Condensed matter physics (Phy 771)
HW #1 - Solution
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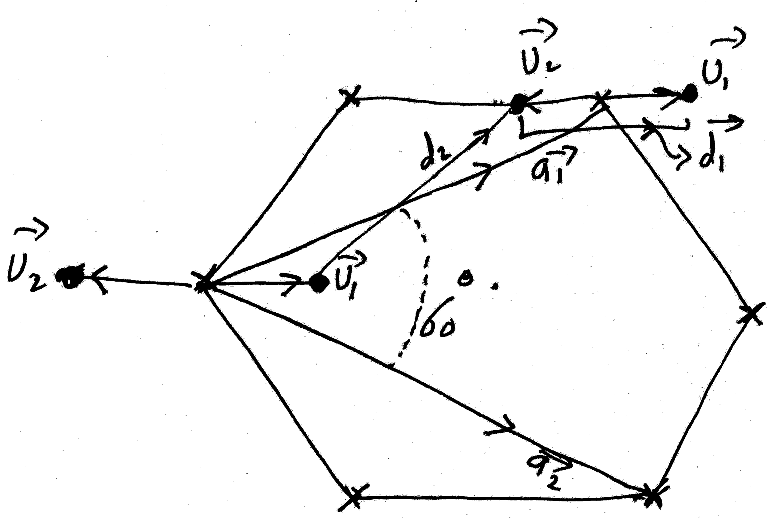
① problem 1.1 Marder!



(Hexagonal lattice)

$\vec{a_1} = a\frac{\sqrt{3}}{2}\hat{i} + \frac{a}{2}\hat{j}$

$\vec{a_2} = a\frac{\sqrt{3}}{2}\hat{i} - \frac{a}{2}\hat{j} \Rightarrow$

$\Rightarrow |\vec{a_1}| = |\vec{a_2}| = a$

where a is lattice constant

and $\vec{U_1} = \frac{a}{2\sqrt{3}}\hat{i}$; $\vec{U_2} = -\frac{a}{2\sqrt{3}}\hat{i}$

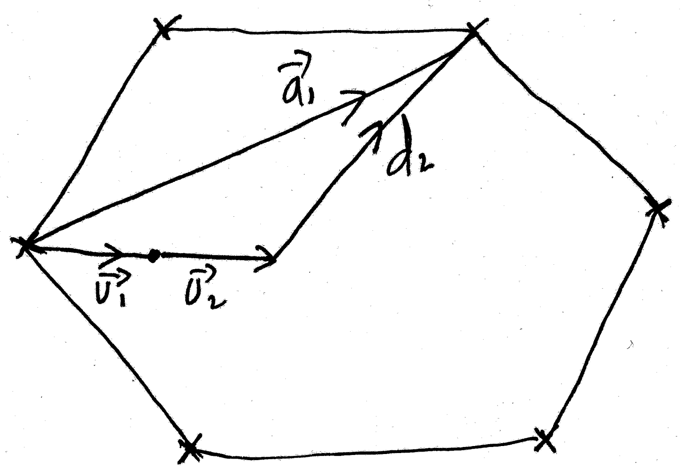
$\Rightarrow |\vec{U_1}| = |\vec{U_2}| = \frac{a}{2\sqrt{3}}$

from eqn 1.5 in textbook

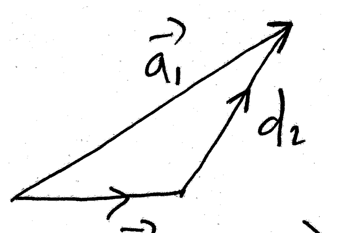
a) to prove that the distance between all neighboring points is identical, it is enough to prove that $d_1 = d_2$ as shown in the figure

$$|\vec{d_1}| = |\vec{U_1} - \vec{U_2}| = \left|\frac{a}{2\sqrt{3}}\hat{i} - \left(\frac{-a}{2\sqrt{3}}\right)\hat{i}\right| = \left|\frac{2a}{2\sqrt{3}}\hat{i}\right| = \frac{a}{\sqrt{3}}$$

Now let us shift or move $\vec{d_2}$ to the right by $\vec{U_1} = \vec{U_2}$, so



$\Rightarrow$



$$\vec{a_1} = 2\vec{U_1} + \vec{d_2}$$

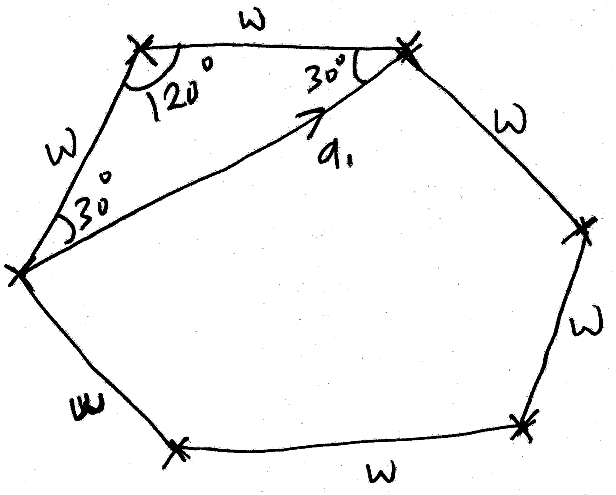
$$\vec{d_2} = \vec{a_1} - 2\vec{U_1}$$

$$= a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) - 2a\left(\frac{1}{2\sqrt{3}}, 0\right)$$

$$= a\left(\frac{\sqrt{3}}{2} - \frac{1}{\sqrt{3}}, \frac{1}{2}\right)$$

$\Rightarrow |\vec{d_2}| = a\sqrt{\frac{3}{4}+\frac{1}{3}-1+\frac{1}{4}} = a\sqrt{\frac{1}{3}} = \frac{a}{\sqrt{3}} \equiv |\vec{d_1}|$ ✓

b)



let w be the distance between nearest neighbors and using the law of sin, we have

$$\frac{|\vec{a_1}|}{\sin 120} = \frac{w}{\sin 30}$$

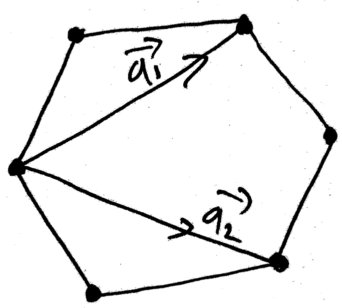
but $|\vec{a_1}| = a \Rightarrow \frac{a}{\frac{\sqrt{3}}{2}} = \frac{w}{\frac{1}{2}} \Rightarrow w = \frac{a}{\sqrt{3}}$

$\Rightarrow w = \frac{2.46\,\text{Å}}{\sqrt{3}} = 1.42\,\text{Å}$

c) for honeycomb lattice, there are 2LP/unit cell

each point is shared with 3 hexagons

$\Rightarrow$



$\Rightarrow 6 \times \frac{1}{3} = 2$ LP/ unit cell

$\Rightarrow \rho = \frac{m}{A} = \frac{2m_c}{|\vec{a_1} \times \vec{a_2}|}$

$= \frac{2 \times 12 \times 1.67 \times 10^{-27} \times 10^{3}\,g}{|a_1|\,|a_2| \sin 60}$; $|a_1| = |a_2| = a = 2.46\,\text{Å}$

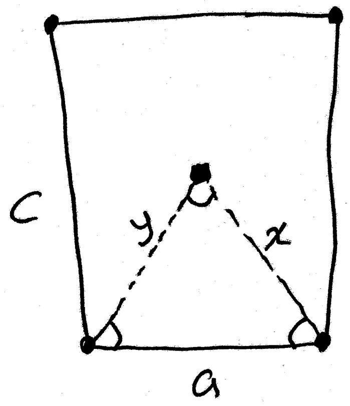
$= \frac{2 \times 12 \times 1.67 \times 10^{-27} \times 10^{3}}{(2.46 \times 10^{-8}\,cm)^2 \frac{\sqrt{3}}{2}}$

$\approx 7.64 \times 10^{-8}\,g/cm^2$

② problem 1.2 Marder:

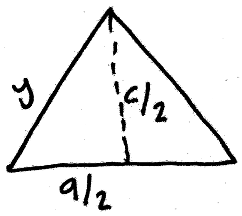
The Hexagonal lattice may be viewed as special case of the centered rectangular lattice shown below

a)



(Fig 1.4)

$\Rightarrow$ from the figure, we see that it becomes Hexagonal if $x = y = a$ that make the triangle equilateral triangle (i.e all three sides have the same length and all three angles are equal (60°).

$\Rightarrow$ 

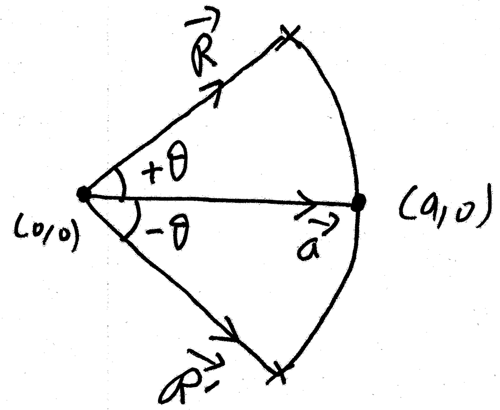
$$\Rightarrow y^2 = \left(\frac{c}{2}\right)^2 + \left(\frac{a}{2}\right)^2 = \frac{c^2}{4} + \frac{a^2}{4} \text{ ; but } y = a$$

$$\Rightarrow a^2 = \frac{c^2}{4} + \frac{a^2}{4} \Rightarrow \frac{c^2}{4} = \frac{3}{4}a^2 \Rightarrow \frac{c}{a} = \sqrt{3}$$

b) the symmetry operations that leave both lattices invariant are summarized below

Hexagonal lattice (2D)	Centered rectangular lattice (2D)
- translation by Bravais lattice vectors $(\vec{a_1}, \vec{a_2})$	- translation by Bravais lattice vectors $(\vec{a_1}, \vec{a_2})$
- Identity	- Identity
- Inversion	- Inversion
- Rotation: 60°, 120°, 180°, 270°, 360°	- Rotation: 180° only
- Reflections: six mirror planes	- Reflections: horizontal and vertical mirror planes

③ problem 1.4 Marder!



let basis vectors be $\vec{a}_1 = (a,0) = \begin{pmatrix} a \\ 0 \end{pmatrix}$

$\vec{a}_2 = (A,B) = \begin{pmatrix} A \\ B \end{pmatrix}$

, Now $R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$; to get $R_{-\theta}$

just replace θ by $-\theta$, so

$$R_{-\theta} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$\Rightarrow$

$\vec{R} = R_\theta \vec{a}_1$

$$= \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} a \\ 0 \end{pmatrix} = \begin{pmatrix} a\cos\theta \\ a\sin\theta \end{pmatrix} \equiv n_1 \vec{a}_1 + n_2 \vec{a}_2$$

must hold for any Bravias lattice

$$= n_1 \begin{pmatrix} a \\ 0 \end{pmatrix} + n_2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} n_1 a + n_2 A \\ n_2 B \end{pmatrix}$$

$\Rightarrow$ $a\cos\theta = n_1 a + n_2 A$ ---(1)

$a\sin\theta = n_2 B$ ---(2)

similarly

$$\vec{R'} = R_{-\theta}\vec{a}_1 = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} a \\ 0 \end{pmatrix} = \begin{pmatrix} a\cos\theta \\ -a\sin\theta \end{pmatrix} \equiv m_1 \vec{a}_1 + m_2 \vec{a}_2$$

$$= m_1 \begin{pmatrix} a \\ 0 \end{pmatrix} + m_2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} m_1 a + m_2 A \\ m_2 B \end{pmatrix}$$

$\Rightarrow$ $a\cos\theta = m_1 a + m_2 A$ ---(3)

$-a\sin\theta = m_2 B$ ---(4)

now substitute (4) in (2), we get $-m_2 B = n_2 B \Rightarrow m_2 = -n_2$

now eqn (3) becomes

$a\cos\theta = m_1 a - n_2 A$ ---(5) , Now add (1) and (5)

$\Rightarrow$ $2a\cos\theta = (n_1 + m_1)a$ $\Rightarrow$ $\cos\theta = \frac{1}{2}\underbrace{(n_1 + m_2)}_{\text{integer}}$

i.e $\cos\theta$ is half-integer.

$\therefore \quad \cos\theta = \frac{1}{2}(n_1 + m_2)$; where $n_1 + m_2 = 0, \pm 1, \pm 2, \pm 3, \ldots$

but because $-1 \leq \cos\theta \leq 1$, the only possible values of $m_1 + n_1$ are $0, \pm 1, \pm 2$ only

$\Rightarrow n_1 + m_1 = 0, +1, -1, +2, -2$

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

$\theta = 90^\circ, 60^\circ, 120^\circ, 0, 180^\circ$

now using $n = \frac{360^\circ}{\theta}$, we get

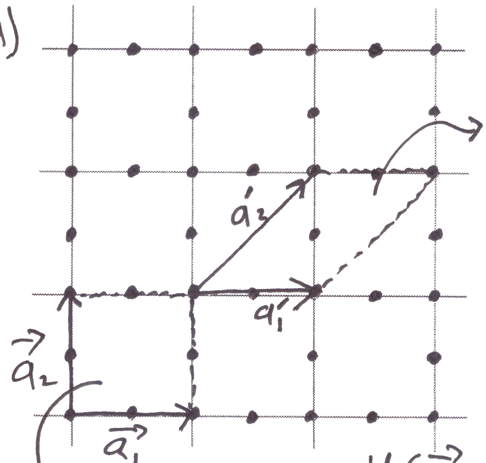
$n = 4, 6, 3, 1, 2$

or $= 1, 2, 3, 4, 6$ as expected

See that the 5-fold symmetry is impossible to occur in Bravais lattice.

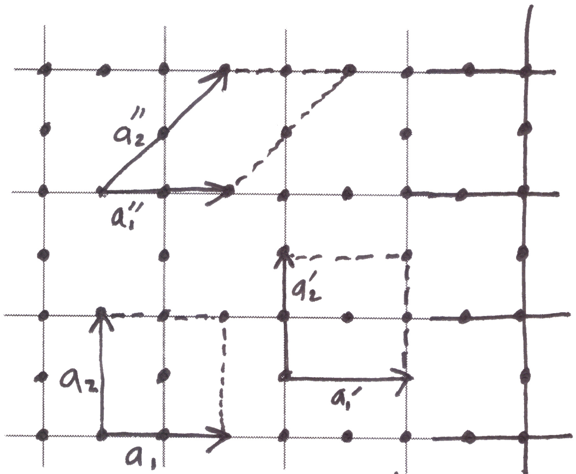
(4)

a)



primitive cell $(\vec{a}_1', \vec{a}_2')$ with 3 LP (2^{nd} choice)

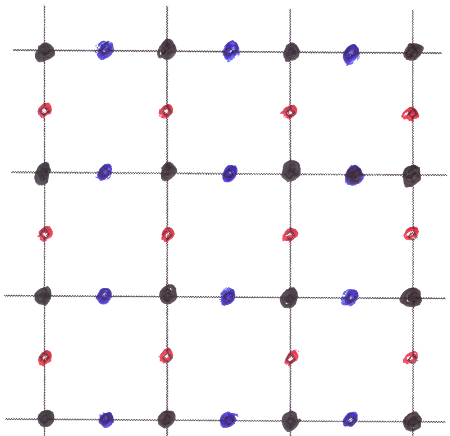
primitive cell $(\vec{a}_1, \vec{a}_2)$ with 3 LP (1^{st} choice)



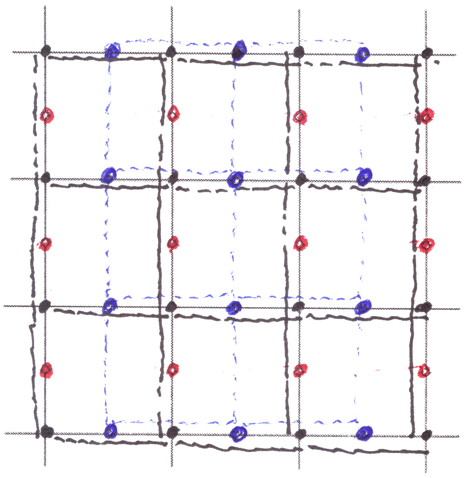
other choices of lattice vectors $(\vec{a}_1, \vec{a}_2)$, (a_1', a_2'), (a_1'', a_2'')

$$\# \text{ of LP} = N_c + N_f = 4 \times \frac{1}{4} + 4 \times \frac{1}{2} = 1 + 2 = 3$$

N_c: corner points; N_f: face points



b) the black, red, and blue lattice points are not equivalent since the environment is different at each site. Therefore, the lattice is Not BL



c) we can see that the non-Bravais lattice may be described as three square Bravais lattices, which are shown in black, red, and blue

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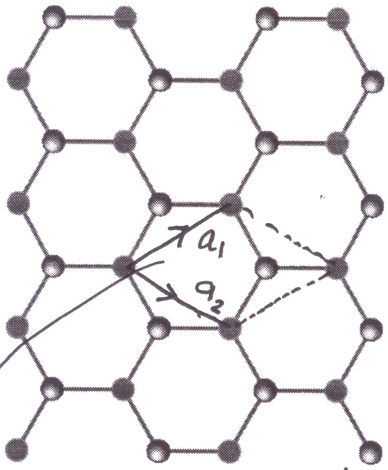
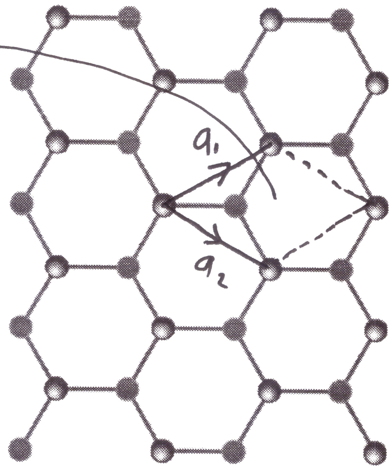
a)



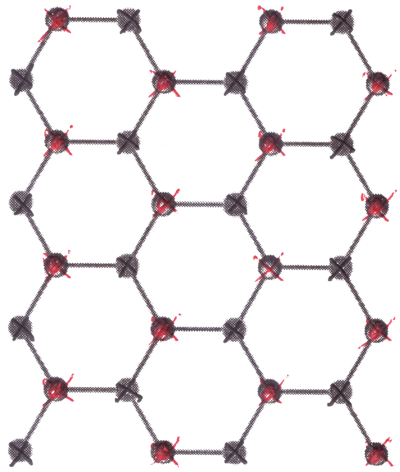
primitive cell $(\vec{a_1}, \vec{a_2})$ (2^{nd} choice) with 2 LP



primitive cell (1^{st} choice) $(\vec{a_1}, \vec{a_2})$ with 2 LP

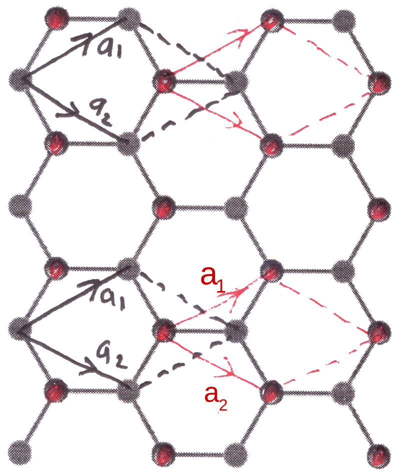
# of LP $= N_c + N_I = 4 \times \frac{1}{4} + 1 = 2$

N_c: corner points; N_I: interior point



b) the black and red lattice points are not equivalent since the environment is different at each site. Therefore, the lattice is not BL

c) we can see that the non-Bravais lattice may be described as two Bravais lattices, which are shown in black and red



6

6. (a) Consider a cube of side length 2 as shown in Figure 3, with the origin of coordinates at the center. Write down the transformation matrix that takes the point (1, -1, 1) into the point (1, -1, -1) using the following symmetry operations in order: first, a 90-degree clockwise rotation around the z-axis, then a reflection across the xz-plane, and finally an inversion about the cube's center.

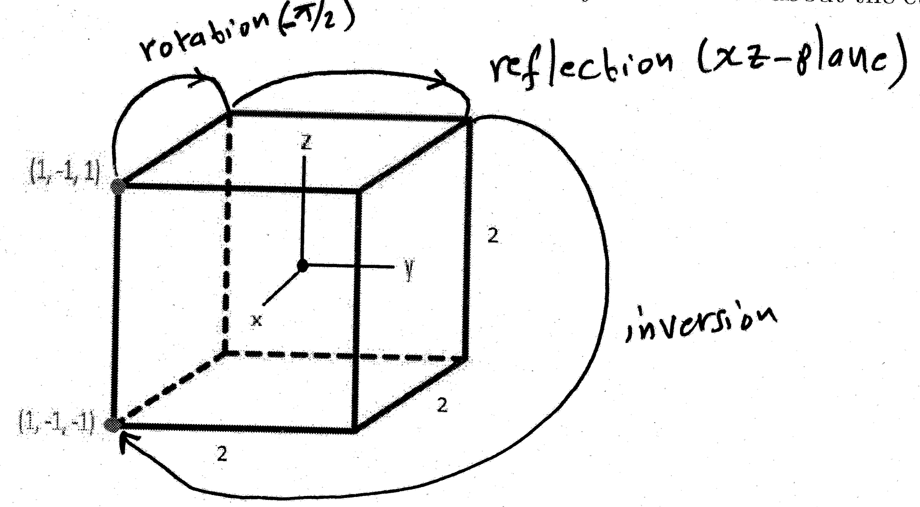


Figure 3:

let the transformation matrix be M

$$\Rightarrow M = \text{inversion} \times \text{reflection} \times \text{rotation}$$

$$= i(0) \times \sigma_{xz} \times R_z(-\pi/2) \; ; \quad R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

clockwise

$$= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

check $\quad M \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} \checkmark$

⑦ $R = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$;

a) $\begin{vmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{vmatrix} = 1 \begin{vmatrix} 0 & -1 \\ 1 & 0 \end{vmatrix} = 0 - (-1) = +1$

$\Rightarrow$ so it is a rotational matrix

b) to find the axis of rotation, we set $R\vec{r} = \vec{r}$ as any vector on the axis of rotation is not affected by rotation

$$\Rightarrow \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{matrix} +z = x \\ -y = y \Rightarrow 2y = 0 \Rightarrow y = 0 \\ +x = z \end{matrix}$$

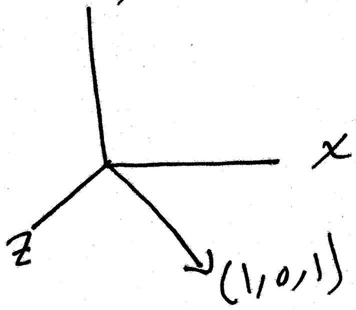
x or z is arbitrary, so let $x = 1 \Rightarrow z = +1$

$\Rightarrow$ the axis of rotation is $(1, 0, +1) = \hat{i} + \hat{k}$

$\Rightarrow$ to find angle of rotation, set

$Tr = 2\cos\theta + 1 = -1 \Rightarrow \cos\theta = -1$

$\Rightarrow \theta = \pm\pi$



c) $\hat{i} = (1, 0, 0)$; $\hat{j} = (0, 1, 0)$, $\hat{k} = (0, 0, 1)$

$$\Rightarrow \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \text{i.e. } \hat{i} \to \hat{k} \checkmark$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 0 \end{pmatrix}; \quad \hat{j} \to -\hat{j}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; \quad \hat{k} \to \hat{i}$$

as expected

⑧

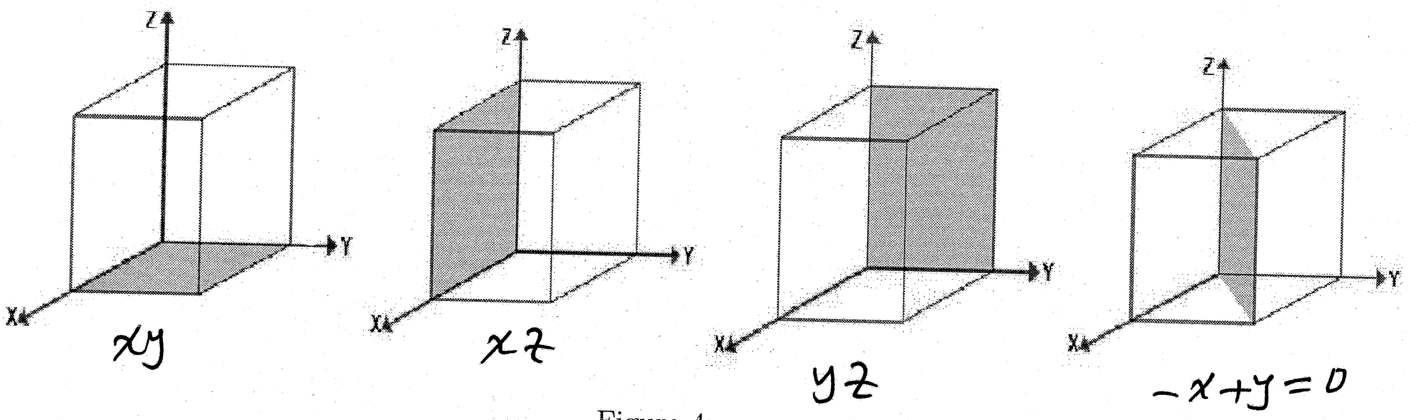


Figure 4:

a) the equation of the xy plane is $z=0 \Rightarrow h=0,\ k=0,\ l=1$

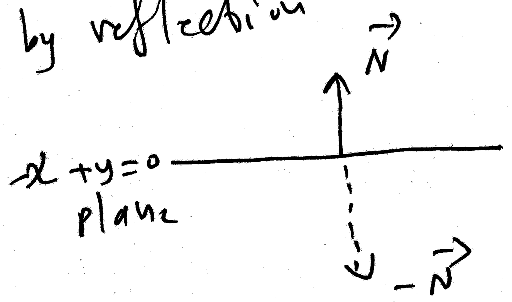
$$\Rightarrow \sigma_{xy} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$; for xz plane $y=0 \Rightarrow h=0,\ l=0,\ k=1$

$$\Rightarrow \sigma_{xz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$; for yz plane $x=0 \Rightarrow k=0,\ l=0,\ h=1$

$$\Rightarrow \sigma_{yz} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

b) $-x+y=0 \Rightarrow h=-1,\ k=1,\ l=0$

$$\Rightarrow \sigma = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$; to verify that this matrix is a reflection matrix through $-x+y=0$ plane, we use the fact that the normal vector $\vec{N}=(-1,1,0)$ is reversed by reflection



$\Rightarrow \sigma\vec{N} = -\vec{N}$

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix} \Rightarrow$$

$y=-x$

$x=-y$

$z=-z \Rightarrow 2z=0 \Rightarrow z=0$

set $x=1 \Rightarrow y=-1$

$\Rightarrow \vec{N}=(x,y,z)=(1,-1,0)$

and using $hx+ky+lz=0$

$x-y=0$, or

$-x+y=0$ ✓

c) $$\sigma\begin{pmatrix} 1 \\ 0 \\ 1/2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1/2 \end{pmatrix}$$ as expected.