FIP10604 - Text 08 - Mean-field approximation I

Spin Hamiltonians involving exchange interactions describe an interacting many-body problem. Hence, very few particular cases exist with exact solution (we will address some later on). As we saw in Text 07 for the Heisenberg model, it is possible to study the thermodynamic behavior at very low temperatures based on non-interacting *magnon*-type elementary excitations. But this is only applicable when the spontaneous (or sublattice) magnetization does not depart very much from its maximum value. To achieve a comprehensive description of the overall thermodynamic behavior, with a disordered phase at high temperatures, an ordered phase at low temperatures, and a phase transition from one to the other, we need to resort to approximation methods.

Among the most common approaches is the **Mean Field Approximation**, also known as *Mean Field Theory* and, for historical reasons, *Molecular Field Theory* (or *Approximation*). We will study here (and in the next Text) its application to the Heisenberg model.

Heisenberg Hamiltonian with applied field

First of all, we add to the Heisenberg Hamiltonian a Zeeman term, i.e., interaction with an external magnetic field, writing

$$\mathcal{H} = -\sum_{ij} J_{ij} \,\mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H}_i \cdot \mathbf{S}_i \,. \tag{1}$$

We continue to use the simplified notation introduced in Text 07, with spin measured in units of \hbar and magnetization in units of $-g\mu_B$ per atom, which leads to the relationship

$$\mathbf{M}_i = \langle \mathbf{S}_i \rangle. \tag{2}$$

Mean-field approximation

The Mean-field approximation consists in using the decomposition

$$\mathbf{S}_{i} = \mathbf{M}_{i} + (\mathbf{S}_{i} - \mathbf{M}_{i}) \equiv \mathbf{M}_{i} + \Delta \mathbf{S}_{i}$$
(3)

and neglecting quadratic terms in the spin deviation from its average value, $\Delta \mathbf{S}_i$. Thus

$$\mathbf{S}_i \cdot \mathbf{S}_j \simeq \mathbf{M}_i \cdot \mathbf{S}_j + \mathbf{S}_i \cdot \mathbf{M}_j - \mathbf{M}_i \cdot \mathbf{M}_j .$$
(4)

The mean-field (MF) Hamiltonian is then

$$\mathcal{H}_{\rm MF} = -2\sum_{ij} J_{ij} \,\mathbf{M}_j \cdot \mathbf{S}_i - \sum_i \mathbf{H}_i \cdot \mathbf{S}_i + \sum_{ij} J_{ij} \,\mathbf{M}_i \cdot \mathbf{M}_j \,. \tag{5}$$

The last term does not contain operators, and may be removed from the Hamiltonian, since it has no influence on the evaluation of average values (it only needs to be included when calculating the total energy). With this procedure, the interaction term has been linearized, and we now have formally a problem of **independent spins** in the presence of an **effective magnetic field**

$$\mathbf{H}_{i}^{\text{eff}} = \mathbf{H}_{i} + 2\sum_{j} J_{ij}\mathbf{M}_{j} .$$
(6)

Note that Eq. (2) is a **self-consistency relationship**, since we must evaluate the the spin's average value in the presence of a "magnetic field" that includes this same average value (at sites that interact with the reference site).

It should be noted that in Mean Field Theory, when dealing with the paramagnetic phase, there is no difference between the Heisenberg and Ising models since the MF Hamiltonian does not depend on spin components perpendicular to the magnetization. This changes in the ordered phase, when we can apply a field perpendicular to the spontaneous magnetization.

FM case

Let us consider, as usual, the nearest-neighbor approximation. In the FM system we have J > 0.

Spontaneous magnetization

In the absence of external field ($\mathbf{H} = 0$) but in the presence of ferromagnetic order, and choosing $\mathbf{M} = (0, 0, M)$, Eq. (6) results in the effective field intensity

$$H^{\text{eff}} = 2zJM , \qquad (7)$$

where z is the coordination number.

We can directly apply the solution obtained for independent magnetic moments (Text 03), which takes the form

$$M = SB_S(2zJSM/T) . (8)$$

Note that, besides the already mentioned simplifications in notation, we are also not including the Boltzmann constant k_B , which means that energies (and in particular the exchange constant J) are measured in temperature units.

Equation (8) is an implicit relation for M, whose temperature-dependent solution is a function M(T). Two graphical solutions are sketched in Fig. 1. For each T, the solution is given by the intersection point of the curve $y_1(M) = SB_S(2zJSM/T)$ with the unit-slope

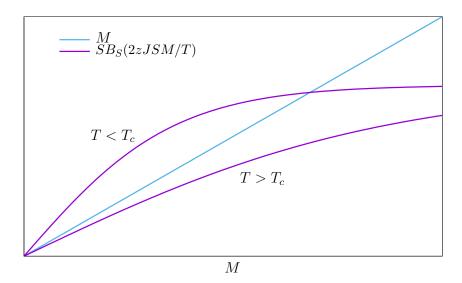


Figure 1: Example graphical solutions of Eq. (8).

straight line $y_2(M) = M$. In practice, this solution is obtained numerically by iterations: for a given value of T, starting from an initial value M_1 , successive approximations

$$M_{n+1} = SB_S(2zJSM_n/T) \tag{9}$$

are generated. When the number of iterations n is sufficiently large, M_n approaches the value of M(T) with the desired accuracy.

Figure 1 shows two distinct regimes:

- $T < T_c$: initial slope of $SB_S(2zJSM/T) > 1 \Rightarrow$ intersection in $M(T) \neq 0$.
- $T > T_c$: initial slope of $SB_S(2zJSM/T) < 1 \Rightarrow$ intersection only for M(T) = 0. Note that M = 0 is always a solution, but it is unstable when there is a solution $M(T) \neq 0$.

The boundary between these two regimes, which occurs at $T = T_C^{\text{MF}}$, corresponds to $SB_S(2zJSM/T)$ with initial slope exactly equal to 1. Making the expansion of $SB_S(x)$ for $x \to 0$,

$$SB_S(x) = \frac{S+1}{3}x + \mathcal{O}(x^3)$$

we have

$$T_C^{\rm MF} = \frac{2}{3} z J S(S+1) .$$
 (10)

Paramagnetic susceptibility for J > 0

In the paramagnetic phase, where there is no spontaneous magnetization, the relation $M = \chi H$ holds in the presence of a sufficiently weak applied magnetic field H. On the other hand, the mean-field approximation views M as the response of **independent** moments to an **effective** field, i.e., $M = \chi_0 H^{\text{eff}}$, where $\chi_0 = C/T$, as obtained in Text 03. In our unit system the Curie constant is simply C = S(S+1)/3. Using these two forms of writing the magnetization and considering that the effective field, Eq. (6), takes the simple form $H^{\text{eff}} = H + 2zJM$, we obtain

$$\chi = \frac{\chi_0}{1 - 2zJ\chi_0} = \frac{C}{T - \theta} , \qquad (11)$$

where $\theta = 2zJC$. This equation reproduces the *Curie-Weiss law*, which agrees with experimental observations for $T \gg T_C$. However, in mean-field theory this form holds for any $T > \theta$, that is, in the entire paramagnetic phase, since $\theta = T_C^{\text{MF}}$ [see Eq. (10)]. Note that C and θ are easily obtained from a straight-line fitting of experimental data for χ^{-1} at high temperatures. This allows to obtain the exchange interaction J. Furthermore, given that the "true" Curie constant depends also on the g factor, we can infer the value of this quantity if the atomic spin is known.

Figure 2 qualitatively summarizes the mean-field results (M and χ^{-1}) for a FM system.

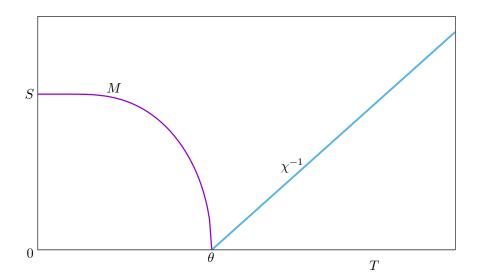


Figure 2: Magnetization and inverse paramagnetic susceptibility as functions of temperature for a FM system in the MF approximation.

AF case

For a bipartite lattice, the system is divided into two identical sublattices, A and B, so that $\mathbf{R}_{i+\delta} \in B$ if $\mathbf{R}_i \in A$. Assuming a Néel-type magnetic order, by choosing $M_i \equiv M$ for $i \in A$ we have $M_{i+\delta} = -M$. Here M is called **sublattice magnetization** instead of spontaneous magnetization. In the absence of external field, the effective field at a site i is $H_i^{\text{eff}} = 2zJM_{i+\delta}$. Remembering that J < 0, the effective field at sites of the A sublattice is $H_A^{\text{eff}} = 2z|J|M$, while in the B sublattice we have $H_B^{\text{eff}} = -H_A^{\text{eff}}$. Thus

$$M = SB_S(2z|J|SM/T) . (12)$$

This equation has the same form as in the FM case [Eq. (8)]. Therefore, the Néel temperature has the same value as T_C^{MF} for J's of the same absolute value, being given by

$$T_N^{\rm MF} = \frac{2}{3}z|J|S(S+1).$$
(13)

Paramagnetic susceptibility (J < 0)

In the PM phase, the effective field still has the form $H^{\text{eff}} = H + 2zJM$. However, since J < 0 the mean field due to nearest neighbors now **opposes** the external field. With the same development as before, we obtain

$$\chi = \frac{\chi_0}{1 - 2zJ\chi_0} = \frac{\chi_0}{1 + 2z|J|\chi_0} = \frac{C}{T + |\theta|} .$$
(14)

A plot equivalent to Fig. 2 for the AF case is shown in Fig. 3.

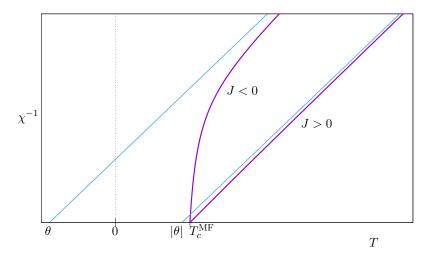


Figure 3: Magnetization and inverse paramagnetic susceptibility as functions of temperature for the AF case in the MF approximation.

As previously remarked, the uniform susceptibility of an AF system does not diverge at any physically meaningful temperature (T > 0) because there is no transition to **uniform** magnetic ordering.

Ferrimagnetic case

Let us consider the same geometry of the AF case but with the two sublattices containing spins of different magnitudes, S_A and S_B , while J may be positive or negative.

We will restrict ourselves to the paramagnetic case. In the presence of an applied field H, the magnetizations of the two sublattices are given by the set of equations

$$M_{A} = \chi_{0}^{A} [H + 2zJM_{B}] ,$$

$$M_{B} = \chi_{0}^{B} [H + 2zJM_{A}] ,$$
(15)

resulting in

$$M_{A} = \frac{\chi_{0}^{A} [1 + 2zJ\chi_{0}^{B}]}{1 - (2zJ)^{2}\chi_{0}^{A}\chi_{0}^{B}}H,$$

$$M_{B} = \frac{\chi_{0}^{B} [1 + 2zJ\chi_{0}^{A}]}{1 - (2zJ)^{2}\chi_{0}^{A}\chi_{0}^{B}}H.$$
(16)

The net magnetization (per unit cell) is $M = (M_A + M_B)$ and must satisfy the general relation $M = \chi H$. Thus,

$$\chi = \frac{\chi_0^A + \chi_0^B + 4zJ\chi_0^A\chi_0^B}{2[1 - (2zJ)^2\chi_0^A\chi_0^B]} \,. \tag{17}$$

Using $\chi_0^A = C_A/T$ and $\chi_0^B = C_B/T$, it follows that

$$\chi^{-1} = \frac{T^2 - (2zJ)^2 C_A C_B}{\bar{C}T + 2zJ C_A C_B} , \qquad (18)$$

where $\bar{C} \equiv (C_A + C_B)$.

Equation (18) shows that, for any sign of J, χ^{-1} vanishes at

$$T_c^{\rm MF} = 2z|J|\sqrt{C_A C_B} = \frac{2}{3}z|J|\sqrt{S_A (S_A + 1)S_B (S_B + 1)} .$$
(19)

It reproduces the transition temperature of the FM or AF cases when $S_A = S_B$.

For high temperatures, neglecting terms of order T^{-1} or higher in Eq. (18), we obtain

$$\chi^{-1} = \frac{1}{\bar{C}} \left[T - 2zJ \frac{C_A C_B}{\bar{C}} \right] . \tag{20}$$

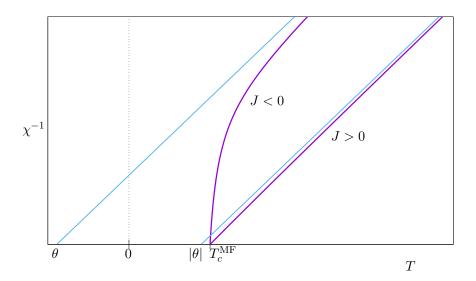


Figure 4: Inverse PM susceptibility as a function of temperature for a ferrimagnetic system. The spins are $S_A = 1$ and $S_B = 1$. Two cases are shown for the same absolute value of J, choosing the scale such that $T_c^{\text{MF}} = 1$.

It can be seen that the ferrimagnetic susceptibility at high temperatures has the FM form $\chi = \bar{C}/(T - \theta)$ for J > 0 and the AF form, $\chi = \bar{C}/(T + |\theta|)$ for J < 0. In both cases,

$$|\theta| = 2z|J|\frac{C_A C_B}{\bar{C}} = T_c^{\rm MF} \frac{\sqrt{C_A C_B}}{\bar{C}} . \tag{21}$$

We can see that $|\theta| \leq T_C^{\text{MF}}$, the equality happening only when the spins are identical, i.e., when the FM or AF cases are reproduced.

The behavior of χ^{-1} for both signs of J is illustrated in Fig. 4.