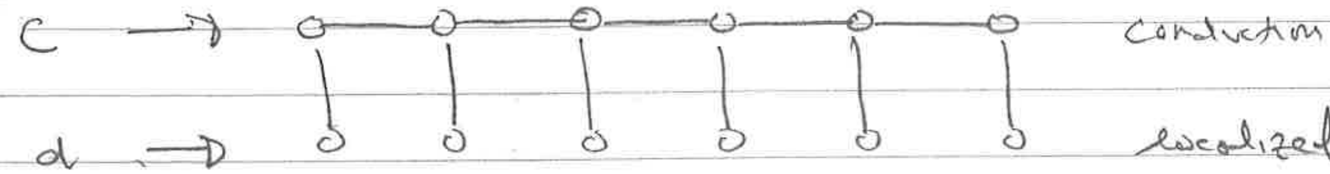
DAM-1

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



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

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

$$\rightarrow \sum_k \epsilon_k c^\dagger_k c_k + t'\sum\left(c^\dagger_k d_k + d^\dagger_k c_k\right)$$

$$= \sum_k \begin{pmatrix} c^\dagger_k & d^\dagger_k \end{pmatrix}\begin{pmatrix} \epsilon_k & t' \\ t' & 0 \end{pmatrix}\begin{pmatrix} c_k \\ d_k \end{pmatrix}$$

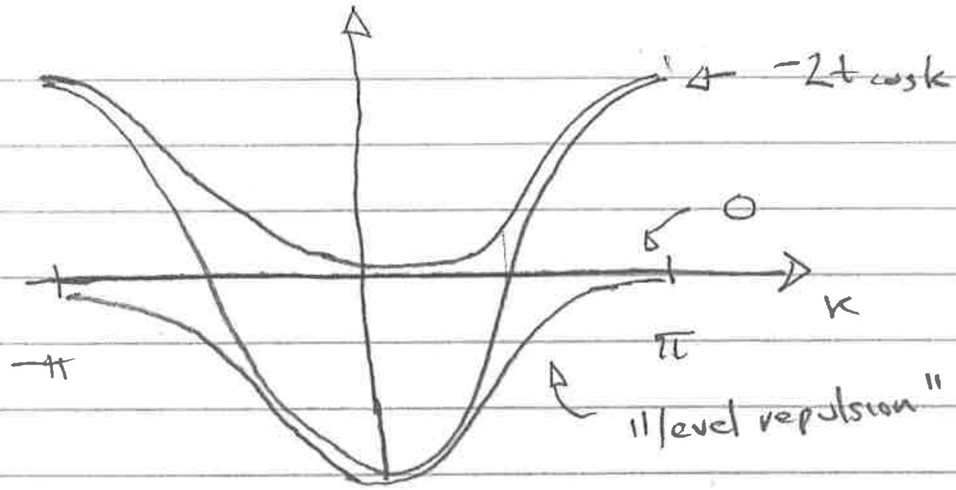
Diagonalize

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

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

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

PAM-2



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

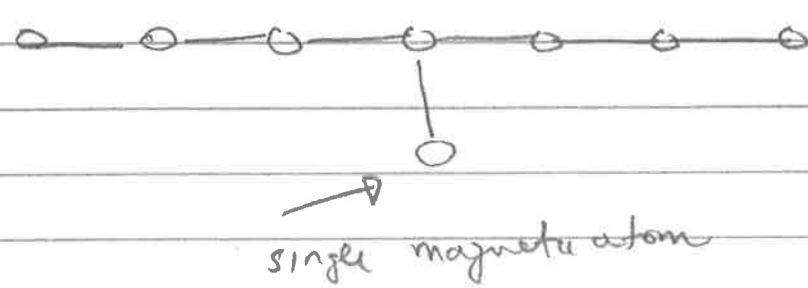
$+2t\left[1+t'^2/t^2\right]^{1/2} \qquad \approx t'^2/2t$

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

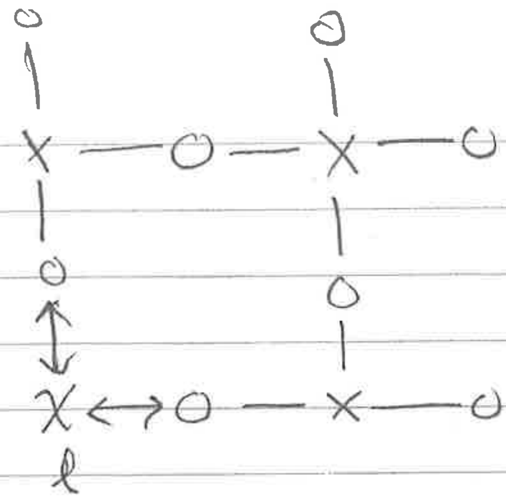
$k=\pi/2 \qquad \lambda = \frac{1}{2}\left[0 \pm \sqrt{4t'^2}\right] = \pm t'$

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

AIM as homework



CuO_2 - 1



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

$$d_l = \frac{1}{\sqrt{N}} \sum_k e^{ikl} d_k$$

$$p_{xl} = \frac{1}{\sqrt{N}} \sum_k e^{ikl} p_{xk}$$

$$p_{yl} = \frac{1}{\sqrt{N}} \sum_k e^{ikl} p_{yk}$$

$CuO_2 - 2$

$$\mathcal{H} = -\frac{t}{N} \sum_{\ell} \sum_{k} \sum_{k'} \left\{ e^{-ik\ell} e^{ik'\ell} \quad d_k^\dagger p_{xk'} + p_{xk}^\dagger d_{k'} \right.$$

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

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

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

t_p

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

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

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

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

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 $\epsilon_p >> t$

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

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

$$\lambda_+ \approx \epsilon_p$$

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

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

& "2nd order perturbation theory"