Physics 431 - Homework 1

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September 2022

1 Problem 1

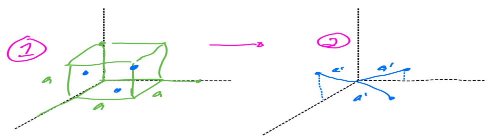
The basis of the $NaCl$ crystal structure on pg 13 consists of one Na^+ ion and one Cl^- ion. The lattice constant, a, describes the length of the basis vectors (in a cubic crystal structure) and will bring us from one Na^+ (Cl^-) ion to the next Na^+ (Cl^-). The Cl^- ion will be positioned at half of the distance between the two Na^+ ions and therefore the distance is:

$$Distance = \frac{a}{2}$$
$$= 0.2815nm$$

Where $a = 0.563nm$

2 Problem 2

2.1



Starting at the origin, we find that we have 3 nearest neighbors. In 3d, we can place another cube in each octant of the three dimensional space. $3 * 8 = 24$, but since we know each of our nearest neighbors to be on the face of a given cube, it will be shared with another cube. Therefore we can take $\frac{24}{2}$ to get the correct number of nearest neighbors in an FCC lattice.

please excuse the poor drawing - I intended to use graphing software but could not figure it out how to illustrate my point using any software.

2.2

Given our known symmetries in from the definition of the FCC lattice, we know that our nearest neighbor sits in the center of a face on the fcc lattice (not every face has a nearest neighbor). We can construct a triangle as we know that projecting this point onto the basis vectors of the unit cell will give us a length of $\frac{a}{2}$. From there, we can use Pythagorean theorem to deduce:

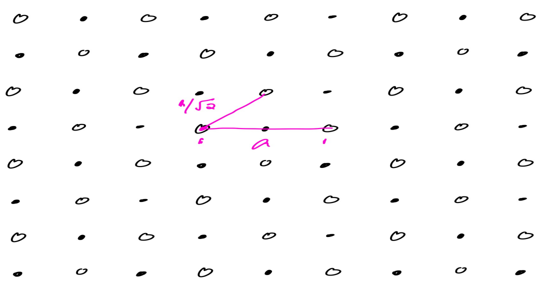
$$Distance = \frac{\sqrt{2}}{2}a$$

3 Problem 3

The HCP structure is not a Bravais lattice because because if you construct a basis with an origin at any given lattice point, there will be lattice point in the structure that cannot be defined as a linear combination of the basis vectors. This is a violation of the definition of Bravais lattices.

4 Problem 4

4.1



4.2

$$T_1 = a\hat{x} + 0\hat{y} \tag{1}$$
$$T_2 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} \tag{2}$$

5 Problem 5

5.1

This is a geometric argument. To explain since I do not have graphs - take a' to be the length from the center lattice point in the 2d plane to the edge of the HCP lattice. From this dimension we can construct a'' knowing that at $\frac{2a'}{3}$ and $\frac{c}{2}\hat{z}$. From this point, we can construct a triangle from a'', a and c and use pythagreom therom to get the ratio between a and c.

5.2

$$a = 1$$
$$c = \sqrt{\frac{8}{3}}$$
$$V_{sphere} = \frac{4}{3}\pi r^3$$
$$V_{hex} = 3c\sqrt{2}$$

$$n_{spheres} = 17$$

$$\begin{aligned} V_{max} &= \frac{V_{hex}}{V_{sphere} * n_{spheres}} \\ &= \frac{V_{hex}}{V_{sphere} * n_{spheres}} \end{aligned} \tag{3}$$

The number resulting from this calculation does not make physical sense.