Mean-field Theory of Anti-ferromagnetic instability of Fermions on square lattice.

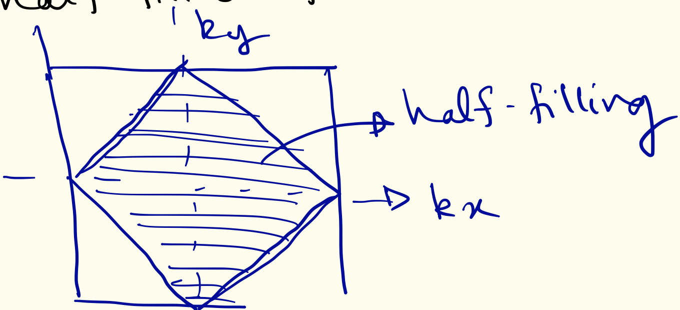
$$H = \sum_k \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} + U\sum_i (\hat{n}_i - 1)^2$$

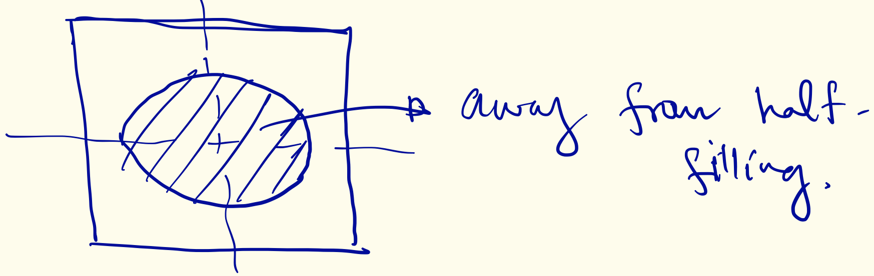
$$n_i = \sum_i c^\dagger_{i\sigma} c_{i\sigma}$$

$$\varepsilon_k = -2t\,(\cos(k_x) + \cos(k_y)) - \mu$$

μ = chemical potential. When $\mu = 0$

$\Rightarrow$ half-filled fermi surface.





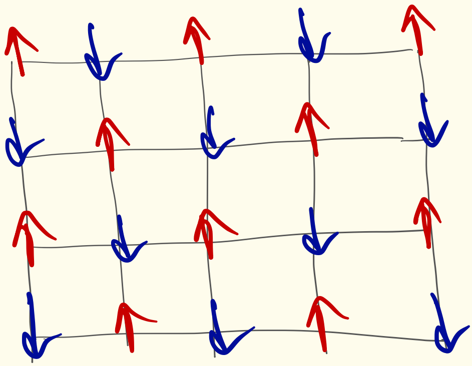
What to expect at half-filling?

First consider the limit $U \gg t$.

As discussed in the lecture, in this limit the effective Hamiltonian is

$$H_{eff} = \frac{4t^2}{U} \sum \vec{S}_i \cdot \vec{S}_j$$

In the ground state of this system spins order antiferromagnetically,



What about the opposite limit $t \gg U$??

Mean-field theory suggests that the system still orders anti-ferromagnetically

At half-filling expect instability for infinitesimal U.

$$U(n_i-1)^2 = -U\left[c^\dagger_i \sigma^z c_i\right]^2 + U$$

$$n_i = 1 \Rightarrow \left[c^\dagger \sigma^z c\right]^2 = 1$$

$$n_i = 0 \Rightarrow \left[c^\dagger \sigma^z c\right]^2 = 0$$

Basic idea of mean-field.

$$(c^\dagger_i \sigma^z c_i)^2 \xrightarrow{\text{Replace}} 2\langle c^\dagger_i \sigma^z c_i\rangle c^\dagger_i \sigma^z c_i - \langle c^\dagger_i \sigma^z c_i\rangle^2$$

Based on physical reasoning $\langle c^\dagger_i \sigma^z c_i\rangle = M(-)^{x+y}$

$$= M(-)^i$$

The mean-field H becomes:

$$H_{M\text{-}F} = \sum_{k\sigma} \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma}$$

$$- 2UM \sum_i (-)^i \, c^\dagger_i \sigma^z c_i$$

$$+ UM^2 N_{site}$$

$$\varepsilon_k = -2t\left[\cos(k_x) + \cos(k_y)\right] - \mu$$

Lets work at $\mu = 0$

$$H_{M\text{-}F} = -2t \sum_k \left(\cos(k_x) + \cos(k_y)\right) c^\dagger_{k\sigma} c_{k\sigma}$$

$$- 2UM \sum_k \left[c^\dagger_k \sigma^z c_{k+Q} + h.c. \right]$$

$$= \sum_k{}' -2t\left[\cos(k_x) + \cos(k_y)\right] c^\dagger_{k\sigma} c_{k\sigma}$$

$$+ \sum_k{}' 2t\left[\cos(k_x) + \cos(k_y)\right] c^\dagger_{k+Q\sigma} c_{k+Q\sigma}$$

$$- 2UM \sum_k \left[c^\dagger_{k} \sigma^z c_{k+Q} + h.c. \right]$$

$$= \sum_{k\sigma} \left[c^{\dagger}_{k\sigma} \; c^{\dagger}_{k+Q\sigma} \right] \begin{bmatrix} \varepsilon_k & -2UM\sigma^z \\ -2UM\sigma^z & -\varepsilon_k \end{bmatrix} \begin{bmatrix} c_{k\sigma} \\ c_{k+Q\sigma} \end{bmatrix}$$

One can diagonalize this 2x2 Matrix.

Eigenvalues $E_k = \pm\sqrt{\varepsilon_k^2 + 4U^2M^2}$

Eigenvectors :

$$\eta_{+\sigma}(k) = -V(k)\, \sigma^z_{\sigma\sigma'}\, c_{\sigma'}(k) + U(k)\, c_\sigma(k+Q)$$

$$\eta_{-\sigma}(k) = U(k)\, c_\sigma(k) + V_k\, \sigma^z_{\sigma\sigma'}\, c_{\sigma'}(k+Q)$$

$$U(k) = \frac{1}{\sqrt{2}}\sqrt{1 - \frac{\varepsilon_k}{E_k}} \qquad V(k) = \sqrt{1 - U(k)^2}$$

$$H = \sum_{k\sigma}{}' E_k \, \eta^{\dagger}_{+\sigma}(k)\, \eta_{+\sigma}(k)$$

$$- \sum_{k\sigma}{}' E_k \, \eta^{\dagger}_{-\sigma}(k)\, \eta_{-\sigma}(k)$$

$$E_k = \sqrt{\varepsilon_k^2 + 4U^2 M^2}$$

$$\boxed{\text{Ground state} = \prod_k \eta^{\dagger}_{-\sigma}(k)|0\rangle}$$

Ground state energy $E_0 =$

$$= -2 \sum_k{}' E_k + N_{site} U M^2$$

To find M, minimize E_0 wrt M

$$\Rightarrow \quad \frac{1}{4} - \frac{U}{N_{site}} \sum_k{}' \frac{1}{E_k} = 0$$

Is there a solution for infinitesimal U?

Yes!

$$U \sum_k{}' \frac{1}{\sqrt{4U^2M^2 + [\cos(k_x) + \cos(k_y)]^2 4t^2}}$$

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

As $U \to 0$ $\displaystyle\sum_k{}' \frac{1}{E_k}$ diverges

So if M was zero for $U < U_c$
$\neq 0$

The above eqn won't make sense.

$\Rightarrow$ $M \neq 0$ as $U \to 0^+$.

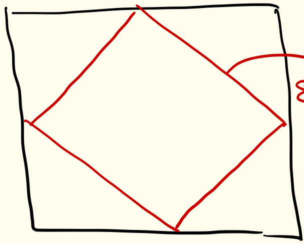
No soln for $U < 0$.

How to solve the self-consistency equation?

$$\frac{U}{N_s} \sum_k{}' \frac{1}{\sqrt{4U^2M^2 + \varepsilon_k^2}} = \frac{1}{4}$$

for small U, M is also small $\Rightarrow$ most contribution comes from $\varepsilon_k \simeq 0$ $\Rightarrow$ fermi surface dominates the integral

Approximately:



$$U \int \frac{d\varepsilon \; N(\varepsilon)}{\sqrt{4U^2M^2 + \varepsilon^2}} = \frac{1}{4}$$

$N(\varepsilon)$ = density of states

= constant at the fermi surface.

limits of integration?

$\varepsilon \simeq -t$ to $\varepsilon \simeq t$, the only scale other than UM

$$2U\,N(\varepsilon_F)\int_0^t \frac{d\varepsilon}{\sqrt{\varepsilon^2 + 4U^2M^2}} = \frac{1}{4}$$

One can do this exactly but when U is small, its even simpler.

$$2 U N(\epsilon_F) \log \frac{t}{2UM} = \frac{1}{4}$$

$$\Rightarrow \quad M \simeq \frac{t}{U} \exp\left[-1/N(\epsilon_F)U\right]$$

Clearly, as $U \to 0$, $M \to 0$.

Superconducting Instability of Fermions.

Above we saw that repulsive interactions at half-filling destabilize a fermi surface and lead to anti-ferromagnetic ordering.

What about attractive interactions i.e., $U < 0$. In this case mean-field theory suggests there is no anti-ferromagnetic ordering. Interestingly, now one finds a "superconducting" instability.

Before we do a mean-field theory for superconductor, let's first understand very basics of a superconductor - heuristically. That will help us to do mean-field theory as well.

What is a superconductor?

In a superconductor, electrons pair up to form a boson, called "cooper pair". (named after Sheldon Cooper from big bang theory).

The easiest way to pair them is to form a boson:

$$b(x) = c^{+}_{\uparrow}(x)\, c^{+}_{\downarrow}(x)$$ so that

the two electrons participating in pairing can be at the same location in the real-space.

In a superconductor, the expectation value of $b(x)$ w.r.t. to the ground state wf^n does not fluctuate much, similar to the ordering of $\langle S^z \rangle$ in an antiferromagnet.

This motivates the following mean-field :

$$\langle c^{\dagger}_{\uparrow}(x)\, c^{\dagger}_{\downarrow}(x) \rangle = \Delta$$

= independent of x.

Question : How can $\langle c^{\dagger}_{\uparrow}(x)\, c^{\dagger}_{\downarrow}(x) \rangle$ be non-zero <u>if</u> the number of particles in the wfn is conserved ?

Answer : It can't but enlarging the Hilbert space to multi-particle space allows it to be non-zero.

Allowing the total number of particles to fluctuate, the wf^n can be written as a superposition of states with different no. of particles :

$$|\psi\rangle = \underbrace{|\phi_{N=1}\rangle}_{\text{1-particle wf}^n} + \underbrace{|\phi_{N=2}\rangle}_{\text{2-particle wf}^n} + \ldots |\phi_{N=\infty}\rangle$$

Within this enlarged Hilbert space, it is now possible for $\langle c^\dagger_\uparrow c^\dagger_\downarrow \rangle$ to be non-zero e.g. $\langle \phi_{N+2} | c^\dagger_\uparrow(x) c^\dagger_\downarrow(x) | \phi_N \rangle$ could in principle be non-zero.

Towards a Mean-Field Theory of a Superconductor

Again consider the same model as the one we studied for anti-ferromagnetic instability of fermi gas:

$$H = \sum_k \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i (\hat{n}_i - 1)^2$$

$$n_i = \sum_i c^\dagger_{i\sigma} c_{i\sigma}$$

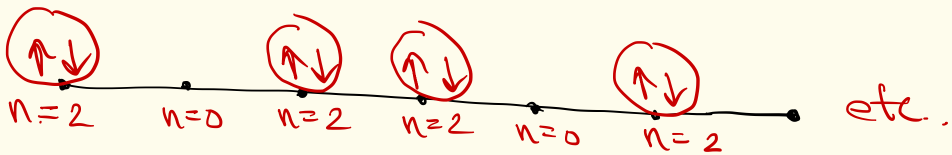
$$\varepsilon_k = -2t\,(\cos(k_x) + \cos(k_y)) - \mu$$

μ = chemical potential.

When U was positive, we found that anti-ferromagnet was favored. We argued this based on the limit $U \to \infty$ where $H_{eff} = \frac{4t^2}{U} \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$.

For getting a superconductor, $U < 0$ is more conducive. To see this, now consider the limit $U \to -\infty$. The term $U(n_i - 1)^2 = -|U|(n_i-1)^2$ will favor $n_i = 0$ and $n_i = 2$.

So the ground state will look like



The bound state of two electons at a given site is precisely the cooper pair $c^\dagger_\uparrow c^\dagger_\downarrow$ responsible for the superconductivity.

Note that, unlike the case of Antiferromagnet in the limit $U \to \infty$, the above argument does not rely on half-filling, and is valid for arbitrary value of the chemical potential μ.

Thus, we write H as: ($\mu' = \mu$ + constant)

$$H = \sum_{k\sigma} (\varepsilon_k - \mu') \, c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

$$= \sum_{k} (\varepsilon_k - \mu) \, c^\dagger_{k\sigma} c_{k\sigma} - U \sum_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\uparrow} c_{i\downarrow}$$

Now, we make a mean-field approximation for the interaction term:

$$-U\, c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\uparrow} c_{i\downarrow}$$

$$\longrightarrow -U \Big[\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle c_{i\uparrow} c_{i\downarrow}$$

$$+ c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \langle c_{i\uparrow} c_{i\downarrow} \rangle$$

$$- \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle \langle c_{i\uparrow} c_{i\downarrow} \rangle \Big]$$

Denoting $\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle = \Delta =$ constant

$$\Rightarrow \langle c_{i\uparrow} c_{i\downarrow} \rangle = -\Delta^*$$

$$H_{\text{Mean-field}} = \sum_{k\sigma} (\varepsilon_k - \mu') c^\dagger_{k\sigma} c_{k\sigma}$$

$\equiv H_{MF}$ henceforth

$$- U \sum_i \Big[\Delta\, c_{i\uparrow} c_{i\downarrow}$$

$$+ \Delta^* c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} \Big] - N_s U |\Delta|^2$$

Note the negative sign

N_s: # of sites

$$= \sum_{k\sigma} (\varepsilon_k - \mu') c^\dagger_{k\sigma} c_{k\sigma}$$

$$- U \sum_k \Big[\Delta^* c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + \Delta\, c_{-k\downarrow} c_{k\uparrow} \Big]$$

$$- U |\Delta|^2 N_s$$

Note that the original Hamiltonian with $U n_{i\uparrow} n_{i\downarrow}$ term had the symmetry

$$c_\sigma \to e^{i\theta} c_\sigma$$ corresponding to

the particle number conservation (recall pset-2). The mean-field H_{MF} breaks this symmetry! The only symmetry left is $c_\sigma \to -c_\sigma$ corresponding to particle no. conservation modulo two.

How to solve the mean-field H_{MF}?

Define
$$c^{+}_{-k\downarrow} = \tilde{c}_{+k\downarrow}$$
$$c^{+}_{k\uparrow} = \tilde{c}^{+}_{k\uparrow}$$

<u>Check:</u> $\tilde{c}_{k\downarrow} \tilde{c}^{+}_{k'\downarrow} + \tilde{c}^{+}_{k'\downarrow} \tilde{c}_{k\downarrow}$

$$= c^{+}_{-k\downarrow} c_{-k'\downarrow} + c_{-k'\downarrow} c^{+}_{-k\downarrow}$$

$$= \delta_{kk'}$$ $\Rightarrow$ $\tilde{c}_{k\sigma}, \tilde{c}^{+}_{k\sigma}$ legitimate fermion operators.

$$\Rightarrow H = \sum_k (\varepsilon_k - \mu') \tilde{c}^\dagger_{k\uparrow} \tilde{c}_{k\uparrow}$$

$$+ \sum_k (\varepsilon_k - \mu') \tilde{c}_{k\downarrow} \tilde{c}^\dagger_{k\downarrow}$$

$$- U \sum_k [\tilde{c}^\dagger_{k\uparrow} \tilde{c}_{k\downarrow} \Delta^* + h.c.]$$

$$- U|\Delta|^2 N_s$$

$$= \sum_k [\tilde{c}^\dagger_{k\uparrow} \quad \tilde{c}_{k\downarrow}] \begin{bmatrix} \varepsilon_k - \mu' & -U\Delta^* \\ -U\Delta & -(\varepsilon_k - \mu') \end{bmatrix} \begin{bmatrix} \tilde{c}_{k\uparrow} \\ \tilde{c}_{k\downarrow} \end{bmatrix}$$

$$- U|\Delta|^2 N_s$$

When $U<0$, this is identical to the mean-field Hamiltonian for the anti-ferromagnetic instability!

eigenvalues $E_k = \pm\sqrt{(\varepsilon_k - \mu')^2 + U^2|\Delta|^2}$

Ground state energy

$$= - \sum_k \sqrt{(\varepsilon_k - \mu')^2 + U^2 |\Delta|^2}$$

$$+ |U| N_s |\Delta|^2$$

Minimizing w.r.t. $|\Delta|$, one again finds

$$|\Delta| \simeq \frac{t}{|U|} \exp\left[-1/N(\varepsilon_F)|U|\right]$$

where $N(\varepsilon_F)$ = density of states at the fermi surface,

exactly as in the case for the anti-ferromagnetic instability.

Thus, a $U > 0$ anti-ferromagnetic instability gets mapped to a $U < 0$ superconducting instability.