}\sin Ka + \cos Ka \approx \frac{-Ha}{\delta+\pi}\delta - 1 \quad \rightsquigarrow \quad \frac{\delta Ha}{\delta+\pi} = -2$



let $Ka - \pi = \delta$

$$\frac{H}{K}\sin(\delta+\pi)$$

$$= -\frac{H}{K}\sin\delta$$

$$\approx -\frac{Ha}{\delta+\pi}\delta$$

$$\delta Ha = -2(\pi+\delta)$$

$$\delta(2+Ha) = -2\pi$$

$$\delta = \frac{-2\pi}{2+Ha} \approx -\frac{2\pi}{Ha}$$

$$Ha = \frac{ma^2}{\hbar^2}V_0$$

$$\Rightarrow \text{width} = \frac{\hbar^2}{2ma^2}\left(\pi^2 - (\pi+\delta)^2\right)$$

$$= \frac{\hbar^2}{2ma^2}(-2\pi\delta)$$

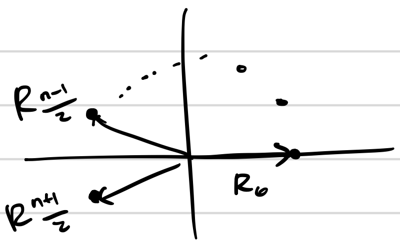
$$= \frac{-\pi\delta}{ma^2}\hbar^2.$$

$$= \boxed{\frac{\pi^2}{ma^2}\frac{2\hbar^2}{2+Ha}}$$

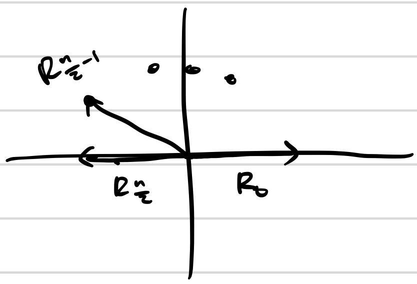
$$\approx \boxed{\frac{2\pi^2\hbar^4}{m^2a^4U_0}}$$

//

5. WLOG, let $R_0 = \hat{x} \equiv \vec{a}_1$ which is shorter than $\vec{a}_2$



n = odd

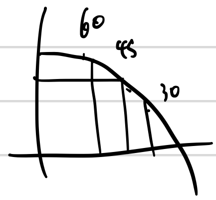


n = even.

(n odd) $\quad R_0 + R_{\frac{n-1}{2}} \in \vec{R} = n a_1 + n a_2$

$\to |R_0 + R_{\frac{n-1}{2}}| \geq 1$

$$\to \left|1 + e^{\frac{2\pi i}{n}\left(\frac{n-1}{2}\right)}\right| = \left(1+\cos\pi\left(1-\frac{1}{n}\right)\right)^2 + \left(\sin\pi\frac{1}{n}\right)^2$$



$$= 1 + 1 - 2\cos\frac{\pi}{n}$$

$$= 2\left(1-\cos\frac{\pi}{n}\right) \geq 1 \qquad \theta \equiv \frac{\pi}{n}$$

$$1 \geq 2\cos\frac{\pi}{n} \to \frac{1}{2} \geq \cos\frac{\pi}{n}$$

$$\to \theta \geq \frac{\pi}{3} \to \boxed{n \leq 3}$$

(n even) $\quad \sim \left|1 + e^{\frac{2\pi i}{n}\left(\frac{n}{2}-1\right)}\right|$

$$= 2\left(1-\cos\frac{2\pi}{n}\right) \geq 1$$

$$\to \theta \geq \frac{\pi}{6} \to \boxed{n \leq 6}$$

$\boxed{\sim n = 2, 3, 4, 6 \text{ are only allowed symr.}}$

6. In 1D, Schrodinger Eqn is 2nd order ODE

$\Rightarrow$ Only allow at most two linearly independent solutions for a given E.

$$\hat{H}\psi = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) \right]\psi = E\psi$$

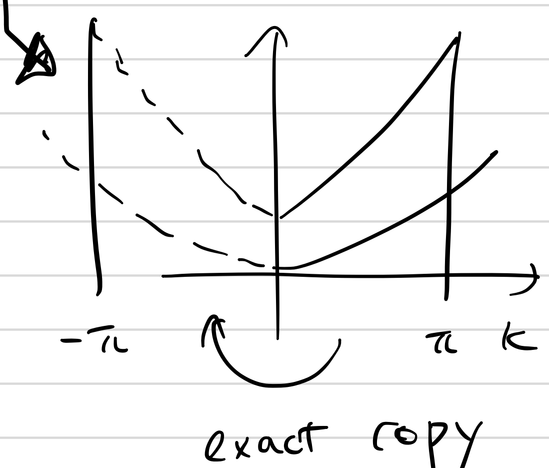
$$(\hat{H} - E)\psi = 0 \rightsquigarrow \text{ODE.}$$

Also, let ψ be solution in the bloch form. (quasi momentum $\vec{k}$)

Then there also exists other solution with $(-k, E)$.

(Assume H is T-invariant)

If there is band overlap, there exists



at least 3-fold degeneracy

$\Rightarrow$ contradiction

$\Rightarrow$ no Band Overlap