IMPRS Focus Course Hubbard Model, November 2018

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1 Mean-field antiferromagnetism in the Hubbard model

Consider the Hubbard model on a bipartite lattice with L sites and periodic boundary conditions,

$$H = \sum_{k,\sigma} \epsilon(k) c_{k,\sigma}^{\dagger} c_{k,\sigma} + U \sum_{i} (n_{i\uparrow} - \frac{1}{2}) (n_{i\downarrow} - \frac{1}{2}).$$
(1)

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

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

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

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

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

$$H_{\uparrow} = \sum_{k} \epsilon(k) c_{k,\uparrow}^{\dagger} c_{k,\uparrow} - U m_0 \sum_{i} (-1)^i (n_{i\uparrow} - \frac{1}{2}), \qquad (4)$$

$$H_{\downarrow} = \sum_{k} \epsilon(k) c_{k,\downarrow}^{\dagger} c_{k,\downarrow} + U m_0 \sum_{i} (-1)^i (n_{i\downarrow} - \frac{1}{2}).$$

$$\tag{5}$$

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 ,

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

Diagonalize H_{\downarrow} by applying a Bogoliubov transformation

$$\alpha_k = u_k \gamma_{k-} + v_k \gamma_{k+}, \beta_k = -v_k \gamma_{k-} + u_k \gamma_{k+}.$$
⁽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 $\langle n_{0\downarrow} - \frac{1}{2} \rangle (m_0)$, the average down-spin density on site 0 as a function of m_0 . Derive the self-consistency equation for the order parameter $\Delta = Um_0$,

$$\Delta = \frac{U}{L} \sum_{k \in Z'_B} \frac{\Delta}{E_k} \tanh(\beta E_k/2), \quad E_k = \sqrt{\epsilon(k)^2 + \Delta^2}.$$
(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 Δ(T = 0) related to T_c from part (d)?
 (ii) take the limit of large U/t ≫ 1, which implies Δ ≫ t. Plot the resulting m₀.