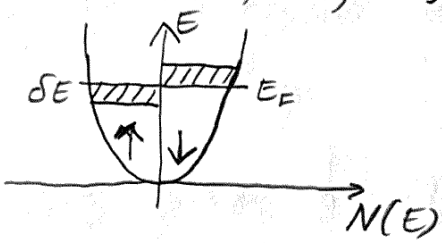
1.9 Magnetism in the Hubbard model

The Hubbard model has ferro- and antiferromagnetic states depending on the lattice structure and band filling.

Rule of thumb: Antiferromagnetism preferred for half-filled band with AB-sublattices (no "frustration").
Ferromagnetism preferred away from half-filling and for large U and high density of states.

Ferromagnetism: Simplest criterion is Stoner criterion (okay but not the whole story for ferromagnetic metals like Fe, Ni, Co). Criterion is $UN(E_F) > 1$



favors unequal ↑ and ↓ populations

Extended discussion: Sigrist lecture notes

Antiferromagnetism (AF): (at half-filling $n=1$) Two limits: (a) strong coupling $\frac{U}{t} \gg 1$
(b) weak coupling $\frac{U}{t} < 1$

(a) Strong coupling: We have found $J = \frac{4t^2}{U} > 0$
⇒ antiferromagnetic exchange interaction in the two-site Hubbard model.

For $\frac{U}{t} \gg 1$ one can derive the AF Heisenberg model from the Hubbard model using a Schrieffer-Wolff transformation: $H_{Heis} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$

The Heisenberg model has an antiferromagnetic ground state in $D \geq 2$ with Néel temperature $T_N \sim J$.

"Mott-Heisenberg antiferromagnet"

(b) Weak coupling: See exercise sheet. We discuss the mean-field solution for the "Slater antiferromagnet".

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

Mean-field ansatz: $\hat{A}\hat{B} = \hat{A}\langle\hat{B}\rangle + \langle\hat{A}\rangle\hat{B} - \langle\hat{A}\rangle\langle\hat{B}\rangle + \delta\hat{A}\,\delta\hat{B}$

$$\delta\hat{X} \equiv \hat{X} - \langle\hat{X}\rangle$$

Mean-field approximation (MFA): $\hat{A}\hat{B} \approx \hat{A}\langle\hat{B}\rangle + \hat{B}\langle\hat{A}\rangle$

$\Rightarrow$ neglect terms $\delta\hat{A}\,\delta\hat{B}$ (fluctuations) and $\langle\hat{A}\rangle\langle\hat{B}\rangle$ (just a number).

(a) Apply MFA to U term:

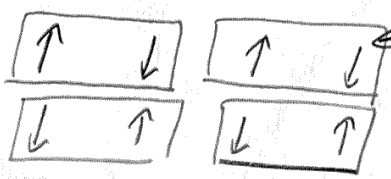
$$(*) \longrightarrow \approx U \sum_j \left(\langle \hat{n}_{j\uparrow} - \tfrac{1}{2} \rangle \left(\hat{n}_{j\downarrow} - \tfrac{1}{2}\right) + \langle \hat{n}_{j\downarrow} - \tfrac{1}{2} \rangle \left(\hat{n}_{j\uparrow} - \tfrac{1}{2}\right) \right) + \text{const.}$$

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

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

with the staggered magnetization $m_0 \equiv \langle \hat{n}_{j\uparrow} - \hat{n}_{j\downarrow} \rangle (-1)^j$.

This doubles the periodicity of the lattice, e.g. on the 2D square lattice one has



Important: The sign of m_0 is not fixed, the symmetry is broken spontaneously! Also we get have to find m_0.

For simplicity we now discuss a 1D chain even though MFA is not really valid in 1D. But key features of the solution can be seen already for the 1D case.

The reduced Brillouin zone $\mathcal{Z}_B'$ for a lattice with $2a$-periodicity is $\mathcal{Z}_B' = \left[-\frac{\pi}{2a}, \frac{\pi}{2a}\right]$. We have

$$H_\uparrow = \sum_k \epsilon(k)\, c_{k\uparrow}^+ c_{k\uparrow} - U m_0 \sum_i (-1)^i \left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)$$

$$H_\downarrow = \sum_k \epsilon(k)\, c_{k\downarrow}^+ c_{k\downarrow} + U m_0 \sum_i (-1)^i \left(\hat{n}_{i\downarrow} - \frac{1}{2}\right)$$

with $H = H_\uparrow + H_\downarrow$. Note that $H_\downarrow = H_\uparrow\left[\uparrow \to \downarrow, m_0 \to -m_0\right]$

$\Rightarrow$ It is sufficient to find m_0 using $H_\downarrow$ (or $H_\uparrow$).

- Introduce new operators α_k, β_k via

$$c_{k\downarrow} = \begin{cases} \alpha_k & k \in \mathcal{Z}_B' \\ \beta_{k-\frac{\pi}{a}} & k \in \left[\frac{\pi}{2a}, \frac{\pi}{a}\right] \\ \beta_{k+\frac{\pi}{a}} & k \in \left[-\frac{\pi}{a}, -\frac{\pi}{2a}\right] \end{cases} \Bigg\} \text{backfolding into } \mathcal{Z}_B'$$

- Diagonalize $H_\downarrow$ by applying a Bogoliubov transformation

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

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

$\Rightarrow$ First write $H_\downarrow$ using α's and β's:

$$\sum_{k \in \mathcal{Z}_B} \epsilon(k)\, n_{k\downarrow} = \sum_{k \in \mathcal{Z}_B'} \epsilon(k)\, \alpha_k^+ \alpha_k + \sum_{k \in \left[\frac{\pi}{2a}, \frac{3\pi}{2a}\right]} \epsilon(k)\, \beta_{k+\frac{\pi}{a}}^+ \beta_{k-\frac{\pi}{a}}$$

$\mathcal{Z}_B$: full BZ

$$= \sum_{k \in \mathcal{Z}_B'} \epsilon(k) \left[\alpha_k^+ \alpha_k - \beta_k^+ \beta_k\right] \qquad \epsilon(k \pm \tfrac{\pi}{a}) = -\epsilon(k)$$

U term:

$$U m_0 \sum_i (-1)^i \left(\hat{n}_{i\downarrow} - \frac{1}{2}\right) = ?$$

First transform to momentum space:

$$c^+_{k\downarrow} = \frac{1}{\sqrt{L}} \sum_i e^{ikr_i} c^+_{i\downarrow}$$

$$c_{k\downarrow} = \frac{1}{\sqrt{L}} \sum_i e^{-ikr_i} c_{i\downarrow}$$

$$c^+_{i\downarrow} = \frac{1}{\sqrt{L}} \sum_k e^{-ikr_i} c^+_{k\downarrow}$$

$$c_{i\downarrow} = \frac{1}{\sqrt{L}} \sum_k e^{ikr_i} c_{k\downarrow}$$

$$\Rightarrow \sum_i (-1)^i \hat{n}_{i\downarrow} = \frac{1}{L} \sum_i \sum_{kk'} (-1)^i e^{-i(k-k')r_i} c^+_{k\downarrow} c_{k'\downarrow} = \ldots$$

$$\frac{1}{L} \sum_i e^{-i(k-k')r_i} \underbrace{(-1)^i}_{= e^{i\frac{\pi}{a} r_i}} = \delta\left(k - k' - \frac{\pi}{a}\right) \Rightarrow k' = k - \frac{\pi}{a}$$

$$\ldots = \sum_k c^+_{k\downarrow} c_{k-\frac{\pi}{a}\downarrow}$$

$\rightarrow$ gives terms $U m_0 \sum_{k \in Z'_B} \left(\alpha^+_k \beta_k + \beta^+_k \alpha_k\right)$

In total: $H_\downarrow = \sum_k{}' \left(\alpha^+_k, \beta^+_k\right) \underbrace{\begin{bmatrix} \epsilon(k) & U m_0 \\ U m_0 & -\epsilon(k) \end{bmatrix}}_{\equiv \underline{\underline{h}}_k} \underbrace{\begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}}_{\equiv \underline{\Psi}_k \text{ spinor}}$.

$\sum_k{}' = \sum_{k \in Z'_B}$

$\Rightarrow$ diagonalize 2x2 via unitary (Bogoljubov transformation).

$$H_\downarrow = \sum_k \underline{\Psi}^+_k \underline{\underline{h}}_k \underline{\Psi}_k = \sum_k \underbrace{\underline{\Psi}^+_k \underline{\underline{U}}_k}_{\underline{\gamma}^+_k} \underbrace{\underline{\underline{U}}^+_k \underline{\underline{h}}_k \underline{\underline{U}}_k}_{\underline{\underline{h}}_k \text{ diag}} \underbrace{\underline{\underline{U}}^+_k \underline{\Psi}_k}_{\underline{\gamma}}$$

Ansatz for unitary: $\alpha_k = u_k \gamma_{k-} + v_k \gamma_{k+}$

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

$\Rightarrow$ two conditions for each pair u_k, v_k by enforcing diagonality and unitarity:

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

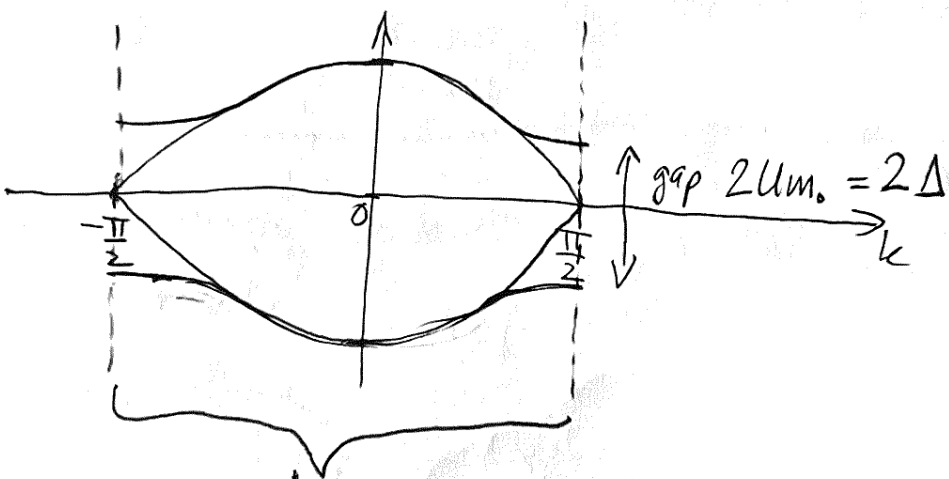
(2) $u_k^2 + v_k^2 = 1$

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

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

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

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



2_B^{11} reduced (antiferromagnetic) Brillouin zone

$\Rightarrow$ opening of energy gap in the magnetically ordered state.

But: We get have to determine the actual value of m_0.

- After diagonalization, observables can be computed in the new basis:

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

↑ local $\downarrow$-occupation on site 0

$$= \frac{1}{L} \sum_k{}' \left((u_k^2 - v_k^2) \underbrace{\langle \gamma_{k-}^\dagger \gamma_{k-} \rangle}_{f(-E_k)} + (u_k^2 + v_k^2) \underbrace{\langle \gamma_{k+}^\dagger \gamma_{k+} \rangle}_{f(+E_k)} \right)$$

Fermi fct.

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

use $\Delta \equiv U m_0$ to rewrite this as the gap equation

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

- One of the most important types of equation in condensed matter physics — also appears in the celebrated Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity — BCS 1957, Nobel prize 1972
- $(*)$ has to be solved self-consistently to obtain Δ — Δ appears on both sides and $(*)$ is not a linear equation. ⇒ approximate solution by linearizing for small Δ (near critical onset temperature T_c) or by iterative numerical integration.

• equation for T_c: set $\Delta = 0 \Rightarrow E_k = |\epsilon(k)|$ (with $\beta_c \equiv \frac{1}{k_B T_c}$)

$$\frac{1}{U} = \frac{1}{L} \sum_k{}' \frac{1}{|\epsilon(k)|} \tanh\left(\frac{\beta_c |\epsilon(k)|}{2}\right) = \dots$$

use density of states (DOS) $n(\epsilon) \equiv \frac{1}{L} \sum_k{}' \delta(\epsilon - \epsilon(k))$

$$\dots = \int_{-\infty}^{\infty} d\epsilon\, n(\epsilon) \frac{\tanh\left(\frac{\beta_c|\epsilon|}{2}\right)}{|\epsilon|} = 2 \int_0^{\infty} d\epsilon\, n(\epsilon) \frac{\tanh\left(\frac{\beta_c|\epsilon|}{2}\right)}{|\epsilon|} \approx \dots$$

↑ particle-hole symmetric DOS

approximate with constant DOS up to energy cutoff Λ:

$\Lambda \approx$ upper band edge

$$\dots \approx 2 n(0) \int_0^{\Lambda} d\epsilon \frac{\tanh\left(\frac{\beta_c|\epsilon|}{2}\right)}{|\epsilon|} \approx \dots$$

$n(0)$: DOS at E_F

Split integral into $\beta_c \epsilon \gg 1$ and $\beta_c \epsilon \ll 1$

$\beta_c \epsilon \gg 1$: $\tanh\left(\frac{\beta_c \epsilon}{2}\right) \approx 1$

$\beta_c \epsilon \ll 1$: $\tanh\left(\frac{\beta_c \epsilon}{2}\right) \approx \frac{\beta_c \epsilon}{2}$

$$\dots \approx 2 n(0) \left[\int_0^{2C/\beta_c} d\epsilon \frac{\beta_c}{2} + \int_{2C/\beta_c}^{\Lambda} d\epsilon \frac{1}{\epsilon} \right]$$

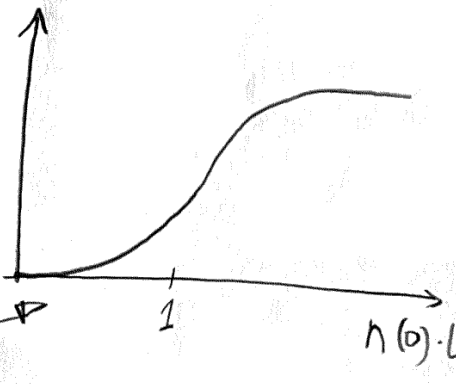
$C = O(1)$ constant

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

$$\Rightarrow \frac{1}{U} \approx n(0) \log\left(\frac{\Lambda \beta_c}{2C'}\right)$$

$C' = O(1)$ constant

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



valid if T_c not too large

* gap at $T=0$: compute Δ in different limits

(i) constant DOS

(ii) large $U/t \Rightarrow \Delta \gg t$

(i) $$\frac{1}{U} \approx n(0) \int_0^{\Lambda'} d\epsilon \frac{1}{\sqrt{\epsilon^2+\Delta^2}} \approx n(0)\left[\int_0^{C\Delta} d\epsilon \frac{1}{\Delta} + \int_{C\Delta}^{\Lambda'} d\epsilon \frac{1}{\epsilon}\right]$$

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

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

Compare with $$T_c \sim e^{-\frac{1}{n(0)U}}$$

$\Rightarrow$ T_c and $\Delta(T=0)$ are proportional to each other.

Important: the result that $T_c \sim e^{-1/x}$ with x the effective dimensionless coupling requires a selfconsistent mean-field approach — it cannot be obtained perturbatively! How to see this?

Try to Taylor expand $e^{-1/x}$ around $x=0$.

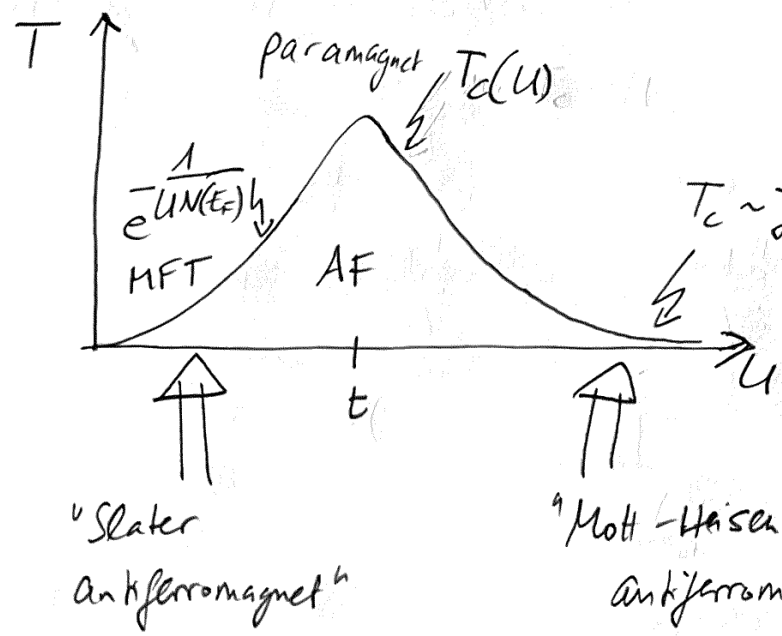
(ii) $U \gg t$: $$\frac{1}{U} = \frac{1}{L}\sum_k{}' \frac{1}{\Delta} = \frac{1}{2\Delta}$$

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

$\Rightarrow$ fully localized spins $\frac{1}{2}$

(but MFT actually breaks down for $U \gg t$)

Overall picture for antiferromagnetic orders in the HH on AB lattice at half-filling:



$T_c \sim J = \frac{4t^2}{U}$ ← cf. chapter 1.7, mapping to Heisenberg model

Difference:

- Slater: metallic bands that gap out due to AF ordering (→ nesting-driven band insulator)
  => metal above T_c, insulator below T_c
- Mott-Heisenberg: Mott insulator due to correlations ($U \gg t$), magnetic ordering is parasitic effect on top of localized-spin physics.
  => insulator even above T_c.