PHY 240A, Condensed Matter Physics: Solutions to Homework Set #1

1. 2D Honeycomb Lattice. 10 points.
The 2D honeycomb lattice has translation vectors

$$\vec{a}_1 = a(\frac{\sqrt{3}}{2}, \frac{1}{2}); \quad \vec{a}_2 = a(\frac{\sqrt{3}}{2}, -\frac{1}{2})$$

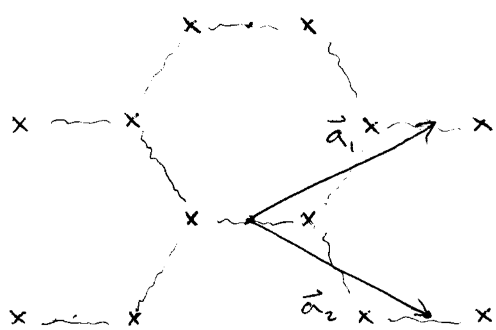
and a basis of two atoms at $\pm a(\frac{1}{2\sqrt{3}}, 0)$.
(a) Show that the distance between all nearest neighbors is the same, and give that distance.
solution
The atom at $a(\frac{1}{2\sqrt{3}}, 0)$ has three nearest neighbors at $a(-\frac{1}{2\sqrt{3}}, 0)$, and $a(\frac{\sqrt{3}}{2} - \frac{1}{2\sqrt{3}}, \pm\frac{1}{2})$. We need to show that the magnitude of vectors to the nearest neighbors are equal.

$$|a(\frac{1}{2\sqrt{3}}, 0) - a(-\frac{1}{2\sqrt{3}}, 0)| = a((\frac{1}{\sqrt{3}})^2 + 0)^{1/2} = \frac{a}{\sqrt{3}}$$

and the other two neighbors

$$\begin{aligned} |a(\frac{1}{2\sqrt{3}}, 0) - a(\frac{\sqrt{3}}{2} - \frac{1}{2\sqrt{3}}, \pm\frac{1}{2})| &= a\left(((\frac{\sqrt{3}}{2} - \frac{1}{\sqrt{3}}))^2 + (\pm\frac{1}{2})^2\right)^{1/2} \\ &= a\left((\frac{1}{2\sqrt{3}})^2 + \frac{1}{4}\right)^{1/2} = a\left(\frac{1}{12} + \frac{1}{4}\right)^{1/2} = \frac{a}{\sqrt{3}} \end{aligned}$$

(b) Sketch the neighborhoods of two particles in the honeycomb lattice which are not identical (i.e. by translation symmetry) and describe the rotation that would be necessary to make them identical.
solution
The neighborhood of one can be rotated into the other by a rotation of $\pi/3$ (60 degrees) about the atom.



2. Cell Volumes. 10 points.
(a) Prove that the reciprocal lattice vectors defined as we have done satisfy

$$\vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3 = \frac{8\pi^3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}.$$

solution
For the proof we will use the vector identities

$$\vec{a} \cdot \vec{b} \times \vec{c} = \vec{b} \cdot \vec{c} \times \vec{a} = \vec{c} \cdot \vec{a} \times \vec{b}$$
$$\vec{a} \times (\vec{b} \times \vec{c}) = (\vec{a} \cdot \vec{c})\vec{b} - (\vec{a} \cdot \vec{b})\vec{c}$$

Our reciprocal lattice vectors are

$$\vec{b}_1 = \frac{2\pi \vec{a}_2 \times \vec{a}_3}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|}$$
$$\vec{b}_2 = \frac{2\pi \vec{a}_3 \times \vec{a}_1}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|}$$
$$\vec{b}_3 = \frac{2\pi \vec{a}_1 \times \vec{a}_2}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|}$$

and we have

$$\begin{aligned}
\vec{b}_1 \cdot \vec{b}_2 \times \vec{b}_3 &= \vec{b}_1 \cdot \frac{(2\pi)^2}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|^2}((\vec{a}_2 \cdot \vec{a}_3 \times \vec{a}_1)\vec{a}_1 - (\vec{a}_1 \cdot \vec{a}_3 \times \vec{a}_1)\vec{a}_2) \\
&= \vec{b}_1 \cdot \frac{(2\pi)^2}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|^2}((\vec{a}_2 \cdot \vec{a}_3 \times \vec{a}_1)\vec{a}_1 - 0) \\
&= \frac{(2\pi)^3}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|^3}(\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3)(\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3) \\
&= \frac{8\pi^3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}
\end{aligned}$$

(b) Prove that the volume of a Bravais lattice cell (i.e. the volume per lattice point) is $V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|$.
solution The volume of a paralleliped is equal to the area of the base times the height. The area of the base is equal to the magnitude of $\vec{a}_2 \times \vec{a}_3$, which is $|a_2 a_3 sin(\hat{a_2}, \hat{a_3})|$, and the height is the projection of $\vec{a}_1$ along the direction of $\vec{a}_2 \times \vec{a}_3$.

$$\begin{aligned}
V &= (\text{height}) * (\text{area of base}) \\
&= (\vec{a}_1 \cdot \frac{\vec{a}_2 \times \vec{a}_3}{|\vec{a}_2 \times \vec{a}_3|}) * (|\vec{a}_2 \times \vec{a}_3|) \\
&= |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|
\end{aligned}$$

3. Hexagonal Lattice. 10 points.
Find the reciprocal lattice vectors of the hexagonal lattice, whose direct lattice vectors are given in A&M Eq. (4.9). What type of lattice is the reciprocal lattice, and what are the lengths of the RLVs?

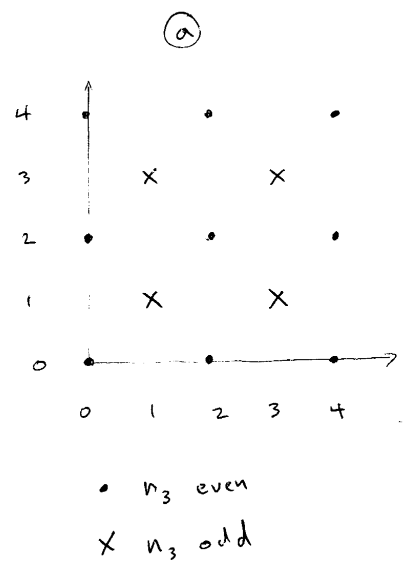
solution
Our reciprocal lattice vectors are

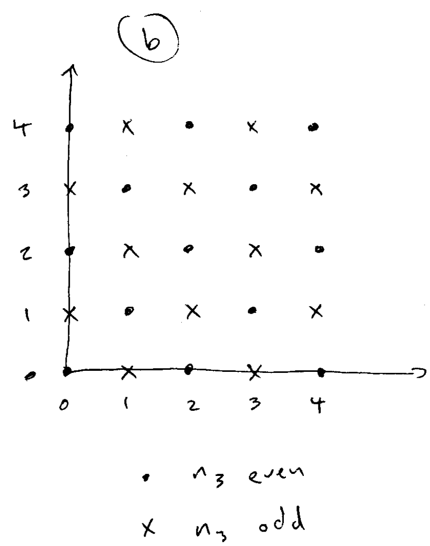
$$\vec{b}_1 = \frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}a}\hat{y}$$
$$\vec{b}_2 = \frac{4\pi}{\sqrt{3}a}\hat{y}$$
$$\vec{b}_3 = \frac{2\pi}{c}\hat{z}$$

Which is again a hexagonal lattice, with lengths

$$|\vec{b}_1| = |\vec{b}_2| = \frac{4\pi}{\sqrt{3}a}$$
$$|\vec{b}_3| = \frac{2\pi}{c}$$

4. Simple Bravais Lattices. 10 points.
What is the Bravais lattice formed by all points (n_1, n_2, n_3) (all integers) such that:
(a) the n_j are all even or all odd?
(b) the sum of the n_j is required to be even?
(These are two separate questions.)
solution
(a) BCC (b) FCC





5. Lattices and Close-Packing. 10 points.
(a) Prove that the ideal c/a ratio for the hexagonal close-packed structure is $\sqrt{8/3} = 1.633....$

solution
The close packing is ideal when the distance between all nearest neighbor lattice points is equal to a. The neighbor on the layer at $z = c/2$ is located directly above the center of the equilateral triangle, which is $a/\sqrt{3}$ away in the plane, by setting the distance of the nearest neighbor to a, we have

$$\begin{aligned}(\frac{a}{\sqrt{3}})^2 + (\frac{c}{2})^2 &= a^2 \\ (\frac{c}{a})^2 &= 4(1-\frac{1}{3}) \\ \frac{c}{a} &= \sqrt{\frac{8}{3}} \qquad (1)\end{aligned}$$

(b) Sodium metal transforms from bcc to hcp at about 23 K (the "martensite transition"). Assume that the density remains constant, and find the lattice constant of the hcp phase, given that the cubic lattice constant is 4.23 $\mathring{A}$ and the c/a ratio is ideal.
solution
Since bcc and hcp both have two atoms in a unit cell. The volume of bcc is simply $(4.23\mathring{A})^3$. The volume of hcp is

$$(\frac{\sqrt{3}a}{2}) * (a) * c = \frac{\sqrt{3}}{2}a^3(\frac{c}{a}) = \frac{\sqrt{3}}{2}a^3 * \sqrt{\frac{8}{3}} = \sqrt{2}a^3$$

And equating the densities

$$\begin{aligned}\frac{2}{V_{hcp}} &= \frac{2}{V_{bcc}} \\ V_{hcp} &= V_{bcc} \\ \sqrt{2}a^3_{hcp} &= (4.23\mathring{A})^3 \\ a_{hcp} &= \left(\frac{1}{\sqrt{2}}\right)^{1/3}(4.23\mathring{A}) = 3.77\mathring{A}\end{aligned}$$