Physics 140A Winter 2011

Homework 2 due Wednesday January 19

1. Consider a plane hkl in a crystal lattice. (a) Prove that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$ is perpendicular to this plane. (b) Prove that this distance between two adjacent planes of this lattice is $d(hkl) = \frac{2\pi}{|\mathbf{G}|}$. (c) Show that for a simple cubic lattice that $d^2 = a^2/(h^2+k^2+l^2)$.

2. The primitive translation vectors of a hexagonal lattice is given by: $\mathbf{a}_1 = \frac{\sqrt{3}a}{2}\mathbf{x} + \frac{a}{2}\mathbf{y}$, $\mathbf{a}_2 = \frac{-\sqrt{3}a}{2}\mathbf{x} + \frac{a}{2}\mathbf{y}$, $\mathbf{a}_3 = c\mathbf{z}$. (In two dimensions, this describes graphene.)(a) Show that the volume of the unit cell is $V_c = \frac{\sqrt{3}}{2}a^2c$. (b) Show that the primitive translation vectors of the reciprocal lattice are: $\mathbf{b}_1 = \frac{2\pi}{\sqrt{3}a}\mathbf{x} + \frac{2\pi}{a}\mathbf{y}$, $\mathbf{b}_2 = -\frac{2\pi}{\sqrt{3}a}\mathbf{x} + \frac{2\pi}{a}\mathbf{y}$, $\mathbf{b}_3 = \frac{2\pi}{c}\mathbf{z}$, so that the lattice is its own reciprocal, but with a rotation of axes. (c) Describe and sketch the first Brillouin zone of the hexagonal space lattice as projected onto the $x-y$ plane.

3. Show that the volume of the first Brillouin zone is is $(2\pi)^3/V_c$, where V_c is the volume of the crystal primitive cell. Recall that the volume of a Brillouin zone is equal to that of the primitive parallelepiped in Fourier space, and that $(\mathbf{c}\times\mathbf{a})\times(\mathbf{a}\times\mathbf{b}) = (\mathbf{c}\cdot\mathbf{a}\times\mathbf{b})\mathbf{a}$.

HW 2 Solutions

Note Title 1/20/2010

1 (a) plane hkl in lattice

intercepts at

15 pts

$$\vec{r}_1 = \frac{1}{h}\vec{a}_1$$

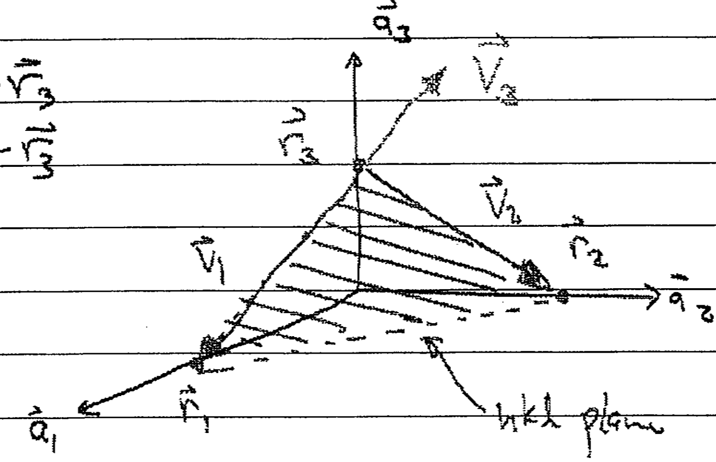
$$\vec{r}_2 = \frac{1}{k}\vec{a}_2 \qquad (\text{where } n = \text{integer})$$

$$\vec{r}_3 = \frac{1}{l}\vec{a}_3$$

consider 2 vectors in this plane:

$$\vec{v}_1 = \vec{r}_1 - \vec{r}_3$$

$$\vec{v}_2 = \vec{r}_2 - \vec{r}_3$$



$\vec{V}_3 = \vec{V}_1 \times \vec{V}_2$ is then perpendicular to the hkl plane

$$= \left(\frac{1}{h}\vec{a}_1 - \frac{1}{l}\vec{a}_3\right) \times \left(\frac{1}{k}\vec{a}_2 - \frac{1}{l}\vec{a}_3\right)$$

$$= \left(\frac{1}{hk}\vec{a}_1 \times \vec{a}_2 - \frac{1}{hl}\vec{a}_1 \times \vec{a}_3 - \frac{1}{lk}\vec{a}_3 \times \vec{a}_2\right)$$

$$\left\{ \begin{aligned} \text{but} \quad \vec{b}_1 &= \frac{2\pi}{V}\left(\vec{a}_2 \times \vec{a}_3\right) \\ \vec{b}_2 &= \frac{2\pi}{V}\left(\vec{a}_3 \times \vec{a}_1\right) \\ \vec{b}_3 &= \frac{2\pi}{V}\left(\vec{a}_1 \times \vec{a}_2\right) \end{aligned} \right\}$$

So

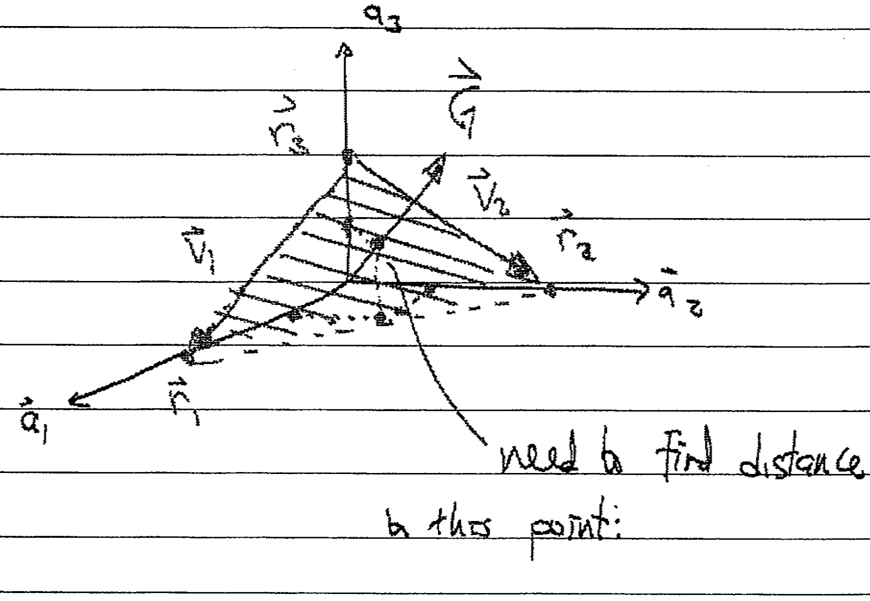
$$\vec{V}_3 = \frac{V}{2\pi}\left(\frac{1}{hk}\vec{b}_3 + \frac{1}{hl}\vec{b}_2 + \frac{1}{lk}\vec{b}_1\right)$$

$$= \frac{V}{2\pi\,(hkl)} \underbrace{\left(h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3\right)}_{\vec{G}} \propto \vec{G}$$

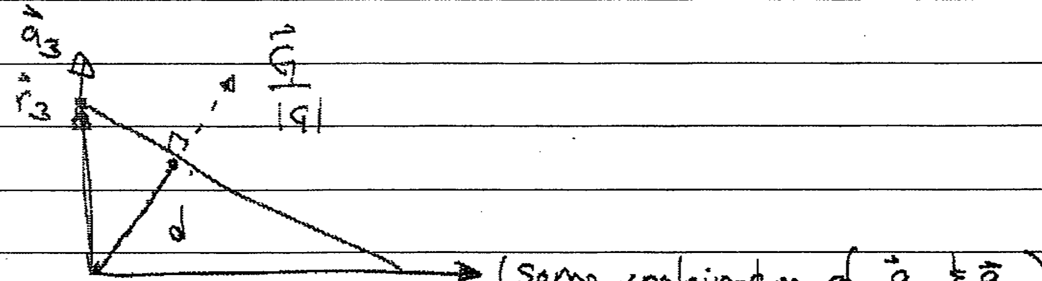
So <u>$\vec{G}$ is $\perp$ to the (hkl) plane</u>

(b) $d(hkl)$ is the distance from the origin to the (hkl) plane along the $\perp$ direction, ie, along $\vec{G}$.

15 pts



$d = \vec{r}_3 \cdot \frac{\vec{G}}{|\vec{G}|}$ (= projection of $\vec{r}_3$ along $\vec{G}$ direction)



we have $\vec{r}_3 = \frac{\vec{a}_3}{l}$, so

$$\vec{r}_3 \cdot \frac{\vec{G}}{|\vec{G}|} = \frac{1}{l}\vec{a}_3 \cdot (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\frac{1}{|\vec{G}|}$$

$$= \frac{2\pi}{l}(l)\frac{1}{|\vec{G}|} = \frac{2\pi}{|\vec{G}|}$$

so $\boxed{d(hkl) = \frac{2\pi}{|\vec{G}|}}$

(c) for a sc lattice, $b_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$, $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

so $\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$

15 pts

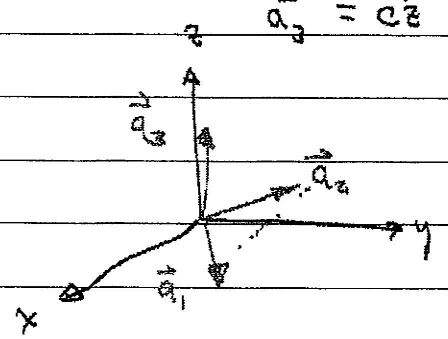
or $d = \frac{2\pi}{\left(\frac{2\pi}{a}\right)^2 (h^2+k^2+l^2)^{\frac{1}{2}}}$

$$\Rightarrow \boxed{d^2 = \frac{a^2}{h^2+k^2+l^2}}$$

(2) hexagonal lattice $\vec{a}_1 = \frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}$

$$\vec{a}_2 = -\frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}$$

$$\vec{a}_3 = c\hat{z}$$



(a) $V_{cell} = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$= \left(\frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}\right)\cdot\left(\frac{-\sqrt{3}a}{2}c(-\hat{y}) + \frac{ac}{2}\hat{x}\right)$$

15 pts

$$= \frac{\sqrt{3}}{4}a^2c + \frac{\sqrt{3}}{4}a^2c$$

$$\boxed{= \frac{\sqrt{3}}{2}a^2c}$$

(b) $\vec{b}_1 = \frac{2\pi}{V}\vec{a}_2\times\vec{a}_3 = \frac{4\pi}{\sqrt{3}a^2c}\left(-\frac{\sqrt{3}a}{2}\hat{x} + \frac{a}{2}\hat{y}\right)\times c\hat{z}$

15 pts

$$= \frac{4\pi}{\sqrt{3}a}\left(-\frac{\sqrt{3}}{2}(-\hat{y}) + \frac{1}{2}\hat{x}\right)$$

$$\Rightarrow \boxed{\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}\left(\hat{x} + \sqrt{3}\,\hat{y}\right)}$$

$$\vec{b}_2 = \frac{4\pi}{\sqrt{3}a^2c}\left(c\hat{z} \times \left(\frac{\sqrt{3}}{2}a\hat{x} + \frac{a}{2}\hat{y}\right)\right)$$

$$\boxed{\vec{b}_2 = \frac{2\pi}{\sqrt{3}a}\left(\sqrt{3}\,\hat{y} - \hat{x}\right)}$$

$$\vec{b}_3 = \frac{4\pi}{\sqrt{3}a^2c}\left(\frac{\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}\right) \times \left(\frac{-\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}\right)$$

$$= \frac{4\pi}{\sqrt{3}c}\left(\frac{\sqrt{3}}{2}\left(\frac{1}{2}\right)\hat{z} + \frac{-\sqrt{3}}{2}\left(\frac{1}{2}\right)\left(-\hat{z}\right)\right)$$

$$\boxed{\vec{b}_3 = \frac{2\pi}{c}\hat{z}}$$

(c) in $\hat{k}$-space, the lattice pts are given by:

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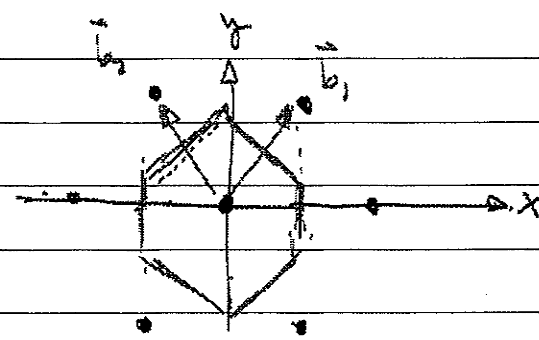
$$\vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$

$$= \frac{2\pi}{\sqrt{3}a}\left((v_1 - v_2)\hat{x} + (v_1 + v_2)\sqrt{3}\,\hat{y} + v_3\hat{z}\right)$$

where $v_1, v_2, v_3 \in \mathbb{Z}$.

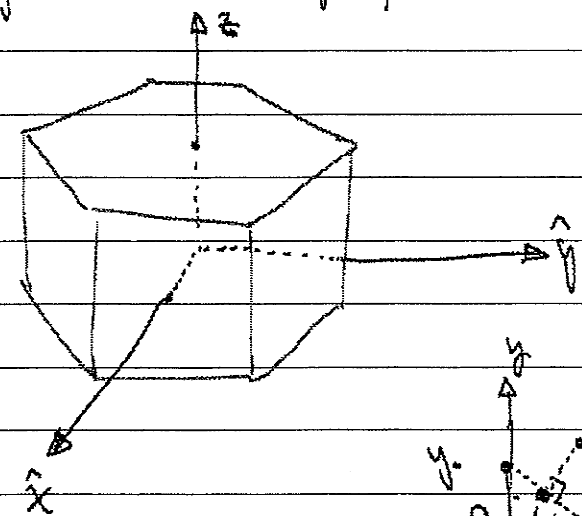
in x-y-plane, we have:



the blue line shows the boundary of the 1st B.Z.

along the $\hat{z}$ - axis, the boundary is at $\pm \frac{c}{a}$.

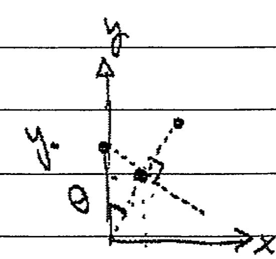
So we have a hexagon in the x-y-plane:



along the x-axis, the boundary is at $\pm \frac{\pi}{\sqrt{3}a}$

along the y-axis the boundary is at

$$y = \pm \frac{\pi}{a}\left(\frac{4}{3}\right)$$



$$\frac{1}{2}\vec{b}_1 = \frac{\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{x} + \hat{y}\right)$$

$$y_0 \cos\theta = \frac{1}{2}|\vec{b}_1|$$

but $\tan\theta = \frac{1}{\sqrt{3}} \Rightarrow \cos\theta = \frac{b_1^y}{|\vec{b}_1|} = \frac{1}{\sqrt{\frac{4}{3}}} = \frac{\sqrt{3}}{2}$

$$y_0 = \frac{\frac{\pi}{a}\left(\frac{2}{\sqrt{3}}\right)}{\frac{\sqrt{3}}{2}} = \frac{\pi}{a}\frac{4}{3}$$

3 Volume of first B.Z. is $\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$

10 pts (here we assume $\vec{a}_1, \vec{a}_2, \vec{a}_3$ & $\vec{b}_1, \vec{b}_2, \vec{b}_3$ are for the <u>primitive</u> lattice!)

but:
$$\begin{cases} \vec{b}_1 = \frac{2\pi}{V_c}(\vec{a}_2 \times \vec{a}_3) \\ \vec{b}_2 = \frac{2\pi}{V_c}(\vec{a}_3 \times \vec{a}_1) \\ \vec{b}_3 = \frac{2\pi}{V_c}(\vec{a}_1 \times \vec{a}_2) \end{cases}$$

$$\Rightarrow V_{BZ} = \left(\frac{2\pi}{V_c}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot \left((\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)\right)$$

$$= \left(\frac{2\pi}{V_c}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot \Big(\underbrace{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}_{= V_c}\, \vec{a}_1\Big)$$

$$= \frac{(2\pi)^3}{V_c^2} \underbrace{(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3))}_{= V_c}$$

$$\boxed{V_{BZ} = \frac{(2\pi)^3}{V_c}}$$