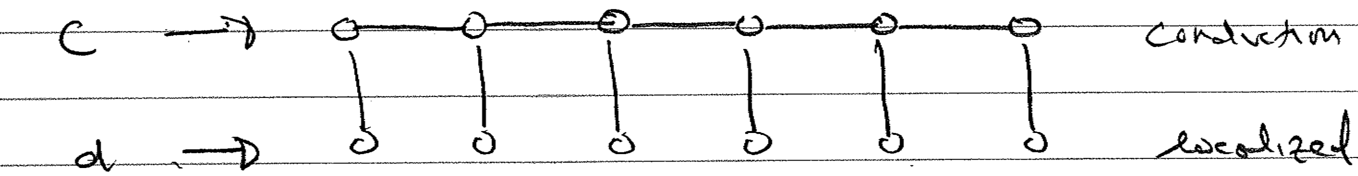
PAM-1

HW problem illustrated how hard it is to get ϵ_k for traditional approach. Let's see how easy it is in 2nd quantized



$$\hat{H} = -t \sum_{l} \left(c^{\dagger}_{l+1} c_l + c^{\dagger}_l c_{l+1} \right) + t' \sum_{l} \left(c^{\dagger}_l d_l + d^{\dagger}_l c_l \right)$$

$$c_l = \frac{1}{\sqrt{N}} \sum c_k e^{ikl} \qquad d_l = \frac{1}{\sqrt{N}} \sum d_k e^{ikl}$$

$$\rightarrow \quad \sum_k \epsilon_k c^{\dagger}_k c_k + t' \sum \left(c^{\dagger}_k d_k + d^{\dagger}_k c_k \right)$$

$$= \sum_k \left(c^{\dagger}_k \; d^{\dagger}_k \right) \begin{pmatrix} \epsilon_k & t' \\ t' & 0 \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

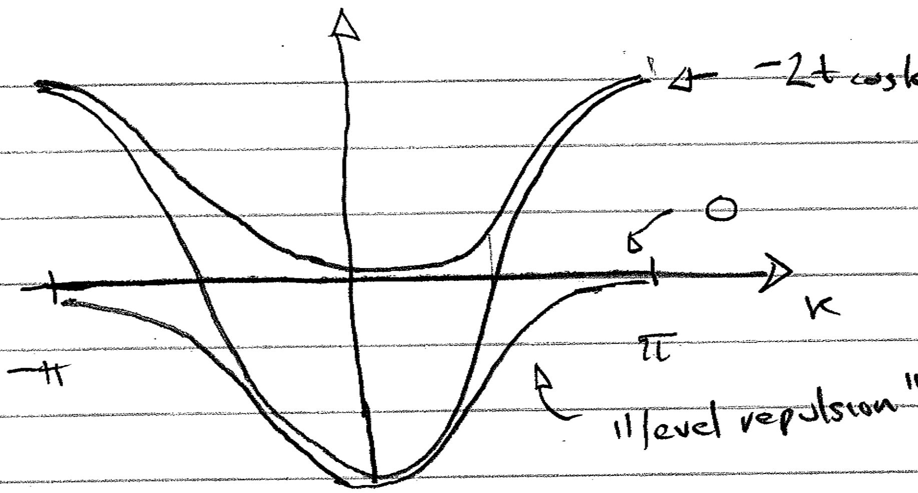
Diagonalize

$$(\epsilon_k - \lambda)(-\lambda) - t'^2 = 0$$

$$\lambda^2 - \epsilon_k \lambda - t'^2 = 0$$

$$\lambda = \frac{1}{2} \left[\epsilon_k \pm \sqrt{\epsilon_k^2 + 4t'^2} \right]$$

PAM-2



$k=0$ $\quad \lambda = \frac{1}{2}\left[-2t \pm \sqrt{4t^2+4t'^2}\right] \approx -2t$

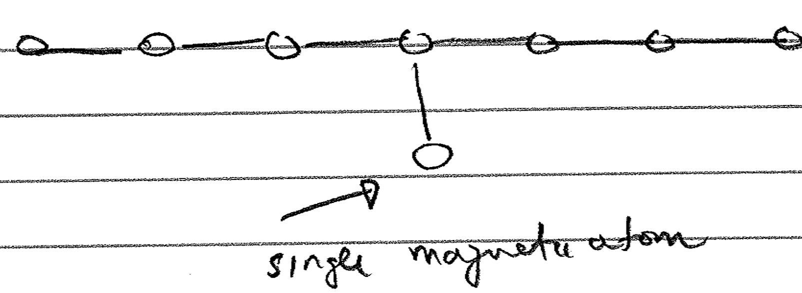
$$+2t\left[1+t'^2/t^2\right]^{1/2} \approx t'^2/2t$$

$$+2t\left[1+\frac{t'^2}{2t^2}\right]$$

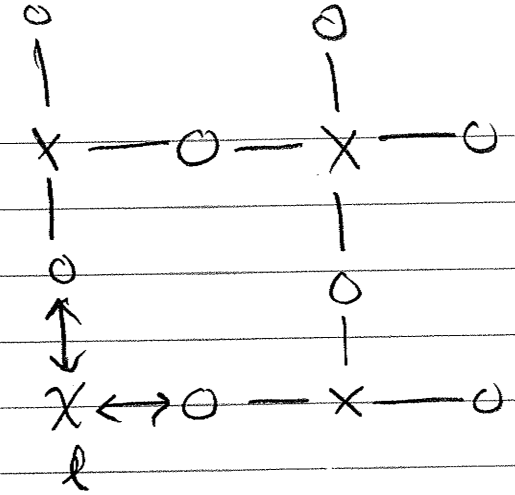
$k=\pi/2$ $\quad \lambda = \frac{1}{2}\left[0 \pm \sqrt{4t'^2}\right] = \pm t'$

Note: We do not have any periodic potential U_e applied here. Just 2 bands because 2 "orbitals" on each site

AIM as homework



CuO_2 - 1



$$H = -t \sum_\ell \Big[\left(d_\ell^\dagger p_{x\ell} + p_{x\ell}^\dagger d_\ell \right) + \left(d_\ell^\dagger p_{y\ell} + p_{y\ell}^\dagger d_\ell \right) + \left(p_{x\ell}^\dagger d_{\ell+\hat{x}} + d_{\ell+\hat{x}}^\dagger p_{x\ell} \right) + \left(p_{y\ell}^\dagger d_{\ell+\hat{y}} + d_{\ell+\hat{y}}^\dagger p_{y\ell} \right) \Big]$$

$$d_\ell = \frac{1}{\sqrt{N}} \sum_k e^{ik\ell} d_k$$

$$p_{x\ell} = \frac{1}{\sqrt{N}} \sum_k e^{ik\ell} p_{xk}$$

$$p_{y\ell} = \frac{1}{\sqrt{N}} \sum_k e^{ik\ell} p_{yk}$$

$CuO_2 - 2$

$$H = -\frac{t}{N} \sum_{l} \sum_{k} \sum_{k'} \Big\{ e^{-ikl} e^{ik'l} \quad d_k^\dagger p_{xk'} + p_{xk}^\dagger d_{k'}$$

$$d_k^\dagger p_{yk'} + p_{yk'}^\dagger d_k$$

$$d_k^\dagger e^{ik_x} p_{xk'} + d_k p_{xk'}^\dagger e^{-ik_x}$$

$$= \left(d_k^\dagger \; p_{xk}^\dagger \; p_{yk}^\dagger \right) \begin{bmatrix} 0 & -t(1+e^{ik_x}) & -t(1+e^{+ik_y}) \\ -t(\;) & 0 & 0 \\ -t(\;) & 0 & 0 \end{bmatrix} \begin{pmatrix} d_k^\dagger \\ p_{xk}^\dagger \\ p_{yk}^\dagger \end{pmatrix}$$

t_p

$$-\lambda(-\lambda)(-\lambda) + t\left(1+e^{ik_x}\right)$$

$$-\cancel{\lambda} \quad -\lambda\left[(\epsilon_p - \lambda)(\epsilon_p - \lambda) - 0\right]$$

$$+ t(1+e^{ik_x})\left[-t(1+e^{-ik_x})(\epsilon_p - \lambda)\right]$$

$$- t(1+e^{ik_y})\left[+t(1+e^{-ik_y})(\epsilon_p - \lambda)\right]$$

CuO_2-3

$$(\epsilon_p-\lambda)\left[-\lambda(\epsilon_p-\lambda)-t^2\left(2+2\cos k_x+2+2\cos k_y\right)\right]$$

$$\lambda=\epsilon_p$$

$$\lambda^2-\lambda\epsilon_p-2t^2\left[1+\cos k_x+\cos k_y\right]=0$$

$$\lambda=\frac{1}{2}\left[\epsilon_p\pm\sqrt{\epsilon_p^2+8t^2[1+\cos k_x+\cos k_y]}\right]$$

If $\epsilon_p \gg t$

$$\lambda \quad \epsilon_p\sqrt{1+\frac{8t^2}{\epsilon_p^2}(1+\cos k_x+\cos k_y)}$$

$$\approx \epsilon_p\left[1+\frac{4t^2}{\epsilon_p}(1+\cos k_x+\cos k_y)\right]$$

$$\lambda_+ \approx \epsilon_p$$

$$\lambda_- \approx \underbrace{-\frac{2t^2}{\epsilon_p}}_{\text{trivial shift in energy}}\underbrace{-\frac{2t^2}{\epsilon_p}(\cos k_x+\cos k_y)}_{\text{2D square lattice } \epsilon_k!}$$

$$t_{eff}\approx\frac{t^2}{\epsilon_p}$$

"2nd order perturbation theory"