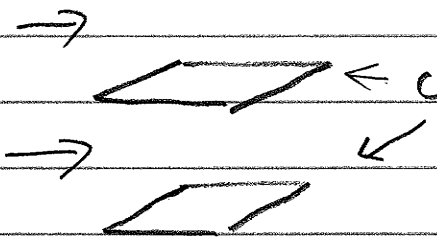
DOS-6

2D square lattice is of particular importance to understand, eg high T_c superconductors

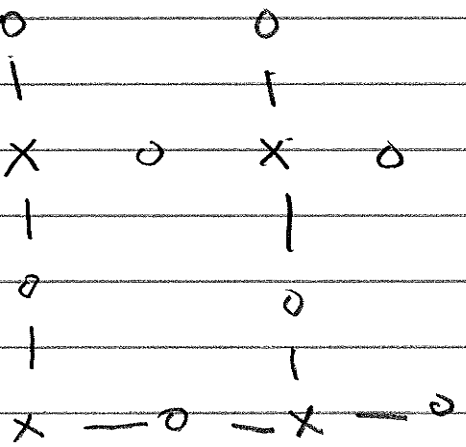


$Y_1Ba_2Cu_3O_7$

$La_{2-x}Sr_xCu_4O_4$

:

Cu atoms in square array, O atoms much higher in energy:



fermions move on square copper lattice

DOS-7

$$E = -2t(\cos k_x + \cos k_y)$$

$$\mathcal{H} = -t \sum_{l_x l_y} \left(c^{+}_{l_x+1, l_y} c_{l_x l_y} + c^{+}_{l_x l_y} c_{l_x+1, l_y} + c^{+}_{l_x l_y+1} c_{l_x l_y} + c^{+}_{l_x l_y} c_{l_x, l_y+1} \right)$$

$$c^{+}_{k_x k_y} = \frac{1}{\sqrt{N}} \sum_{l_x l_y} e^{i(k_x l_x + k_y l_y)} c^{+}_{l_x l_y}$$

generalized $d=1$ result

$$c^{+}_{l_x l_y} = \frac{1}{\sqrt{N}} \sum_{k_x k_y} e^{-i(k_x l_x + k_y l_y)} c^{+}_{k_x k_y}$$

$$-t \sum_{l_x l_y} \sum_{k_x k_y} \sum_{k'_x k'_y} \left[e^{-i(k_x(l_x+1) + k_y l_y)} e^{i(k'_x l_x + k'_y l_y)} + \ldots \right] c^{+}_{k_x k_y} c_{k'_x k'_y}$$

$\sum_{l_x l_y}$ gives $\delta_{k_x k'_x} \delta_{k_y k'_y}$

leftover phases $e^{-ik_x} + e^{+ik_x}$

$+ e^{-ik_y} + e^{+ik_y}$

$$2t(\cos k_x + \cos k_y)$$

Fermi surface?

For free particles $E_{k_x k_y} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$

surfaces of constant E are circles

(spheres in 3D)

what does $-2t(\cos k_x + \cos k_y) = E = \text{constant}$

look like? suppose $E = -4t + \epsilon$

ϵ small #

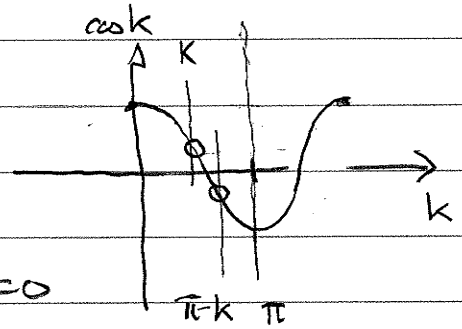
$\cos k_x \sim 1 - \frac{k_x^2}{2}$ $\cos k_y \sim 1 - \frac{k_y^2}{2}$

$k_x^2 + k_y^2 = \epsilon/t$ circles

What about $E_1 = 0$? ← ASIDE: sign of E is impt? Nope. Since bands arise from bound atomic levels expect $E < 0$

$-2t(\cos k_x + \cos k_y) = 0$ zero of energy some

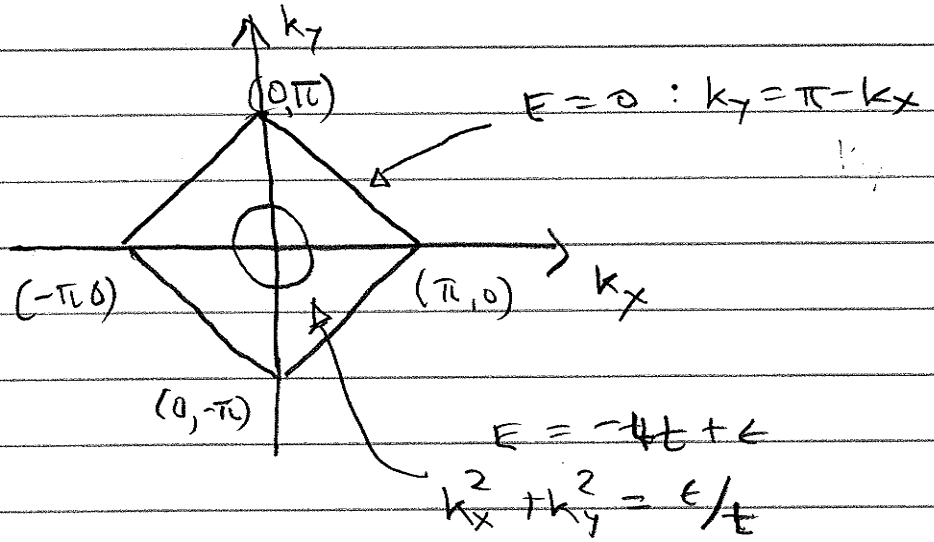
$\cos k_x + \cos k_y = 0$



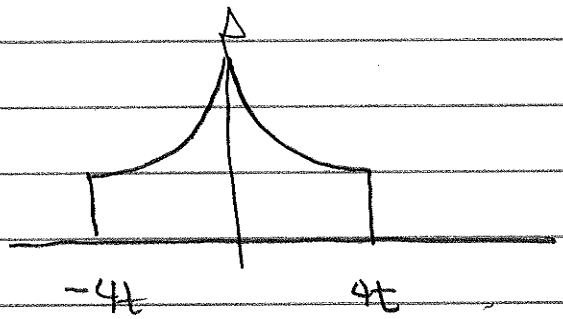
$\cos k = -\cos(\pi - k)$

$\cos\frac{7\pi}{4}$

i.e. $k_y = \pi - k_x$ gives $E = 0$



HW PROBLEM $N(E) = \sum_{k_x k_y} \delta(E - (-2t\cos k_x - 2t\cos k_y))$



NESTING: Given a Fermi surface, is there a $\vec{q}$ value which connects broad regions? If so system will be unstable to order of various sorts at that $\vec{q}$ value

Square lattice has "perfect nesting" at $\vec{q} = (\pi, \pi)$

Sure enough: Unstable to antiferromagnetism

↑ ↓
↓ ↑

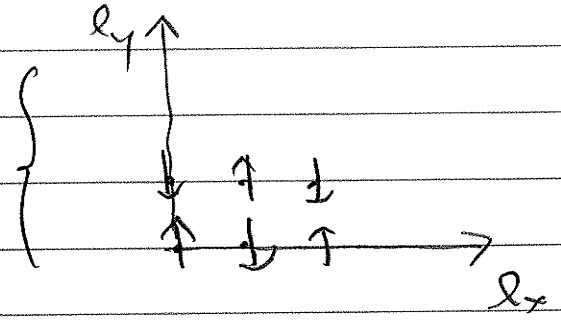
Dos -10

Why is ↑ ↓ ↑ ↓ ↑ ... $q = \pi$?

$$(-1)^{\ell} = e^{i\pi\ell} = e^{iq\ell} \quad \text{with } q = \pi$$

likewise

$$(-1)^{\ell_x + \ell_y}$$



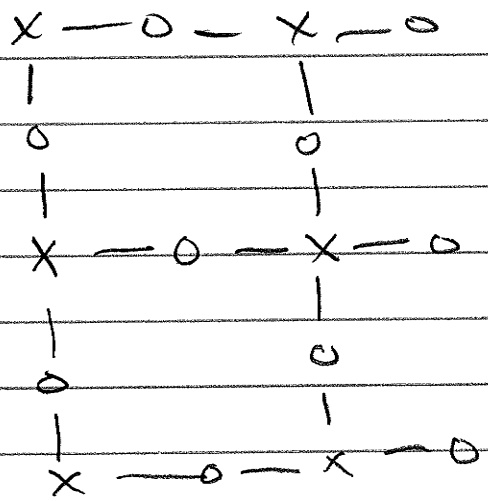
$$= e^{i\pi\ell_x + i\pi\ell_y}$$

$$= e^{i(\pi,\pi)\cdot(\ell_x \ell_y)}$$

$(q_x\, q_y)$

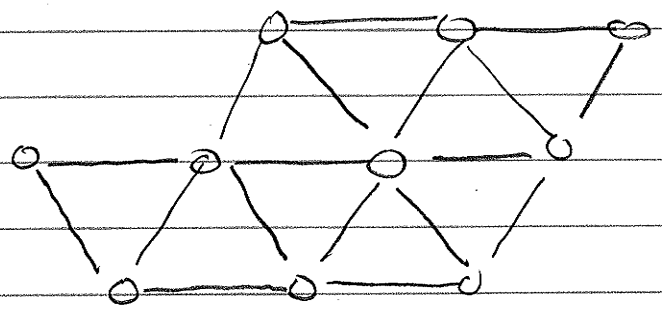
DOS-11

3 band model of Cu_2O_2 planes



$$d^{+}_{l_x l_y} p_{1 l_x l_y} + d^{+}_{l_x l_y} p_{2 l_x l_y}$$

Triangular lattice



$$-t\sum_{R}\Big(c^{+}_{\vec{R}}c_{\vec{R}+a\hat{x}} + c^{+}_{\vec{R}}c_{\vec{R}+\frac{a}{2}\hat{x}+\frac{\sqrt{3}}{2}\hat{y}} + c^{+}_{\vec{R}}c_{\vec{R}-\frac{a}{2}\hat{x}+\frac{\sqrt{3}}{2}\hat{y}} + \text{hc} + \text{hc} + \text{hc}\Big)$$

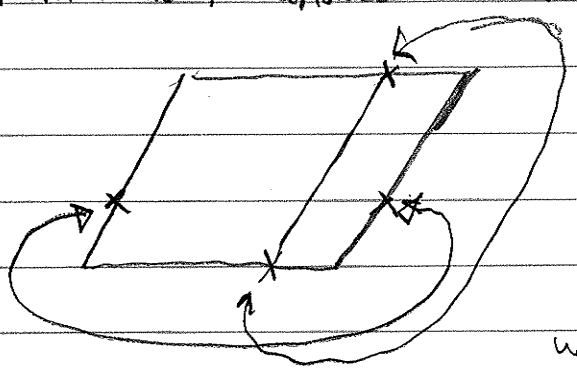
$$c^{+}_{\vec{R}} = \sum_{k} e^{-i\vec{k}\cdot\vec{R}}\, c^{+}_{\vec{k}}$$

Setting $a = 1$

Now get $-2t\left[\cos k_x + \cos\frac{k_x}{2}\cos\frac{\sqrt{3}}{2}k_y + \cos\frac{k_x}{2}\cos\frac{\sqrt{3}}{2}k_y\right]$

$$E_{k_x k_y} = -2t\left[\cos k_x + 2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}}{2}k_y\right]$$

Think about allowed k values



$y \to y$

when $x \to x + L$ want $e^{i\vec{k}\cdot\vec{R}} = 1$

$e^{ik_x L} = 1 \quad k_x = \frac{2\pi}{L} n_x$

when $x \to x + \frac{L}{2}$ $y \to y + \frac{\sqrt{3}}{2}L$

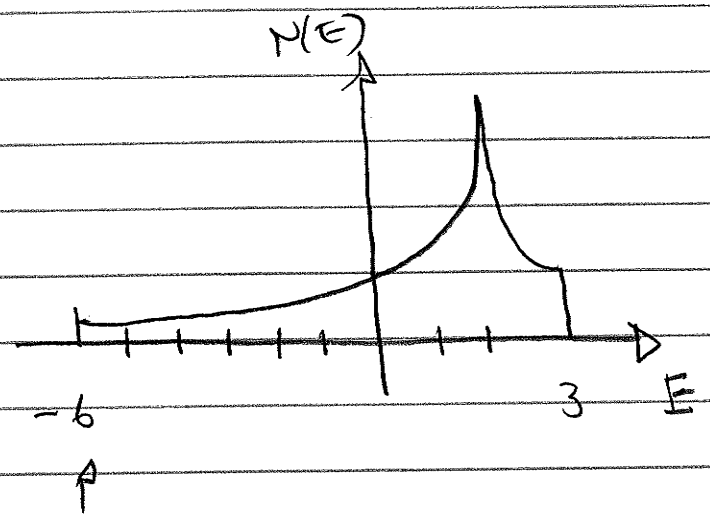
want $e^{i\vec{k}\cdot\vec{R}} = 1$

DOS - 12'

$$k_x \frac{L}{2} + k_y \frac{\sqrt{3}}{2} L = 2\pi l_y$$

$$\rightarrow k_y = \frac{2\pi}{L} \frac{2}{\sqrt{3}} l_y - \frac{1}{\sqrt{3}} k_x$$

$\frac{2\pi}{L} l_x$



$NaCoO_2$ Sodium Cobaltate

Co atoms on triangular lattice

$k_x = k_y = 0$

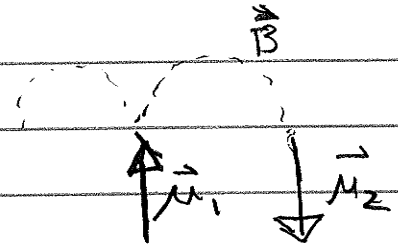
$E = -6t$

$k_x = \pi$
$k_y = \pi$ } $+2t$

How to get $+3t$?

$NdNiO_3$ "Nickelates"
$YNiO_3$
$AgNiO_2$

Ni atoms on triangular lattice



Why AF?

Actually not really correct picture But...

"Frustration"

If neighboring spins like to be antiparallel

how do they manage it