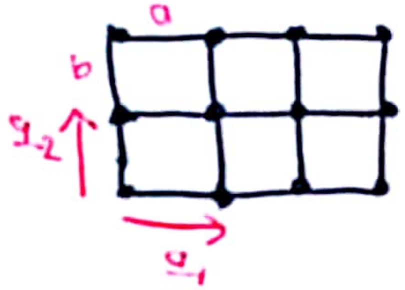
EP402 / MP464 Solid State Physics

Solutions to problems 1–6.

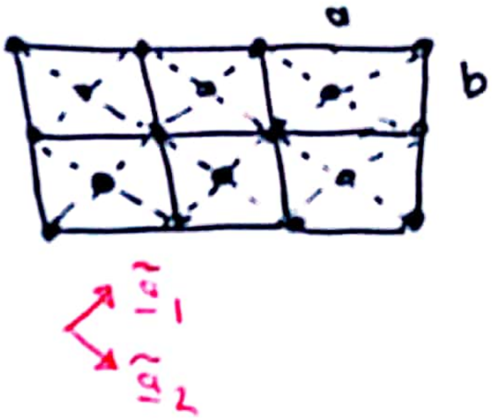
Q1: This was dealt with extensively in a tutorial.

Rectangular lattice:



$\underline{a}_1 = a\hat{\underline{x}}$
$\underline{a}_2 = b\hat{\underline{y}}$

Face-centred rectangular lattice



$$\tilde{\underline{a}}_1 = \tfrac{1}{2}(a\hat{\underline{x}} + b\hat{\underline{y}})$$
$$\tilde{\underline{a}}_2 = \tfrac{1}{2}(a\hat{\underline{x}} - b\hat{\underline{y}})$$

(These are not unique, other choices are possible.)

- The translations and ~~the~~ point groups combine in different ways for these two lattices. For example

$m_1: \underline{a}_1 \to \underline{a}_1$ $\qquad$ $m_1: \tilde{\underline{a}}_1 \to \tilde{\underline{a}}_2$
$m_1: \underline{a}_2 \to -\underline{a}_2$ $\qquad$ $m_1: \tilde{\underline{a}}_2 \to \tilde{\underline{a}}_1$

$m_2: \underline{a}_1 \to -\underline{a}_1$ $\qquad$ $m_2: \tilde{\underline{a}}_1 \to -\tilde{\underline{a}}_2$
$m_2: \underline{a}_2 \to \underline{a}_2$ $\qquad$ $m_2: \tilde{\underline{a}}_2 \to -\tilde{\underline{a}}_1$

Another way of seeing the difference is to observe that all translations of the rectangular lattice, $\underline{L} = n_1\underline{a}_1 + n_2\underline{a}_2$ with n_1 and n_2 integers are also translations of the centred rectangular lattice, but not all translations of the centred rectangular lattice are symmetries of the rectangular lattice — for example

$\underline{\tilde{a}}_1$ and $\underline{\tilde{a}}_2$ are translational symmetries of the centred rectangular lattice, but they are not symmetries of the rectangular lattice.

Q 2: Primitive lattice vectors $\underline{a}_1$ and $\underline{a}_2$

$\Rightarrow$ area of a primitive cell is $|\underline{a}_1 \times \underline{a}_2| = A_c$

area of the parallelogram generated by $\underline{a}_1'$ and $\underline{a}_2'$ is

$$|\underline{a}_1' \times \underline{a}_2'| = |(\alpha_{11}\underline{a}_1 + \alpha_{12}\underline{a}_2) \times (\alpha_{21}\underline{a}_1 + \alpha_{22}\underline{a}_2)|$$

$$= |\alpha_{11}\alpha_{22}(\underline{a}_1 \times \underline{a}_2) + \alpha_{12}\alpha_{21}(\underline{a}_2 \times \underline{a}_1)|$$

$$= (|\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}|)\, |\underline{a}_1 \times \underline{a}_2|$$

$$= (|\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}|)\, A_c$$

$\underline{a}_1'$ and $\underline{a}_2'$ are only primitive if this parallelogram is a primitive cell $\Rightarrow$ it has area A_c

$$\Rightarrow \alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21} = 1$$

$$\Rightarrow \det\begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix} = 1$$

i) $\begin{pmatrix} \underline{a}_1' \\ \underline{a}_2' \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \underline{a}_1 \\ \underline{a}_2 \end{pmatrix}$, $\det\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} = 1$

$\Rightarrow$ $\underline{a}_1'$ and $\underline{a}_2'$ are primitive.

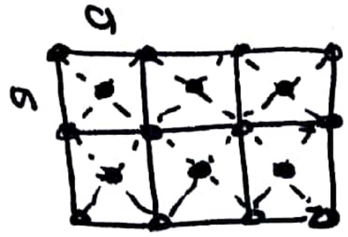
ii) $\begin{pmatrix} \underline{a}_1' \\ \underline{a}_2' \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} \underline{a}_1 \\ \underline{a}_2 \end{pmatrix}$, $\det\begin{pmatrix} 2 & -1 \\ 1 & 1 \end{pmatrix} = 2+1 = 3$

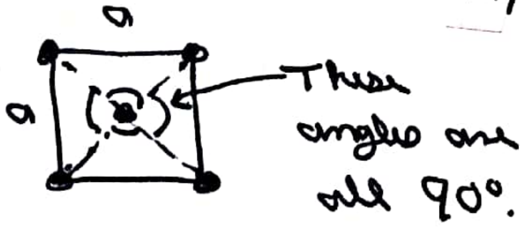
These are not primitive.

iii) $\begin{pmatrix} \underline{a}_1' \\ \underline{a}_2' \end{pmatrix} = \begin{pmatrix} 2 & 5 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} \underline{a}_1 \\ \underline{a}_2 \end{pmatrix}$, $\det\begin{pmatrix} 2 & 5 \\ 1 & 3 \end{pmatrix} = 6-5 = 1$

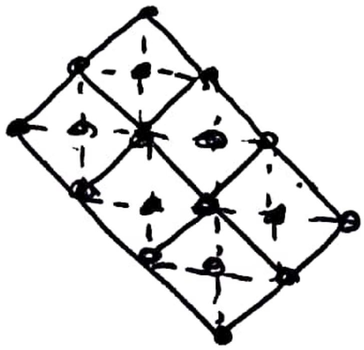
These are primitive.

Q3)



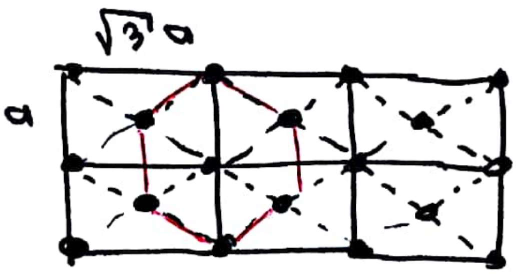


Turn the lattice through 45°

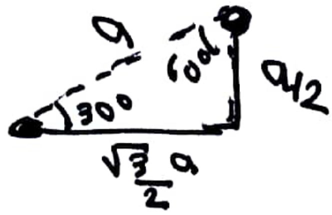


We get a square lattice with lattice spacing $a/\sqrt{2}$.

Q 4.)



← Each triangle here is half of an equilateral triangle.



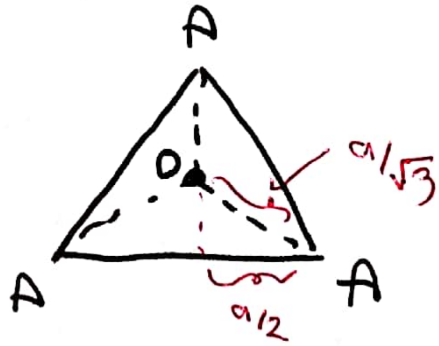
The red figure above is a hexagon - point symmetries include rotations through 60°, this is a hexagonal lattice.

(6)

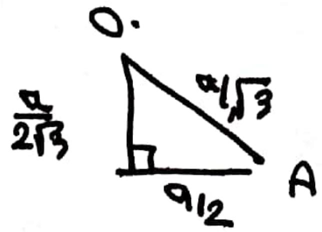
Q5). From the diagram of the ABABA... structure on page 17 of the lecture notes, the distance between two adjacent A–A sites and two adjacent A–B sites is the same, if identical hard spheres are placed at each site and packed together. Hence the figure

is a regular tetrahedron with side a.

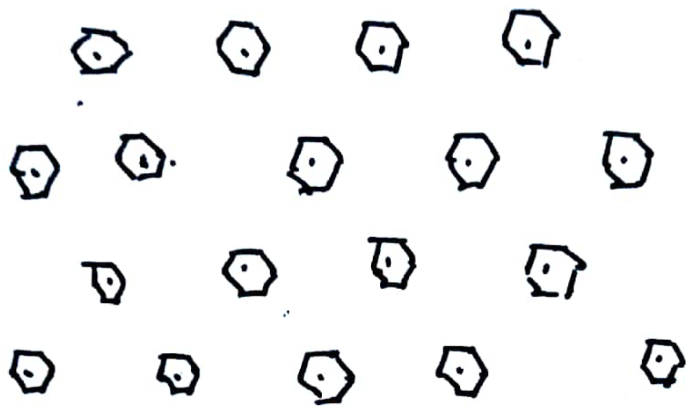
To calculate the height of the tetrahedron, drop a perpendicular from B to the mid-point, O, of the base triangle:



AO has length $a/\sqrt{3}$ and the height of O above the baseline A–A is $\frac{a}{2\sqrt{3}}$, from Pythagoras' theorem



To identify the lattice in the Alhambra Palace tiling, focus on one piece of the pattern, for example the white hexagons



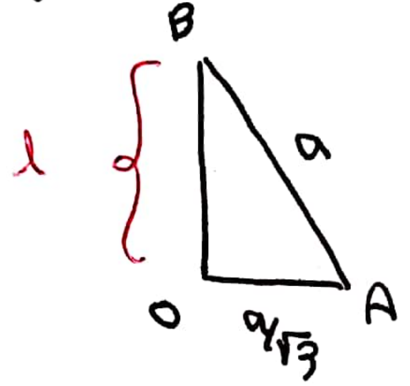
This is a hexagonal lattice with hexagons at the lattice points. The point group is that of the hexagonal lattice: rotations through 60° and multiples thereof, and 6 reflections about the axes

The pattern has a smaller point group though. The basis is the following shape:

BASIS

This has no reflection symmetries and reduces the rotational symmetry from 6-fold to 3-fold. The point group of the crystal is just rotations through 120°, 240° and 360°.

We can now calculate the length of OB, again by Pythagoras

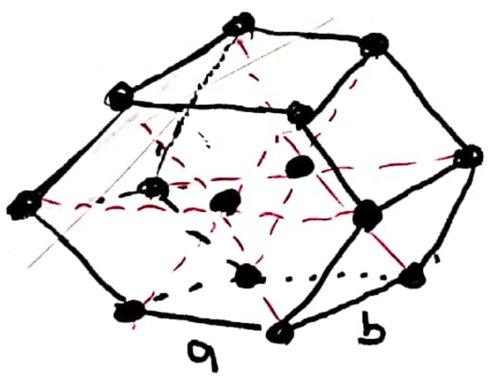


$$l = \sqrt{a^2 - \frac{a^2}{3}} = \sqrt{\frac{2}{3}} \cdot a$$

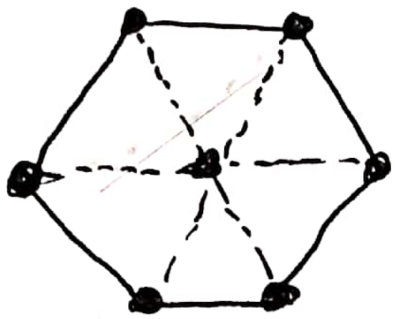
The distance between adjacent A-layers in the figure on page 17 of the lecture notes is

$$c = 2l = 2\sqrt{\frac{2}{3}}\,a = \sqrt{\frac{8}{3}}\,a.$$

Q 6) From the diagram on page 9 of the lecture notes

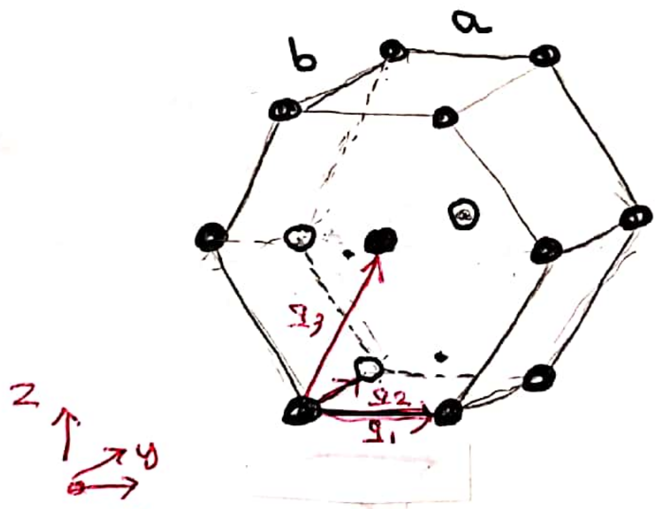


as pieces of a 2-dimensional hexagonal lattice, the front and back hexagons both contain 3 complete lattice points of a 2-dimensional hexagonal lattice.



The 3-dimensional structure on the previous page therefore contains 3 complete lattice points, 3/2 from the front face and 3/2 from the back face.

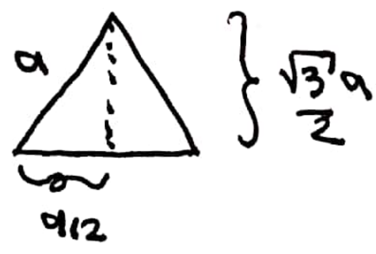
A primitive cell should therefore have 1/3 of the volume of the shape on the previous page.



The area of each hexagonal face is

$$6 \times \left(\frac{\sqrt{3}}{4}a^2\right) = \frac{3\sqrt{3}}{2}a^2$$

where $\frac{\sqrt{3}}{4}a^2$ is the area of an equilateral triangle of side a :



Therefore the volume of the hexagonal box pictured above is $\frac{3\sqrt{3}}{2}a^2 b$ and the volume of a primitive cell should be $\frac{1}{3}$ of this :

$$V_c = \frac{\sqrt{3}}{2}a^2 b$$

Choosing x-y-z axes as shown on the previous page, primitive lattice vectors are:

$$\underline{a}_1 = a\hat{\underline{x}}$$

$$\underline{a}_2 = b\hat{\underline{y}}$$

$$\underline{a}_3 = \frac{a}{2}\hat{\underline{x}} + \frac{\sqrt{3}a}{2}\hat{\underline{z}}$$

(these are not unique — other choices are possible).

To check that these are primitive, calculate the volume

$$\underline{a}_1 \cdot (\underline{a}_2 \times \underline{a}_3) = a\hat{\underline{x}} \cdot \left\{ \frac{ba}{2}\hat{\underline{y}}\times\hat{\underline{x}} + \sqrt{3}\frac{ba}{2}\hat{\underline{y}}\times\hat{\underline{z}} \right\}$$

$$= \frac{\sqrt{3}}{2}ba^2\,\hat{\underline{x}}\cdot(\hat{\underline{y}}\times\hat{\underline{z}}) = \frac{\sqrt{3}}{2}a^2 b$$

which is the volume of a primitive cell.