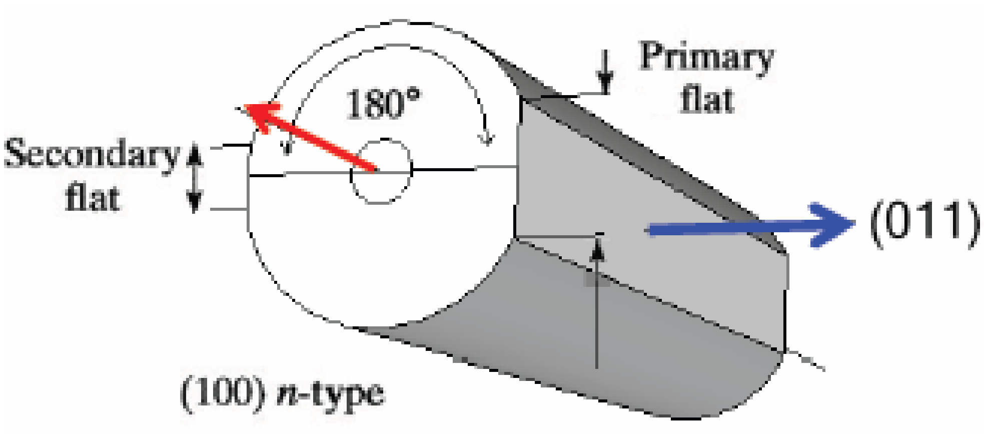
EE 207 : 2018

Tutorial-1

Crystal Structure and Quantum Mechanics

31st July, 2018

1. How do I have to orient my wafer in order to fabricate devices along [020]?



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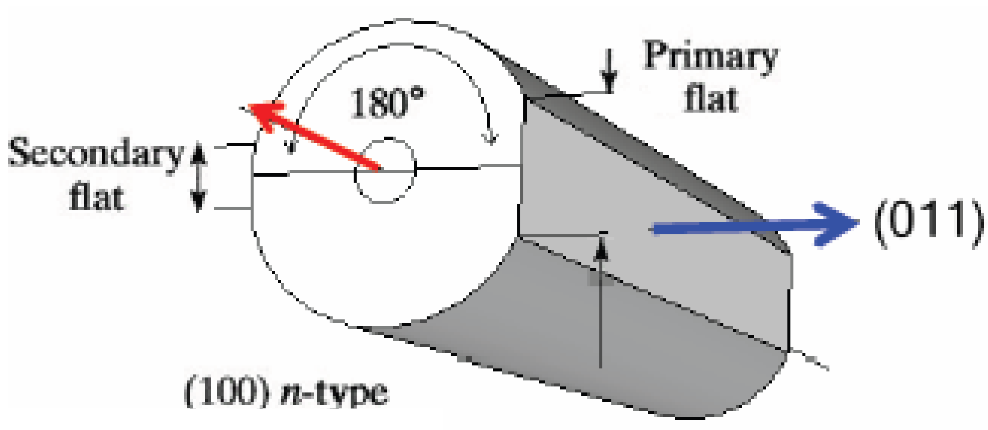

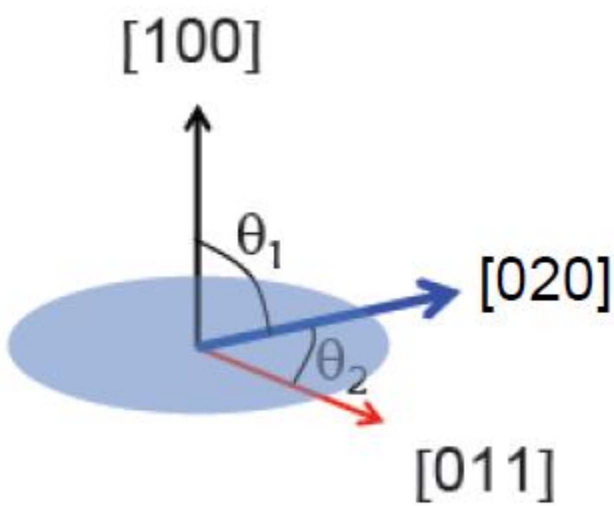

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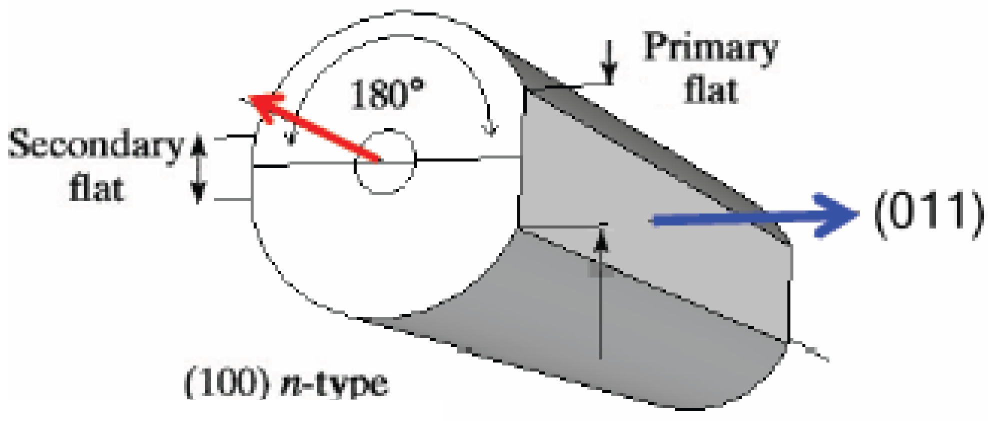

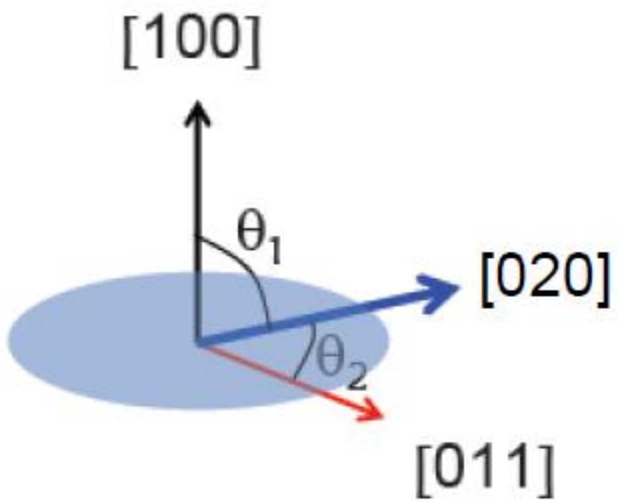

$$\cos\theta_1 = \frac{(1\cdot 0 + 0\cdot 2 + 1\cdot 0)}{1\cdot 2} = 0$$

$$\cos\theta_2 = \frac{(0\cdot 0 + 1\cdot 2 + 1\cdot 0)}{\sqrt{2}\cdot 2} = \frac{1}{\sqrt{2}}$$

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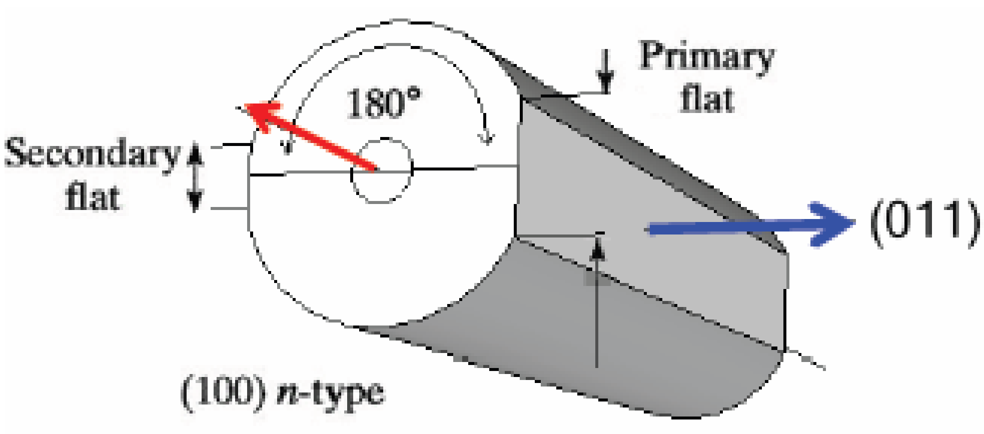

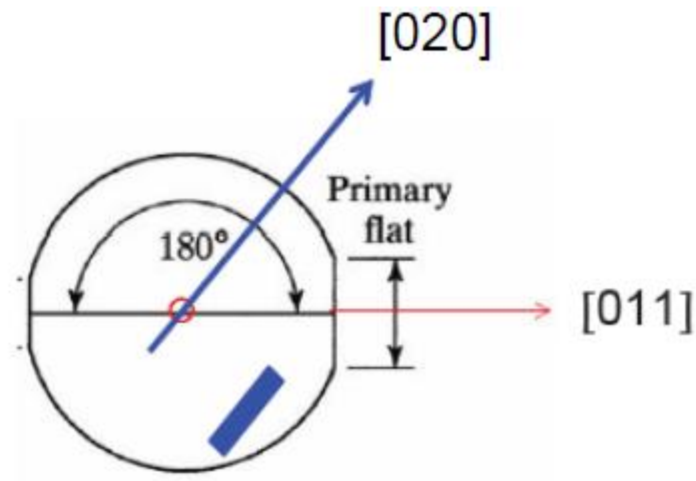

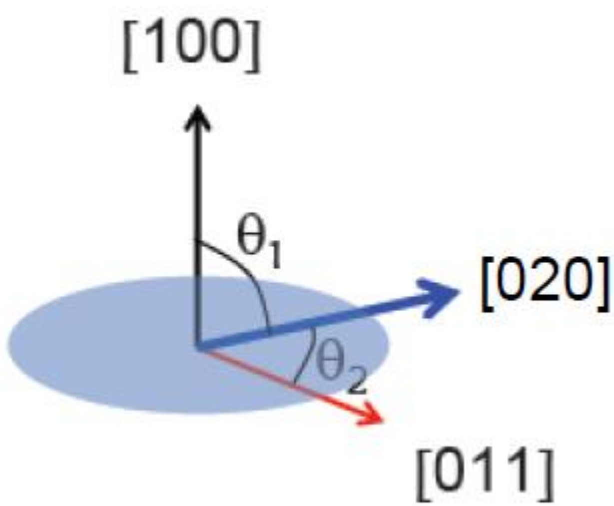

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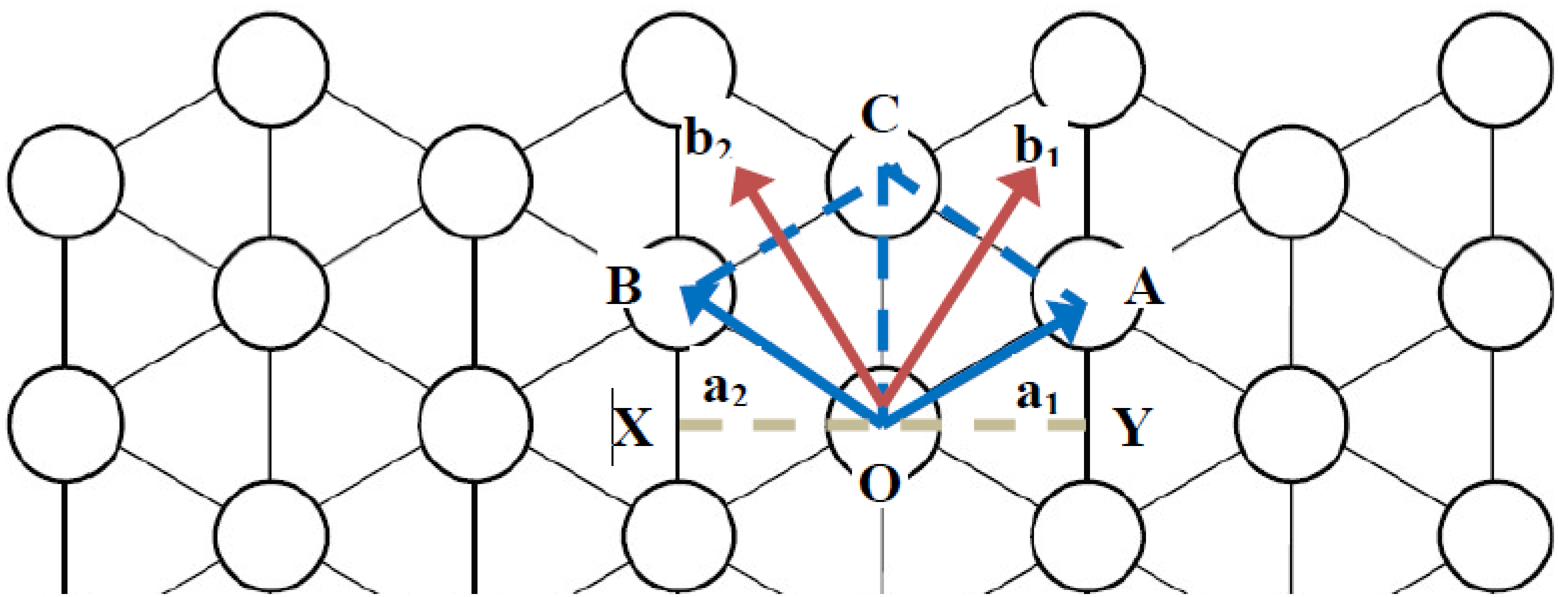
2. Name the kind of lattice with the following set of primitive vectors and derive the reciprocal lattice primitive vectors.

$$a_1 = \frac{a\sqrt{3}}{2}\hat{x} + \frac{a}{2}\hat{y}$$

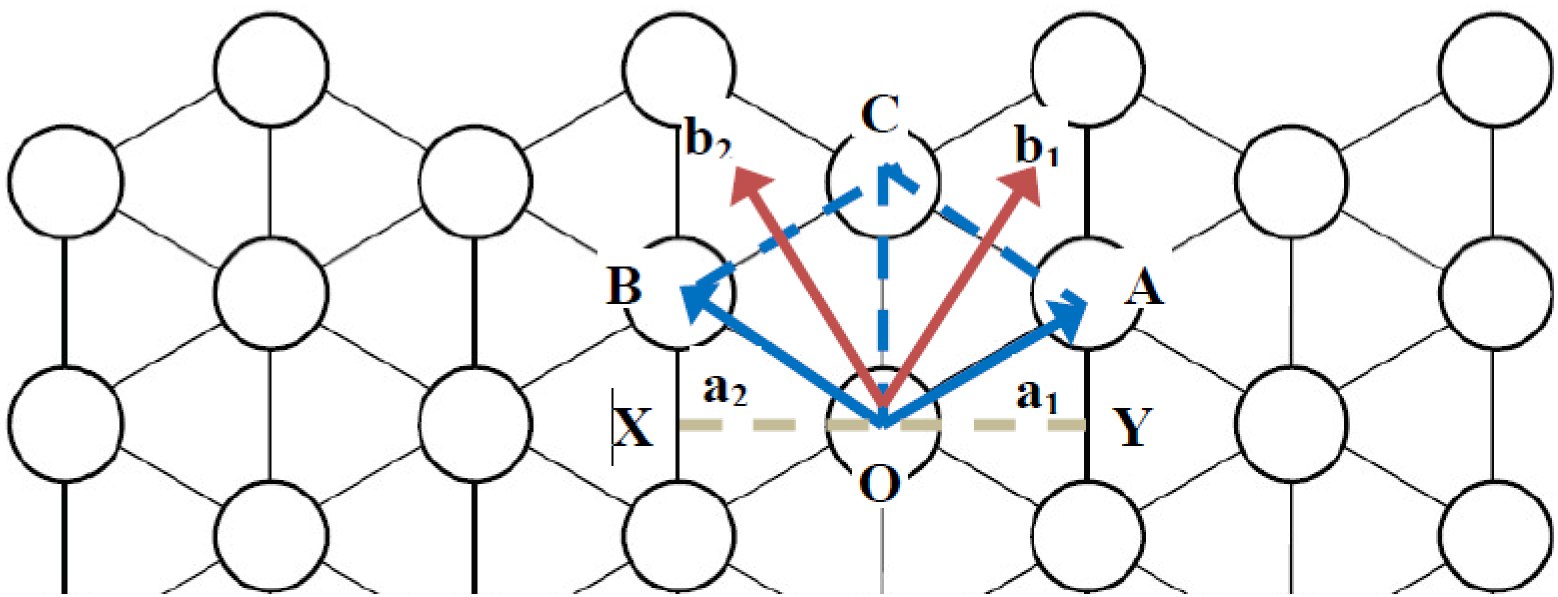
$$a_2 = -\frac{a\sqrt{3}}{2}\hat{x} + \frac{a}{2}\hat{y}$$

$$a_3 = c\hat{z}$$

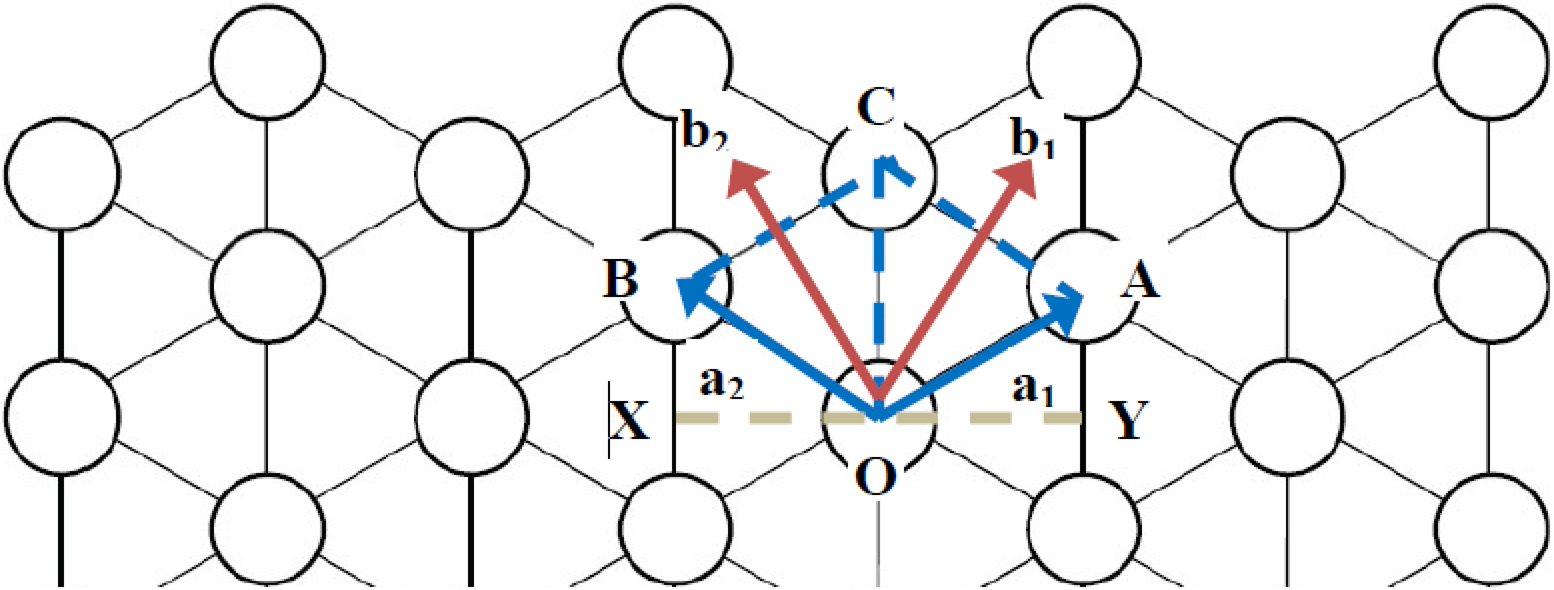


$$\sin(AOY) = \frac{1}{2} \Rightarrow AOY = 30^0 \quad \sin(AOC) = \frac{\sqrt{3}}{2} \Rightarrow AOC = 60^0$$

$$\text{Similarly } \sin(BOC) = \frac{\sqrt{3}}{2} \Rightarrow BOC = 60^0$$



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



What is the orientation of reciprocal lattice w.r.t. real-space lattice?

3. Consider the plane (hkl) in direct lattice of a crystal structure, prove that the reciprocal lattice vector $\boldsymbol{G} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}$ is perpendicular to this plane.

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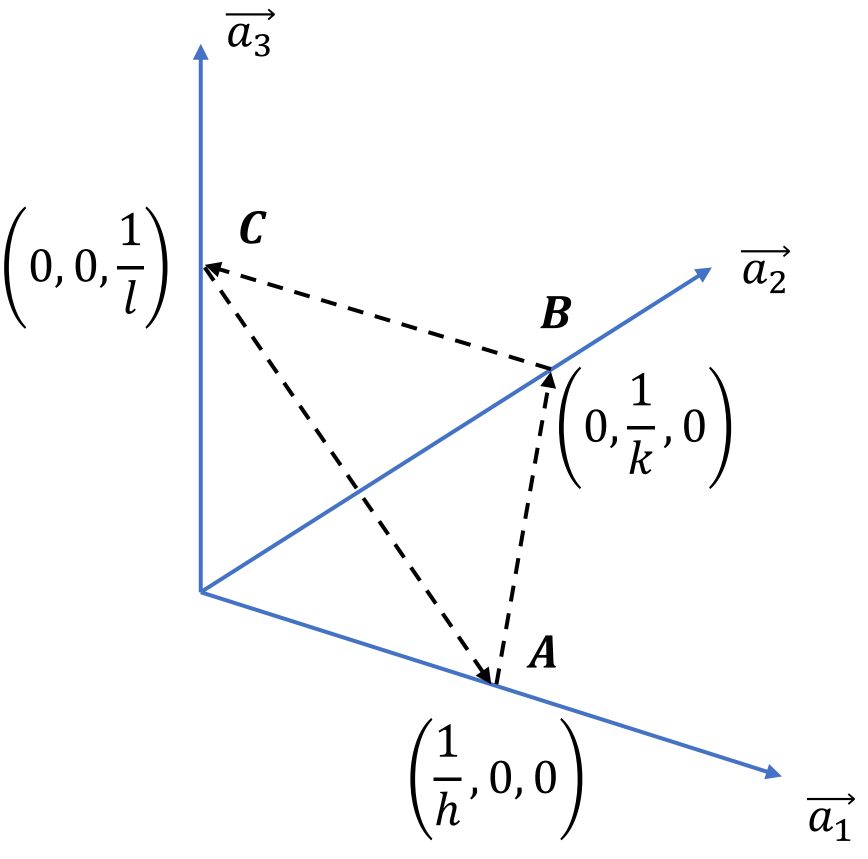

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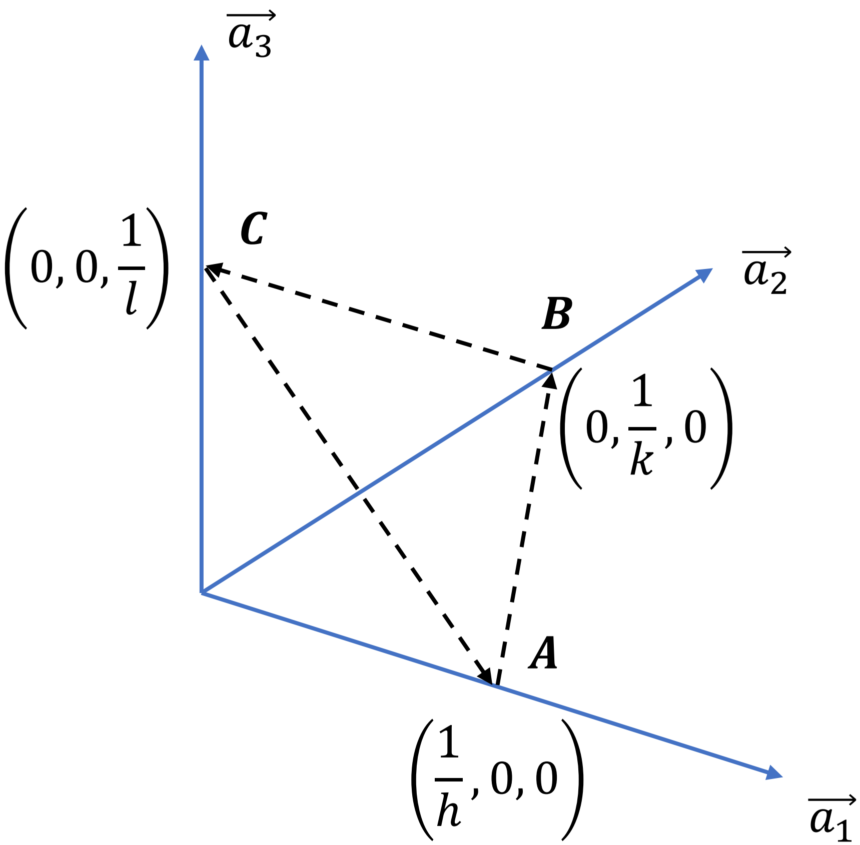

$$\overrightarrow{AB} = \frac{1}{k}\overrightarrow{a_2} - \frac{1}{h}\overrightarrow{a_1}$$

$$\overrightarrow{BC} = \frac{1}{l}\overrightarrow{a_3} - \frac{1}{k}\overrightarrow{a_2}$$

$$\overrightarrow{CA} = \frac{1}{h}\overrightarrow{a_1} - \frac{1}{l}\overrightarrow{a_3}$$

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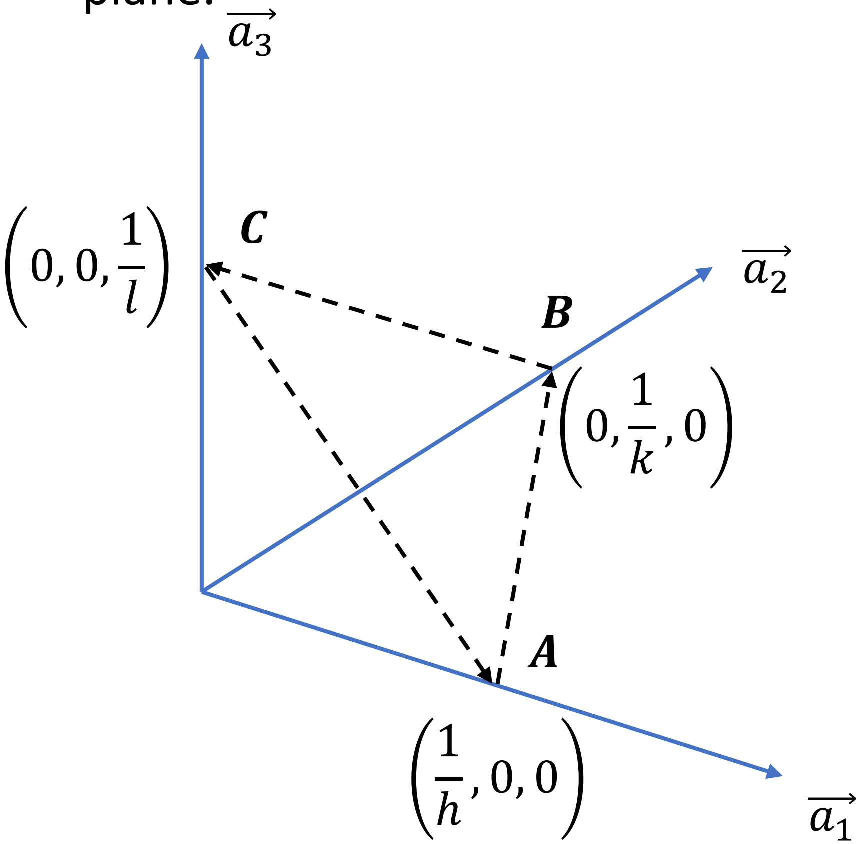

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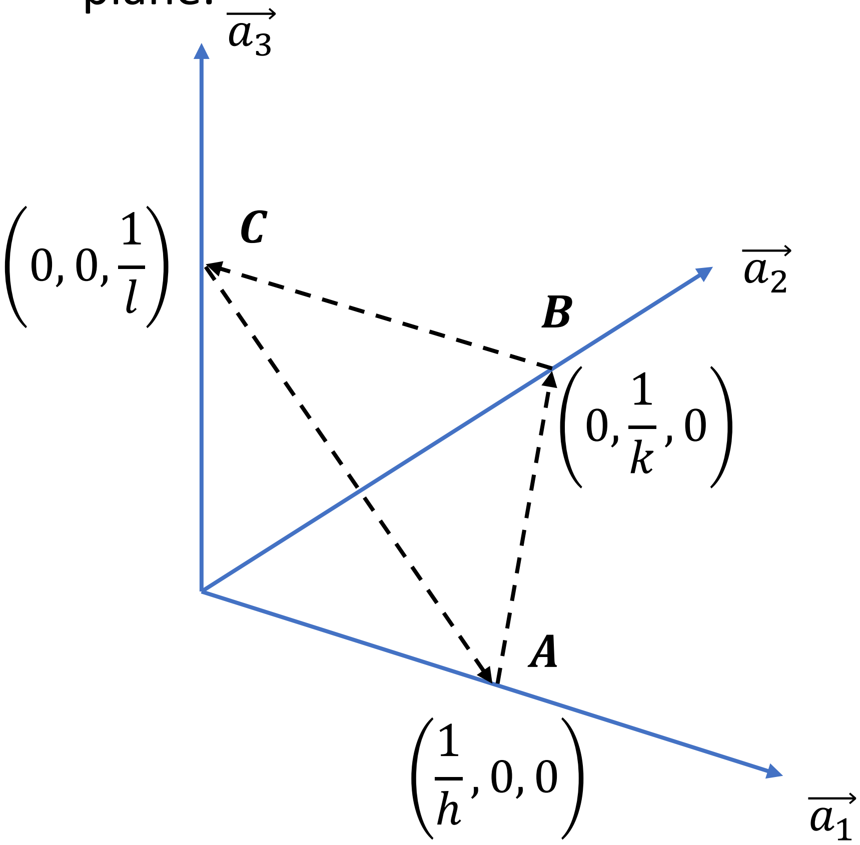
$\boldsymbol{G}.\overrightarrow{AB}$ = ?

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

$$\overrightarrow{b_i} \cdot \overrightarrow{a_j} = 2\pi\delta_{ij}$$

3. Consider the plane (hkl) in direct lattice of a crystal structure, prove that the reciprocal lattice vector $\boldsymbol{G} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}$ is perpendicular to this plane.



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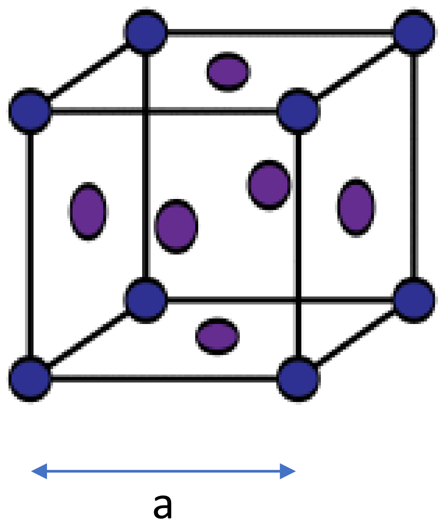
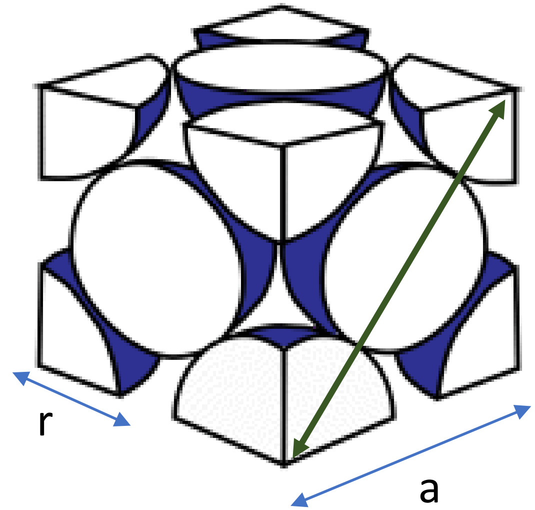
$\boldsymbol{G}.\overrightarrow{AB}$ = ?

$Note\text{: } We\ have\ to\ prove\ that\ G\ is\ perpendicular\ to\ atleast\ \boldsymbol{two}\ vectors$

4. Determine the packing fraction in FCC.





$$4r = a\sqrt{2}$$

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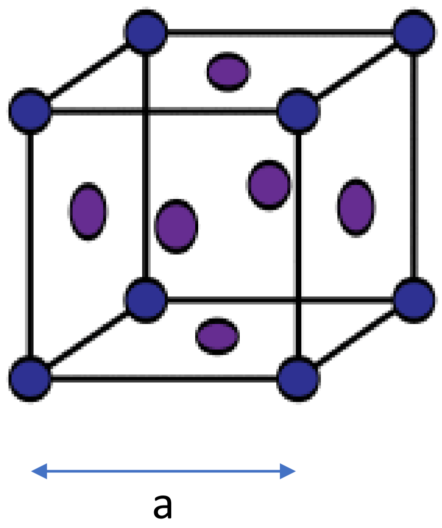
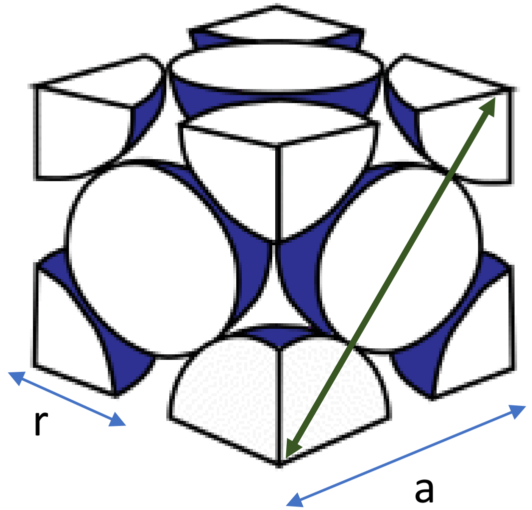


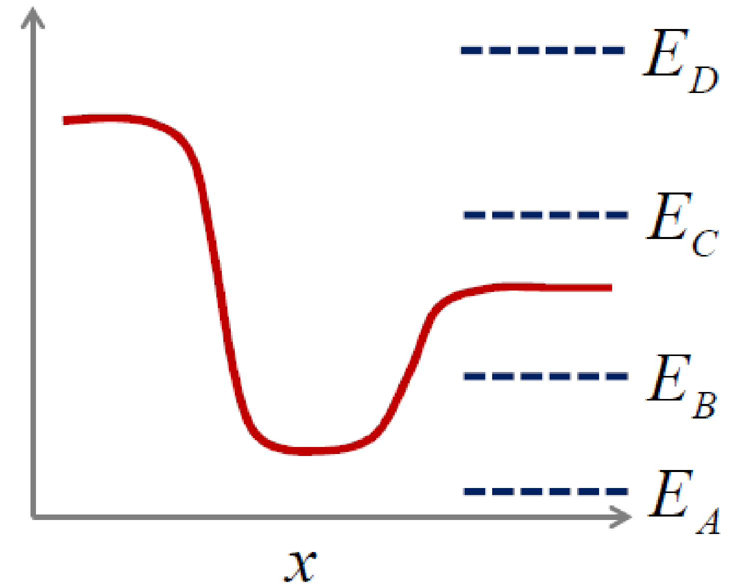


$$4r = a\sqrt{2}$$

$$\eta = \frac{volume\ occupied\ by\ atoms\ in\ unit\ cell}{volume\ of\ unit\ cell}$$

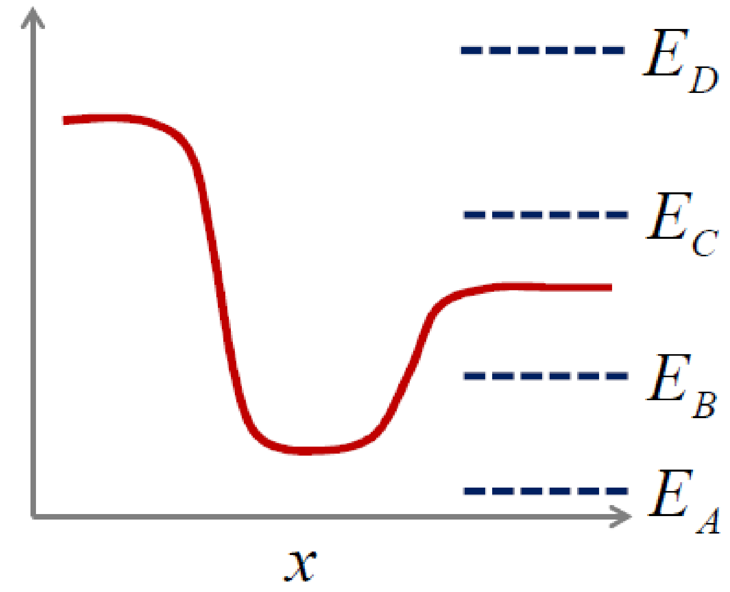
$$\eta = \frac{\left(\left(\frac{1}{8} * 8\right) + \left(\frac{1}{2} * 6\right)\right) * \left(\frac{4}{3}\pi r^3\right)}{a^3} \approx 0.74$$

5. Comment on the nature of the energy states shown in the following figure if they are free/bound/don't exist.

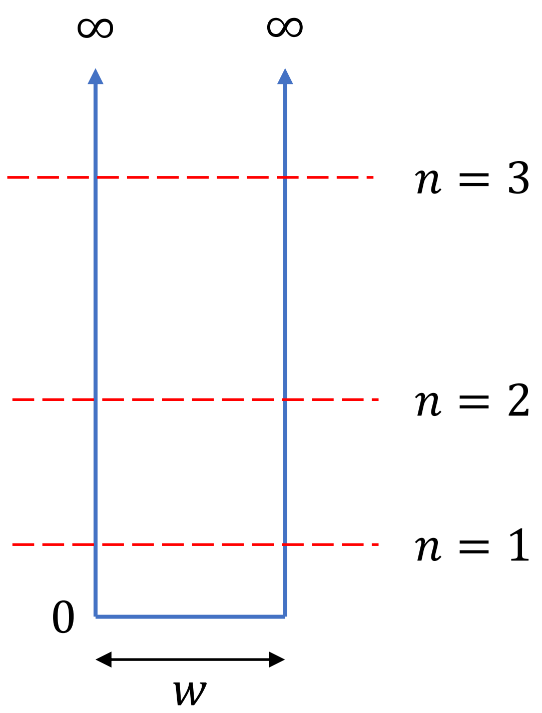


5. Comment on the nature of the energy states shown in the following figure if they are free/bound/don’t exist.

$$E_D:\ Free$$
$$E_C: Free$$
$$E_B: Bound$$
$$E_A: Doesn't\ exist$$



6. Consider an infinite potential well of width *w* having a particle of mass *m*. Find out the relation between *w* and *m* such that the energy separation lowest two energy eigen values is equal to kBT. Assume T = 300 K.

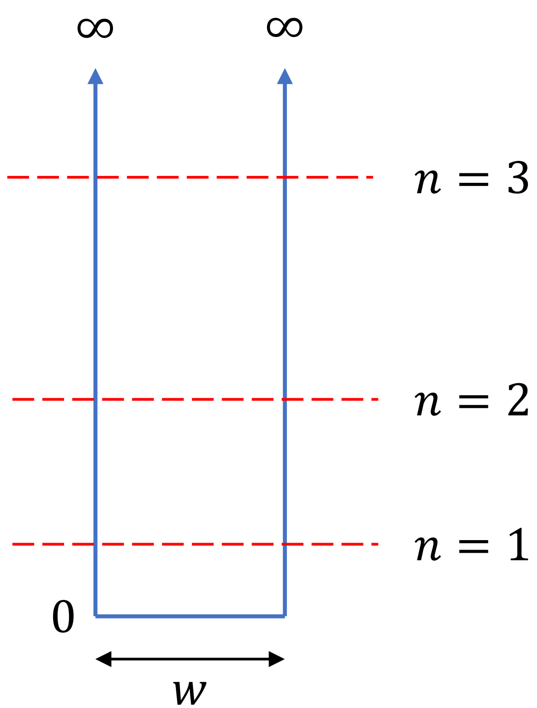


6. Consider an infinite potential well of width *w* having a particle of mass *m*. Find out the relation between *w* and *m* such that the energy separation lowest two energy eigen values is equal to kBT. Assume T = 300 K.

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

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{w}\right)^2$$

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



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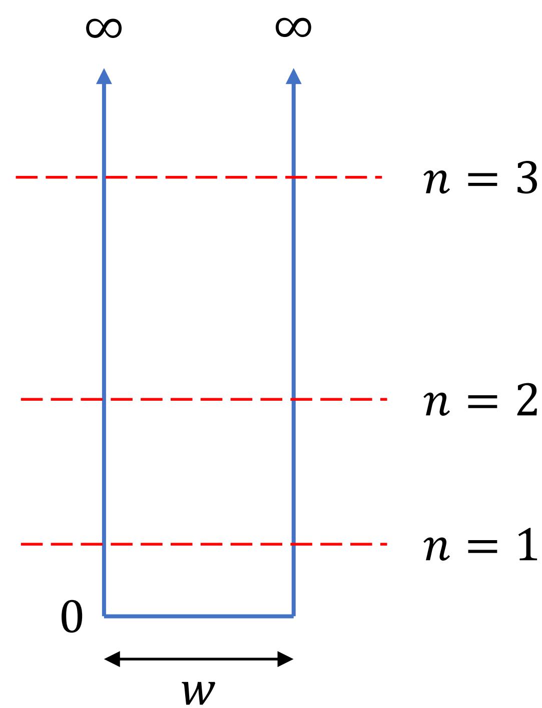
$$E_2 - E_1 = k_B T$$



7. A particle of mass m is in 1D box of width a. The particle is in the state $\psi = \frac{3\phi_2 + 4\phi_9}{\sqrt{25}}$. Find the energy probabilities of the particle, in all energy states E_n.

Total energy, $< E > = < \psi^* \left| \widehat{H} \right| \psi >$

We have $\widehat{H}\phi_i = E\phi_i$

Therefore,

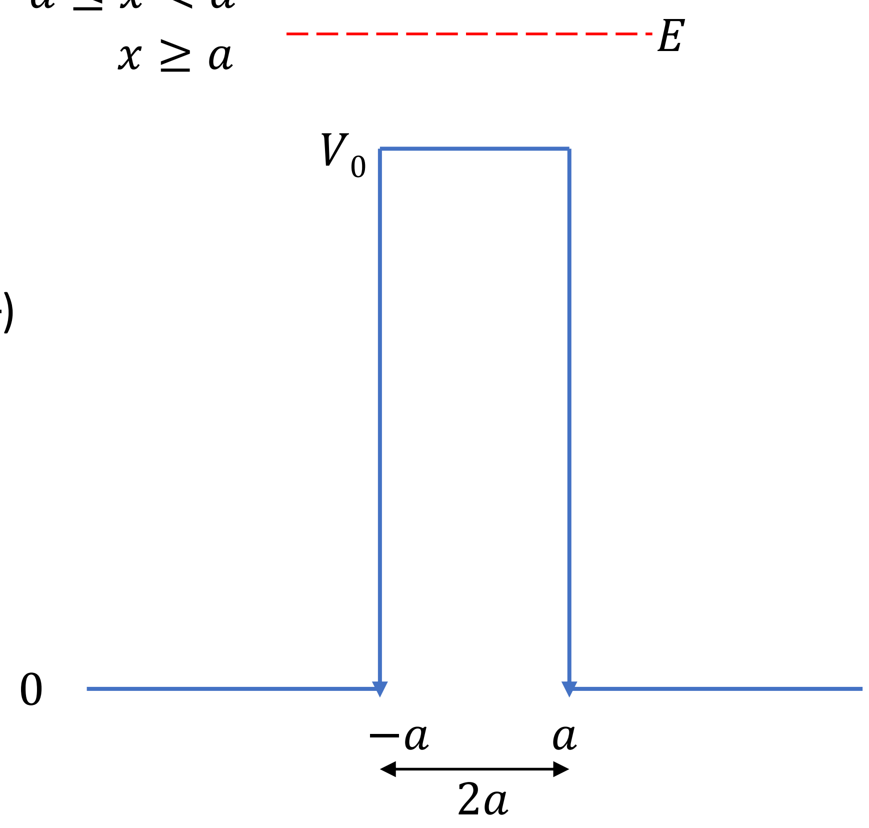
$$< E > = \int_{-\infty}^{\infty} \left(\frac{3\phi_2^* + 4\phi_9^*}{\sqrt{25}} \right) \left(\frac{3E\phi_2 + 4E\phi_9}{\sqrt{25}} \right) dx$$

$\phi_i$are orthogonal. Hence,

$$< E > = \frac{9}{25} E_2 + \frac{16}{25} E_9$$

8.

$$\psi(x) = \begin{cases} A\, exp(ikx) + B \exp(-ikx)\,; & x < -a \\ C \exp(i\alpha x) + D \exp(-i\alpha x)\,; & -a \le x < a \\ F\, exp(ikx); & x \ge a \end{cases}$$



$$Given\ that\colon\ J(x) = \frac{i\hbar}{2m}\,(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx})$$

show that $T = \frac{J_{transmitted}}{J_{incident}} = \frac{|F|^2}{|A|^2}$

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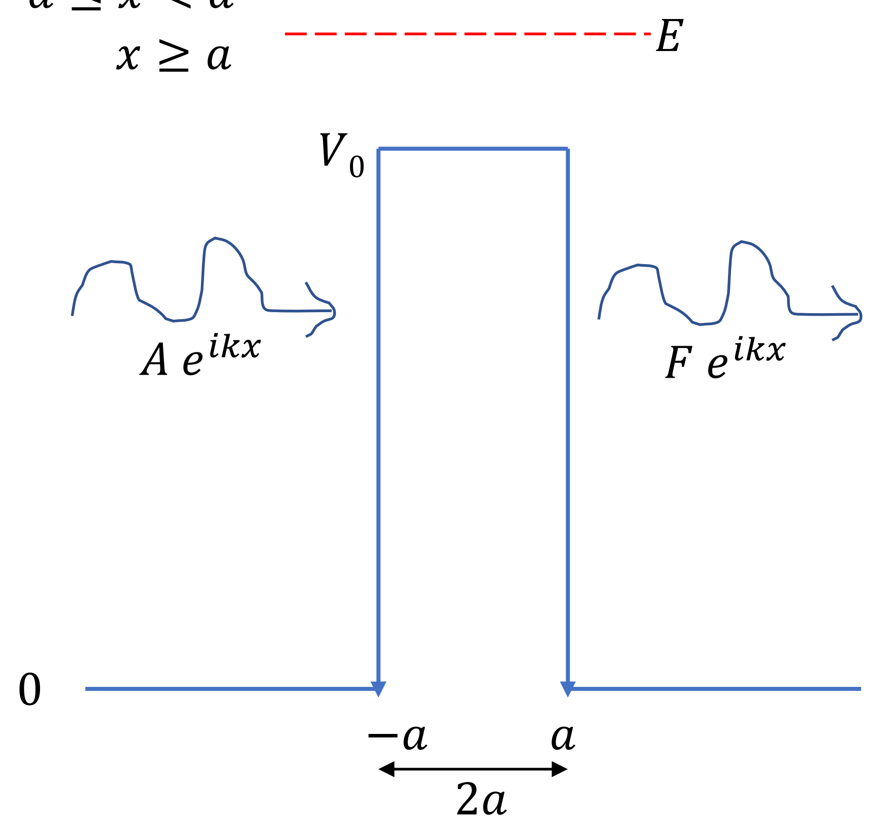

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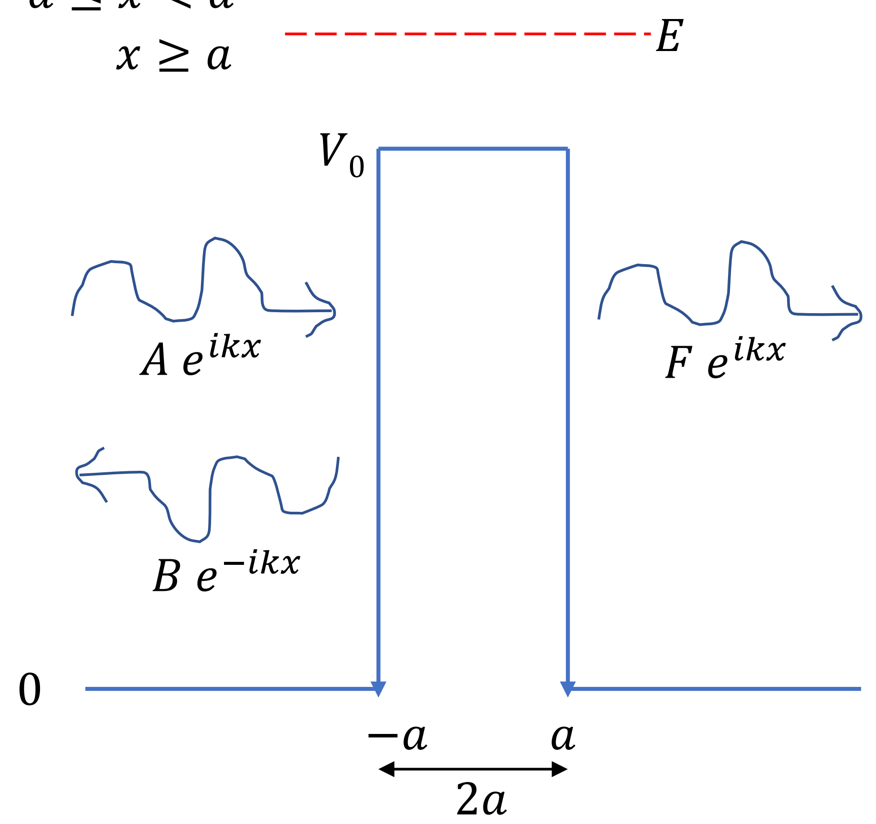

$$J(x) = \frac{i\hbar}{2m}\left(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx}\right)$$

$$\text{Similarly, } R = \frac{J_{reflected}}{J_{incident}} = \frac{|B|^2}{|A|^2}$$