Mathematics 26: The Mean-field Hubbard Model

In this section we will formalise the mean-field theory of magnetism for the Hubbard model. The problem is straightforward, although the single-particle hopping terms are solvable (see 'Phys7'), the two-particle Coulomb interactions are *not* solvable: The effect on one particle depends on whether or not the other particle involved is present. The very complicated motion found in the true solution is too difficult to analyse at this level, and here we will investigate the mean-field or *Hartree-Fock* approximation: The probability of finding the second particle involved in the two-particle interactions is replaced by its average.

For the current Hubbard model repulsion, this approximation amounts to:

$$\begin{aligned} c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}c_{i\uparrow} \mapsto & c^\dagger_{i\uparrow}c_{i\uparrow} < c^\dagger_{i\downarrow}c_{i\downarrow} > + < c^\dagger_{i\uparrow}c_{i\uparrow} > c^\dagger_{i\downarrow}c_{i\downarrow} - < c^\dagger_{i\uparrow}c_{i\uparrow} >< c^\dagger_{i\downarrow}c_{i\downarrow} > \\ & - c^\dagger_{i\uparrow}c_{i\downarrow} < c^\dagger_{i\downarrow}c_{i\uparrow} > - < c^\dagger_{i\uparrow}c_{i\downarrow} > c^\dagger_{i\downarrow}c_{i\uparrow} + < c^\dagger_{i\uparrow}c_{i\downarrow} >< c^\dagger_{i\downarrow}c_{i\uparrow} > \end{aligned}$$

where $< ... >$ denotes an average and the final constant terms are included to ensure that the replacement has the same average. Employing the number and magnetisation representation provides:

$$c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}c_{i\uparrow} \mapsto 2 < \hat{n}_i > \hat{n}_i - 2 < \hat{\mathbf{m}}_i > .\hat{\mathbf{m}}_i - < \hat{n}_i >< \hat{n}_i > + < \hat{\mathbf{m}}_i > . < \hat{\mathbf{m}}_i >$$

which then provides us with an effective single-particle Hamiltonian to approximate the original problem:

$$H_{eff} = -tZ \sum_{\mathbf{k}\sigma} \gamma_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{i\sigma} n_i c^\dagger_{i\sigma} c_{i\sigma} - U \sum_i n_i^2 + U \sum_i \mathbf{m}_i . \mathbf{m}_i$$

$$-U \sum_i \left[m_i^x (c^\dagger_{i\uparrow}c_{i\downarrow} + c^\dagger_{i\downarrow}c_{i\uparrow}) - i m_i^y (c^\dagger_{i\uparrow}c_{i\downarrow} - c^\dagger_{i\downarrow}c_{i\uparrow}) + m_i^z (c^\dagger_{i\uparrow}c_{i\uparrow} - c^\dagger_{i\downarrow}c_{i\downarrow}) \right] \qquad (1)$$

We will consider *spiral magnetism* here:

$$n_i = n \qquad \mathbf{m}_i = m(\cos \mathbf{Q}.\mathbf{R}_i, \sin \mathbf{Q}.\mathbf{R}_i, 0)$$

which involves a uniform rotation of spins with a pitch controlled by the vector $\mathbf{Q}$. This 'ansatz' yields:

$$U \sum_{i\sigma} n_i c^\dagger_{i\sigma} c_{i\sigma} \mapsto \frac{U}{N} \sum_{i\sigma} \sum_{\mathbf{k}\mathbf{k}'} n e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma} = Un \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

and:

$$-U \sum_i \left[m_i^x (c^\dagger_{i\uparrow}c_{i\downarrow} + c^\dagger_{i\downarrow}c_{i\uparrow}) - i m_i^y (c^\dagger_{i\uparrow}c_{i\downarrow} - c^\dagger_{i\downarrow}c_{i\uparrow}) \right] \mapsto$$

$$-\frac{U}{N} \sum_i \sum_{\mathbf{k}\mathbf{k}'} m \left[e^{i(\mathbf{k}-\mathbf{k}'-\mathbf{Q}).\mathbf{R}_i} c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} + e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{Q}).\mathbf{R}_i} c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}'\uparrow} \right] = -Um \sum_{\mathbf{k}} \left(c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} c_{\mathbf{k}\downarrow} + c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}+\mathbf{Q}\uparrow} \right)$$

and so:

$$H_{eff} \mapsto \sum_{\mathbf{k}} \left[c^{\dagger}_{\mathbf{k}+\mathbf{Q}\uparrow} \quad c^{\dagger}_{\mathbf{k}\downarrow} \right] \begin{bmatrix} Un - tZ\gamma_{\mathbf{k}+\mathbf{Q}} & -Um \\ -Um & Un - tZ\gamma_{\mathbf{k}} \end{bmatrix} \left[c_{\mathbf{k}+\mathbf{Q}\uparrow} \quad c_{\mathbf{k}\downarrow} \right] - UN[n^2 - m^2]$$

which must be solved.

There are *two* methods of solution:

(1) Statistical Physics

The 2×2 matrix may be diagonalised to provide two energies:

$$\epsilon_{\mathbf{k}\pm} = Un - \frac{tZ}{2}\left(\gamma_{\mathbf{k}+\mathbf{Q}} + \gamma_{\mathbf{k}}\right) \pm \left[\left(\frac{tZ}{2}\right)^2 \left(\gamma_{\mathbf{k}+\mathbf{Q}} - \gamma_{\mathbf{k}}\right)^2 + (Um)^2 \right]^{1/2}$$

in terms of which the total-energy is:

$$E = \sum_{\mathbf{k}\tau} \epsilon_{\mathbf{k}\tau} f(\epsilon_{\mathbf{k}\tau}) - UN(n^2 - m^2)$$

the free-energy is, $F = E - TS$, and the 'grand potential' is: $G = F - \mu N = E - TS - \mu N$:

$$G = \sum_{\mathbf{k}\tau} (\epsilon_{\mathbf{k}\tau} - \mu) f(\epsilon_{\mathbf{k}\tau}) - UN(n^2 - m^2) + k_B T \sum_{\mathbf{k}\tau} \left(f(\epsilon_{\mathbf{k}\tau}) \log f(\epsilon_{\mathbf{k}\tau}) + [1 - f(\epsilon_{\mathbf{k}\tau})] \log[1 - f(\epsilon_{\mathbf{k}\tau})] \right)$$

in terms of the Fermi-occupation number:

$$f(\epsilon) = \frac{1}{1 + \exp\left[\frac{\epsilon - \mu}{k_B T}\right]}$$

The statistical physics involves minimising the grand potential over the parameters, n and m:

$$0 = \frac{\partial G}{\partial n} = \sum_{\mathbf{k}\tau} U f(\epsilon_{\mathbf{k}\tau}) - 2UNn + \sum_{\mathbf{k}\tau} \frac{\partial f}{\partial n} \left(\epsilon_{\mathbf{k}\tau} - \mu + k_B T \log \frac{f(\epsilon_{\mathbf{k}\tau})}{[1 - f(\epsilon_{\mathbf{k}\tau})]} \right)$$

and so:

$$n = \frac{1}{2N} \sum_{\mathbf{k}\tau} f(\epsilon_{\mathbf{k}\tau}) \tag{2}$$

while:

$$0 = \frac{\partial G}{\partial m} = \sum_{\mathbf{k}\tau} \tau \frac{2U^2 m}{\epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}-}} f(\epsilon_{\mathbf{k}\tau}) + 2UNm + \sum_{\mathbf{k}\tau} \frac{\partial f}{\partial m} \left(\epsilon_{\mathbf{k}\tau} - \mu + k_B T \log \frac{f(\epsilon_{\mathbf{k}\tau})}{[1 - f(\epsilon_{\mathbf{k}\tau})]} \right)$$

and so:

$$m = Um \frac{1}{N} \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}-}) - f(\epsilon_{\mathbf{k}+})}{\epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}-}} \tag{3}$$

Equations (2) and (3) are 'self-consistent' equations for n and m in principle, although in practice n is decided and μ must be found.

(2) Hartree-Fock

The second method involves solving the effective Hamiltonian (1), calculating the average values of the parameters involved in the two-particle interactions, and then finding solutions for which these parameters are equal to the values obtained in the effective single-particle theory.

In the theory we have:

$$< c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} > = \delta_{\mathbf{k},\mathbf{k}'+\mathbf{Q}} < c^\dagger_{\mathbf{k}'+\mathbf{Q}\uparrow} c_{\mathbf{k}'\downarrow} >$$

which is real, and so:

$$\begin{aligned}
< \hat{m}^x_i > &= \frac{1}{2}\left[< c^\dagger_{i\uparrow} c_{i\downarrow} > + < c^\dagger_{i\downarrow} c_{i\uparrow} > \right] \\
&= \frac{1}{2}\left[\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} < c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} > + \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} < c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}'\uparrow} > \right] \\
&= \frac{1}{2}\left[\frac{1}{N}\sum_{\mathbf{k}'} e^{i\mathbf{Q}.\mathbf{R}_i} < c^\dagger_{\mathbf{k}'+\mathbf{Q}\uparrow} c_{\mathbf{k}'\downarrow} > + \frac{1}{N}\sum_{\mathbf{k}} e^{-i\mathbf{Q}.\mathbf{R}_i} < c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}+\mathbf{Q}\uparrow} > \right] \\
&= \cos \mathbf{Q}.\mathbf{R}_i \frac{1}{N}\sum_{\mathbf{k}} < c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} c_{\mathbf{k}\downarrow} >
\end{aligned}$$

and hence the 'self-consistent' equation is:

$$m = \frac{1}{N}\sum_{\mathbf{k}} < c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} c_{\mathbf{k}\downarrow} >$$

which may be recast using the eigenvectors as:

$$c^\dagger_{\mathbf{k}+} = u_{\mathbf{k}} c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}-} \qquad c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} = u^*_{\mathbf{k}} c^\dagger_{\mathbf{k}+} - v_{\mathbf{k}} c^\dagger_{\mathbf{k}-}$$

$$c^\dagger_{\mathbf{k}-} = -v^*_{\mathbf{k}} c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} + u^*_{\mathbf{k}} c^\dagger_{\mathbf{k}-} \qquad c^\dagger_{\mathbf{k}\downarrow} = v^*_{\mathbf{k}} c^\dagger_{\mathbf{k}+} + u_{\mathbf{k}} c^\dagger_{\mathbf{k}-}$$

to obtain:

$$m = \frac{1}{N}\sum_{\mathbf{k}} \left[u^*_{\mathbf{k}} v_{\mathbf{k}} f(\epsilon_{\mathbf{k}+}) - v_{\mathbf{k}} u^*_{\mathbf{k}} f(\epsilon_{\mathbf{k}-}) \right]$$

and the eigenvectors, $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ satisfy:

$$\begin{bmatrix} Un - tZ\gamma_{\mathbf{k}+\mathbf{Q}} & -Um \\ -Um & Un - tZ\gamma_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} u^*_{\mathbf{k}} \\ v^*_{\mathbf{k}} \end{bmatrix} = \epsilon_{\mathbf{k}+} \begin{bmatrix} u^*_{\mathbf{k}} \\ v^*_{\mathbf{k}} \end{bmatrix}$$

$$\begin{bmatrix} Un - tZ\gamma_{\mathbf{k}+\mathbf{Q}} & -Um \\ -Um & Un - tZ\gamma_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} -v_{\mathbf{k}} \\ u_{\mathbf{k}} \end{bmatrix} = \epsilon_{\mathbf{k}-} \begin{bmatrix} -v_{\mathbf{k}} \\ u_{\mathbf{k}} \end{bmatrix}$$

and so, with a bit of algebra:

$$v_{\mathbf{k}} u^*_{\mathbf{k}} (\epsilon_{\mathbf{k}+} - Un + tZ\gamma_{\mathbf{k}+\mathbf{Q}}) + Um \mid v \mid^2_{\mathbf{k}} = 0$$

$$v_{\mathbf{k}} u^*_{\mathbf{k}} (\epsilon_{\mathbf{k}-} - Un + tZ\gamma_{\mathbf{k}+\mathbf{Q}}) - Um \mid u \mid^2_{\mathbf{k}} = 0$$

$$\Rightarrow v_{\mathbf{k}} u^*_{\mathbf{k}} = \frac{Um}{\epsilon_{\mathbf{k}-} - \epsilon_{\mathbf{k}+}}$$

and so:

$$m = Um \frac{1}{N} \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}-}) - f(\epsilon_{\mathbf{k}+})}{\epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}-}}$$

exactly as before. Also:

$$\begin{aligned} n =& \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{2} \left[< c^\dagger_{\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} > + < c^\dagger_{\mathbf{k}+\mathbf{Q}\uparrow} c_{\mathbf{k}+\mathbf{Q}\downarrow} > \right] \\ =& \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{2} \left(\mid u \mid^2_{\mathbf{k}} + \mid v \mid^2_{\mathbf{k}} \right) \left(f(\epsilon_{\mathbf{k}+}) + f(\epsilon_{\mathbf{k}-}) \right) \\ =& \frac{1}{2} \frac{1}{N} \sum_{\mathbf{k}} \left(f(\epsilon_{\mathbf{k}+}) + f(\epsilon_{\mathbf{k}-}) \right) \end{aligned}$$

exactly as before.

The problem for general $\mathbf{Q}$ is therefore:

$$n = \frac{1}{2N} \sum_{\mathbf{k}\tau} f(\epsilon_{\mathbf{k}\tau}) \tag{2}$$

$$m = Um \frac{1}{N} \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}-}) - f(\epsilon_{\mathbf{k}+})}{\epsilon_{\mathbf{k}+} - \epsilon_{\mathbf{k}-}} \tag{3}$$

$$\begin{aligned} G =& \sum_{\mathbf{k}\tau} (\epsilon_{\mathbf{k}\tau} - \mu) f(\epsilon_{\mathbf{k}\tau}) - UN(n^2 - m^2) + k_B T \sum_{\mathbf{k}\tau} \left(f(\epsilon_{\mathbf{k}\tau}) \log f(\epsilon_{\mathbf{k}\tau}) + [1 - f(\epsilon_{\mathbf{k}\tau})] \log[1 - f(\epsilon_{\mathbf{k}\tau})] \right) \\ =& k_B T \frac{1}{N} \sum_{\mathbf{k}\tau} \log[1 - f(\epsilon_{\mathbf{k}\tau})] - U(n^2 - m^2) \end{aligned}$$

with:

$$f(\epsilon) = \frac{1}{1 + \exp\left[\frac{\epsilon - \mu}{k_B T}\right]} \qquad 1 - f(\epsilon) = \frac{1}{1 + \exp\left[\frac{\mu - \epsilon}{k_B T}\right]}$$

in terms of:

$$\epsilon_{\mathbf{k}\pm} = Un - \frac{tZ}{2} \left(\gamma_{\mathbf{k}+\mathbf{Q}} + \gamma_{\mathbf{k}} \right) \pm \left[\left(\frac{tZ}{2} \right)^2 \left(\gamma_{\mathbf{k}+\mathbf{Q}} - \gamma_{\mathbf{k}} \right)^2 + (Um)^2 \right]^{1/2}$$

and:

$$\gamma_{\mathbf{k}} = \frac{1}{Z} \sum_{<0n>} e^{i\mathbf{k}.\mathbf{R}_n}$$

If we further restrict attention to paramagnetism versus ferromagnetism versus *bipartite* antiferromagnetism, then the problem may be reduced with the density of states. The simplification is that one only needs to consider the function $\gamma_{\mathbf{k}}$. For ferromagnetism $\mathbf{Q} = \mathbf{0}$, and so $\gamma_{\mathbf{k}+\mathbf{Q}} = \gamma_{\mathbf{k}}$, and for bipartite antiferromagnetism, $\gamma_{\mathbf{k}+\mathbf{Q}} = -\gamma_{\mathbf{k}}$. The problem therefore reduces to:

$$n = \int_{\mathbf{R}} d\gamma \rho(\gamma) \frac{1}{2} \left[f(\epsilon_+) + f(\epsilon_-) \right]$$

$$m = Um \int_{\mathbf{R}} d\gamma \rho(\gamma) \frac{f(\epsilon_-) - f(\epsilon_+)}{\epsilon_+ - \epsilon_-}$$

$$g \equiv \frac{G}{N} = k_B T \int_{\mathbf{R}} d\gamma \rho(\gamma) \sum_{\tau} \log[1 - f(\epsilon_\tau)] - U(n^2 - m^2)$$

and for ferromagnetism:

$$\epsilon_\pm = Un - tZ\gamma \pm Um$$

while for bipartite antiferromagnetism:

$$\epsilon_\pm = Un \pm \left[(tZ\gamma)^2 + (Um)^2 \right]^{1/2}$$