Field theory for nonequilibrium systems, WS 2016/17

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Sheet 4
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1 Self-consistent mean-field theory for Slater antiferromagnetism

Consider the Hubbard model

$$H = \sum_{k,\sigma} \epsilon(k) c^\dagger_{k,\sigma} c_{k,\sigma} + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2). \tag{1}$$

(a) Perform a mean field decoupling $H \to H_{\mathrm{MF}}$ around the site-dependent mean field

$$\langle n_{j\uparrow} - 1/2 \rangle = (-1)^j m_0, \tag{2}$$

$$\langle n_{j\downarrow} - 1/2 \rangle = -(-1)^j m_0. \tag{3}$$

What is the motivation for choosing this site dependence? What is the periodicity of H_{MF}?

(b) The mean-field Hamiltonian can be written as $H_{\mathrm{MF}} = H_\uparrow + H_\downarrow$ with

$$H_\uparrow = \sum_k \epsilon(k) c^\dagger_{k,\uparrow} c_{k,\uparrow} - U m_0 \sum_i (-1)^i (n_{i\uparrow} - 1/2), \tag{4}$$

$$H_\downarrow = \sum_k \epsilon(k) c^\dagger_{k,\downarrow} c_{k,\downarrow} + U m_0 \sum_i (-1)^i (n_{i\downarrow} - 1/2). \tag{5}$$

Now assume a 1D system with dispersion $\epsilon(k) = -2t\cos(ka)$. Introduce new operators α_k, β_k in $H_\downarrow$ in the reduced Brillouin zone Z'_B,

$$c_{k\downarrow} = \begin{cases} \alpha_k, & k \in [-\pi/2a, \pi/2a] \\ \beta_{k-\pi/a}, & k \in [\pi/2a, \pi/a] \\ \beta_{k+\pi/a}, & k \in [-\pi/a, -\pi/2a]. \end{cases} \tag{6}$$

Diagonalize $H_\downarrow$ by applying a Bogoliubov transformation

$$\alpha_k = u_k \gamma_{k-} + v_k \gamma_{k+}, \beta_k = -v_k \gamma_{k-} + u_k \gamma_{k+}. \tag{7}$$

Why is it sufficient to do this for $H_\downarrow$?

(c) Use the diagonalized form of $H_\downarrow$ to solve at finite T for $\langle n_{0\downarrow} - 1/2 \rangle(m_0)$, the average up-spin density on site 0 as a function of m_0. Derive the self-consistency equation for the order parameter $\Delta = U m_0$,

$$\Delta = \frac{U}{\Omega} \sum_{k \in Z'_B} \frac{\Delta}{E_k} \tanh(\beta E_k/2), \quad E_k = \sqrt{\epsilon(k)^2 + \Delta^2}. \tag{8}$$

(d) Write down the equation which determines T_c and take the continuum limit. Solve the equation for a constant density of states and plot T_c versus U ($U > 0$). *Hint*: You can split the integral over energy ϵ into two parts, (i) $\beta\epsilon \ll 1$, and (ii) $\beta\epsilon \gg 1$, to simplify the tanh in the integrand.

(e) At $T = 0$, compute Δ in different limits:
(i) take constant density of states and split the integral over energy. How is the resulting $\Delta(T = 0)$ related to T_c from part (d)?
(ii) take the limit of large $U/t \gg 1$, which implies $\Delta \gg t$.
Plot the resulting m_0.

2) Mean-field AF in Hubbard

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

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

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

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

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)

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

Potential term (3.127):

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

(see also Sheet 6)

$\Rightarrow$ Hamiltonian has the form

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

$$A(k) \equiv -\varepsilon(k) > 0 \text{ for } k \in Z_B'$$
$$V = U m_0$$

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:

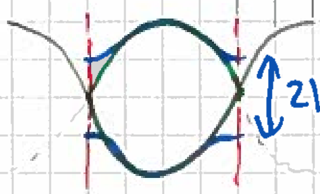
$$V(u_k^2 - v_k^2) - 2A(k) u_k v_k = 0$$

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

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

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

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



(c) Calculation of observables → translate to new basis

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

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

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

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.

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

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

$$\Rightarrow \boxed{\underbrace{\left\langle n_{0\downarrow} - \frac{1}{2}\right\rangle}_{=-m_0} = -\frac{1}{\Omega}\sum_{k\in Z_B}\frac{Um_0}{\sqrt{\varepsilon(k)^2+(Um_0)^2}}\tanh\left(\frac{\beta E_k}{2}\right)}$$

$\Delta \equiv Um_0$ 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: $\beta_c \varepsilon \gg 1$, $\beta_c \varepsilon \ll 1$

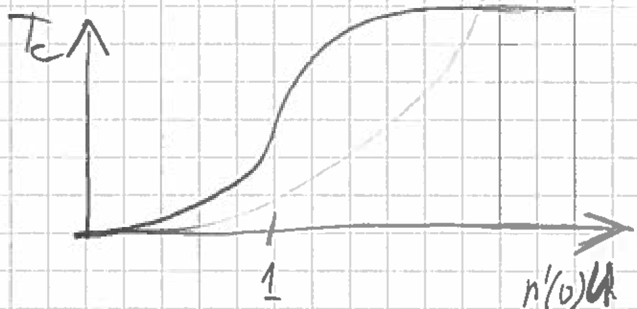
$\tanh\left(\frac{\beta_c \varepsilon}{2}\right) \approx 1$ $\quad$ $\tanh\left(\frac{\beta_c \varepsilon}{2}\right) \approx \frac{\beta_c \varepsilon}{2}$

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

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

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

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



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

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

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

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

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 $1/2$