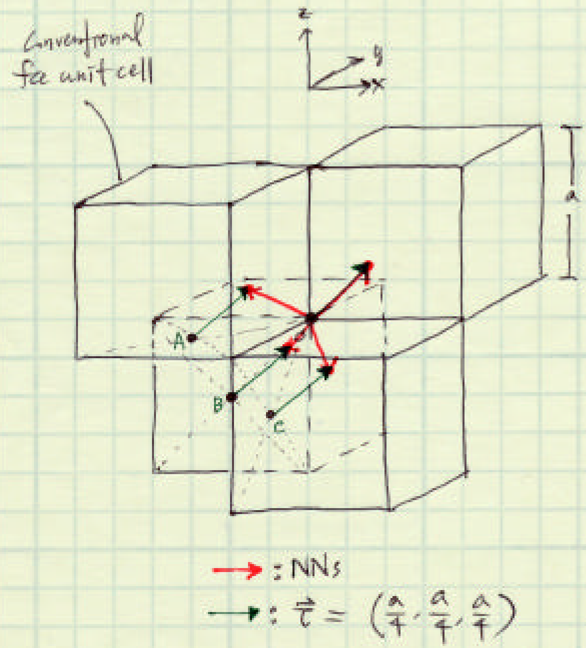
1. (i) The diamond lattice consists of two interpenetrating fcc lattices, where the 2nd basis point is located at $(a/4, a/4, a/4)$ (the first is at the origin). So we can define the unit cell to have 2 atoms — one from each fcc lattice, & one displaced

$$\vec{\tau} = \left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$$

from the other.



Each atom has 4 NNs — one in the same unit cell & the other three in 3 different adjacent unit cells, which have the following coordinates:

$$\vec{R}_1 = \left(-\frac{a}{4}, -\frac{a}{4}, \frac{a}{4}\right) - \vec{\tau}$$

$$= \frac{a}{2}(-1, -1, 0) \quad \cdots \text{(Pt. A)}$$

$$\vec{R}_2 = \left(-\frac{a}{4}, \frac{a}{4}, -\frac{a}{4}\right) - \vec{\tau}$$

$$= \frac{a}{2}(-1, 0, -1) \quad \cdots \text{(Point B)}$$

$$\vec{R}_3 = \left(\frac{a}{4}, -\frac{a}{4}, -\frac{a}{4}\right) - \vec{\tau}$$

$$= \frac{a}{2}(0, -1, -1) \quad \cdots \text{(Point C)}$$

Get the Hamiltonian:

$$H_{11} = H_{22} = \epsilon_s$$

$$H_{12} = t\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}$$

$$= t\left\{\exp\left[-\frac{ia}{2}(k_x+k_y)\right] + \exp\left[-\frac{ia}{2}(k_z+k_x)\right] + \exp\left[-\frac{ia}{2}(k_y+k_z)\right] + \underbrace{1}_{\vec{R}=\vec{0}}\right\}$$

$$H_{21} = H_{12}^*$$

$$\text{So} \quad H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

Get the eigenvalues:

$$\begin{vmatrix} \epsilon_s - E & H_{12} \\ H_{21} & \epsilon_s - E \end{vmatrix} = 0 \longrightarrow E^2 + 2E\epsilon_s + \epsilon_s^2 - |H_{12}|^2 = 0 \rightarrow E = \epsilon_s \pm \sqrt{|H_{12}|^2}$$

$$|H_{12}|^2 = \Big[4 + 2\cos\frac{a}{2}(k_x+k_y) + 2\cos\frac{a}{2}(k_y+k_z) + 2\cos\frac{a}{2}(k_z+k_x)$$

$$+ 2\cos\frac{a}{2}(k_x-k_y) + 2\cos\frac{a}{2}(k_y-k_z) + 2\cos\frac{a}{2}(k_z-k_x)\Big]t^2$$

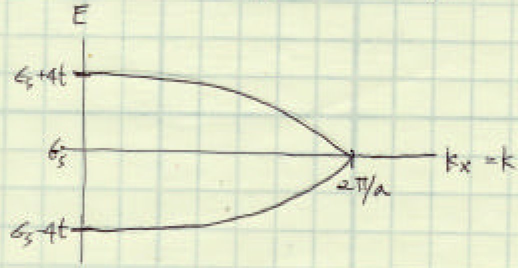
$$= 4t^2\left(\cos\frac{ak_x}{2}\cos\frac{ak_y}{2} + \cos\frac{ak_y}{2}\cos\frac{ak_z}{2} + \cos\frac{ak_z}{2}\cos\frac{ak_x}{2} + 1\right)$$

$$\therefore E = \epsilon_s \pm 2t\sqrt{\cos\frac{ak_x}{2}\cos\frac{ak_y}{2} + \cos\frac{ak_y}{2}\cos\frac{ak_z}{2} + \cos\frac{ak_z}{2}\cos\frac{ak_x}{2} + 1}$$

Plot along (100) : (0, 0, 0) to ($2\pi/a$, 0, 0)

set $k_y = k_z = 0$

$$E = \epsilon_s \pm 2t\sqrt{2 + 2\cos\frac{ak_x}{2}}$$

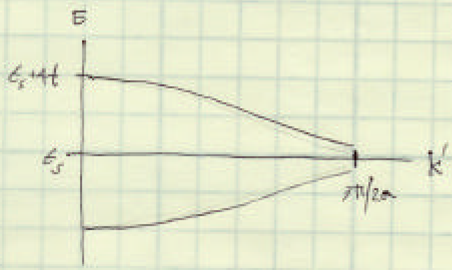


Plot along (110) : (0, 0, 0) to ($3\pi/2a$, $3\pi/2a$, 0)

$k_z = 0$; $k_x = k_y \equiv k'$

$$E = \epsilon_s \pm 2t\sqrt{1 + \cos^2\frac{ak'}{2} + 2\cos\frac{ak'}{2}}$$

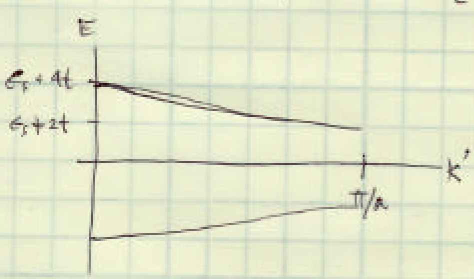
$$= \epsilon_s \pm 2t\left(1 + \cos\frac{ak'}{2}\right)$$



Plot along (111) : (0, 0, 0) to (π/a, π/a, π/a)

$k_x = k_y = k_z \equiv k'$

$$E = \epsilon_s \pm 2t\sqrt{1 + 3\cos^2\frac{ak}{2}}$$



(ii)

$$\mathcal{S} = \begin{bmatrix} 1 & \frac{s}{t} H_{12} \\ \frac{s}{t} H_{21} & 1 \end{bmatrix}$$

$$|\hat{H} - E\hat{S}| = 0.$$

$$\begin{vmatrix} \epsilon_s - E & \left(1 - \frac{s}{t}\right) H_{12} \\ \left(1 - \frac{s}{t}\right) H_{21} & \epsilon_s - E \end{vmatrix} = 0$$

$$\therefore (\epsilon_s - E)^2 = 4(t-s)^2 \left(1 + \cos\frac{ak_x}{2}\cos\frac{ak_y}{2} + \cos\frac{ak_z}{2}\cos\frac{ak_z}{2} + \cos\frac{ak_z}{2}\cos\frac{ak_x}{2}.\right)$$