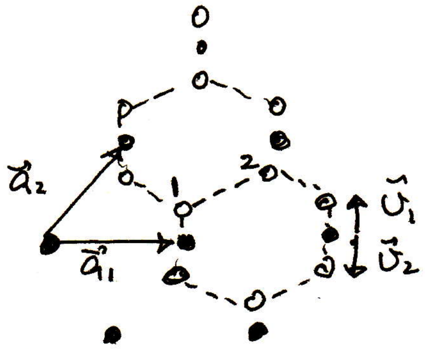
Physics 211A — HW 1 Solutions — Fall 2014

## Problem 1




Add basis:

$$\vec{u}_1 = a\left(0, \frac{1}{2\sqrt{3}}\right)$$

$$\vec{u}_2 = a\left(0, -\frac{1}{2\sqrt{3}}\right)$$

Bravais lattice:

$$\vec{a}_1 = a(1,0)$$

$$\vec{a}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$$

Distance between points vertically:

$$d = 2a \cdot \frac{1}{2\sqrt{3}} = \frac{a}{\sqrt{3}}$$

Distance between points 1 and 2 in figure:

$$1 = a\left(0, \frac{1}{2\sqrt{3}}\right) \quad ; \quad 2 = \vec{a}_2 + \vec{u}_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2} - \frac{1}{2\sqrt{3}}\right) \Rightarrow$$

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

$$\Rightarrow |2-1| = a\sqrt{\frac{1}{4} + \frac{1}{12}} = a\sqrt{\frac{4}{12}} = \frac{a}{\sqrt{3}}$$

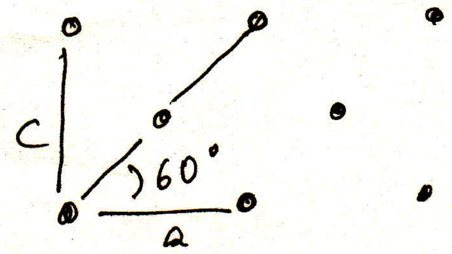
points 1 and 2 are not identical. e.g. there is a point at distance d above 2 and not above 1.

(b) $a = 2.46\,\mathring{A}$, $d = a/\sqrt{3} = 1.42\,\mathring{A}$

(c) Unit cell area $= a^2\frac{\sqrt{3}}{2}$, 2 atoms / unit cell. $m_c = 12 \times 1.66 \cdot 10^{-27}\,kg$

$$\rho = \frac{M}{A} = \frac{2 \times m_c}{a^2\frac{\sqrt{3}}{2}} = \frac{4}{\sqrt{3}} \cdot \frac{12 \times 1.66 \times 10^{-27} \times 10^3\,g}{2.46^2 \times (10^{-8}\,cm)^2} = 7.6 \times 10^{-8}\,\frac{g}{cm^2}$$

# Problem 2

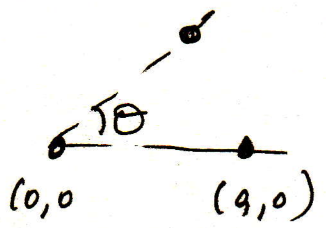



$\tan 60° = \sqrt{3} = c/a$

<u>Hexagonal</u>: 2, 3, 6-fold rotations; inversion; x, y reflections, reflections about 30°, 60° axis

<u>Centered tetragonal</u>: no 3, 6-fold rotations, no reflections about 30°, 60° axis

Problem 4




rotate by $\theta$: $(a,0) \to (a\cos\theta, a\sin\theta)$

rotate by $-\theta$: $(a,0) \to (a\cos\theta, -a\sin\theta)$

vector connecting these points is in BL $\Rightarrow$

$(a\cos\theta, a\sin\theta) - (a\cos\theta, -a\sin\theta) = (0, 2a\sin\theta)$

If we use as primitive vectors

$$\vec{a}_1 = (a,0), \quad \vec{a}_2 = (a\cos\theta, a\sin\theta)$$

$\Rightarrow \quad (0, 2a\sin\theta) = n_1\vec{a}_1 + n_2\vec{a}_2$ for some integers $a_1, a_2$

$$\Rightarrow \quad 0 = n_1 + n_2\cos\theta \quad \Rightarrow \quad \cos\theta = -\frac{n_1}{n_2}$$

$$2a\sin\theta = n_2 a\sin\theta \quad \Rightarrow \quad n_2 = 2$$

$$\Rightarrow \quad \cos\theta = -\frac{n_1}{2} \quad \Rightarrow$$

$$\cos\theta = 0, \pm\frac{1}{2}, \pm 1$$

$$\Rightarrow \quad \theta = \frac{\pi}{2}, \frac{\pi}{6}, \frac{\pi}{3}, \pi$$

$\Rightarrow$ 2, 3, 4, 6 fold rotations only

## Problem 5

Find minimum of $\phi(r) = e^{-r}\left(\frac{1}{r^3} - 1\right)$

$$\phi' = -\left(\frac{1}{r^3} - 1\right) - \frac{3}{r^4} = 0 \Rightarrow \frac{1}{r^3} - 1 + \frac{3}{r^4} = 0 \Rightarrow$$

$$r^4 - r - 3 = 0 \Rightarrow \boxed{r = 1.45} \quad \text{(numerically)}$$

hexagonal has 6 nn, square has 4 nn $\Rightarrow$ hexagonal has lower energy, equilibrium lattice spacing is $a = 1.45$.

(b) If $\phi(r) = \phi_0 e^{-r}\left(\frac{1}{2r} - 1\right)$

$n$ = density = # of points per unit area

$$\sum_j \phi(r_{0j}) = \int d^2r\, n\, \phi(r)$$ is interaction energy for atom at $r=0$

$$= n \cdot 2\pi \int_0^R d^2r\, e^{-r}\left(\frac{1}{2r} - 1\right) \cdot \phi_0 \quad ; \quad R = 1.5$$

If the integral is negative, the energy becomes lower the larger $n$ is, and the system would collapse into a state of high density. So need to calculate

$$I = \int_0^R dr \cdot r \cdot e^{-r}\left(\frac{1}{2r} - 1\right) \equiv I_1 - I_2$$

$$I_1 = \int_0^R dr\, \frac{1}{2} e^{-r} = -\frac{1}{2} e^{-r} \Big]_0^R = \frac{1}{2} - \frac{1}{2} e^{-R}$$

$$I_2 = \int_0^R dr\, r e^{-r} = -r e^{-r} \Big]_0^R + \int_0^R dr\, e^{-r} =$$

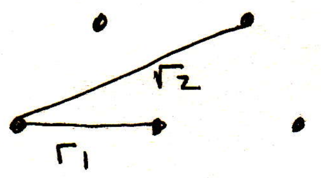
$$= -Re^{-R} - e^{-r} \Big]_0^R = -Re^{-R} - e^{-R} + 1 = 1 - e^{-R} - Re^{-R} \Rightarrow$$

$$I = I_1 - I_2 = \frac{1}{2} - \frac{1}{2} e^{-R} - 1 + e^{-R} + Re^{-R} = -\frac{1}{2} + \frac{1}{2} e^{-R} + Re^{-R} =$$

$$= -\frac{1}{2} + e^{-R}\left(R + \frac{1}{2}\right) = -0.5 + 2e^{-1.5} = -0.5 + 0.446$$

$$= -0.054 < 0 \Rightarrow \text{system will collapse.}$$

(c)




$$\phi(r) = \phi_0 e^{-r}\left(\frac{1}{r^3} - 1\right)$$

For $r_1 = 1.45$, $\phi(r_1) = -0.158$, there are 6 nn

The 2nd nn distance is $r_2 = \sqrt{3}\, r_1 = 2.51$, there are 6 nnn

$\phi(r_2) = -0.078$

The 3rd nn distance is $r_3 = 2r_1 = 2.90$, there are 6 3rd nn.

$\phi(r_3) = -0.053$

decays slowly $\Rightarrow$ solve by computer