Physics 560A HW 1

Solutions

1.3) $\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 \in BL$

a) and

$\vec{R} + L\hat{x} \in BL$, where

L is the circumference of the cylinder, whose axis coincides with the y-axis.

$$L\hat{x} = m_1 \vec{a}_1 + m_2 \vec{a}_2$$

$L\hat{x} \cdot \vec{b}_i = 2\pi m_i$, where $\vec{b}_i$ are reciprocal lattice vectors.

$$\boxed{\hat{x} \cdot \vec{b}_i = \frac{2\pi m_i}{L}}$$

b) $L_1\hat{x} \in BL$ & $L_2\hat{y} \in BL$

$$L_1\hat{x} = m_1\vec{a}_1 + m_2\vec{a}_2$$

and

$$L_2\hat{y} = n_1\vec{a}_1 + n_2\vec{a}_2$$

$$\Rightarrow \quad \hat{x}\cdot\vec{b}_i = \frac{2\pi m_i}{L_1}$$

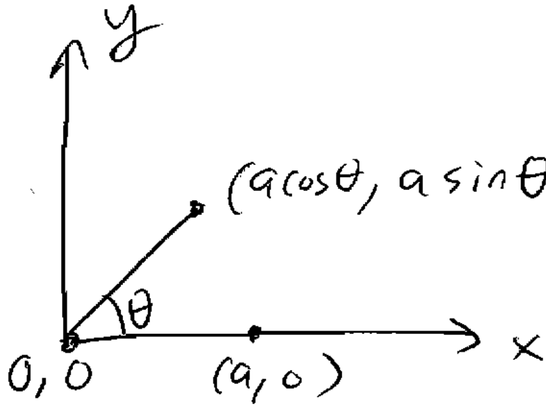
$$\hat{y}\cdot\vec{b}_i = \frac{2\pi n_i}{L_2}$$

$$\vec{b}_i = \left(\frac{2\pi m_i}{L_1}, \frac{2\pi n_i}{L_2}\right)$$

and

$$\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$$

1.4) a)



$\vec{a}_1 = (a, 0)$

let $\vec{a}_2 = (a\cos\theta, a\sin\theta)$

then $(a\cos\theta, -a\sin\theta) = n_1 \vec{a}_1 + n_2 \vec{a}_2$

$= (n_1 a + n_2 a\cos\theta, \; n_2 a\sin\theta)$

$\cos\theta = n_1 + n_2 \cos\theta$

$-\sin\theta = n_2 \sin\theta \quad \Rightarrow \quad n_2 = -1$

$\cos\theta = n_1 - \cos\theta \qquad \theta \neq 0, 2\pi$

$n_1 = 2\cos\theta$, $\Rightarrow n_1 = -1, 0, 1$

also -2

$$\cos\theta = 0, \pm\frac{1}{2}, -1$$

$$\theta = \frac{\pi}{2}, \frac{\pi}{3}, \frac{2\pi}{3}, \pi$$

b)

$$\theta = 2\pi\left(\frac{1}{4}, \frac{1}{6}, \frac{1}{3}, \frac{1}{2}\right)$$

2-fold, 3-fold, 4-fold, and 6-fold rotational axes are possible.

A five-fold symmetry axis would have $\theta = \frac{2\pi}{5}$ and

$$2\cos\theta = 0.618 \notin \mathbb{Z}$$ (not possible).

2.1) a) Body-centered cubic

needs two basis vectors:

$(0,0,0)$ and $\left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right)$

(corner and body center).

fcc needs four basis vectors:

$(0,0,0)$, $\left(\frac{a}{2}, \frac{a}{2}, 0\right)$, $\left(0, \frac{a}{2}, \frac{a}{2}\right)$

and $\left(\frac{a}{2}, 0, \frac{a}{2}\right)$ (corner and three face centers).

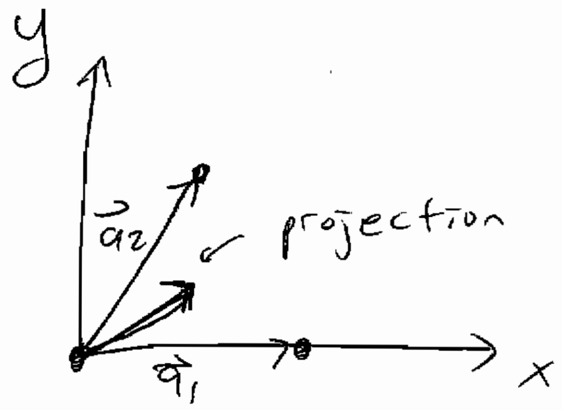
b) bcc: $a^3 = 2V_c$

fcc: $a^3 = 4V_c$

2.4) hcp $\quad \vec{a}_1 = (a, 0, 0)$

$\vec{a}_2 = \left(\frac{a}{2}, \frac{a\sqrt{3}}{2}, 0\right)$

from Eq. (2.4)



$\vec{V_2} = \left(\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2}\right)$

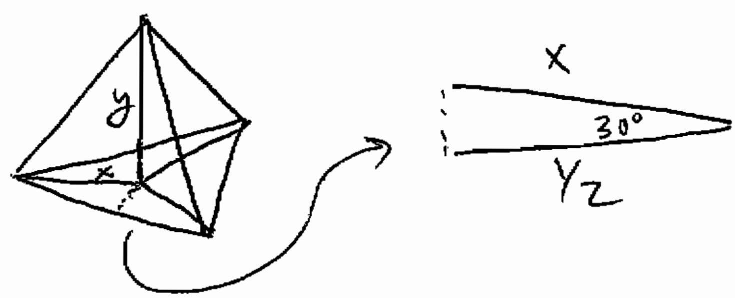
← projection of $\vec{V_2}$ in the x-y plane

$$\vec{V_2} \cdot \vec{a_1} = \frac{a^2}{2} = \frac{1}{2}\, \vec{a_1} \cdot \vec{a_1}$$

$$\vec{V_2} \cdot \vec{a_2} = \frac{a^2}{4} + \frac{a^2}{4} = \frac{a^2}{2} = \frac{1}{2}\, \vec{a_2} \cdot \vec{a_2}$$

$\Rightarrow$ The projection of $\vec{V_2}$ on the xy plane lies at the center of the equilateral triangle whose vertices are $\vec{0}$, $\vec{a_1}$, and $\vec{a_2}$.

b) $\frac{c}{a}$ = twice the height of a regular tetrahedron of unit edge:



$$\frac{1/2}{x} = \cos 30^\circ = \frac{\sqrt{3}}{2}$$

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$$x = \frac{1}{\sqrt{3}}, \quad y = \sqrt{1-x^2} = \sqrt{2/3}$$

$$\frac{c}{a} = 2y = \sqrt{8/3}$$ ✓

2.6) simple cubic: The sphere inscribes the cube.

$$V_{sphere} = \frac{4}{3}\pi r^3$$

$$V_{cube} = (2r)^3 = 8r^3$$

$$f = \frac{V_{sphere}}{V_{cube}} = \frac{4\pi}{3 \cdot 8} = \frac{\pi}{6} \simeq 0.52$$

bcc: Twice the sphere's diameter = cube body diagonal

$$2d = \sqrt{3}a \qquad d = \frac{\sqrt{3}a}{2} \qquad r = \frac{\sqrt{3}}{4}a$$

$$V_{sphere} = \frac{4\pi}{3}r^3 = \frac{\pi\sqrt{3}}{16}a^3$$

$$f = \frac{V_{sphere}}{V_c} = \frac{\pi\sqrt{3}}{16}a^3 \Big/ \frac{a^3}{2} = \frac{\pi\sqrt{3}}{8} = 0.68$$

fcc: Twice the sphere's diameter
= face diagonal of cube

$2d = \sqrt{2}\,a \qquad d = \frac{a}{\sqrt{2}} \qquad r = \frac{a}{2\sqrt{2}}$

$$V_{sphere} = \frac{4\pi r^3}{3} = \frac{\pi}{12\sqrt{2}}\,a^3$$

$$f = \frac{V_{sphere}}{V_c} = \frac{V_{sphere}}{a^3/4} = \frac{\pi}{3\sqrt{2}} \simeq 0.74$$

hcp: $f_{hcp} = f_{fcc}$ since they both correspond to close packing of hard spheres, with consecutive planes with hexagonal packing arranged according to ABABAB ... (hcp) or ABCABC ... (fcc), where B and C are the interstices of the hexagonal lattice of close-packed spheres.

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<u>diamond</u> the lattice is fcc with basis vectors $(0,0,0)$ and $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$.

The diameter of close-packed spheres is thus

$$d^2 = 3\left(\frac{a}{4}\right)^2 = \frac{3a^2}{16}$$

$$d = \frac{\sqrt{3}\,a}{4}, \quad r = \frac{\sqrt{3}\,a}{8}$$

$$V_{sphere} = \frac{4\pi}{3} r^3 = \frac{4\pi}{3}\,\frac{3\sqrt{3}}{512}\,a^3$$

$$= \frac{\sqrt{3}}{128}\pi a^3$$

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

$$f = \frac{2V_{sphere}}{V_c} = \frac{8}{a^3}\,\frac{\sqrt{3}\pi a^3}{128} = \frac{\sqrt{3}\pi}{16}$$

$$\simeq 0.34$$