Answere to the question No-1

If The vectors to define the primitive unit cells are $\vec{a_1}, \vec{a_2}$ and $\vec{a_3}$. then the volume of this primitive unit cell is $|\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})|$

for fcc

$$\vec{a_1} = \frac{1}{2}a(\hat{x}+\hat{y})$$
$$\vec{a_2} = \frac{1}{2}a(\hat{y}+\hat{z})$$
$$\vec{a_3} = \frac{1}{2}a(\hat{z}+\hat{x})$$

$$\vec{a_2}\times\vec{a_3} = \left(\frac{1}{2}a\right)^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix}$$

$$= \left(\frac{1}{2}a\right)^2(\hat{x}+\hat{y}-\hat{z})$$

$$\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3}) = \left(\frac{1}{8}a^3\right)\left[(\hat{x}+\hat{y})\cdot(\hat{x}+\hat{y}-\hat{z})\right]$$

$$= \frac{a^3}{8}\cdot(1+1-0)$$

$$= \frac{a^3}{4}.$$

$$\therefore \text{Ratio} = \frac{a^3/4}{a^3} = \frac{1}{4} \quad \text{for fcc.}$$

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for bcc

$\vec{a_1} = \frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$

$\vec{a_2} = \frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z})$

$\vec{a_3} = \frac{1}{2}a(\hat{x}-\hat{y}+\hat{z})$

$$\vec{a_2}\times\vec{a_3} = \frac{1}{4}a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix}$$

$$= \frac{1}{4}a^2\left[2\hat{x} + 2\hat{y}\right]$$

$$= \frac{1}{2}a^2(\hat{x}+\hat{y})$$

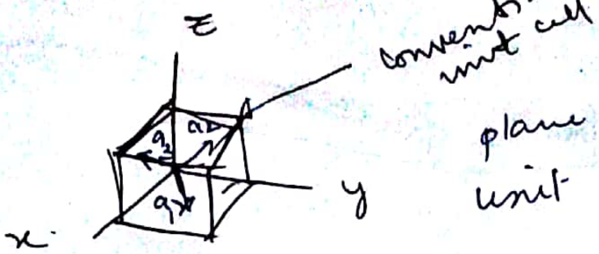
$$\therefore \vec{a_1}\cdot(\vec{a_2}\times\vec{a_3}) = \frac{1}{4}a^3(\hat{x}+\hat{y}-\hat{z})\cdot(\hat{x}+\hat{y})$$

$$= \frac{1}{4}a^3 \times 2$$

$$= \frac{a^3}{2}$$

$$\therefore \text{Ratio} = \frac{a^3/2}{a^3} = 1/2 \text{ Ans}$$

(b)



plane (1 0 0) wrt the conce unit is parallel to $\vec{a}_2$

for (1 0 0)

Intercept with $\vec{a_1}$ = $2|\vec{a_1}|$

" " $\vec{a_3}$ = $2|\vec{a_3}|$

" " $\vec{a_2}$ = ∞

$\therefore$ Indices wrt $(a_1\ a_2\ a_3)$

$= \frac{1}{2}\ \frac{1}{\infty}\ \frac{1}{2}$

$= (1\ 0\ 1)$

for (0 0 1) || a_1

similarly (0 1 1) Answer.

Answer to the question No-2

$$1 = \int \psi(r)^* \, \psi(r) \, dv$$

$$\int \psi(r)^* \, \psi(r) \, dv$$

dv (in sphrepical coordinate) $= r^2 \sin\varphi \, dr \, d\varphi \, d\theta$

$$= \int_{r=0}^{\infty} \int_{\varphi=0}^{\pi} \int_{\theta=0}^{2\pi} A^2 \exp\left(-\frac{2Zr}{a}\right) r^2 \sin\varphi \, dr \, d\varphi \, d\theta$$

$$\cancel{= A^2 \int_{r=0}^{\infty} r^2 \left\{ \int_{\varphi=0}^{\pi} \int_{\theta=0}^{2\pi} \exp\left(-\frac{2Zr}{a}\right) \sin\varphi \, d \right.}$$

$$= A^2 \int_{r=0}^{\infty} r^2 \exp\left(-\frac{2Zr}{a}\right) \left\{ \int_{\varphi=0}^{\pi} \int_{\theta=0}^{2\pi} \sin\varphi \, d\varphi \, d\theta \right\} dr$$

$$= A^2 \, 4\pi \int_0^{\infty} r^2 \exp\left(-\frac{2Zr}{a}\right) dr$$

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$$\int_0^\infty r^2 e^{-\frac{2Zr}{a}} dr$$

$$= r^2 \int_0^\infty e^{-\frac{2Zr}{a}} dr - \int \left\{ \frac{d}{dr} r^2 \int e^{-\frac{2Zr}{a}} dr \right\} dr$$

$$= \frac{r^2 \cdot e^{-\frac{2Zr}{a}}}{-\frac{2Z}{a}} - \int \frac{2r\, e^{-\frac{2Zr}{a}}}{-\frac{2Z}{a}} dr$$

This part will go to zero when limit is put

$$= -\frac{r^2 a}{2Z} e^{-\frac{2Zr}{a}} + \int \frac{ra}{Z} e^{-\frac{2Zr}{a}} dr$$

$$\int r e^{-\frac{2Zr}{a}} dr$$

$$= r \int e^{-\frac{2Zr}{a}} dr - \int \left\{ \frac{dr}{dr} \int e^{-\frac{2Zr}{a}} dr \right\} dr$$

$$= \frac{r e^{-\frac{2Zr}{a}}}{-\frac{2Z}{a}} + \int \frac{a}{2Z} \cdot e^{-\frac{2Zr}{a}} dr$$

This part will be zero when limit is put.

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This part will be zero when limit is put

$$= -\left(\frac{a}{2z}\right) r e^{-\frac{2zr}{a}} - \left(\frac{a}{2z}\right)^2 e^{-\frac{2zr}{a}}$$

By putting limits we get

$$\int_0^\infty r^2 e^{-\frac{2rz}{a}} dr = \frac{a}{z}\left(\frac{a^2}{2z}\right)$$

$$\therefore \quad A^2 \cdot 4\pi \frac{a}{z}\left(\frac{a}{2z}\right)^2 = 1$$

$$\Rightarrow A^2 \cdot \cancel{4}\pi \cdot \frac{a^3}{\cancel{4} z^3} = 1$$

$$\therefore \quad A^2 = \frac{z^3}{\pi a^3}$$

$$\therefore A = \left(\frac{z^3}{\pi a^3}\right)^{1/2}$$

$$\therefore \quad \boxed{A = \left(\frac{z^3}{\pi a^3}\right)^{1/2}}$$

Answer to the question No-3.

(a)

$$E(k) = E_0 \{ 1 - \exp(-2a^2k^2) .$$

$$\frac{dE}{dk} = E_0 \cdot (2a^2)\, e^{-2a^2k^2} \cdot (2k) = (E_0\, 4a^2) k e^{-2a^2k^2}$$

$$\frac{d^2E}{dk^2} = (E_0 4a^2) \left[e^{-2a^2k^2} - k e^{-2a^2k^2} \cdot (2a^2 \cdot 2k) \right] .$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2}$$

$$\therefore\; m^* \text{ @ } k=0 = \frac{\hbar^2}{4E_0 a^2}$$

(b)

$$V_g = \frac{1}{\hbar} \frac{dE}{dk} .$$

For Max V_g $\quad \frac{d^2E}{dk^2} = 0 .$

$$\therefore\; (4E_0 a^2) \left[e^{-2a^2k^2} - 4a^2k^2 e^{-2a^2k^2} \right] = 0$$

$$\therefore\; k^2 = \frac{1}{4a^2}$$

$$\therefore\; \boxed{k = \pm \frac{1}{2a}}$$

(c) ~~At~~ the ~~ez~~ edge of Brouilline zone $k = \pm \frac{\pi}{a}$

Just put $k = \pm \frac{\pi}{a}$ @ the expression of $\frac{d^2E}{dk^2}$.