1)

$$\boxed{\begin{gathered} V(\vec{r}+\vec{R}_N) = V(\vec{r}) \\ \psi_k(\vec{r}) = u_{\vec{k}}(\vec{r})\, e^{i\vec{k}\cdot\vec{r}} \\ \text{for } u_k(\vec{r}+\vec{R}_n) = u_k(\vec{r}) \end{gathered}}$$

define translation operator $\hat{\vec{T}}_n$

$$\hat{T}_N f(\vec{r}) = f(\vec{r}+\vec{R}_N)$$

$$\boxed{\hat{T}_N V(\vec{r}) = V(\vec{r}+\vec{R}_N) = V(\vec{r})}$$, checks out with periodic potential

$$\hat{T}_N \psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r}+\vec{R}_N)$$

$$= \underbrace{\lambda_{\vec{k}}}_{\text{eigenvalue } = e^{i\vec{k}\cdot\vec{R}_N}} \psi_{\vec{k}}(\vec{r})$$

$$\boxed{\Rightarrow \psi_{\vec{k}}(\vec{r}+\vec{R}_N) = e^{i\vec{k}\cdot\vec{R}_N} \cdot \psi_{\vec{k}}(\vec{r})}$$

2)i

$$a_1 = \left(\frac{a\sqrt{3}}{2}, \frac{1}{2}\right) = \frac{a}{2}(\sqrt{3}, 1)$$

$$a_2 = \frac{a}{2}(\sqrt{3}, -1)$$

2ii)

$$a_3 = (0, 0, 1)$$

$$a_2 \times a_3 = \begin{vmatrix} \frac{a}{2}\sqrt{3} & -\frac{a}{2} & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

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

$$b_1 = \frac{2\pi (a_2 \times a_3)}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi\left(-\frac{a}{2}, -\frac{a}{2}\sqrt{3}\right)}{-\frac{a^2}{4}\sqrt{3} + \frac{-a^2\sqrt{3}}{4}}$$

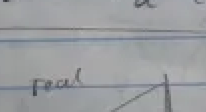
$$= \frac{2\pi\left(-\frac{a}{2}, -\frac{a}{2}\sqrt{3}\right)}{\frac{-2a^2\sqrt{3}}{4}} = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, 1\right)$$

$$= b_1$$

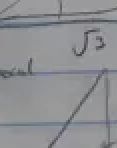
$$b_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, -1\right)$$

$$M @ \left(\frac{2\pi}{a\sqrt{3}}, 0\right)$$

R



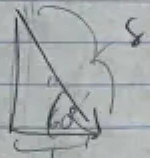
$$\frac{\sqrt{3}}{1} = \frac{\frac{2\pi}{\sqrt{3}a}}{k_y} \Rightarrow k_y = \frac{2\pi}{3a}$$



$$K @ \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, \frac{1}{3}\right)$$

$$K' @ \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}, -\frac{1}{3}\right)$$

2iii) $\frac{x}{2} = a_{i,y}$



$$|\delta| = \frac{\frac{a}{2}}{\sin(60^\circ)} = \frac{a}{\sqrt{3}}$$

$$\frac{\sqrt{3}}{2}$$

$$x = \frac{a}{2}\,\frac{1}{\tan 60^\circ} = \frac{a}{2\sqrt{3}}$$

$$\Rightarrow \quad \delta_1 = \frac{a}{2}\left(\frac{1}{\sqrt{3}},\ 1\right) = \left(\frac{a}{2\sqrt{3}},\ \frac{a}{2}\right)$$

$$\delta_2 = \frac{a}{2}\left(\frac{1}{\sqrt{3}},\ -1\right) = \left(\frac{a}{2\sqrt{3}},\ \frac{-a}{2}\right)$$

$$\delta_3 = \frac{a}{2}\left(\frac{-2}{\sqrt{3}},\ 0\right) = \left(\frac{-a}{\sqrt{3}},\ 0\right)$$

$$\Delta k = \sum e^{ik\delta_n}$$

$$= e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3}$$

$$= e^{ik\delta_3}\left[e^{ik(\delta_1-\delta_3)} + e^{ik(\delta_2-\delta_3)} + 1\right]$$

$$= e^{-ik_x\frac{a}{\sqrt{3}}}\left[e^{-ik\left(\frac{a}{2}\frac{3}{\sqrt{3}},\ \frac{a}{2}\right)} + e^{ik\left(\frac{a}{2}\frac{3}{\sqrt{3}},\ -\frac{a}{2}\right)} + 1\right]$$

$$= e^{-ik_x\frac{a}{\sqrt{3}}}\left[e^{ik_x\frac{\sqrt{3}}{2}a}\,2\cos\left(\frac{k_y}{2}a\right) + 1\right]$$

$$E = \pm t\sqrt{\Delta k\,\Delta k^*}$$

$$= \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right) + 4\cos^2\left(\frac{1}{2}k_y a\right)}$$

(alternatively, multiply everything by $\sqrt{3}$ $\left(D_{cc} = \sqrt{3}\cdot a\right)$)

2) iii $\delta_1 = \frac{a}{2}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$

$$\delta_2 = a\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)$$

$$\delta_3 = a\left(-1, 0\right)$$

$$\Delta k = \sum e^{ik\delta_n}$$

$$= e^{ik\cdot\delta_1} + e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3}$$

$$= e^{ik\delta_3}\left[e^{ik(\delta_1-\delta_3)} + e^{ik(\delta_2-\delta_3)} + 1\right]$$

$$= e^{-ik_xa}\left[e^{ik\cdot\left(\frac{3}{2}a, \frac{\sqrt{3}}{2}a\right)} + e^{ik\cdot\left(\frac{3}{2}a, -\frac{\sqrt{3}}{2}a\right)} + 1\right]$$

$$= e^{-ik_xa}\left[e^{ik_x\frac{3}{2}a} e^{ik_y\frac{\sqrt{3}}{2}a} + e^{ik_x\frac{3}{2}a} e^{-ik_y\frac{\sqrt{3}}{2}a} \ldots\right.$$

$$= e^{-ik_xa}\left[e^{ik_x\frac{3}{2}a}\left(e^{ik_y\frac{\sqrt{3}}{2}a} + e^{-ik_y\frac{\sqrt{3}}{2}a}\right) + 1\right]$$

$$2\cos\left(\frac{\sqrt{3}}{2}k_y a\right)$$

$$\Delta E = \pm t\sqrt{\Delta k \Delta k^*}$$

$$= \pm t\sqrt{1 + 2e^{-ik_xa\frac{3}{2}}\cos\left(\frac{\sqrt{3}}{2}k_y a\right) + 2e^{ik_xa\frac{3}{2}}\cos\left(\frac{\sqrt{3}}{2}\ldots\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}k_y a\right)}$$

$$= \pm t\sqrt{1 + 4\cos\left(\frac{3}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}k_y a\right)}$$

(Same as formula on slide 5)

2v)

K @ $\left(\frac{2\pi}{a\sqrt{3}}, \frac{2\pi}{a}\frac{1}{3}\right)$

$$E_K = \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}\frac{2\pi}{a\sqrt{3}}a\right)\cos\left(\frac{1}{2}\frac{2\pi}{a}\frac{1}{3}a\right) + 4\cos^2\left(\frac{1}{2}\frac{2\pi}{a}\frac{1}{3}a\right)}$$

$$= \pm t\sqrt{1 + 4\underbrace{\cos(\pi)}_{-1}\underbrace{\cos\left(\frac{\pi}{3}\right)}_{0.5} + 4\underbrace{\cos^2\left(\frac{\pi}{3}\right)}_{0.25}}$$

$$= \pm t\sqrt{1 + (-2) + 1}$$

$$= 0$$

K' @ $\left(\frac{2\pi}{a\sqrt{3}}, -\frac{2\pi}{a}\frac{1}{3}\right)$

$$E_{K'} = \pm t\sqrt{1 + 4\cos(\pi)\underbrace{\cos\left(-\pi/3\right)}_{0.5} + 4\underbrace{\cos^2\left(\pi/3\right)}_{0.25}}$$

$$= 0$$

M @ $\left(\frac{2\pi}{a\sqrt{3}}, 0\right)$

$$E_M = \pm t\sqrt{1 + 4\underbrace{\cos\left(\frac{\sqrt{3}}{2}\frac{2\pi}{a\sqrt{3}}a\right)}_{-1}\underbrace{\cos(0)}_{1} + 4\underbrace{\cos(0)}_{1}}$$

$$= \pm t$$

2,v)

$$\Delta_k = 1 + e^{ika_1} + e^{ika_2} -$$

$$k = K + q \Rightarrow \Delta_{k+q} = 1 + e^{i(k+q)a_1} + e^{i(k+q)a_2}$$

(Euler 1st order Taylor expansion)

$$= 1 + e^{ik\cdot a_1}(1 + iq\cdot a_1) + e^{ik\cdot a_2}(1 + iq\cdot a_2)$$

$$a_1 = \left(\frac{a\sqrt{3}}{2}, \frac{a}{2}\right) \qquad a_2 = \left(\frac{a\sqrt{3}}{2}, -\frac{a}{2}\right)$$

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

$$\Delta_{K+q} = 1 + e^{i\frac{4\pi}{3}}\left(1 + i\left(\frac{a\sqrt{3}}{2}q_x + \frac{a}{2}q_y\right)\right) + e^{i\frac{2\pi}{3}}\left(1 + i\left(\frac{a\sqrt{3}}{2}q_x - \frac{a}{2}q_y\right)\right)$$

$$= -\frac{\sqrt{3}}{2}a(iq_x + q_y)$$

$$E = \pm t\sqrt{\Delta_k \Delta_k^*} = \pm t|\Delta_K|$$

$$= \pm t\sqrt{\frac{3}{4}a^2(q_x^2 + q_y^2)} = \pm\left(\frac{\sqrt{3}}{2}a|q|\right)t$$

2vi)

$$E = \pm t\underbrace{|\Delta k|}_{\text{nearest}} + t'\underbrace{|\Delta k'|}_{\text{next nearest}}$$

$$\Delta k' = e^{ik\cdot\left(\frac{-a\sqrt{3}}{2}, \frac{a}{2}\right)} + e^{ik\cdot\left(\frac{-a\sqrt{3}}{2}, \frac{-a}{2}\right)}$$

$$= \left[\left(\cos\left(\frac{-a\sqrt{3}}{2}k_x\right) + i\sin\left(-k_x\frac{a\sqrt{3}}{2}\right)\right)\left(\cos\left(k_y\frac{a}{2}\right) + i\sin\left(k_y\frac{a}{2}\right)\right)\right]$$

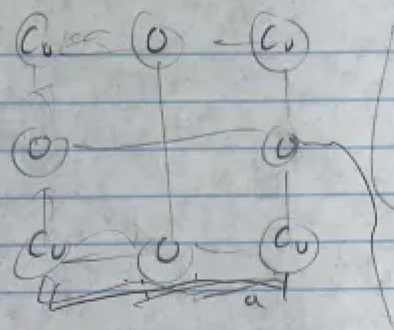
$$+ \left[\left(\cos\left(-\frac{a\sqrt{3}}{2}k_x\right) + i\sin\left(\frac{a\sqrt{3}}{2}k_x\right)\right)\left(\cos -k_y\frac{a}{2}\right)\left(i\sin -k_y\frac{a}{2}\right)\right]$$

$$= 2\cos\left(\frac{a\sqrt{3}K_x}{2}\right)\cos\left(k_y\frac{a}{2}\right) + 2i\sin\left(-k_x\frac{a\sqrt{3}}{2}\right)\cos\left(k_y\frac{a}{2}\right)$$

$$E = \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{1}{2}k_y a\right) + 4\cos^2\left(\frac{1}{2}k_y a\right)}$$

$$\pm t' \, 2\sqrt{\cos^2\left(\frac{a\sqrt{3}}{2}k_x\right)\cos^2\left(k_y\frac{a}{2}\right) + \sin\left(-k_x\frac{a\sqrt{3}}{2}\right)\cos\left(k_y\frac{a}{2}\right)}$$

3a) Unit cell

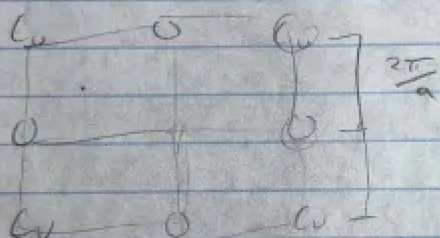


Per cell

$4 \cdot \frac{1}{4} = 1$ Cu

$4 \cdot \frac{2}{4} = 2$ O

Reciprocal lattice



3b) $\Delta k = e^{ik\cdot(\frac{a}{2},0)} + e^{ik\cdot(-\frac{a}{2},0)} + e^{ik\cdot(0,\frac{a}{2})} + e^{ik\cdot(0,-\frac{a}{2})}$

$= e^{ik_x \frac{a}{2}} + e^{ik_x -\frac{a}{2}} + e^{ik_y \frac{a}{2}} + e^{ik_y(-\frac{a}{2})}$

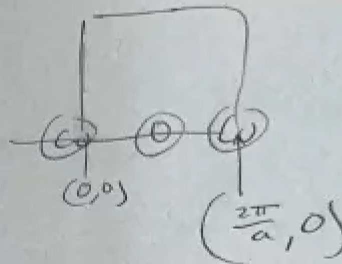
$= 2\cos k_x \frac{a}{2} + 2\cos k_y \frac{a}{2}$

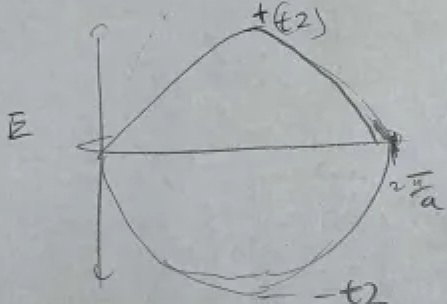
$\Rightarrow \boxed{E = \pm t 2\sqrt{\cos^2(k_x \frac{a}{2}) + \cos^2(k_y \frac{a}{2})}}$

3 bands: p_x, p_y, and $d_{x^2-y^2}$ orbital

3 b2)

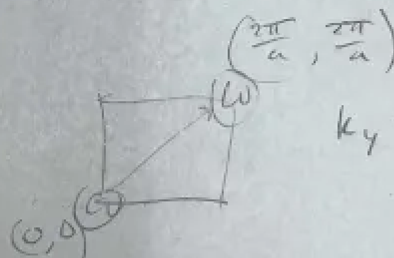
[1 0]



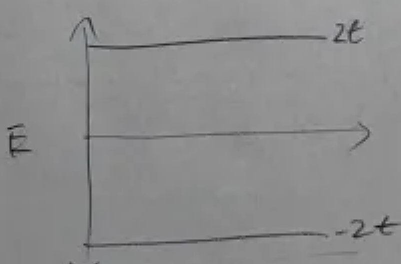


$E = \pm t2 \cos(k \frac{a}{2})$

[1, 1]



$k_y = k_x = k$



$E = \pm 2t \sqrt{\cancelto{1}{\cos^2(k\frac{a}{2}) + \sin^2(k\frac{a}{2})}}$

3c) Two e^- in Cu orbital ⇒ four valence e^- per unit cell, two bands occupied in first BZ, fermi level somewhere in band gap

One e^- ⇒ no band gap, fermi level at intersection between $E \pm t2\sqrt{\cos^2 + \sin^2}$ bands