Solution to Sheet 1

(1) Mean-field antiferromagnetism in the Hubbard model

$$\hat{H} = \underbrace{\sum_{k\sigma} \epsilon(k)\, c^{\dagger}_{k\sigma} c_{k\sigma}}_{\hat{T}} + \underbrace{U \sum_{j} (\hat{n}_{j\uparrow} - \tfrac{1}{2})(\hat{n}_{j\downarrow} - \tfrac{1}{2})}_{(*)}$$

Mean-field decoupling : $\boxed{\hat{A}\hat{B} \xrightarrow{MF} \hat{A}\langle\hat{B}\rangle + \langle\hat{A}\rangle\hat{B}}$

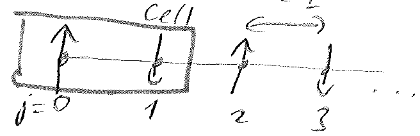
(but can be important for free energy) $\leftarrow$ drop $\leftarrow$ = const. number $\leftarrow$ $-\langle\hat{A}\rangle\langle\hat{B}\rangle + \cancel{\delta\hat{A}\,\delta\hat{B}}$

$\delta\hat{A} \equiv \hat{A} - \langle\hat{A}\rangle$ etc.

(a) $(*) \xrightarrow{MF} U \sum_j \left(\langle \hat{n}_{j\uparrow} - \tfrac{1}{2}\rangle (\hat{n}_{j\downarrow} - \tfrac{1}{2}) + \langle \hat{n}_{j\downarrow} - \tfrac{1}{2}\rangle (\hat{n}_{j\uparrow} - \tfrac{1}{2}\right) + \text{const.}$

(b) using $\langle \hat{n}_{j\uparrow} - \tfrac{1}{2}\rangle = (-1)^j m_0$

$\langle \hat{n}_{j\downarrow} - \tfrac{1}{2}\rangle = -(-1)^j m_0$



$m_0 \equiv \langle \hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}\rangle$ on even sublattice

= staggered magnetization (order parameter of Slater antiferromagnet)

periodicity of $\hat{H}_{MF} = \hat{H}_{\uparrow} + \hat{H}_{\downarrow}$ is $2a$ instead of a

$\Rightarrow$ Brillouin zone goes from $Z_B = [-\frac{\pi}{a}, \frac{\pi}{a})$ to $Z_B' = [-\frac{\pi}{2a}, \frac{\pi}{2a})$

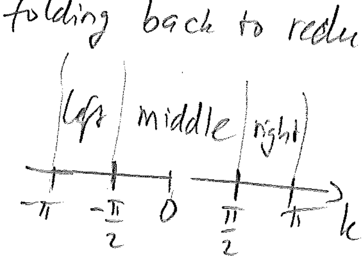
$$H_{\uparrow} = \sum_k \epsilon(k)\, c^{\dagger}_{k\uparrow} c_{k\uparrow} - U m_0 \sum_j (-1)^j (\hat{n}_{j\uparrow} - \tfrac{1}{2})$$

$$H_{\downarrow} = H_{\uparrow}\left[\uparrow \to \downarrow,\ m_0 \to -m_0\right] \quad \text{symmetry-related}$$

(c) In Z_B' introduce new operators by folding back to reduced zone

1D:
$\epsilon(k) = -2t\cos(k)$

$$c_{k\downarrow} = \begin{cases} \alpha_k & k \in \text{middle} \\ \beta_{k-\pi} & k \in \text{right} \\ \beta_{k+\pi} & k \in \text{left} \end{cases}$$



Rewrite $\hat{H}_{\downarrow} = \hat{T}_{\downarrow} + \hat{a}_{MF,\downarrow}$:

$\epsilon(k \pm \pi) = -\epsilon(k)$

$$\hat{T}_{\downarrow} = \sum_{\substack{k \\ k \in Z_B}} \epsilon(k)\, c^{\dagger}_{k\downarrow} c_{k\downarrow} = \sum_{\substack{k \\ k \in Z_B'}}' \epsilon(k) \left(\alpha_k^{\dagger}\alpha_k - \beta_k^{\dagger}\beta_k \right)$$

$$\hat{U}_{MF,\downarrow} = \sum_j U m_0 \underbrace{(-1)^j}_{=e^{i\pi j}} (n_{j\downarrow} - \tfrac{1}{2})$$

drop the "$-\frac{1}{2}$", const and cancels against the one in $\hat{U}_{MF,\uparrow}$

$$\hat{=} U m_0 \sum_{kk'} \underbrace{\frac{1}{L}\sum_j e^{i\pi j} e^{ikj} e^{-ik'j}}_{\delta_{k'=k+\pi}} c^\dagger_{k\downarrow} c_{k'\downarrow}$$

$$= U m_0 \sum_k c^\dagger_{k\downarrow} c_{k+\pi\downarrow}$$

$$= U m_0 \sum_k{}' (\alpha_k^\dagger \beta_k + \beta_k^\dagger \alpha_k)$$

$$\Rightarrow \boxed{H_\downarrow = \sum_k{}' (\alpha_k^\dagger \ \beta_k^\dagger) \underbrace{\begin{pmatrix} \epsilon(k) & U m_0 \\ U m_0 & -\epsilon(k) \end{pmatrix}}_{\equiv \underline{\underline{h}}_k} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}} \qquad \underline{\Psi}_k \equiv \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} \text{ spinor}$$

$\Rightarrow$ diagonalize! Bogoliubov transformation $\underline{\underline{U}}_k = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix}$

such that

$$H_k = \sum_k \underline{\Psi}_k^\dagger \underline{\underline{h}}_k \underline{\Psi}_k \qquad \underline{\underline{U}}_k \underline{\underline{U}}_k^\dagger = \mathbb{1} \text{ (unitary)}$$

$$= \sum_k \underbrace{\underline{\Psi}_k^\dagger \underline{\underline{U}}_k}_{\equiv \underline{\gamma}_k^\dagger} \underbrace{\underline{\underline{U}}_k^\dagger \underline{\underline{h}}_k \underline{\underline{U}}_k}_{\equiv \underline{\underline{h}}_{diag,k}} \underbrace{\underline{\underline{U}}_k^\dagger \underline{\Psi}_k}_{\equiv \underline{\gamma}_k}$$

using Ansatz

$$\alpha_k = u_k \gamma_{k-} + v_k \gamma_{k+}$$
$$\beta_k = -v_k \gamma_{k-} + u_k \gamma_{k+}$$

$\rightarrow$ two conditions for each pair of u_k, v_k ("coherence factors" $\leftrightarrow$ BCS theory) by enforcing diagonality and unitarity

(1) $U m_0 (u_k^2 - v_k^2) + 2\epsilon(k) u_k v_k = 0$

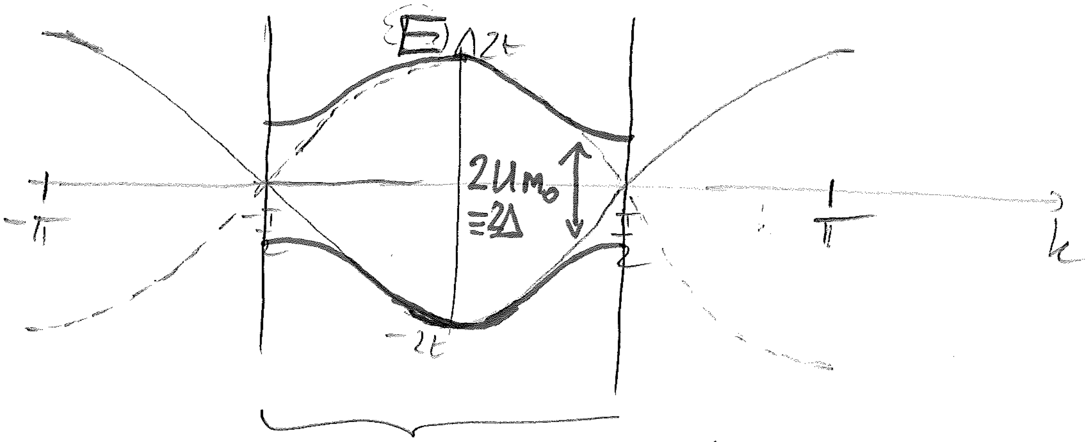
(2) $u_k^2 + v_k^2 = 1$

(2) automatically fulfilled by $u_k = \cos(\theta_k)$, $v_k = \sin(\theta_k)$

$$\Rightarrow \left.\begin{matrix} u_k \\ v_k \end{matrix}\right\} = \left[\frac{1}{2}\left(1 \mp \frac{\epsilon(k)}{\sqrt{\epsilon(k)^2 + U^2 m_0^2}}\right)\right]^{1/2}$$

$$\Rightarrow E_\pm(k) = \pm\left(-\epsilon(k)\,(u_k^2 - v_k^2) + 2U m_0 u_k v_k\right)$$

$$= \pm\sqrt{\epsilon(k)^2 + U^2 m_0^2}$$



Z_B'

$\Rightarrow$ opening of energy gap in ordered state

(c) observables $\rightarrow$ new basis

$$\langle \hat{n}_{0\downarrow} \rangle = \langle c_{0\downarrow}^\dagger c_{0\downarrow} \rangle = \frac{1}{L} \sum_k{}' \left\langle \begin{pmatrix} \alpha_k^\dagger \\ \beta_k^\dagger \end{pmatrix}^T \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} \right\rangle$$

$$= \dots = \frac{1}{L} \sum_k{}' \Big((u_k^2 - v_k^2) \underbrace{\langle \gamma_{k-}^\dagger \gamma_{k-} \rangle}_{\substack{f(-E_k) \\ \text{Fermi fct.}}} + (u_k^2 + v_k^2) \underbrace{\langle \gamma_{k+}^\dagger \gamma_{k+} \rangle}_{f(E_k)} \Big)$$

$$\Rightarrow \underbrace{\langle \hat{n}_{0\downarrow} - \tfrac{1}{2} \rangle}_{= -m_0} = -\frac{1}{L} \sum_k{}' \frac{U m_0}{\sqrt{\epsilon(k)^2 + U^2 m_0^2}} \tanh\left(\frac{\beta E_k}{2}\right)$$

using $\Delta = U m_0$

self-consistency condition

$$\boxed{\Delta = \frac{U}{L} \sum_k{}' \frac{\Delta}{\sqrt{\epsilon(k)^2 + \Delta^2}} \tanh\left(\frac{\beta\sqrt{\epsilon(k)^2 + \Delta^2}}{2}\right)}$$