FIP10604 – Text 10 — Beyond mean field

Critical view of the Mean Field Approximation

In Texts 08 and 09 we introduced the mean-field approach to study magnetic properties of systems described by the Heisenberg Hamiltonian (with or without anisotropy). This method, being an approximation, has strengths and weaknesses that we now discuss.

Virtues:

- Qualitatively reproduces the behavior of real (3D) magnetic insulators throughout the observable temperature range.
- Obtains the Curie-Weiss law in a quantitatively correct form, allowing estimation of the exchange interaction (when a single one is relevant) from the θ constant.

Drawbacks:

- The Curie-Weiss law is wrongly predicted as valid in the entire PM phase. Experiments show that the transition temperature is always below θ (for FM interactions). This is an effect of spin fluctuations, which are neglected in the mean-field (MF) approximation. These fluctuations also cause the PM susceptibility near T_C to behave as $(T - T_C)^{-\gamma}$ with $\gamma \neq 1$.
- In the ordered phase, although the mean-field $M(T)$ curve is qualitatively correct, it ends at a temperature $T_{C(N)}^{\mathrm{MF}} = |\theta| > T_{C(N)}$. Furthermore, the functional form of the magnetization with temperature is incorrect. In particular, (i) an exponential deviation is predicted near saturation for $T \to 0$, but we know from the magnon theory that the deviation follows a power law; (ii) the behavior for $T \to T_{C(N)}$ is of type $(T_{C(N)} - T)^{\beta}$, which is qualitatively correct, but $\beta = 1/2$ in MF, while the experimental observations for 3D Heisenberg systems indicate $\beta \sim 1/3$.
- The average energy is simply $E = -Nz|J|M^2$. Therefore, the mean-field specific heat is null in the PM phase (in contrast to experimental observations), and tends exponentially to zero for $T \to 0$, when it should follow a power law, as we saw in the study of spin waves.
- The Néel state **is** the ground state of $\mathcal{H}^{MF}$ for AF interactions, although it is not an eigenstate of the Heisenberg Hamiltonian.

- The mean-field results do not take correctly into account effects of spatial dimensionality of the system, obtaining a phase transition at finite temperature for any dimension. We had indications that this is not correct in a low-temperature analysis using spin waves.

Validity

Based on this criticism, it is relevant to investigate under what conditions would the mean-field approximation be valid.

It is easy to see that MF becomes **exact** in the limit of infinite coordination number ($z \to \infty$), or equivalently, in the limit where the exchange interactions have infinite range so that each spin interacts with all the other spins of the lattice. The argument can be summarized as follows:

- MF considers a single spin in the presence of a mean field due to its neighbors.
- Corrections to MF are due to fluctuations of the effective field around its mean value.
- The contribution of each neighbor to the fluctuations is finite because the spin component responsible for the effective field can only fluctuate between $\pm S$.
- The average field can be seen as a sum of random variables (the contributions of each neighbor). When $z \gg 1$, this sum is a random variable with Gaussian distribution (*Central Limit Theorem*).
- Therefore, fluctuations of the effective field are proportional to $1/\sqrt{z}$, and vanish in the limit $z \to \infty$.

Note that the characteristic energy scale is given by $T_C^{\mathrm{MF}} \sim z|J|$. Then one must take the double limit $z \to \infty$, $|J| \to 0$, keeping the product $z|J|$ constant.

Alternatives to Mean Field

Considering the difficulties that are inherent to a many-body problem (here, interacting magnetic moments), there are few alternatives to the mean-field approximation. The main ones are listed below.

1. **High-temperature series** - They allow to obtain thermodynamic quantities in the PM phase as power series in $1/T$, providing corrections to the mean-field results.
2. **Exact (analytic) solutions** - Some solutions exist, for simplified low-dimensional models.

3. **Numerical solutions** - They are restricted to finite-size systems (usually very small and low-dimensional). The more "direct" method is to diagonalize the Hamiltonian matrix in an appropriate basis (e.g., all possible products of local states). Also extensively used are *Monte Carlo* methods, based on averages over random spin configurations or dynamical evolution between these configurations to search for the one that minimizes the energy.

4. **Theories of phase transitions and critical phenomena** - They explore concepts of *universality* and *scaling laws* to study in a rigorous way the system's behavior near the transition between ordered and paramagnetic phases.

We will explore (without much detail) the first two alternatives listed above.

High-temperature series

This method applies to the evaluation of physical quantities in the paramagnetic phase, particularly specific heat and susceptibility.

The basic relations are

$$c_m = -\left.\frac{T}{N}\frac{\partial^2 F}{\partial T^2}\right|_0 , \quad \chi = -\left.\frac{1}{N}\frac{\partial^2 F}{\partial H^2}\right|_0 , \tag{1}$$

$$F = -T \ln Z , \qquad Z = \mathrm{Tr}\ \mathrm{e}^{-\mathcal{H}/T} , \tag{2}$$

and the high-temperature series consists in the expansion

$$\mathrm{e}^{-\mathcal{H}/T} = 1 - \frac{\mathcal{H}}{T} + \frac{1}{2!}\frac{\mathcal{H}^2}{T^2} - \frac{1}{3!}\frac{\mathcal{H}^3}{T^3} + \dots \tag{3}$$

This allows to write

$$\frac{Z}{Z_\infty} = 1 - \frac{\langle\mathcal{H}\rangle}{T} + \frac{1}{2!}\frac{\langle\mathcal{H}^2\rangle}{T^2} - \frac{1}{3!}\frac{\langle\mathcal{H}^3\rangle}{T^3} + \dots , \tag{4}$$

defining

$$\langle X\rangle \equiv \frac{\mathrm{Tr}\, X}{Z_\infty}. \tag{5}$$

$Z_\infty = \mathrm{Tr}\,\mathbb{1}$ is the partition function in the limit $T \to \infty$, with $\mathbb{1}$ being the identity matrix in spin space. The average values that appear in Eq. (4) are also calculated in this limit, as explicitly indicated in Eq. (5).

In the presence of magnetic field, it is convenient to write

$$\mathcal{H} = \mathcal{H}_0 + \bar{\mathcal{H}}_1 H , \tag{6}$$

where $\mathcal{H}_0$ is the Hamiltonian in zero field and $\bar{\mathcal{H}}_1 = -\sum_i S_i^z$. Note that $\mathcal{H}_0$ has dimension of energy, but $\bar{\mathcal{H}}_1$ is dimensionless.

Given that spin operators at different sites commute, the trace is taken independently for each site. Consequently, the average of a product of spin operators is given by the product of averages at each of the involved sites. For a single-site, $\mathrm{Tr}\,\mathbb{1} = 2S+1$. Since any spin component has zero trace, $\langle\mathcal{H}_0\rangle = \langle\bar{\mathcal{H}}_1\rangle = 0$.

Series for the susceptibility

Using the set of relations (1–6), we obtain the series

$$\chi = \frac{1}{T}\frac{1}{N}\langle\bar{\mathcal{H}}_1^2\rangle - \frac{1}{T^2}\frac{1}{N}\langle\mathcal{H}_0\bar{\mathcal{H}}_1^2\rangle + \frac{1}{6T^3}\frac{1}{N}\left(\langle\mathcal{H}_0\bar{\mathcal{H}}_1\mathcal{H}_0\bar{\mathcal{H}}_1\rangle + 2\langle\mathcal{H}_0^2\bar{\mathcal{H}}_1^2\rangle - 3\langle\mathcal{H}_0^2\rangle\langle\bar{\mathcal{H}}_1^2\rangle\right) + \dots \quad (7)$$

This series can be compared to that obtained from the Curie-Weiss law

$$\chi = \frac{C}{T-\theta} = \frac{C}{T}\left(1-\frac{\theta}{T}\right)^{-1} = \frac{C}{T} + \frac{C\theta}{T^2} + \frac{C\theta^2}{T^3} + \dots \quad (8)$$

We can evaluate

$$\frac{1}{N}\langle\bar{\mathcal{H}}_1^2\rangle = \frac{1}{N}\sum_{ij}\langle S_i^z S_j^z\rangle = \langle(S_i^z)^2\rangle = \frac{1}{3}S(S+1)\,, \quad (9)$$

reproducing the Curie constant C, which shows that the first term is coincident in series (7) and (8).

It is also not difficult to verify that

$$\frac{1}{N}\langle-\mathcal{H}_0\bar{\mathcal{H}}_1^2\rangle = \frac{J}{N}\sum_{\substack{i\delta\\ jl}}\langle(\mathbf{S}_i\cdot\mathbf{S}_{i+\delta})S_j^z S_l^z\rangle = 2zJ\langle(S_i^z)^2\rangle\langle(S_{i+\delta}^z)^2\rangle = 2zJC^2\,. \quad (10)$$

Comparing the second term in the series (7) and (8), we see that they are also coincident if $\theta = 2zJC$, which is in agreement with the mean-field results. Starting at order $1/T^3$ the terms of the two series present differences, thereby introducing corrections to the mean-field susceptibility.

Critical temperature

We know that the paramagnetic susceptibility diverges at T_C, which implies that its high-temperature series is no longer convergent at that point. Thus, one can estimate T_C by using the fact that a series ceases to be convergent when the ratio between successive terms ceases to be less than unity. Writing $\chi = \sum_n a_n T^{-n}$, we can determine T_C through the relation

$$\lim_{n\to\infty}\frac{a_n T_C^{-n}}{a_{n-1}T_C^{-(n-1)}} = 1\,, \quad (11)$$

which leads to

$$T_C = \lim_{n\to\infty} \frac{a_n}{a_{n-1}} \, . \tag{12}$$

Results obtained by this method indicate a significant reduction of T_C in comparison to $T_C^{\rm MF}$. The following table shows the ratio $T_C/T_C^{\rm MF}$ for the three-dimensional FM Heisenberg model in cubic lattices for some values of the local spin.

S	sc (z=6)	bcc (z=8)	fcc (z=12)
1	0.57	0.65	0.69
1	0.66	0.71	0.75
3	0.68	0.73	0.77
2	0.69	0.75	0.775

One can see the expected effect of the number of neighbors, as the ratio becomes closer to 1.0 with increasing z. One also observes a growing ratio for increasing spin magnitude. In this case, we are approaching the classical limit ($S \to \infty$). Actually, the high-temperature series can be applied to the classical Heisenberg model up to much higher orders than in the quantum case, so that a good estimate of the critical temperature can be achieved. In particular, the best values for a three-component classical spin in the sc and bcc lattices correspond to ratios $T_C^{\rm cl}/T_C^{\rm MF}$ of 0.72 and 0.77, respectively (J is rescaled so that $JS^2 = 1$)). We can see from the above table that $S = 2$ is already close to the classical limit.

We only presented the high-temperature-series calculation of the susceptibility for the symmetric Heisenberg model with nearest-neighbor interactions. However, the general method expressed by Eqs. (1–6) can be applied even when $\mathcal{H}_0$ includes anisotropy terms and/or more complex exchange interactions. In these cases, the Curie-Weiss law is not enough to determine the system parameters from fitting of experimental data, and it is necessary to use more terms of the high-temperature series.

Exact solutions

The simplest magnetic model that admits exact solution in the thermodynamic limit is the Ising model in one dimension, which we will discuss in the following.

1D Ising model

Consider a chain of N sites, with periodic boundary conditions and nearest-neighbor interaction. Redefining the exchange constant ($2JS^2 \to J$), the Hamiltonian becomes

$$\mathcal{H} = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} \, , \qquad \sigma_{N+1} = \sigma_1 \, , \quad \sigma_i = \pm 1 \, . \tag{13}$$

Rigorously, this formulation applies to $S = 1/2$, but it can used for $S > 1/2$ if the system presents strong easy-axis anisotropy ($-DS_{iz}^2$), since the $\pm S$ states are favored.

The partition function is given by

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta\mathcal{H}} = \mathrm{Tr} \prod_{i=1}^{N} \mathrm{e}^{\beta J \sigma_i \sigma_{i+1}} = \mathrm{Tr}\, \mathbf{P}^N \ , \tag{14}$$

where we introduce the **transfer matrix**, $\mathbf{P}$, whose elements are

$$P_{ij} = \mathrm{e}^{\beta J \sigma_i \sigma_j} \ . \tag{15}$$

As it happens with any matrix, we have

$$\mathrm{Tr}\, \mathbf{P}^N = \sum_n \lambda_n^N \ , \tag{16}$$

where the λ_n's are the matrix eigenvalues.

In our present case,

$$\mathbf{P} = \begin{pmatrix} \mathrm{e}^{\beta J} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta J} \end{pmatrix} \ , \tag{17}$$

and the eigenvalues are

$$\lambda_\pm = \mathrm{e}^{\beta J} \pm \mathrm{e}^{-\beta J} = \begin{cases} 2\cosh(\beta J) \\ 2\ \sinh(\beta J) \end{cases} \tag{18}$$

Therefore,

$$Z = 2^N \cosh^N(\beta J) \left[1 + \tanh^N(\beta J)\right] \tag{19}$$

From the partition function, we obtain the free energy

$$F = -\frac{1}{\beta} \ln Z \ . \tag{20}$$

After a simple algebra, we can write

$$\frac{F}{N} = -\frac{1}{\beta} \left\{ \ln[2\cosh(\beta J)] + \frac{1}{N} \ln[1 + \tanh^N(\beta J)] \right\} \ . \tag{21}$$

We must have an even number of sites to allow for periodic boundary conditions in the AF case. Therefore, $\tanh^N(\beta J)$ is always a number in the range $[0, 1]$, and the last term on the right-hand side of Eq. (21) disappears in the thermodynamic limit ($N \to \infty$). So, in this limit the free energy per site is

$$\frac{F}{N} = -T \ln[2\cosh(J/T)] \ . \tag{22}$$

Note that this result is equivalent to writing $Z = \lambda_{\max}^N$, where $\lambda_{\max}$ is the maximum eigenvalue of the transfer matrix, which dominates the sum in Eq. (16). Even if this eigenvalue is degenerate in some limit (such as $T \to 0$ in the present case, when $\lambda_+ = \lambda_-$), this degeneracy introduces a finite factor (i.e., not of order N) in Z, which does not contribute to F/N when $N \to \infty$.

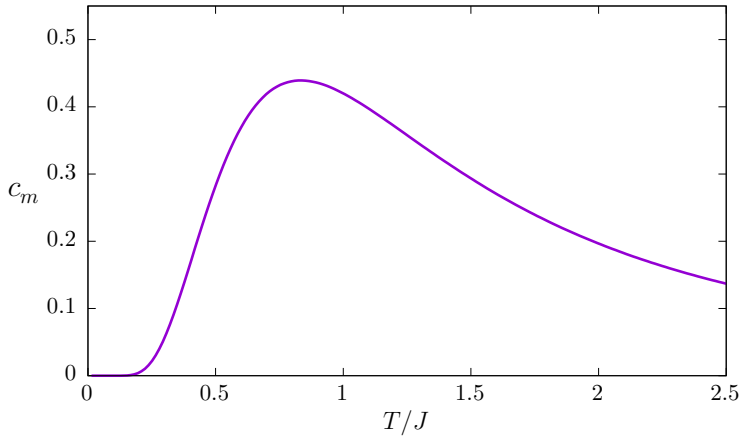

Figure 1: Specific heat as a function of temperature for the 1D Ising model.

Specific heat

Evaluating the specific heat from the magnetic free energy, we obtain

$$c_m = -\frac{T}{N}\frac{\partial^2 F}{\partial T^2} = \left(\frac{J}{T}\right)^2 \operatorname{sech}^2\left(\frac{J}{T}\right) . \tag{23}$$

A plot of c_m as a function of T is shown in Fig. 1. One can see that, despite the existence of a maximum slightly below $T = J$, the specific heat shows no singularity, indicating the absence of phase transition. It is worth remarking that c_m is independent of the sign of J, which means that the same result applies to both FM and AF systems.

Magnetization and susceptibility

To obtain the magnetization and the magnetic susceptibility we need to add an external-field term to the Hamiltonian (13), which becomes

$$\mathcal{H} = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - H\sum_i \sigma_i . \tag{24}$$

We use the same procedure as before. Now, however, the elements of the transfer matrix are

$$P_{12} = \mathrm{e}^{\beta[J\sigma_1\sigma_2 + \frac{H}{2}(\sigma_1+\sigma_2)]} . \tag{25}$$

Therefore,

$$\mathbf{P} = \begin{pmatrix} \mathrm{e}^{\beta(J+H)} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta(J-H)} \end{pmatrix} , \tag{26}$$

with eigenvalues

$$\lambda_{\pm} = \mathrm{e}^{\beta J}\cosh(\beta H) \pm \sqrt{\mathrm{e}^{2\beta J}\cosh^2(\beta H) - 2\,\sinh(2\beta J)}\ . \tag{27}$$

As happened without applied field, in the thermodynamic limit the free energy per spin is given by

$$\frac{F}{N} = -\frac{1}{\beta}\ln\lambda_+\ , \tag{28}$$

which can be written as

$$\frac{F}{N} = -T\ln\Lambda(H,T)\ , \tag{29}$$

with the definitions

$$\begin{aligned}\Lambda(H,T) &= \mathrm{e}^{J/T}\cosh(H/T) + R(H,T)\ ,\\ R(H,T) &= \sqrt{\mathrm{e}^{2J/T}\left[\cosh^2(H/T) - 1\right] + \mathrm{e}^{-2J/T}}\ .\end{aligned} \tag{30}$$

The magnetization is then

$$M(H,T) = -\frac{1}{N}\frac{\partial F}{\partial H} = \frac{\mathrm{e}^{J/T}\,\sinh(H/T)}{R(H,T)}\ . \tag{31}$$

One observes that

$$\begin{aligned}\lim_{H\to 0} M(H,T) &= 0 \qquad \text{for any } T>0,\\ \lim_{T\to 0} M(H,T) &= 1 \qquad \text{for any } H>0\ .\end{aligned} \tag{32}$$

Therefore, **there is no ordered phase at finite temperature**, but we obtain a FM ground-state taking the limit $T\to 0$ **before** the limit $H\to 0$.

To evaluate the magnetic susceptibility in the linear response regime we use

$$\chi = \left.\frac{\partial M}{\partial H}\right|_{H=0}\ , \tag{33}$$

which results in

$$\chi = \frac{1}{T}\frac{\mathrm{e}^{J/T}}{R(0,T)} = \frac{1}{T}\,\mathrm{e}^{2J/T}\ . \tag{34}$$

Expanding the exponential, we obtain a Curie-Weiss law at high temperature (Fig. 2), with $\theta = 2J$. We recognize the mean-field result if we take into account the redefinition of J [before Eq. (13)] and the fact that the Curie constant C is given by S^2 instead of $S(S+1)/3$ in the Ising case. Once more, simply changing $J\to -J$ reproduces the mean-field limit in the AF case. Although the high-temperature Curie-Weiss limit yields a finite θ, the inverse FM susceptibility goes (exponentially) to zero only at $T=0$. In contrast, in the AF case it is χ that goes to zero at zero temperature, so that χ^{-1} diverges.

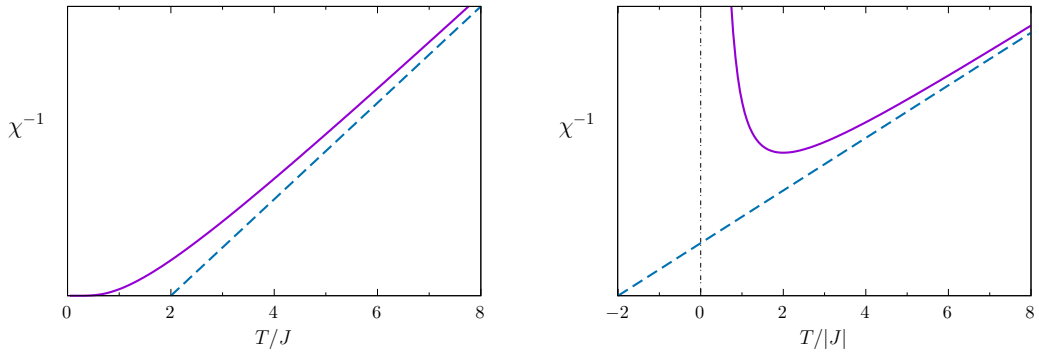

Figure 2: Inverse of the magnetic susceptibility as a function of temperature for the 1D Ising model in the FM (left) and AF (right) cases.

Entropy and order at low dimensions

The absence of magnetic order at finite temperature observed in the 1D Ising model can be understood in terms of a simple argument.

The FM state minimizes exchange energy in **all** bonds. In an excited state with only one bond not minimized, all spins point up on one side and all point down on the other side of that bond. This configuration is called a *kink*. The bond energy at the kink is J, while all the other bonds have energy $-J$. So, the energy difference to the ground state is positive ($2J$). However, as the kink can be located between any two of the N lattice sites, we have a configuration entropy equal to $\ln N$. Then, the change in free energy due to the presence of a kink is

$$\Delta F = 2J - T \ln N \ , \tag{35}$$

which is **negative** for any $T > 0$ in the thermodynamic limit. Thus, the system tends to form a *kink gas*, suppressing magnetic order.

2D Ising model

The above arguments can be applied to a two-dimensional system (e.g., a square lattice). In this case, the equivalent of a kink is a region of inverted spins limited by a polygonal line of length L. The energy balance indicates L non-minimized links, yielding $\Delta E = 2LJ$. To evaluate the entropy, we first note that each "step" along the polygonal line has three possible choices (at least for the first half of the *round trip*, since the choice of subsequent steps is restricted by the condition of closing the path). Therefore, the configuration entropy will be close to (but smaller than) $\ln 3^L$, so that

$$\Delta F \gtrsim L(2J - T \ln 3) \ . \tag{36}$$

This free-energy difference changes sign at a critical temperature $T_c \gtrsim 2J/\ln 3$, allowing us to expected an FM phase to be stable below this temperature.

In 1944, Onsager solved exactly the Ising model on the square lattice. We will not reproduce here this solution, which generalizes the use of transfer matrices to the two-dimensional case. From Onsager's results we highlight the Curie-temperature value,

$$T_C = \frac{2J}{\ln(1+\sqrt{2})} \, , \tag{37}$$

for comparison with the above discussion, and the fact that the specific heat has a **logarithmic** divergence at T_C.

Heisenberg chain

Another one-dimensional model with exact solution is the (quantum) Heisenberg model. This solution, employing the so-called *Bethe ansatz*, is significantly more complex than what we have shown here for the Ising model. For this reason, we will present it in a separate text (Text 11).