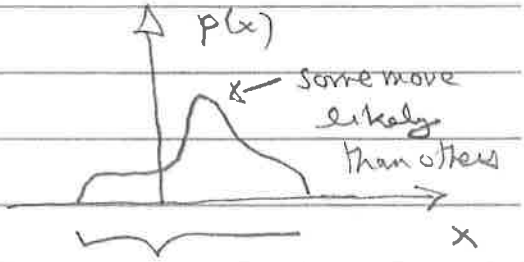
Density of States

Energy band ← continuous set of energy levels.

But not all energies in band are equally likely.

analogy: probability distribution



$p(x)dx$ = probability measure $(x, x+dx)$

For example for free particles in 3D

$$E = \frac{\hbar^2 k^2}{2m}$$

$$N = 2 \frac{V}{(2\pi)^3} \int d^3k = 2 \frac{V}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk$$

2 ← spin

$\left(\frac{2\pi}{L}\right)^3$ ← volume per k point

$$= \frac{V}{\pi^2} \frac{k_F^3}{3}$$

$$k_F = (3\pi^2 p)^{1/3}$$

$n(k)dk \equiv$ # $\vec{k}$ vectors with $|\vec{k}|$ between k and $k+dk$

$$= \underbrace{\frac{V}{(2\pi)^3} 4\pi k^2 dk}_{n(k)} = n(E)dE$$

$$E = \frac{\hbar^2 k^2}{2m} \qquad dE = \frac{\hbar^2 k}{m} dk$$

$$n(k)dk = \frac{V}{(2\pi)^3} 4\pi k^2 \frac{m dE}{\hbar^2 k}$$

$$= \frac{V}{2\pi^2} \frac{m}{\hbar^2} \left(\frac{2mE}{\hbar^2}\right)^{1/2} dE$$

$$\underbrace{\qquad\qquad}_{n(E)}$$

(Sometimes add factor of 2 for spin.)

$N(E) \sim E^{1/2}$ for free fermions

↑ proportionality constant involves mass

Why impt? Recall $C \sim \gamma T$ for fermions

because only states within $k_B T$ of Fermi surface can respond to increase in temperature.

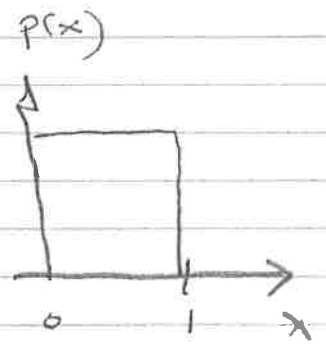
$$C = \frac{3}{2} N k_B \quad \text{classical}$$

$$\downarrow$$

$$N \frac{k_B T}{E_F} k_B$$

Exact result is $\frac{\pi^2}{2} \frac{k_B T}{E_F} N k_B$

Mathematical Aside



Suppose x is uniform on $[0,1]$

ie $p(x) = 1 \quad 0 < x < 1$

You use these x values to generate $y = x^2$.

What is $\tilde{p}(y)$? Is it uniform?

$x =$	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0
$y =$	.01	.04	.09	.16	.25	.36	.49	.64	.81	1.0

$\frac{3}{10}$ values interval $0 < y < .1$

Seems like y small more likely

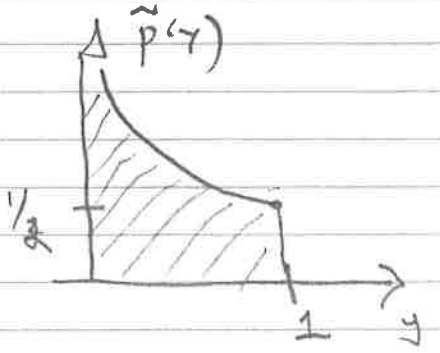
Method to get $\tilde{p}(y)$ is very simple

$$\tilde{p}(y)\,dy = p(x)\,dx \qquad y = x^2 \quad dy = 2x\,dx$$

$$\downarrow \qquad \downarrow$$

$$\tilde{p}(y)\,dy = 1 \cdot dy/2\sqrt{y}$$

$$\therefore \tilde{p}(y) = \frac{1}{2\sqrt{y}}$$



NB $\int_0^1 \tilde{p}(y)\,dy = 1$ ✓

It's not completely obvious $p(y)dy = p(x)dx$

Here's another argument:

$\tilde{p}(y)dy \equiv$ prob get value between y and $y+dy$

For this to happen x must be between $\sqrt{y}$ and $\sqrt{y+dy}$

But $\sqrt{y+dy} = \sqrt{y(1+dy/y)} = \sqrt{y}\,(1+dy/y)^{1/2}$

$$\doteq \sqrt{y}\left(1+\frac{dy}{2y}\right) = \sqrt{y} + \frac{dy}{2\sqrt{y}}$$

The likelyhood x is in any range x_1, x_2 is $x_2 - x_1$

so the probability is just $\frac{dy}{2\sqrt{y}} = \tilde{p}(y)dy$

this yields same answer $\tilde{p}(y) = \frac{1}{2\sqrt{y}}$

Bottom line if you have x with $p(x)$

and $y = f(x)$ and you want $\tilde{p}(y)$

just set $p(x)\,dx = \tilde{p}(y)dy$

$dy = f'(x)dx$ ↘ eliminate all references to x.

States within $k_B T$ of E_F involves $N(E_F)$

$C \sim N(E_F)$

* Many responses of solid involve $N(E_F)$ and indeed became larger as $N(E_F)$ increases (more e^- are free to participate) $\chi = dM/dB \sim N(E_F)$

χ ← magnetic susceptibility

Superconductivity

$T_c \sim \omega_{phonon} e^{-1/VN(E_F)}$

V ← electron phonon interaction energy

"Heavy" fermions Curro, Treve:

$CeAl_2$, $CeAl_3$, $CeCoIn_5$, $CeRhIn_5$, $CeIrIn_5$

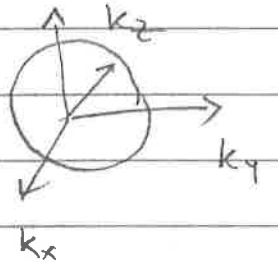
"115" materials

$N(E_F)$ is abnormally large → interesting physics

$$N(E) = \frac{V}{2\pi^2} \frac{m}{\hbar^2} \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

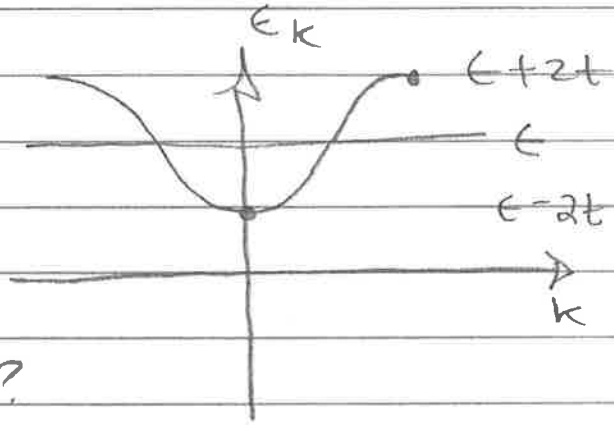
ascribe large $N(E)$ & large effective mass "heavy"

$N(E) \sim E^{1/2}$ ← more k points as Fermi sphere gets bigger



Do also our 1-d example

$\Delta = 0$ first



Where are there more k points?

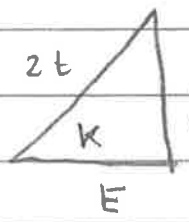
Set $\epsilon = 0$ for simplicity

$N(E)dE = n(k)dk$

↑ flat one k point per $\frac{2\pi}{L}$

$E = -2t\cos k$

$dE = 2t \sin k \, dk$



$\cos k = \frac{E}{2t}$

$\sin k = \frac{\sqrt{4t^2-E^2}}{2t}$

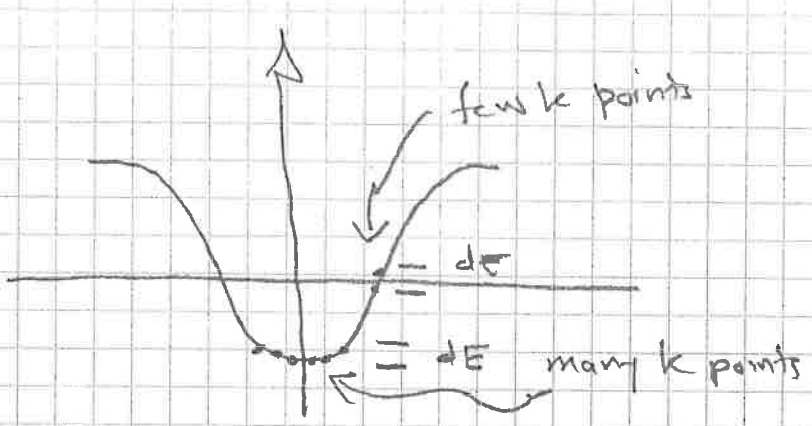
$N(E)dE = \frac{L}{2\pi} \frac{dE}{2t \sin k}$

$= \frac{L}{2\pi} \frac{dE}{\sqrt{4t^2-E^2}}$

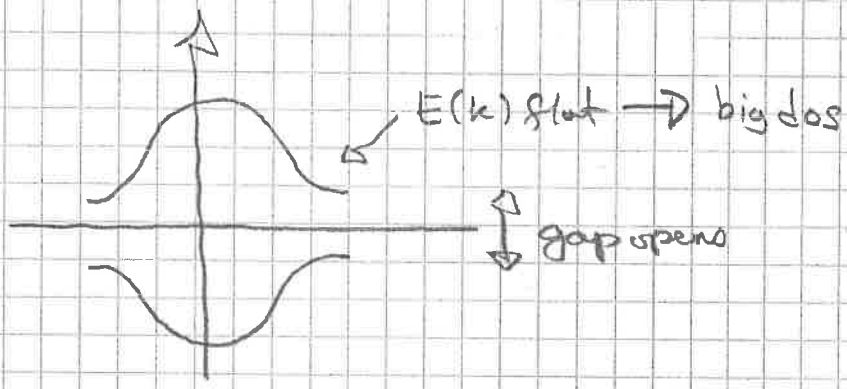
$N(E) = \frac{L}{2\pi} \frac{1}{\sqrt{4t^2-E^2}}$

peaks at $E = \pm 2t$

Physically:

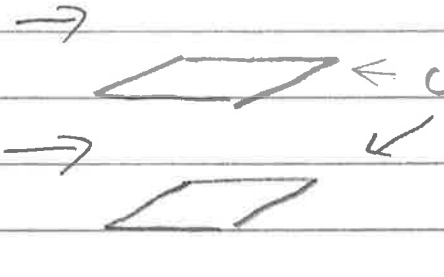


what if $\Delta \neq 0$



DOS-6

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



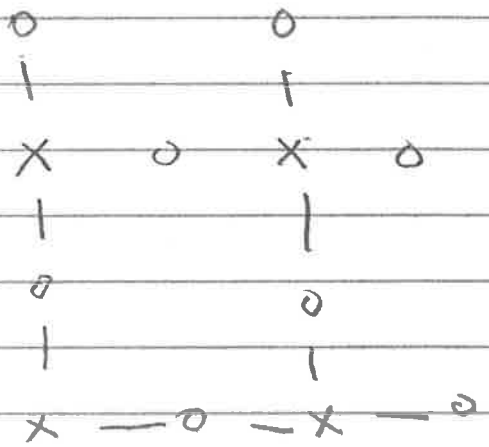
$Y_1Ba_2Cu_3O_7$

$La_{2-x}Sr_xCuO_4$

⋮

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

fermions move on square copper lattice



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

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

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

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

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

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

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 #

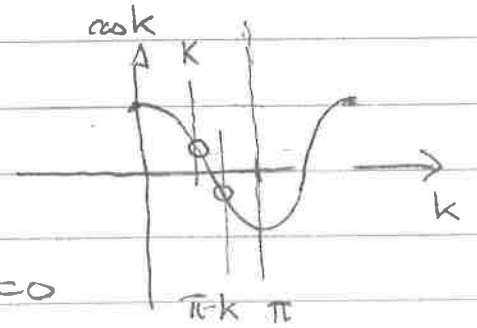
$\cos k_x \sim 1 - \frac{k_x^2}{2}$ $\cos k_y \sim 1 - \frac{k_y^2}{2}$

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

what about $E_f = 0$? ← ASIDE: sign of E is impt? Nope. Zero of energy is some ↑ since bands arise from bound atomic levels expect E<0

$-2t(\cos k_x + \cos k_y) = 0$

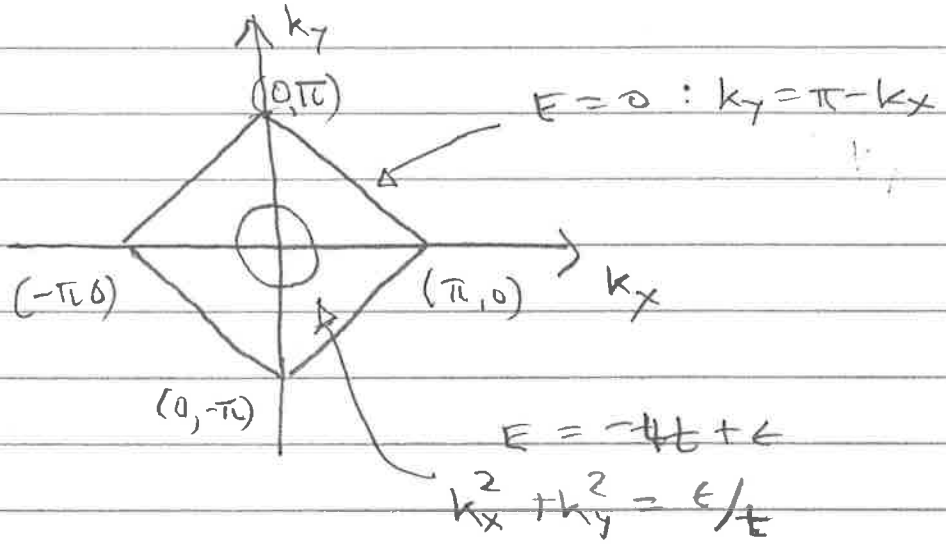
$\cos k_x + \cos k_y = 0$



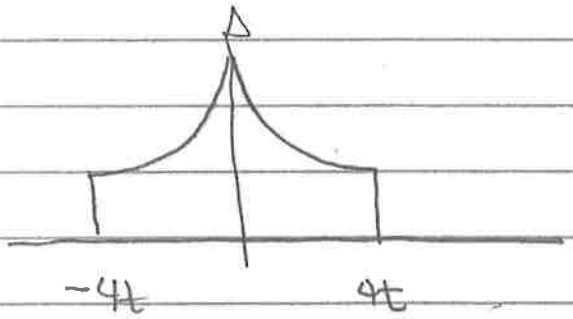
$\cos k = -\cos(\pi - k)$

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

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



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



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

↓ ↑

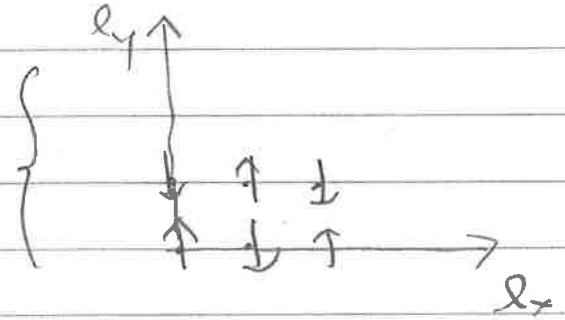
DOS-10

Why is ↑ ↓ ↑ ↓ ↑ ... $q = \pi$?

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

likewise

$$(-1)^{l_x + l_y}$$

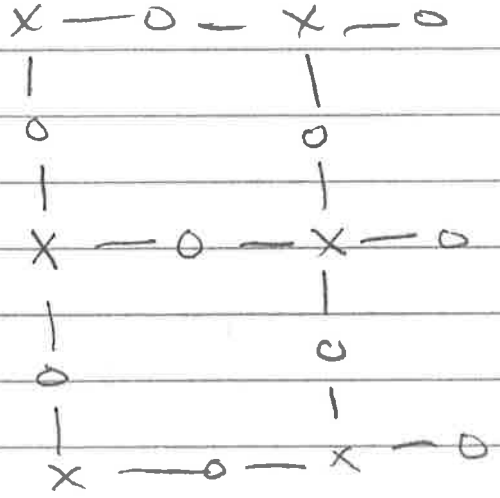


$$= e^{i\pi l_x + i\pi l_y}$$

$$= e^{i(\pi,\pi)\cdot(l_x, l_y)}$$

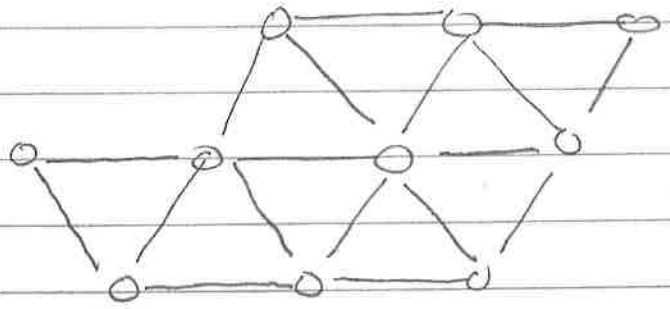
$$(q_x, q_y)$$

3 band model of $Cu O_2$ 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



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

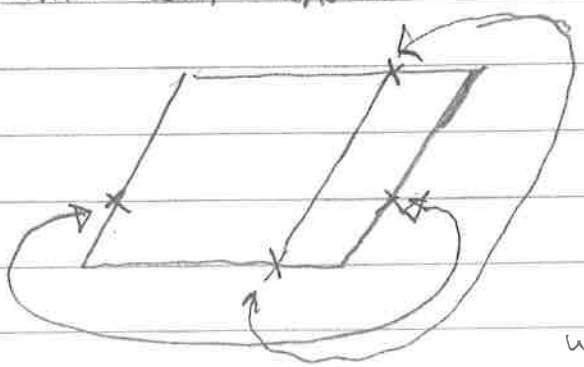
$$c^{\dagger}_{\vec{R}} = \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}} c^{\dagger}_{\vec{k}}$$

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

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

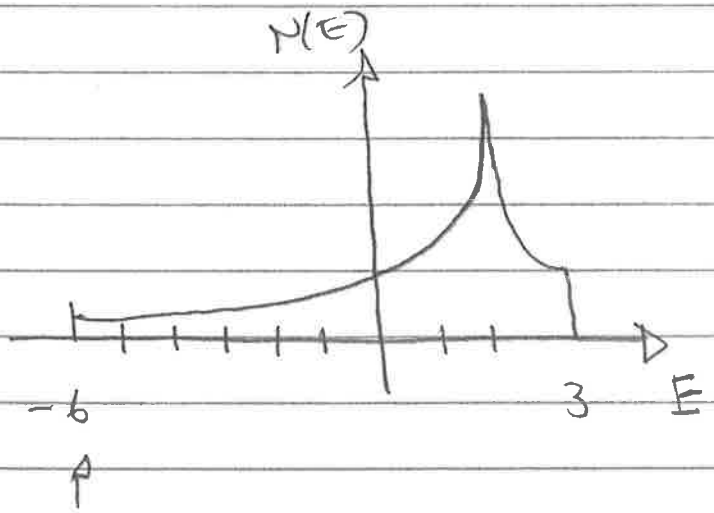
when $x \to x + \frac{L}{2}$ $y \to y + \frac{\sqrt{3}}{2}L$

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

DOS - 12'

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

$$\Rightarrow k_y = \frac{2\pi}{L} \frac{2}{\sqrt{3}} l_y - \frac{1}{\sqrt{3}} \underbrace{k_x}_{\frac{2\pi}{L} l_x}$$



$k_x = k_y = 0$

$E = -6t$

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

How to get $+3t$?

$NaCoO_2$ Sodium cobaltate

Co atoms on triangular lattice

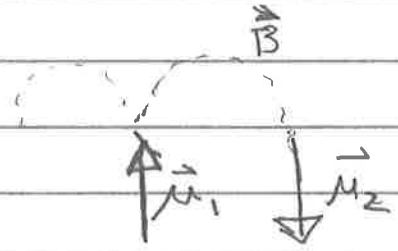
$NdNiO_3$ "Nickelates"

$YNiO_3$

$AgNiO_2$

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