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

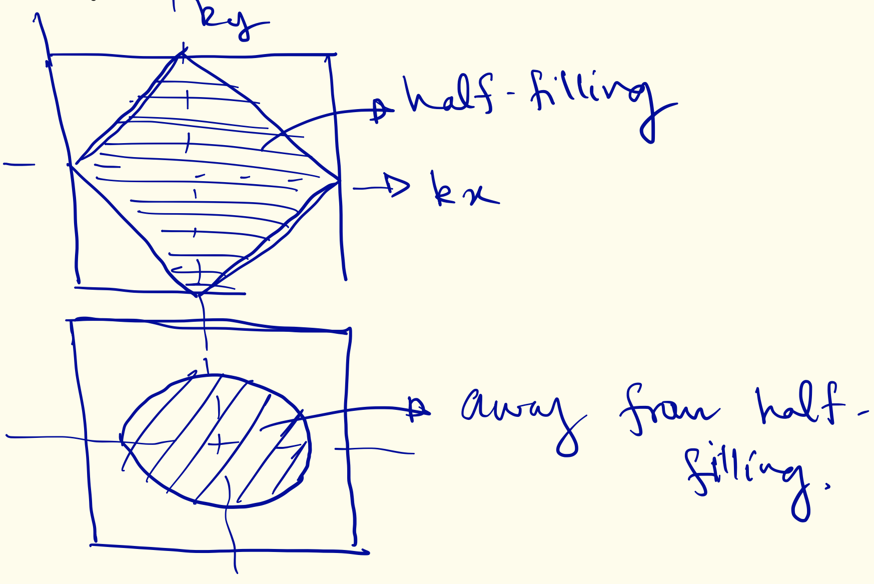
$$H = \sum_k \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i (\hat{n}_i - 1)^2$$

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

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

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

$\Rightarrow$ half-filled fermi surface.



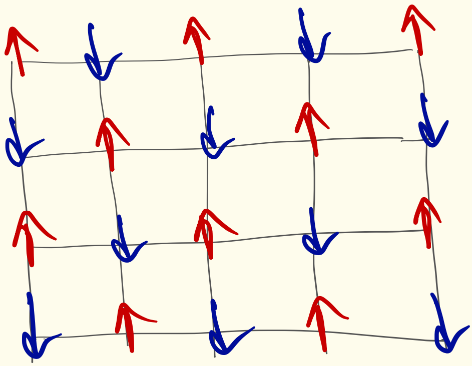
What to expect at half-filling?

First consider the limit $U >> t$.

As you will show in pset-4, 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 $t >> U$??

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

At half-filling expect instability for infinitesimal U.

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

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

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

Basic idea of mean-field.

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

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

$$= M(-)^i$$

The mean-field H becomes:

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

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

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

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

Lets work at $\mu = 0$

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

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

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

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

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

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

One can diagonalize this 2x2 Matrix.

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

Eigenvectors :

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

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

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

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

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

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

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

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

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

The above eqn won't make sense.

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

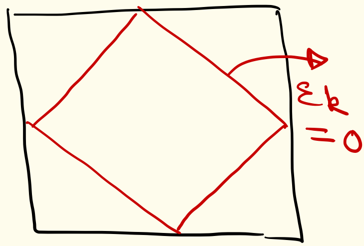
No soln for $U < 0$.

How to solve the self-consistency equation?

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

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, it's 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, lets 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 wfn does not fluctuate much, similar to the ordering of $\langle S^z \rangle$ in an antiferromagnet.