(7.1) bl-d!

$$H = -t\sum_{\langle i,j\rangle,\sigma}\left(c^\dagger_{i\sigma}c_{j\sigma}+h.c.\right)+U\sum_i n_{i\uparrow}n_{i\downarrow}-\mu\sum_i\left(n_{i\uparrow}+n_{i\downarrow}\right).$$

Hartree-Fock decoupling: $AB \to \langle A\rangle B + A\langle B\rangle - \langle A\rangle\langle B\rangle$.

here: $n_{i\uparrow}n_{i\downarrow} \to \langle n_{i\uparrow}\rangle n_{i\downarrow} + n_{i\uparrow}\langle n_{i\downarrow}\rangle - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle$

Using the ansatz:

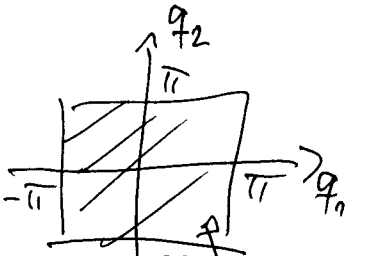
$$\langle n_{i\uparrow}\rangle = n + (-1)^i m$$
$$\langle n_{i\downarrow}\rangle = n - (-1)^i m$$

(anti-ferromagnet Néel order)

$$\Rightarrow H_{HF} = -t\sum_{\langle i,j\rangle,\sigma}\left(c^\dagger_{i\sigma}c_{j\sigma}+h.c.\right)+U\sum_i\Big[\left(n+(-1)^i m\right)n_{i\downarrow} + \left(n-(-1)^i m\right)n_{i\uparrow} - \underbrace{\left(n+(-1)^i m\right)\left(n-(-1)^i m\right)}_{=n^2-m^2}\Big] - \mu\sum_{i,\sigma} n_{j\sigma}$$

Quadratic Ham (after decoupling), can be diagonalized by Bloch functions

$$c_{j\sigma} = \frac{1}{\sqrt{N_L}}\sum_{q\in BZ} e^{iqx_j}\,c_{q\sigma}.$$



with $\vec{Q}=(\pi,\pi)$. $(a=1)$.

Write $(-1)^{j_1+j_2} = \exp\left[i\pi(j_1+j_2)\right] = e^{i\vec{Q}\cdot\vec{x}_j}$ with $\vec{x}_j = j_1\vec{a}_1 + j_2\vec{a}_2$.

$$\Rightarrow H_{HF} = \sum_{\substack{q\in BZ\\ \sigma}}\Big[\varepsilon_q\,c^\dagger_{q\sigma}c_{q\sigma} + UM\,c^\dagger_{q\sigma}c_{q\sigma} + UM\left(c^\dagger_{q+Q,\uparrow}c_{q\uparrow} - c_{q+Q,\downarrow}c_{q,\downarrow}\right)\Big] - UN_L\left(n^2-m^2\right).$$

We have introduced $\xi_q = \varepsilon_q - \mu$ and $\varepsilon_q = -2t(\cos q_1 + \cos q_2)$.

Writing as a <u>symmetric</u> matrix:

$$H_{HF} = \frac{1}{2}\sum_{q\in BZ} \left(c^\dagger_{q\uparrow}\, c^\dagger_{q\downarrow}\, c^\dagger_{q+Q,\uparrow}\, c^\dagger_{q+Q,\downarrow}\right) \begin{pmatrix} \tilde{\xi}_q & 0 & Um & 0 \\ 0 & \tilde{\xi}_q & 0 & -Um \\ Um & 0 & \tilde{\xi}_{q+Q} & 0 \\ 0 & -Um & 0 & \tilde{\xi}_{q+Q} \end{pmatrix} \begin{pmatrix} c_{q\uparrow} \\ c_{q\downarrow} \\ c_{q+Q\uparrow} \\ c_{q+Q,\downarrow} \end{pmatrix}$$

from Symmetrization.

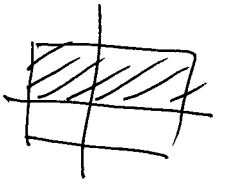
with $\tilde{\xi}_q = \xi_q + nU$.

This can be brought to block-matrix structure via

$$H_{HF} = \sum_{\substack{q>0 \\ q\in BZ}} \vec{c}^{\,\dagger}_q \begin{pmatrix} \tilde{\xi}_q & \Delta & 0 & 0 \\ \Delta & \tilde{\xi}_{q+Q} & 0 & 0 \\ 0 & 0 & \tilde{\xi}_q & -\Delta \\ 0 & 0 & -\Delta & \tilde{\xi}_{q+Q} \end{pmatrix} \vec{c}_q$$

with (reordered) vector $\vec{c}_q = \left(c_{q\uparrow}, c_{q+Q,\uparrow}, c_{q,\downarrow}, c_{q+Q,\downarrow}\right)^T$.

Summation is over half of BZ:



Choose chemical potential $\mu = Um$ to remain at half-filling.

Then, $\tilde{\xi}_{q+Q} = -\tilde{\xi}_q$ for $\mu = Um$.

and we find spectrum

$$H_{HF} = \sum_{\substack{q_1>0 \\ q\in B^2 \\ \sigma}} \sum_{a=\pm} a E_q \, d^\dagger_{q,\sigma,a} d_{q,\sigma,a} - \underbrace{U N_L (n^2 - m^2)}_{= \frac{N_L}{U}(U^2 n^2 - \Delta^2)}$$

↑ two bands

with $E_q = \sqrt{\varepsilon_q^2 + \Delta^2}$.

Now minimize free energy F at $T=0$: $F = \langle H_{HF} \rangle$ w.r.t. Δ. This self-consistency equation for Δ is called the gap equation:

$$\frac{\delta \langle H_{HF} \rangle}{\delta \Delta} = \sum_{q\in B^2, q_1>0} \sum_{\sigma, a} a \, \delta_{a,-1} \frac{\Delta}{\sqrt{\varepsilon_q^2 + \Delta^2}} + \frac{2N_L}{U}\Delta \overset{!}{=} 0.$$

↑ only lower band filled

$\langle d^\dagger_{q,\sigma,a} d_{q,\sigma,a} \rangle = \delta_{a,-1}$.

$$\Leftrightarrow 0 = -\sum_{q;\, q_1>0} \overbrace{\sum_{\sigma}}^{=2} \frac{\Delta}{\sqrt{\varepsilon_q^2 + \Delta^2}} + \frac{2N_L}{U}\Delta$$

$$\Leftrightarrow \boxed{\frac{2}{2} N_L \Delta \int \frac{d^2q}{(2\pi)^2} \frac{1}{\sqrt{\varepsilon_q^2 + \Delta^2}} = \frac{2N_L \Delta}{U}}$$

$$\sum_{\substack{q;\, q_1>0 \\ B^2}} = \frac{1}{2} \sum_{q\in B^2} = \frac{1}{2} N_L \int \frac{d^2q}{(2\pi)^2}$$

Gap equation: ← all filled states

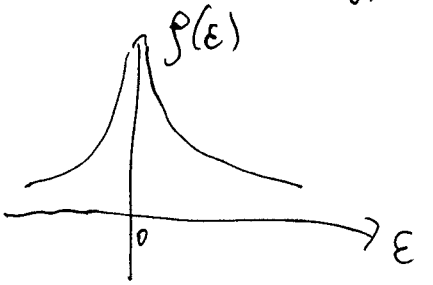
$$1 = \frac{U}{2} \int \frac{d^2q}{(2\pi)^2} \frac{1}{\sqrt{\varepsilon_q^2 + \Delta^2}}$$ with "gap" $\Delta = U m$.

$$\Leftrightarrow \quad 1 = \frac{U}{2} \int_{-4t}^{0} d\varepsilon \; \rho(\varepsilon) \frac{1}{\sqrt{\varepsilon^2 + \Delta^2}}$$

↖ at $T=0$ and half-filling only lower band is occupied.

We have calculated the DoS $\rho(\varepsilon)$ before. To logarithmic accuracy, it reads

$$\rho(\varepsilon) \simeq \underbrace{\frac{1}{2\pi^2 t}}_{= N_0} \log\left(\frac{16t}{\varepsilon}\right)$$



$$\Rightarrow \boxed{1 = \frac{N_0 U}{2} \int_{-4t}^{0} d\varepsilon \; \frac{\log\left(\frac{16t}{\varepsilon}\right)}{\sqrt{\varepsilon^2 + \Delta^2}}}$$

Approx. this integral by splitting it into $\int_{-4t}^{0} = \int_{-4t}^{\Delta} + \int_{\Delta}^{0}$

and approx. the integrand as $\varepsilon \gg \Delta$ and $\varepsilon \ll \Delta$, respectively.

$$\Rightarrow (A) = \int_{\Delta}^{4t} d\varepsilon \; \frac{\log\left(16t/\varepsilon\right)}{\varepsilon} = -\frac{1}{2}\left\{\left[\log 4\right]^2 - \log\left[\frac{16t}{\Delta}\right]^2\right\} \simeq$$

$$\simeq \frac{1}{2}\left[\log\left(\frac{16}{\Delta}\right)\right]^2 .$$

$\rho_{\Delta \to 0}$

$$(B) = \int_{0}^{\Delta} d\varepsilon \; \frac{\log\left(16/\varepsilon\right)}{\Delta} = \left[\varepsilon + \varepsilon \log \frac{16t}{\varepsilon}\right]\Big|_{0}^{\Delta} = \text{finite and subdominant}$$

compared to $\left[\log\left(\frac{16t}{\Delta}\right)\right]^2$ divergence for $\Delta \to 0$.

$\Rightarrow$ extracting the dominant divergent part (A) yields for gap equation:

$$1 = \frac{N_0 U}{2} \cdot \frac{1}{2}\left[\log\left(\frac{16t}{\Delta}\right)\right]^2$$

$$\Leftrightarrow \frac{8\pi^2 t}{U} = \left[\log\left(\frac{16t}{\Delta}\right)\right]^2 \Leftrightarrow 2\pi\sqrt{\frac{2t}{U}} = \log\left(\frac{16t}{\Delta}\right)$$

$$\Leftrightarrow \boxed{\Delta = 16\, t \exp\left[-2\pi\sqrt{2}\sqrt{\frac{t}{U}}\right].}$$

$N_0 = \frac{1}{2\pi^2 t}$

We find that $\Delta > 0$ for any parameter t and U_2 (at $T=0$). $\Rightarrow$ the system can lower its (free) energy by developing a non-zero Δ, i.e., a spin-density wave (order parameter m).

(1) (1a) The interaction Ham-n

$$\hat{H}_{int} = \int \hat{\rho}(r)\, V(r-r')\, \hat{\rho}(r')\, dr\, dr' = g \int \hat{\rho}(r)\, \hat{\rho}(r)\, dr$$

$$\hat{\rho}_\sigma(r) = \hat{\psi}^+_\sigma(r)\, \hat{\psi}_\sigma(r)$$

$$\downarrow \quad \hat{\psi}(r) = \frac{1}{\sqrt{V}} \sum_k e^{ikr}\, \hat{a}_{k\sigma}$$

$$\hat{\rho}_\sigma(r) = \frac{1}{V} \sum_{k,k'} e^{i(k'-k)r}\, \hat{a}^+_{k\sigma}\, \hat{a}_{k'\sigma}$$

$$\hat{H}_{int} = g \sum_{\substack{k,k' \\ p,p' \\ \sigma,\tau}} \frac{1}{V^2} \int e^{i(k'-k)r + i(p'-p)r}\, \hat{a}^+_{k\sigma} \hat{a}_{k'\sigma}\, \hat{a}^+_{p\tau}\, \hat{a}_{p'\tau}\, dr = .$$

(spins)

$$= \boxed{\frac{g}{V} \sum_{\substack{k,k' \\ p,p' \\ \sigma,\tau}} \hat{a}^+_{k\sigma}\, \hat{a}_{k'\sigma}\, \hat{a}^+_{p\tau}\, \hat{a}_{p'\tau}\, \delta_{k'+p'-k-p} = \hat{H}_{int}}$$

(1b) There are 2 types of contributions to the energy correction in the lowest order in interaction (self-energy part)

1. Hartree

$$\langle \hat{a}^+_{k\sigma}\, \hat{a}_{k'\sigma} \rangle \longrightarrow \delta_{kk'} \left(N^F_\uparrow(k) + N^F_\downarrow(k) \right)$$

($N^F_\uparrow(k)$: occupation number of electrons with spin ↑ and momentum k)

$$H_{int} \leftarrow \frac{1}{V} g \sum_k \left[N^F_\uparrow(k) + N^F_\downarrow(k) \right] \sum_{p\tau} \hat{a}^+_{p\tau}\, \hat{a}_{p\tau} =$$

$$= g\,(n_\uparrow + n_\downarrow) \sum_{p\sigma} \hat{a}^+_{p\sigma}\, \hat{a}_{p\sigma} \qquad (1)$$

2. Fock

$$\langle \hat{a}_{k'\sigma}\, \hat{a}^+_{p\tau} \rangle \rightarrow -\langle \hat{a}^+_{p\tau} a_{k'\sigma} \rangle = \delta_{pk'}\, \delta_{\tau\sigma}\, N^F_\tau(p)$$

We do not care of spin-independent constants which only shift the overall energy

$$\delta_{pk'}\,\delta_{k'+p'-k-p} = \delta_{pk'}\,\delta_{p'k}$$

$$H_{int} \leftarrow -\frac{g}{V}\sum_{k\sigma}\hat{a}^{+}_{k\sigma}\hat{a}_{k\sigma}\sum_{p} n^{F}_{\sigma}(p) = -g\sum_{k\sigma}\hat{a}^{+}_{k\sigma}\hat{a}_{k\sigma}\,n_{\sigma} =$$

$$= -g\sum_{k}\left(\hat{a}^{+}_{k\uparrow}\hat{a}_{k\uparrow}\,n_{\uparrow} + \hat{a}^{+}_{k\downarrow}\hat{a}_{k\downarrow}\,n_{\downarrow}\right) \qquad (2)$$

$$(1)+(2) = $$

$$= g\sum_{k}\left(\hat{a}^{+}_{k\uparrow}\hat{a}_{k\uparrow}\,n_{\downarrow} + \hat{a}^{+}_{k\downarrow}\hat{a}_{k\downarrow}\,n_{\uparrow}\right)$$

Thus, $\boxed{\delta E_{\uparrow} = g\,n_{\downarrow},\ \delta E_{\downarrow} = g\,n_{\uparrow}}$ $\boxed{\gamma = 1}$

(1c)

$$\begin{cases} \frac{p_{\uparrow}^2}{2m} + \mu B + g\,n_{\downarrow} = E_F \\ \frac{p_{\downarrow}^2}{2m} - \mu B + g\,n_{\uparrow} = E_F \end{cases}$$

$$n_{\uparrow} = \frac{1}{(2\pi)^3}\,\frac{4}{3}\,\pi p_{\uparrow}^3$$

$$n_{\downarrow} = \frac{1}{(2\pi)^3}\,\frac{4}{3}\,\pi p_{\downarrow}^3$$

Introduce small deviations of all the quantities from those at $B=0$

$$\delta E_{\uparrow} + \mu B + g\,\delta n_{\downarrow} = 0 \qquad \delta E_{\downarrow} - \mu B + g\,\delta n_{\uparrow} = 0$$

$$\delta n_{\uparrow} = \nu_0\,\delta E_{\uparrow} \qquad \delta n_{\downarrow} = \nu_0\,\delta E_{\downarrow}$$

$$\begin{cases} \delta n_{\uparrow} = \nu_0(-\mu B - g\,\delta n_{\downarrow}) \\ \delta n_{\downarrow} = \nu_0(\mu B - g\,\delta n_{\uparrow}) \end{cases}$$

$$\delta n_{\uparrow} = -\nu_0\mu B - (\nu_0 g)\,\nu_0\mu B + (g\nu_0)^2\,\delta n_{\uparrow}$$

$$\delta n_{\uparrow} = -\nu_0\mu B\,\frac{1+\nu_0 g}{1-(\nu_0 g)^2} = -\frac{\nu_0\mu B}{1-\nu_0 g}$$

Similarly, $\delta n_{\downarrow} = \dfrac{\nu_0\mu B}{1-\nu_0 g}$

$$M = -\mu(\delta n_{\uparrow} - \delta n_{\downarrow}) = \frac{2\mu^2\nu_0 B}{1-g\nu_0}$$

$$\boxed{\chi = \frac{2\mu^2\nu_0}{1-g\nu_0}}$$

Qualitative interpretation: because the interaction is contact and because two electrons with the same spin cannot sit at the same point, each electron is sensitive only to the density of electrons with the opposite spin. That is why $\delta E_{\uparrow} \sim g\,n_{\downarrow}$ and $\delta E_{\downarrow} \sim g\,n_{\uparrow}$