2) Mean-field AF in Hubbard

$$H = \sum_{k\sigma} \varepsilon(k)\, c^\dagger_{k\sigma} c_{k\sigma} + \overbrace{U \sum_i \left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right)}^{H_U}$$

(a) $\langle n_{j\uparrow} - \frac{1}{2} \rangle = (-1)^j m_0 \;,\; \langle n_{j\downarrow} - \frac{1}{2}\rangle = -(-1)^j m_0$

$$\Rightarrow H_U \Rightarrow H_{U,MF} = U \sum_i \Big[\underbrace{(-1)^i m_0 \left(n_{i\downarrow} - \tfrac{1}{2}\right)}_{\text{only for } \downarrow} - \underbrace{(-1)^i m_0 \left(n_{i\uparrow} - \tfrac{1}{2}\right)}_{\text{only for } \uparrow} \Big]$$

$$H_\uparrow = \sum_k \varepsilon(k)\, c^\dagger_{k\uparrow} c_{k\uparrow} - U m_0 \sum_i (-1)^i \left(n_{i\uparrow} - \tfrac{1}{2}\right)$$

$$H_\downarrow = \sum_k \varepsilon(k)\, c^\dagger_{k\downarrow} c_{k\downarrow} + U m_0 \sum_i (-1)^i \left(n_{i\downarrow} - \tfrac{1}{2}\right)$$

periodicity is $2a$ (instead of a) $\rightarrow$ reduces BZ by $1/2$

(b) Diagonalize $H_\downarrow$:

$$c_{k\downarrow} = \begin{cases} \alpha_k & k \in \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right] \\ \beta_{k-\frac{\pi}{a}} & k \in \left[\frac{\pi}{2a}, \frac{\pi}{a}\right] \\ \beta_{k+\frac{\pi}{a}} & k \in \left[-\frac{\pi}{a}, -\frac{\pi}{2a}\right] \end{cases}$$

Using $\varepsilon(k \pm \frac{\pi}{a}) = -\varepsilon(k)$: (3.126)

$$\sum_k \varepsilon(k)\, c^\dagger_k c_k = \sum_{k \in Z_B'} \varepsilon(k) \left[\alpha^\dagger_k \alpha_k - \beta^\dagger_k \beta_k\right]$$

Potential term (3.127): (see also sheet 6)

$$\sum_k c^\dagger_{k+\frac{\pi}{a}\downarrow} c_{k\downarrow} = \sum_{k \in Z_B'} \left(\alpha^\dagger_k \beta_k + \beta^\dagger_k \alpha_k\right)$$

$\Rightarrow$ Hamiltonian has the form

$$H_\downarrow = \sum_{k \in Z_B'} \begin{pmatrix} \alpha^\dagger_k \\ \beta^\dagger_k \end{pmatrix}^T \begin{pmatrix} -A(k) & V \\ V & A(k) \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}$$

$A(k) = -\varepsilon(k) > 0$ for $k \in Z_B'$

$V = U m_0$

New operators: $\begin{pmatrix} \gamma_{k-} \\ \gamma_{k+} \end{pmatrix} = \overbrace{\begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix}}^{\mathcal{U}_k} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}$

with unitary transformation $\mathcal{U}_k$ chosen such that

$$H = \sum_{k \in Z_B'} \begin{pmatrix} \gamma_{k-}^+ \\ \gamma_{k+}^+ \end{pmatrix}^T \tilde{h}(k) \begin{pmatrix} \gamma_{k-} \\ \gamma_{k+} \end{pmatrix}$$

with $\tilde{h}(k)$ diagonal. Shorthand: $\begin{cases} \gamma_k = \begin{pmatrix} \gamma_{k-} \\ \gamma_{k+} \end{pmatrix} \\ X_k = \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} \end{cases}$

$$\gamma_k = \mathcal{U}_k X_k \Rightarrow X_k = \mathcal{U}_k^+ \gamma_k$$

$$H = \sum_{k \in Z_B'} X_k^+ h(k) X_k = \sum_{k \in Z_B'} \gamma_k^+ \underbrace{\mathcal{U}_k h(k) \mathcal{U}_k^+}_{\equiv \tilde{h}(k)} \gamma_k$$

$\Rightarrow$ defines $\mathcal{U}_k$ as matrix of eigenvectors; condition:

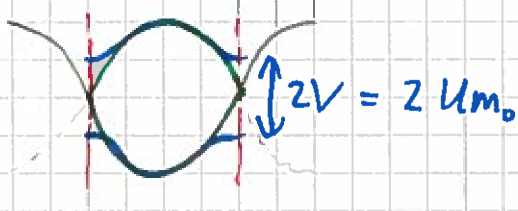
$$V(u_k^2 - v_k^2) - 2A(k) u_k v_k = 0$$

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

parametrization $u_k = \cos\theta_k$, $v_k = \sin\theta_k$

$$\Rightarrow \quad u_k(v_k) = \left[\frac{1}{2}\left(1 \underset{(-)}{+} \frac{A(k)}{\sqrt{A(k)^2 + V^2}}\right)\right]^{1/2}$$

$$\Rightarrow \quad E_\pm(k) = \pm\left[A(k)(u_k^2 - v_k^2) + 2Vu_kv_k\right] = \pm\sqrt{A(k)^2 + V^2}$$



(c) Calculation of observables → translate to new basis

$$\langle n_{0\downarrow} \rangle = \langle c_{0\downarrow}^+ c_{0\downarrow} \rangle = \ldots$$

$$c_{0\downarrow}^+ = \sum_k c_{k\downarrow}^+ = \sum_{k \in Z_B'} (\alpha_k^+ + \beta_k^+)$$

$$\ldots = \frac{1}{\Omega} \sum_{kk'}' \langle (\alpha_k^+ + \beta_k^+)(\alpha_{k'} + \beta_{k'}) \rangle$$

H does not mix k and k' $\Rightarrow$ $k \overset{!}{=} k'$

$$\langle n_{0\downarrow} \rangle = \frac{1}{\Omega} \sum_k{}' \left\langle \begin{pmatrix} \alpha_k^+ \\ \beta_k \end{pmatrix}^T \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} \right\rangle = \ldots$$

Transform to γ-basis:

$$\ldots = \frac{1}{\Omega} \sum_k{}' \left\langle \begin{pmatrix} \gamma_{k-}^+ \\ \gamma_{k+}^+ \end{pmatrix}^T \mathcal{U}_k \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \mathcal{U}_k^+ \begin{pmatrix} \gamma_{k-} \\ \gamma_{k+} \end{pmatrix} \right\rangle = \ldots$$

$$\mathcal{U}_k \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \mathcal{U}_k^+ = \begin{pmatrix} (u_k - v_k)^2 & u_k^2 - v_k^2 \\ u_k^2 - v_k^2 & (u_k + v_k)^2 \end{pmatrix}$$

Need only contributions diagonal in γ's:

$$\langle \gamma_{k-}^+ \gamma_{k-} \rangle = f(-E_k)$$

$$\langle \gamma_{k+}^+ \gamma_{k+} \rangle = f(E_k) \qquad E_k \equiv \sqrt{A(k)^2 + V^2}$$

$$\Rightarrow \langle n_{0\downarrow} \rangle = \frac{1}{\Omega} \sum_k{}' \left((u_k - v_k)^2 f(-E_k) + (u_k + v_k)^2 f(E_k) \right)$$

$$= \frac{1}{\Omega} \sum_k{}' \left(1 - \frac{V}{\sqrt{A(k)^2 + V^2}} \tanh\left(\frac{\beta E_k}{2}\right) \right)$$

$$\Rightarrow \boxed{\underbrace{\left\langle n_{0\downarrow} - \frac{1}{2} \right\rangle}_{= -m_0} = -\frac{1}{\Omega} \sum_{k \in Z_B} \frac{U m_0}{\sqrt{\varepsilon(k)^2 + (U m_0)^2}} \tanh\left(\frac{\beta E_k}{2}\right)}$$

$\Delta \equiv U m_0$ self-consistency condition

$$\boxed{\Delta = \frac{U}{\Omega} \sum_{k \in Z_B} \frac{\Delta}{\sqrt{\varepsilon_k^2 + \Delta^2}} \tanh\left(\frac{\beta \sqrt{\varepsilon(k)^2 + \Delta^2}}{2}\right)}$$

(d) Equation for T_c: $\Delta(T_c) = 0$

$$\Rightarrow \frac{1}{U} = \frac{1}{\Omega} \sum_k{}' \frac{1}{\sqrt{\varepsilon(k)^2}} \tanh\left(\frac{\beta_c \sqrt{\varepsilon(k)^2}}{2}\right)$$

$$= \frac{1}{\Omega} \sum_k{}' \frac{\tanh\left(\frac{\beta_c \varepsilon_k}{2}\right)}{\varepsilon_k}$$

$$= \int d\varepsilon \, n(\varepsilon) \frac{\tanh\left(\frac{\beta_c \varepsilon}{2}\right)}{\varepsilon} \cong n(0) \int_{-\Lambda}^{\Lambda} d\varepsilon \frac{\tanh\left(\frac{\beta_c \varepsilon}{2}\right)}{\varepsilon}$$

Split integral: $\beta_c \varepsilon \gg 1$, $\beta_c \varepsilon \ll 1$

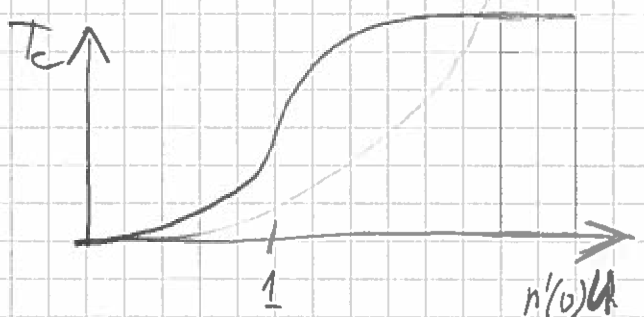
$\tanh\left(\frac{\beta_c\varepsilon}{2}\right) \approx 1$ $\quad$ $\tanh\left(\frac{\beta_c\varepsilon}{2}\right) \approx \frac{\beta\varepsilon}{2}$

$$\Rightarrow 2n(0)\int_{-\Omega}^{\Lambda} d\varepsilon \, \frac{\tanh\left(\frac{\beta\varepsilon}{2}\right)}{\varepsilon} \approx 2n(0)\left[\int_0^{2C/\beta_c} d\varepsilon \, \frac{\beta}{2} + \int_{2C/\beta_c}^{\Lambda} d\varepsilon \, \frac{1}{\varepsilon}\right] \quad C = \mathcal{O}(1)$$

$$= n(0)\left[C + \log\left(\frac{\Lambda\beta_c}{2C}\right)\right]$$

$$\frac{1}{U} \approx n'(0)\log\left(\frac{\Lambda\beta}{2C'}\right) \qquad C' = \mathcal{O}(1)$$

$$\Rightarrow \quad T_c = \frac{1}{\beta_c} \approx \frac{\Lambda}{2C'} e^{-\frac{1}{n(0)U}}$$



(e) $\underline{\underline{T=0}}$; Δ in different limits

(i) $$\frac{1}{U} = n(0)\int_0^{\Lambda'} d\varepsilon \, \frac{1}{\sqrt{\varepsilon^2+\Delta^2}}$$

$$\approx n(0)\left(\int_0^{C\Delta} d\varepsilon \, \frac{1}{\Delta} + \int_{C\Delta}^{\Lambda'} d\varepsilon \, \frac{1}{\varepsilon}\right)$$

$$= C + \log\frac{\Lambda'}{C\Delta} = \log\frac{\Lambda'}{\Delta}$$

small Δ: $\Delta(T=0) \approx \Lambda'' e^{-1/n(0)U}$

(BCS: $2\Delta(T=0) = 3.52\, T_c$)

(ii) $U \gg t$

$$\frac{1}{U} = \frac{1}{\Omega} \sum_{k \in Z_B'} \frac{1}{\Delta} = \frac{1}{2\Delta}$$

$$\Rightarrow \quad \Delta = \frac{U}{2} \quad \Rightarrow \quad m_0 = \frac{\Delta}{U} = \frac{1}{2}$$

$\Rightarrow$ localized spins $1/2$