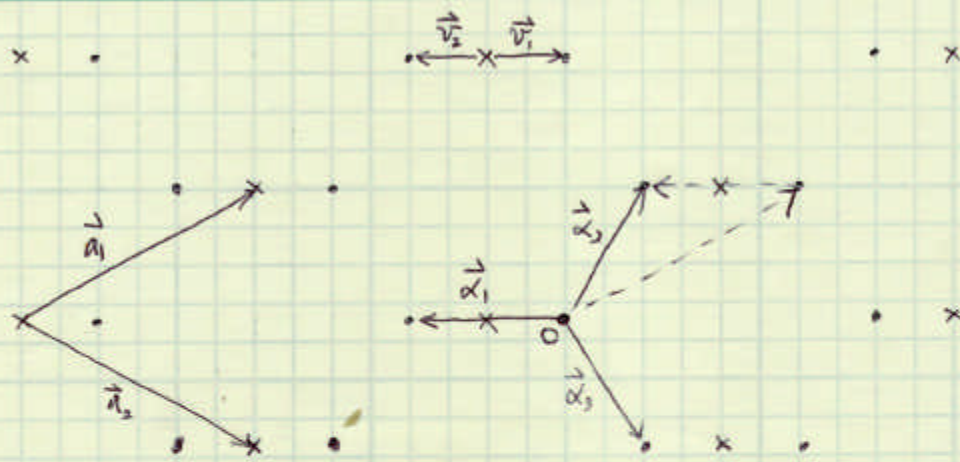


(a)



x Hex lattice pt.  
• Basis points

Each point in a honeycomb lattice has three nearest neighbors.  
E.g., point 0 has them at  $\vec{\alpha}_1, \vec{\alpha}_2, \vec{\alpha}_3$ .

i)  $\alpha_1$ .

$$\alpha_1 = |\vec{\alpha}_1|$$

$$\vec{\alpha}_1 = \vec{v}_2 - \vec{v}_1$$

$$= -\frac{1}{\sqrt{3}} \vec{x}$$

(I'm letting  $a=1$ )

$$\therefore \alpha_1 = \frac{1}{\sqrt{3}}$$

ii)  $\alpha_2$ .

$$\vec{\alpha}_2 = \vec{a}_1 + \vec{\alpha}_1$$

$$= \frac{\sqrt{3}}{2} \vec{x} + \frac{1}{2} \vec{y} - \frac{1}{\sqrt{3}} \vec{x}$$

$$= \frac{1}{2\sqrt{3}} \vec{x} + \frac{1}{2} \vec{y}$$

$$\therefore \alpha_2 = \frac{1}{\sqrt{3}}$$

iii)  $\alpha_3$ .

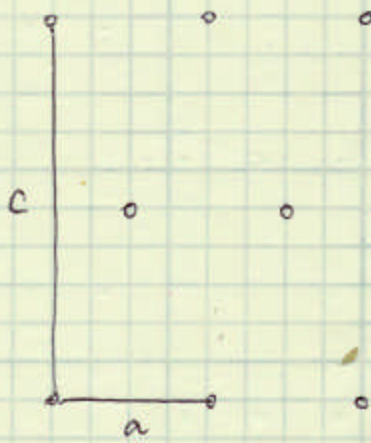
$$\vec{\alpha}_3 = \vec{a}_2 + \vec{\alpha}_1$$

$$= \frac{1}{2\sqrt{3}} \vec{x} - \frac{1}{2} \vec{y}$$

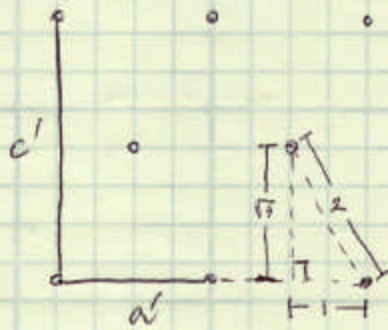
$$\therefore \alpha_3 = \frac{1}{\sqrt{3}} = \alpha_1 = \alpha_2$$

Do similarly for the other basis point ~~of~~ the same lattice point, & you will get the same results. Since the lattice is a Bravais lattice (hex), we will get the same results for all the points of the honeycomb. Hence, the distance between all neighboring points for all points on the honeycomb lattice is identical.

2.(a)



<centered rect.>



<Hex>

From the trigonometric properties of an equilateral triangle, we know that

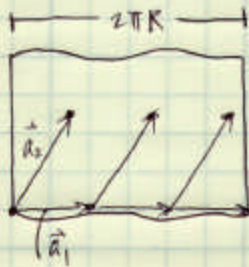
$$\frac{c'}{a'} = \sqrt{3}. \quad (\text{see above})$$

So, the  $c/a$  ratio for which the centered rectangular lattice becomes hex is  $\sqrt{3}$ .

1.(a) Infinite cylinder:



unfold



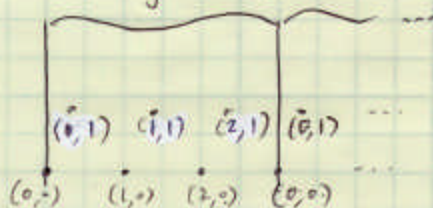
$\vec{a}_1, \vec{a}_2$ : primitive vectors

As long as

$$n|\vec{a}_1| = 2\pi R,$$

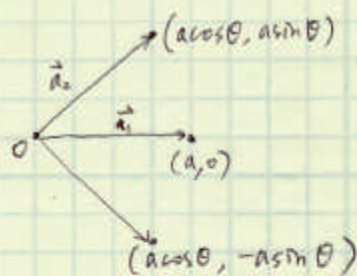
where  $n \equiv$  integer &  $R \equiv$  radius of cylinder, any 2D Bravais lattice could live on the surface of a cylinder.  $R$  can be defined to fit any lattice, so all 5 of the 2D Bravais lattices fit this description.

The set of all lattices can be indexed by two integers, one being the number of lattice points away from the origin in the  $x$  direction, the other being that in the  $y$  direction:

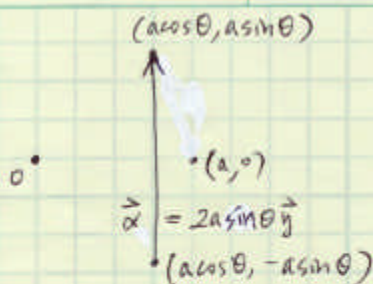


After  $n$  times along the  $x$  direction, indexing begins again, meaning we get to the same point of the cylinder.

f(a)



&lt;Fig. 1&gt;



&lt;Fig. 2&gt;

The problem requires all 4 of the points in Fig. 1 are on the Bravais lattice. So, by definition of the Bravais lattice,  $\vec{\alpha}$  of Fig. 2 can be represented by ~~integer~~ the sum of integer multiples of 2 linearly independent lattice vectors, e.g.

$$\vec{a}_1 = n\vec{x} \quad \# \quad \text{linearly independent.}$$

$$\vec{a}_2 = a \cos \theta \vec{x} + a \sin \theta \vec{y}$$

Letting  $a=1$ ,

$$n\vec{a}_1 + m\vec{a}_2 = \vec{\alpha} \quad (n, m \text{ ints})$$

$$(n + m \cos \theta)\vec{x} + m \sin \theta \vec{y} = 2 \sin \theta \vec{y} \quad \leftarrow \text{Ans.}$$

$$\therefore m = 2$$

$$n + 2 \cos \theta = 0$$

$$\cos \theta = -\frac{n}{2}$$

Since  $|\cos \theta| \leq 1$ ,  $n = 0, \pm 1, \pm 2$ . So

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

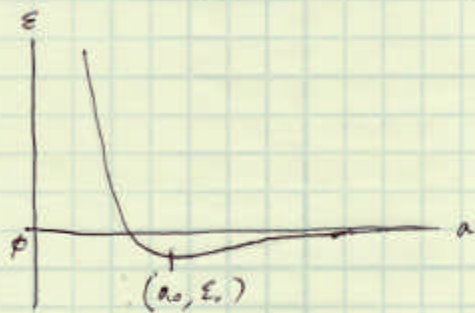
$$\therefore \theta = \frac{\pi}{2}, \frac{2\pi}{3}, \frac{\pi}{3}, 0, \pi$$

↑	↑	↑	↑
4-fold	3-fold	6-fold	2-fold

Rest for part (b)

(a) i) Square lattice: 4 NNs

$$\varepsilon = \frac{1}{2} \varphi_0 e^{-a} (a^{-3} - 1) \times 4, \quad a = \text{lattice spacing}$$



$a_0 =$  equilibrium lattice spacing

$\varepsilon_0 =$  min. energy

Minimize:  $\left. \frac{d\varepsilon}{da} \right|_{a_0} = 0$

$$0 = -e^{-a_0} (a_0^{-3} - 1) - e^{-a_0} \cdot 3a_0^{-4}$$

$$\therefore a_0 \approx 1.453 \quad (\text{which is } < 1.5, \text{ so we're good})$$

$$\therefore \varepsilon_0 \approx -0.315$$

ii) Hex lattice: 6 NNs

$$\varepsilon = \frac{1}{2} \varphi_0 e^{-a} (a^{-3} - 1) \times 6$$

From i), we know

$$a_0 = 1.453$$

$$\therefore \varepsilon_0 \approx -0.473$$

So the hex structure has the minimal energy state.