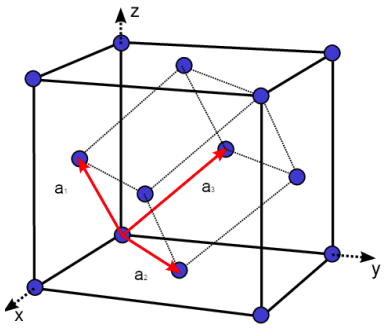
Condensed Matter Physics 2023
Quiz 3 (Week 10)

1. (a) Find the primitive reciprocal lattice vectors of a face-centered-cubic (fcc) lattice. What type of lattice is the reciprocal lattice?

   (b) The primitive vectors of a hexagonal lattice can be taken as $\mathbf{a}_1 = \frac{a\sqrt{3}}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}$, $\mathbf{a}_2 = -\frac{a\sqrt{3}}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}$ and $\mathbf{a}_3 = c\hat{\mathbf{z}}$. Determine the volume of the primitive cell, the primitive reciprocal lattice vectors and what type of lattice is the reciprocal lattice.

(a) As shown in the figure below, the unit vectors of the fcc lattice can be written as:

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{z}}) = \frac{a}{2}(1,0,1); \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}) = \frac{a}{2}(1,1,0); \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}) = \frac{a}{2}(0,1,1)$$



The volume of the fcc lattice is:

$$V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{8}\begin{pmatrix}1\\0\\1\end{pmatrix} \cdot \begin{pmatrix}1\\1\\0\end{pmatrix} \times \begin{pmatrix}0\\1\\1\end{pmatrix} = \frac{a^3}{4}$$

The primitive reciprocal lattice vectors can then be found as:

$$\mathbf{b}_1 = \frac{2\pi}{V}\,\mathbf{a}_2 \times \mathbf{a}_3 = \frac{8\pi}{a^3}\frac{a^2}{4}\begin{pmatrix}1\\1\\0\end{pmatrix} \times \begin{pmatrix}0\\1\\1\end{pmatrix} = \frac{8\pi}{a^3}\frac{a^2}{4}\begin{pmatrix}1\\-1\\1\end{pmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

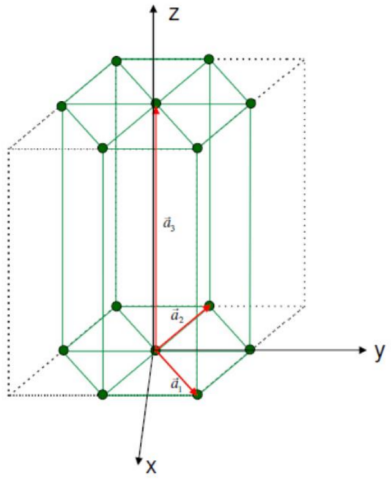
$$\mathbf{b}_2 = \frac{2\pi}{V}\,\mathbf{a}_3 \times \mathbf{a}_1 = \frac{8\pi}{a^3}\frac{a^2}{4}\begin{pmatrix}0\\1\\1\end{pmatrix} \times \begin{pmatrix}1\\0\\1\end{pmatrix} = \frac{8\pi}{a^3}\frac{a^2}{4}\begin{pmatrix}1\\1\\-1\end{pmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\1\\-1\end{pmatrix}$$

$$\mathbf{b}_3 = \frac{2\pi}{V}\,\mathbf{a}_1 \times \mathbf{a}_2 = \frac{8\pi}{a^3}\frac{a^2}{4}\begin{pmatrix}1\\0\\1\end{pmatrix} \times \begin{pmatrix}1\\1\\0\end{pmatrix} = \frac{8\pi}{a^3}\frac{a^2}{4}\begin{pmatrix}-1\\1\\1\end{pmatrix} = \frac{2\pi}{a}\begin{pmatrix}-1\\1\\1\end{pmatrix}$$

These vectors correspond to the primitive vectors of a bcc lattice.

(b) A possible choice of the primitive vectors is already given in the exercise and shown below:

$$\mathbf{a}_1 = \frac{a\sqrt{3}}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}; \quad \mathbf{a}_2 = -\frac{a\sqrt{3}}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}; \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$



Using the same formulas as in (a), the volume of the hexagonal primitive cell is:

$$V = \begin{pmatrix} a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} -a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} = \begin{pmatrix} a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} ac/2 \\ ac\sqrt{3}/2 \\ 0 \end{pmatrix} = \frac{\sqrt{3}}{2} a^2 c$$

And the primitive reciprocal lattice vectors are:

$$\mathbf{b}_1 = \frac{4\pi}{\sqrt{3}a^2 c} \begin{pmatrix} -a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} = \frac{4\pi}{\sqrt{3}a^2 c} \begin{pmatrix} ac/2 \\ ac\sqrt{3}/2 \\ 0 \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} 1/\sqrt{3} \\ 1 \\ 0 \end{pmatrix}$$

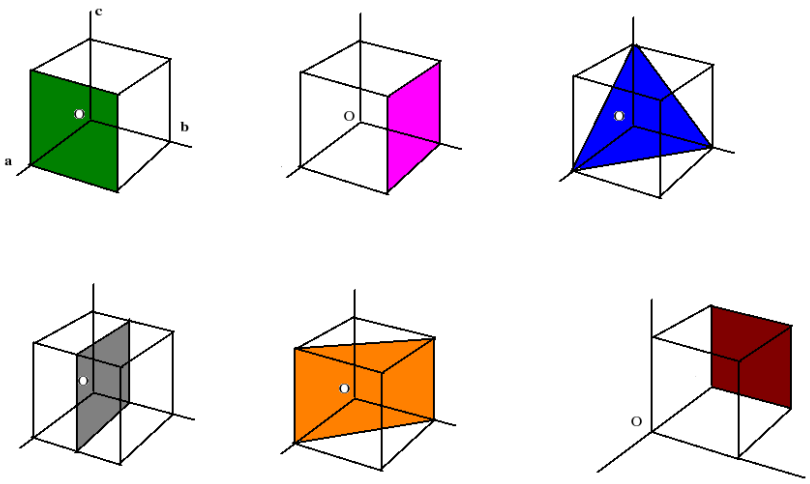
$$\mathbf{b}_2 = \frac{4\pi}{\sqrt{3}a^2 c} \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} \times \begin{pmatrix} a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} = \frac{4\pi}{\sqrt{3}a^2 c} \begin{pmatrix} -ac/2 \\ ac\sqrt{3}/2 \\ 0 \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} -1/\sqrt{3} \\ 1 \\ 0 \end{pmatrix}$$

$$\mathbf{b}_3 = \frac{4\pi}{\sqrt{3}a^2 c} \begin{pmatrix} a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} \times \begin{pmatrix} -a\sqrt{3}/2 \\ a/2 \\ 0 \end{pmatrix} = \frac{4\pi}{\sqrt{3}a^2 c} \begin{pmatrix} 0 \\ 0 \\ a^2\sqrt{3}/2 \end{pmatrix} = \frac{2\pi}{c} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The reciprocal lattice is again a hexagonal lattice. For example, you can check that the angle between $\mathbf{b}_1$ and $\mathbf{b}_2$ is 60^o:

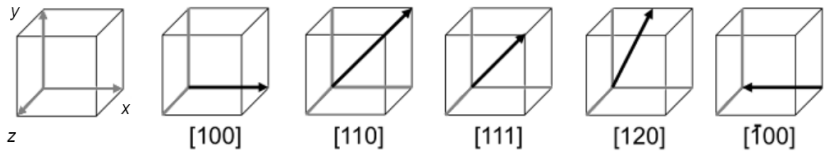
$$\cos\theta = \frac{\mathbf{b}_1 \cdot \mathbf{b}_2}{|\mathbf{b}_1||\mathbf{b}_2|} = \frac{\frac{4\pi^2}{a^2}\frac{2}{3}}{\frac{4\pi^2}{a^2}\sqrt{1/3+1}\sqrt{1/3+1}} = \frac{1}{2} \quad \Rightarrow \quad \theta = 60^o$$

2. Consider a simple cubic crystal of side a.
   (a) Give the Miller indices of the planes shown in the figure below.
   (b) Draw the [100], [110], [111], [120] and $[\bar{1}00]$ directions.
   (c) Write all possible $\langle 001 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions.
   (d) The first Brillouin zone boundary in the [111] reciprocal space direction occurs at $\frac{2\pi}{a}(0.5, 0.5, 0.5)$. Is this correct, and why?



(a) From left to right, the Miller indices for the first row are: (100), (010), (111); and for the second row: (020), (110), $(\bar{1}00)$.

(b) The [100], [110], [111], [120] and $[\bar{1}00]$ directions are shown below.



(c) $\langle 001\rangle$: [001], $[00\bar{1}]$, [100], $[\bar{1}00]$, [010], $[0\bar{1}0]$;
$\langle 110\rangle$: [110], $[1\bar{1}0]$, $[\bar{1}10]$, $[\bar{1}\bar{1}0]$, [101], $[\bar{1}0\bar{1}]$, $[10\bar{1}]$, $[\bar{1}01]$, [011], $[0\bar{1}\bar{1}]$, $[0\bar{1}1]$, $[01\bar{1}]$;
$\langle 111\rangle$: [111], $[\bar{1}\bar{1}\bar{1}]$, $[11\bar{1}]$, $[\bar{1}\bar{1}1]$, $[1\bar{1}\bar{1}]$, $[\bar{1}11]$, $[\bar{1}1\bar{1}]$, $[1\bar{1}1]$.

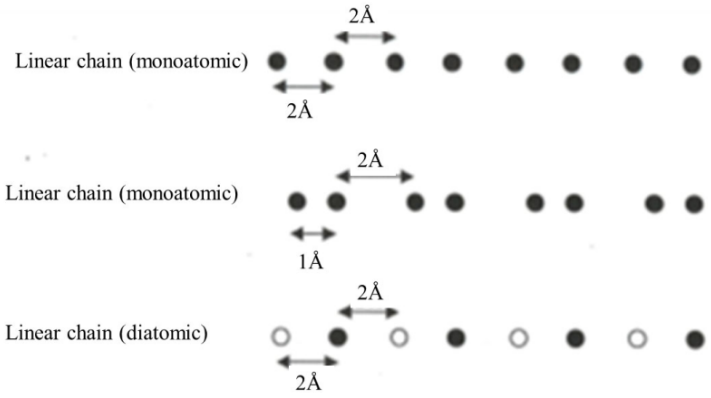
(d) This is correct. Along the [111] direction, the shortest reciprocal lattice vector is $\mathbf{G} = \frac{2\pi}{a}(1,1,1)$. The first Brillouin zone boundary is the plane perpendicular to the reciprocal lattice vector and bisecting it, so in this direction, the first BZ boundary occurs at $\frac{2\pi}{a}(0.5, 0.5, 0.5)$.

3. Define the Wigner-Seitz cell and explain how to construct it. What is the Wigner-Seitz cell of the reciprocal lattice?

The Wigner-Seitz cell is a special choice of primitive unit cell that corresponds to the region of points closer to a given lattice point than to any other. To construct the Wigner-Seitz cell of a given lattice, pick a lattice point and draw lines connecting it to all nearby lattice points, then draw the perpendicular planes bisecting each line. The smallest volume enclosed in this way is the Wigner–Seitz primitive cell.

The Wigner-Seitz cell of the reciprocal lattice is the first Brillouin zone. When plotting the electron or phonon band structures of solids, one generally plots energy vs. k along line cuts in the first Brillouin zone.

4. Mainstream only. Find the reciprocal lattice vectors for the three lattices below (include units in your answers).



In 1D, the lattice vectors are given by $R = na$ and the reciprocal lattice vectors by $G = \frac{2\pi}{a}n$, where n is an integer.
(i) In the first case, the periodicity of the lattice is $a = 2$ Å, so the reciprocal lattice points are spaced by $\frac{2\pi}{2} = \pi$ Å^{-1}.
(ii) In the second case, the crystal consists of a two-atom basis (of the same species), and the periodicity of the lattice is $a = 3$ Å. The reciprocal lattice spacing is then $\frac{2\pi}{3}$ Å^{-1}.
(iii) Also in this case the crystal consists of a two-atom basis, with the atoms of different species. The lattice periodicity is $a = 4$ Å, and the reciprocal lattice spacing is $\frac{2\pi}{4} = \frac{\pi}{2}$ Å^{-1}.

5. Advanced only. Consider a two-dimensional (2D) monoatomic solid measuring $L \times L$ in which the atoms are arranged in a square lattice with lattice parameter a (L is an integer multiple of a). Each atom in the solid contributes one electron to the electron (Fermi) sea.
   (a) Compute the Fermi wavevector k_F. (Hint: find the number of k points contained in the Fermi circle, by knowing that the area per k point is $(2\pi/L)^2$, then consider the total number of electrons in the solid.)
   (b) Make a 2D sketch of the reciprocal lattice and indicate the Fermi circle. In particular, compare the size of the Fermi circle with the size of the first Brilloin zone.

(a) As reminded in the hint, the area per k point is $(2\pi/L)^2$. In 2D we have a Fermi circle instead of a Fermi sphere, with area πk_F^2. Hence, the number of states in the Fermi circle is $\pi k_F^2/(2\pi/L)^2 = L^2 k_F^2/(4\pi)$ and each state can accommodate 2 electrons. The number of electrons in the solid is $(L/a)^2 \times 1$, so accommodating 2 electrons in each state we have the equation $(L/a)^2 = 2L^2 k_F^2/(4\pi)$. Solving for k_F we obtain $k_F = \sqrt{2\pi}/a$.

(b) A sketch of the reciprocal lattice and the Fermi circle is below. The Fermi circle (i.e. the occupied states at $T = 0$ K) is entirely inside the first Brillouin zone, since $k_F = \sqrt{2\pi}/a < \pi/a$.