FIP10604 – Text 09 — MEAN-FIELD APPROXIMATION - II

Heisenberg Hamiltonian in wavevector space

As we saw in Text 08, the uniform susceptibility does **not** diverge in the case of an AF system. However, if we could apply a magnetic field that changed sign between neighboring lattice sites, we should expect the corresponding susceptibility to diverge at T_N. This situation is best described in terms of Fourier components of the relevant physical quantities.

For a lattice of N sites with periodic boundary conditions, we have a discrete Fourier transform. For the magnetization, it is defined by the relations

$$\begin{aligned} \mathbf{M}_i &= \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \mathbf{M}(\mathbf{q}) \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{R}_i} \ , \\ \mathbf{M}(\mathbf{q}) &= \frac{1}{\sqrt{N}} \sum_{i} \mathbf{M}_i \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{R}_i} \ , \end{aligned} \tag{1}$$

where the wavevector sum spans the N vectors belonging to the 1st BZ (Brillouin zone). Similar equations can be written for the magnetic field, the spin operators, etc.

The Heisenberg Hamiltonian on a lattice,

$$\mathcal{H} = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H}_i \cdot \mathbf{S}_i \ , \tag{2}$$

can be rewritten in wavevector space as

$$\mathcal{H} = -\sum_{\mathbf{q}} J(\mathbf{q})\, \mathbf{S}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q}) - \sum_{\mathbf{q}} \mathbf{H}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q}) \ , \tag{3}$$

where we used the previous definition (Text 07),

$$J(\mathbf{q}) = \sum_j J_{ij} \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} = J \sum_{\delta} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\delta} \ . \tag{4}$$

The last equality implies restriction to nearest-neighbor interactions.

Mean-field Hamiltonian

Using the same procedure employed in Text 08 for site-dependent quantities, we obtain the mean-field Hamiltonian as

$$\mathcal{H}_{\mathrm{MF}} = -\sum_{\mathbf{q}} \mathbf{H}^{\mathrm{eff}}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q}) \ , \tag{5}$$

with

$$\mathbf{H}^{\mathrm{eff}}(\mathbf{q}) = \mathbf{H}(\mathbf{q}) + 2J(\mathbf{q})\mathbf{M}(\mathbf{q}) \ . \tag{6}$$

Staggered magnetization

The Néel-type AF order is characterized by a magnetization that alternates between neighboring sites of a bipartite lattice, so that $\mathbf{M}_{i+\delta} = -\mathbf{M}_i$. This is usually called *staggered* magnetization. Fourier transforming, this leads to

$$\sum_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{R}_i}\mathbf{M}(\mathbf{q})\left[\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\delta}+1\right] = 0\ . \tag{7}$$

The condition $\mathbf{M}(\mathbf{q}) \neq 0$ can only be satisfied for a wavevector $\mathbf{q} = \mathbf{Q}$ chosen so that

$$\mathbf{Q}\cdot\delta = \pi \tag{8}$$

for any δ that connects neighboring sites. Therefore, the only nonzero Fourier component of the magnetization is $\mathbf{M}(\mathbf{Q})$. In a simple-cubic lattice, $\mathbf{Q} = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$.

Generalized susceptibility

Considering a static but position dependent magnetic field, we have

$$\delta\mathbf{M}_i = \sum_j \chi_{ij}\mathbf{H}_j \quad \Rightarrow \quad \delta\mathbf{M}(\mathbf{q}) = \chi(\mathbf{q})\mathbf{H}(\mathbf{q})\ , \tag{9}$$

where $\delta\mathbf{M}_i$ is the part of the magnetization induced by the applied field (which is not the whole magnetization if there is magnetic order), and

$$\chi(\mathbf{q}) = \sum_i \chi_{ij}\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\ . \tag{10}$$

As used for $J(\mathbf{q})$, the right-hand side of the above equation is independent of j due to invariance under lattice translations (with periodic boundary conditions).

The tensor $\chi(\mathbf{q})$ has components

$$\chi_{\alpha\beta}(\mathbf{q}) = \left.\frac{\partial M_\alpha(\mathbf{q})}{\partial H_\beta(\mathbf{q})}\right|_0\ , \tag{11}$$

where the index 0 indicates zero external field, and Greek indices refer to the usual orthogonal components of a vector.

Besides these general relations, in the context of Mean Field Theory we expect the magnetization of an intrinsically isotropic system to point in the direction of the **effective** field. We can then define a **scalar** quantity

$$\chi_L(\mathbf{H}^{\mathrm{eff}}) \equiv \frac{M(\mathbf{q})}{H^{\mathrm{eff}}(\mathbf{q})}\ , \tag{12}$$

known as *Langevin susceptibility*, so that

$$\mathbf{M}(\mathbf{q}) = \chi_L(\mathbf{H}^{\text{eff}})\mathbf{H}^{\text{eff}}(\mathbf{q}) \; . \tag{13}$$

Note that the Langevin susceptibility is **not** a linear-response coefficient.

Still considering an intrinsically isotropic system, the breakdown of isotropy introduced by magnetic order should keep the tensor $\chi(\mathbf{q})$ in diagonal form, with distinct parallel and perpendicular components relative to the ordering direction. We simplify the notation of these components to $\chi_\alpha(\mathbf{q})$, $\alpha = \parallel, \perp$. Using Eqs. (11) and (13), we have

$$\chi_\alpha(\mathbf{q}) = \frac{\partial M_\alpha(\mathbf{q})}{\partial H_\alpha^{\text{eff}}(\mathbf{q})} \frac{\partial H_\alpha^{\text{eff}}(\mathbf{q})}{\partial H_\alpha(\mathbf{q})} \equiv \chi_\alpha^{\text{eff}} \frac{\partial H_\alpha^{\text{eff}}(\mathbf{q})}{\partial H_\alpha(\mathbf{q})} \, , \tag{14}$$

where the limit $H \to 0$ is implied. With $\mathbf{H}^{\text{eff}}$ given by Eq. (6), we obtain

$$\frac{\partial H_\alpha^{\text{eff}}(\mathbf{q})}{\partial H_\alpha(\mathbf{q})} = 1 + 2J(\mathbf{q}) \frac{\partial M_\alpha(\mathbf{q})}{\partial H_\alpha(\mathbf{q})} = 1 + 2J(\mathbf{q})\chi_\alpha(\mathbf{q}) \; . \tag{15}$$

Therefore,

$$\chi_\alpha(\mathbf{q}) = \frac{1}{(\chi_\alpha^{\text{eff}})^{-1} - 2J(\mathbf{q})} \, , \tag{16}$$

with

$$\chi_\alpha^{\text{eff}} = \left[\chi_L(\mathbf{H}^{\text{eff}}) + \frac{\partial \chi_L(\mathbf{H}^{\text{eff}})}{\partial H_\alpha^{\text{eff}}} H_\alpha^{\text{eff}} \right]_0 \; . \tag{17}$$

Note that χ_α^{eff} does not depend on $\mathbf{q}$. Being related to the response of a single magnetic moment, it is a local quantity.

PM phase

If there is no spontaneous magnetization, the second term on the right-hand side of Eq. (17) is null, and $\chi_\alpha^{\text{eff}} = \chi_0 = C/T$, independent of direction, which results in the scalar susceptibility

$$\chi(\mathbf{q}) = \frac{C}{T - 2J(\mathbf{q})C} \; . \tag{18}$$

Choosing $\mathbf{Q}$ such that

$$J(\mathbf{Q}) = \max[J(\mathbf{q})] \, , \tag{19}$$

$\chi(\mathbf{Q})$ **diverges** at the temperature $T_{\mathbf{Q}}^{\text{MF}} = 2J(\mathbf{Q})C$. For a FM system, $\mathbf{Q} = \mathbf{0}$, while the AF case corresponds to $\mathbf{Q}$ given by Eq. (8). In both cases, $J(\mathbf{Q}) = z|J|$ in the nearest-neighbor approximation, and $T_{\mathbf{Q}}^{\text{MF}}$ reproduces T_C^{MF} or T_N^{MF}.

Ordered phase

In the presence of magnetic order, the effective field is not null at zero external field. Its components are

$$H_{0\parallel}^{\rm eff} = H_0^{\rm eff} = 2J(\mathbf{Q})M_0 \ , \qquad H_{0\perp}^{\rm eff} = 0 \ , \tag{20}$$

where M_0 is the magnitude of the spontaneous (FM) or sublattice (AF) magnetization.

The perpendicular susceptibility is easily determined, since

$$\chi_\perp^{\rm eff} = \chi_L(H_0^{\rm eff}) = \frac{M_0}{H_0^{\rm eff}} = \frac{1}{2J(\mathbf{Q})} \ , \tag{21}$$

so that Eq. (16) results in

$$\chi_\perp(\mathbf{q}) = \frac{1}{2[J(\mathbf{Q}) - J(\mathbf{q})]} \ . \tag{22}$$

This equation indicates that

- with FM order, the perpendicular uniform susceptibility diverges throughout the ordered phase (which reflects the possibility of rotating the magnetization direction without energy cost, due to the system's isotropy);
- in the AF case, $\chi_\perp(\mathbf{Q})$ diverges throughout the ordered phase ($\mathbf{Q}$ being the wavevector that defines the AF order), while the perpendicular **uniform** susceptibility is constant:

  $$\chi_\perp = \frac{1}{2[J(\mathbf{Q}) - J(\mathbf{0})]} \ .$$

  Note that this coincides with the uniform PM susceptibility [see Eq. (18)] at the transition temperature $T_N^{\rm MF}$.

It is somewhat more complicated to evaluate the parallel susceptibility in the ordered phase because the last term in Eq. (17) does not vanish. We must differentiate $\chi_L(\mathbf{H}^{\rm eff})$ with respect to the effective field before setting the external field to zero. It is simpler to use

$$\chi_\parallel^{\rm eff} = \frac{\partial M_0}{\partial H_0^{\rm eff}} = \beta S^2 B_S'(\beta S H_0^{\rm eff}) \ , \tag{23}$$

where the prime means derivative with respect to the function's argument, and $B_S(x)$ is the Brillouin function, introduced as $B_J(x)$ in Text 3, for magnetic moments associated to the total angular momentum. From what we have seen there about this function, we can write

$$B_S'(0) = \frac{S+1}{3S} = \frac{C}{S^2} \ , \tag{24}$$

C being the Curie constant. Then, defining

$$b_S \equiv \frac{B_S'(\beta S H_0^{\rm eff})}{B_S'(0)} \ , \tag{25}$$

and using Eq. (16), we can write

$$\chi_{\parallel}(\mathbf{q}) = \frac{C\, b_S}{T - 2J(\mathbf{q}) C\, b_S} \,. \tag{26}$$

Note that $b_S \to 1$ when $T \to T_C^{\rm MF}$ (or $T_N^{\rm MF}$), indicating the **same** divergence as in the PM phase (or continuity of the uniform susceptibility at $T_N^{\rm MF}$ in the AF case). On the other hand, b_S tends **exponentially** to zero for $T \to 0$, indicating that the parallel component of the susceptibility goes to zero in this limit, since the spins are close to their maximum average value.

FM system with finite applied field

With a finite applied field, the relation $M = SB_S(\beta S H^{\rm eff})$ shows that M only vanishes for $\beta \to 0$, i.e., $T \to \infty$, because the external field is a lower limit for $H^{\rm eff}$. Therefore, **there is no phase transition**, i.e., there is no critical temperature separating regions with $M = 0$ and $M \neq 0$. It should be noted that, as a consequence of this, the **experimental** curves of magnetization versus temperature are always "rounded", not giving a very accurate indication of the critical temperature, since measurements are made with a finite (although weak) applied field.

Anisotropic AF system with finite applied field

Unlike the FM case, a finite magnetic field yields a highly nontrivial situation at low temperatures with AF interactions. We will generalize the discussion by including an easy-axis anisotropy of type $D(S_i^z)^2$.

The most noticeable characteristic is that the uniform magnetization as a function of applied field shows a *metamagnetic* behavior at low temperatures. This means that there is a critical value of the applied magnetic field for which the magnetization jumps from a very low value to a sizable one.

There are different scenarios, depending on the relative importance of anisotropy and exchange interaction, as detailed below.

Weak anisotropy

- ***Field parallel to the easy axis*** – For low fields, the magnetization rises slowly with the field intensity, as the alignment of magnetic moments parallel to the field is strengthened, but the opposite orientation of the other sublattice does not allow much gain in Zeeman energy. At a critical field, the system undergoes a ***spin-flop*** transition: the AF order becomes **perpendicular** to the applied field (and hence, to the easy axis). This preserves the exchange energy, but the magnetic moments are tilted, developing a non-zero component parallel to the field. This

tilting increases until saturation, when the Zeeman energy is dominant even over the exchange interaction, and the spins are fully aligned with the magnetic field. It is interesting to notice that the AF phase for zero anisotropy is of spin-flop type for any non-zero applied field.

- ***Field perpendicular to the easy axis*** – Here the situation is essentially equivalent to the spin-flop phase, but without transition. The magnetization grows (almost linearly) with field until saturation.

Strong anisotropy

- ***Field parallel to the easy axis*** – In this case, the spin-flop transition does not occur because the orientation of moments parallel to the anisotropy axis is favored. However, when the field is sufficiently strong so that the Zeeman energy exceeds the exchange interaction, a ***spin-flip*** transition occurs: the magnetic moments of the down sublattice are reversed to parallel orientation with the field. Therefore, the magnetization jumps to near saturation.

- ***Field perpendicular to the easy axis*** – The behavior is the same as for weak anisotropy, but with a smaller slope.

Taking into account the effect of temperature, phase diagrams can be constructed as shown in Figs. 1 and 2. In these figures, solid lines are used for second-order transitions, and dashed lines for first-order ones. Note that the spin-flip and spin-flop transitions are first order since there is a discontinuity of the magnetization in both cases.

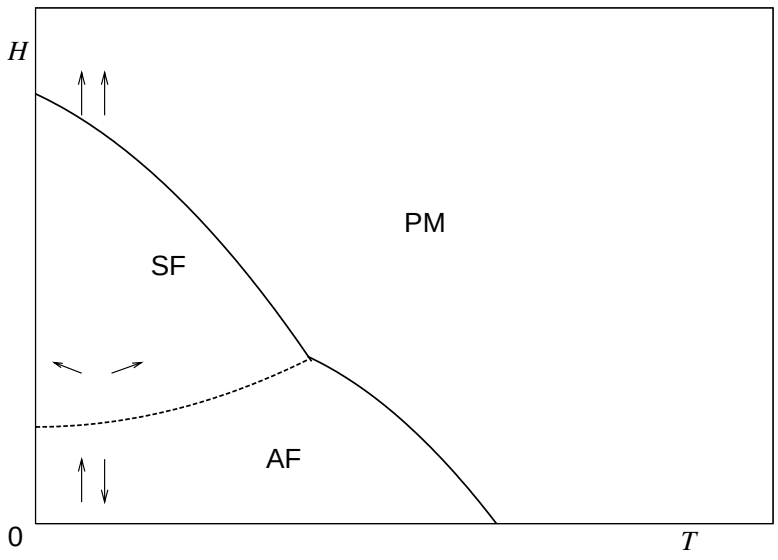

Figure 1: Schematic phase diagram for weak anisotropy. SF indicates the *spin-flop* phase.

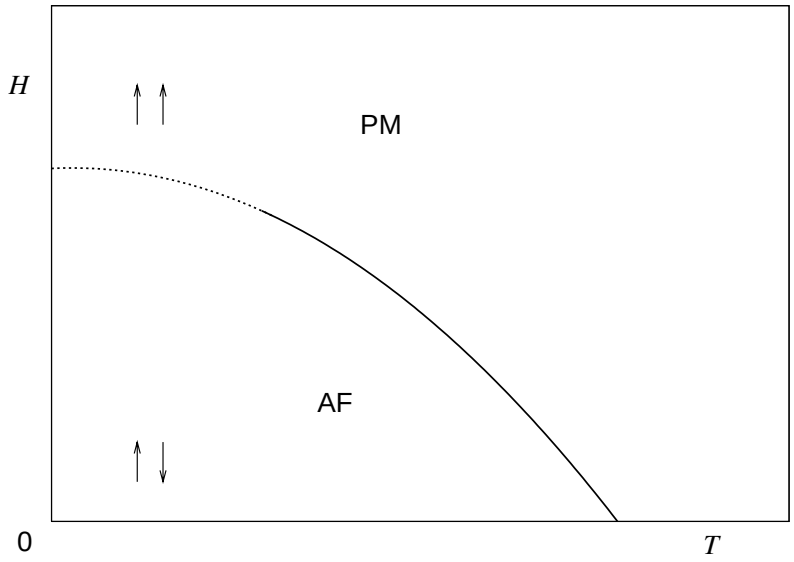

Figure 2: Schematic phase diagram for strong anisotropy (*spin-flip* case).

In Fig. 1, the two second-order lines (PM-AF, PM-SF) end at the same point at which a first-order line (AF-SF) also ends, characterizing a *bicritical point*. On the other hand, Fig. 2 shows the second-order line (PM-AF) ending at a *tricritical point*. It is called so because if we assumed the presence of a *staggered* field, with intensity and sign displayed on a third axis of the phase diagram, there would exist two additional second-order lines ending at this tricritical point.

Susceptibility and correlation functions

All points on second-order lines of type PM-AF (Figs. 1 and 2) are points where $\chi_{\parallel}(\mathbf{Q})$ diverges, while $\chi_{\perp}(\mathbf{Q})$ diverges at all points of a PM-SF line (Fig. 1). Although these susceptibility components refer to the PM phase, their evaluation is not trivial. The presence of anisotropy and of a finite applied field explicitly break rotational symmetry, preventing the use of Langevin's susceptibility.

In general, susceptibility components are related to spin correlation functions, as briefly commented at the end of Text 03. Here we must go back to it more carefully, because different spin components do not commute.

In the presence of a perturbative applied field, the Hamiltonian of a generic magnetic system can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \ , \quad \mathcal{H}_1 = -\sum_{i\alpha} H_i^{\alpha} S_i^{\alpha} \ , \tag{27}$$

where $\mathcal{H}_0$ contains all terms that do not vanish when the perturbative field goes to zero. These non-vanishing terms might even include a fixed finite field.

The magnetization components are given by

$$M_i^\alpha = \langle S_i^\alpha \rangle = \frac{\mathrm{Tr} e^{-\beta\mathcal{H}} S_i^\alpha}{\mathrm{Tr} e^{-\beta\mathcal{H}}} \, . \tag{28}$$

We need to make an expansion in powers of $\mathcal{H}_1$ in order to extract a linear term in the perturbative field. To do this we follow the usual procedure (interaction representation in Quantum Mechanics):

$$e^{-\beta\mathcal{H}} \equiv e^{-\beta\mathcal{H}_0}\mathcal{U}(\beta) \, , \tag{29}$$

$$\mathcal{U}(\tau) = e^{\mathcal{H}_0\tau} e^{-\mathcal{H}\tau} \, , \tag{30}$$

$$\frac{\partial\mathcal{U}}{\partial\tau} = -\mathcal{H}_1(\tau)\mathcal{U} \, , \quad \mathcal{H}_1(\tau) = e^{\mathcal{H}_0\tau}\mathcal{H}_1 e^{-\mathcal{H}_0\tau} \, , \quad \mathcal{U}(0) = 1 \, . \tag{31}$$

The solution is an **ordered** exponential,

$$\mathcal{U}(\tau) = \hat{T}_\tau \, e^{-\int_0^\tau d\tau' \, \mathcal{H}_1(\tau')} \, . \tag{32}$$

Explicitly writing $\mathcal{U}(\beta)$ as a perturbation series, and keeping only up to linear terms in $\mathcal{H}_1$, we have

$$\mathcal{U}(\beta) = 1 - \int_0^\beta d\tau \mathcal{H}_1(\tau) + \ldots \tag{33}$$

We are interested in the initial susceptibility, whose components are

$$\chi_{ij}^{\alpha\alpha'} = \left. \frac{\partial M_i^\alpha}{\partial H_j^{\alpha'}} \right|_0 \, . \tag{34}$$

The development (28 - 33), with $\mathcal{H}_1$ as given in Eq. (27), yields

$$\chi_{ij}^{\alpha\alpha'} = \int_0^\beta d\tau \left[\langle S_i^\alpha(\beta) S_j^{\alpha'}(\tau) \rangle_0 - \langle S_i^\alpha(\beta) \rangle_0 \langle S_j^{\alpha'}(\tau) \rangle_0 \right] \, , \tag{35}$$

where the subscript zero indicates unperturbed average. The right-hand side of this last equation was rearranged to reflect the order of subscripts on the left-hand side, which took one of the spins to the largest possible *time* β.

When applying this formalism to mean-field theory, one must note that the interaction part is turned into a magnetization-dependent term. This causes $\mathcal{H}_1$ to assume a more complex form than in Eq. (27),

$$\mathcal{H}_1 = -\sum_{i\alpha} \left[H_i^\alpha + 2\sum_l J_{il} \, \delta M_l^\alpha \right] S_i^\alpha = -\sum_{ij} \sum_{\alpha\alpha'} \left(\delta_{ij}\delta_{\alpha\alpha'} + 2\sum_l J_{il} \chi_{lj}^{\alpha\alpha'} \right) H_j^{\alpha'} S_i^\alpha \, , \tag{36}$$

where we used the first equality of Eq. (9). Rewriting in terms of wavevectors, and assuming axial symmetry, we have

$$\mathcal{H}_1 = -\sum_{\mathbf{q}\alpha} \left[1 + 2J(\mathbf{q})\chi_\alpha(\mathbf{q})\right] H_\alpha(\mathbf{q}) S_\alpha(-\mathbf{q}) \; . \tag{37}$$

Skipping some calculation details, we remark that the additional term in $\mathcal{H}_1$ yields the susceptibility as in Eq. (16), with $\chi_\alpha^{\rm eff}$ being determined by Eq. (35) **for the single-site effective problem**. Since we are interested in the PM-AF and PM-SF transitions, with an applied field H parallel to the easy axis (notice that it is **not** the perturbative field, which has already been set to zero), the unperturbed Hamiltonian takes the form

$$\mathcal{H}_0 = -H_0^{\rm eff} S_z - D S_z^2 \; , \quad D > 0 \; , \tag{38}$$

with $H_0^{\rm eff} = H - 2z|J|M_0$ (in the nearest-neighbor approximation), and $M_0 = \langle S_z \rangle_0$, which is nonzero even in the PM phase due to the presence of the applied field. Since S_z commutes with $\mathcal{H}_0$, evaluation of the z component is trivial, resulting in

$$\chi_z^{\rm eff} = \beta[\langle S_z^2 \rangle_0 - M_0^2] \, . \tag{39}$$

Here, in contrast to the isotropic case, $\langle S_z^2 \rangle_0$ does not have the constant value $S(S+1)/3$. The transverse component can be obtained from

$$\chi_x^{\rm eff} = \int_0^\beta d\tau \langle {\rm e}^{\mathcal{H}_0 \tau} S_x {\rm e}^{-\mathcal{H}_0 \tau} S_x \rangle_0 \; . \tag{40}$$

Using a basis of S_z eigenvectors, and the relation $S_x = (S^+ + S^-)$, the functions $\chi_z^{\rm eff}(T,H)$ and $\chi_x^{\rm eff}(T,H)$ can be evaluated (obviously also depending on the value of D). The result, inserted into Eq. (16), allows to obtain the transition temperatures and fields along second-order lines by solving the equation

$$2J(\mathbf{Q})\chi_\alpha^{\rm eff}(T_N, H) = 1 \; . \tag{41}$$

The highest T_N for a given H determines the actual transition temperature, while the susceptibility component and $\mathbf{Q}$ value indicate the type of order, remembering that $\mathbf{Q}$ is the value of $\mathbf{q}$ for which $J(\mathbf{q})$ is maximum. For the case illustrated in Fig. 1, $\chi_z^{\rm eff}$ gives larger values of T_N in the low-field region, while $\chi_x^{\rm eff}$ leads to the largest T_N at high fields.