Lecture note Magnetism (8)

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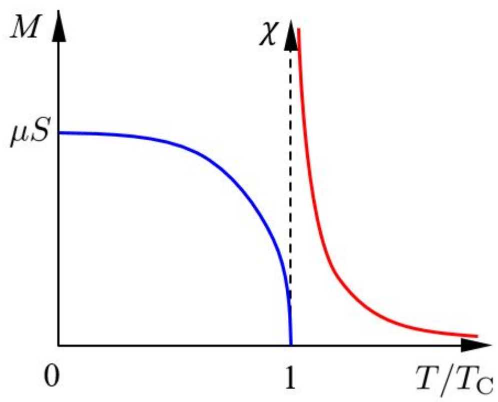


Fig. 5.1 Schematic drawing of susceptibility χ above T_C and spontaneous magnetization M below T_C for a ferromagnet.

Last week we introduced the Heisenberg model for magnetic insulators. In mean field (molecular field) approximation, the power series expansion of the Brillouin function (eq. (5.6)) gives the equation, which leads to the Curie-Weiss law:

$$\chi = \frac{\mu^2 S(S+1)}{k_B} \frac{1}{T - T_C}. \tag{5.8}$$

In the region $T < T_C$, the solutions of $M \neq 0$ exists for $B = 0$, i.e., the **spontaneous magnetization** appears. In the vicinity of T_C, the term of M^3 in eq. (5.6) is included to give the spontaneous magnetization as

$$M = \mu\sqrt{\frac{10}{3}} \frac{S(S+1)}{\sqrt{(S+1)^2 + S^2}} \sqrt{1 - \frac{T}{T_C}}. \tag{5.9}$$

On the other hand, at $T \ll T_C$, we use the asymptotic expression

$$B_S(x) \sim 1 - \frac{1}{S}\exp\left(-\frac{x}{S}\right) + \left[\frac{2S+1}{S}\exp\left(-\frac{2S+1}{S}x\right)\right] \tag{5.10}$$

for $x \gg 1$. The first two leading terms give

$$M = \mu\left[S - \exp\left(-\frac{3}{S+1}\frac{T_C}{T}\right)\right], \tag{5.11}$$

which approaches the perfect magnetization μS with $T \to 0$. The temperature dependences of χ and M obtained above are summarized schematically in Fig. 5.1.

5.2 Phenomenology of ferromagnetic transition: the GL theory

The above simple results still contains characteristic features of **cooperative phenomena**. For example, in eq. (5.8), $T \approx T_C$, we can write

$$\chi \propto \frac{1}{1 - (T_C/T)} = 1 + \frac{T_C}{T} + \left(\frac{T_C}{T}\right)^2 + \left(\frac{T_C}{T}\right)^3 + \cdots,$$

which expresses the following process: the effective field by the neighboring sites gives the excess polarization proportional to T_C/T, while the neighboring sites get the same excess polarizations that give the feedback of $(T_C/T)^2$. This series continues infinitely. The series reaches the radius of convergence at $T = T_C$ and the spontaneous magnetization appears there.

We know that even such a simple model includes a mechanism of the appearance of ferromagnetism. Then, here, we have a look on a very general properties of phase transitions and try to find the correspondence with the mean field approximation.

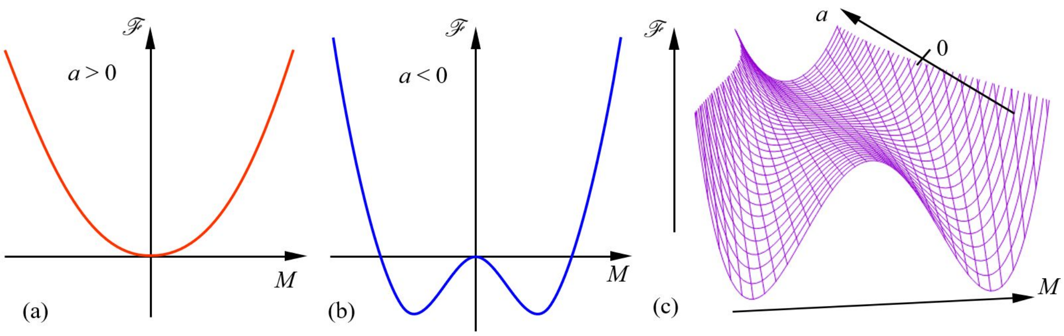


Fig. 5.2 Illustration of power expansion formula for the free energy $\mathscr{F}$ by M eq. (5.14). (a) Case $a \geq 0$. (b) case $a < 0$. In (c), a varies continuously through 0, and $\mathscr{F}$ is plotted in a wireframe.

5.2.1 Free energy

Here we introduce the **Ginzburg-Landau (GL)** theory of phase transition[1, 2]. This was constructed to understand superconductivity and superconducting transition phenomenologically. The GL theory, however, can be applied to a wide range of phase transition phenomena, and naturally have hugely been affecting the study of critical phenomena[3, 4]. In the theory, the free energy of the system is a function of physical quantities. In an equilibrium, the free energy should be at a minimum for the parameters "adjustable" by the system such as magnetization. In other words, the parameters take the values that make the free energy take a minimum. Let $\mathscr{F}$ be the free energy per spin, then we consider the functional form of $\mathscr{F}(M)$, where M is the magnetization per spin.

In order to consider the symmetry of the system, we turn off the magnetic field in the Hamiltonian in eq. (5.1), which reduces the symmetry. Now we perform a kind of symmetry operation of spin inversion on all sites, namely

$$\forall i \;\; \boldsymbol{S}_i \to -\boldsymbol{S}_i.$$

For this operation, the Hamiltonian in eq. (.1) with $\boldsymbol{B} = 0$ is invariant. Accordingly $\mathscr{F}$ is unchanged. On the other hand, from the definition,

$$\boldsymbol{M} = \langle \boldsymbol{S}_i \rangle \to \langle -\boldsymbol{S}_i \rangle = -\boldsymbol{M}, \tag{5.12}$$

that is the parameter M is inverted. The above inference leads to

$$\mathscr{F}(M) = \mathscr{F}(-M), \tag{5.13}$$

namely $\mathscr{F}$ is an even function of M. Therefore we can expand $\mathscr{F}$ to the power series of small M (hence close to the transition) to the forth order as

$$\mathscr{F}(M) = \mathscr{F}_0 + aM^2 + bM^4. \tag{5.14}$$

First in eq. (5.14), to have a stable point of $\mathscr{F}$ at finite M, b should be positive ($b > 0$). Under this condition, a positive a ($a \geq 0$) always gives $M = 0$ as the stable point of $\mathscr{F}$ as in Fig. 5.2(a). For $a < 0$, two finite values of M give energy minima, hence are stable points, lower than the energy for $M = 0$ as in Fig. 5.2(b). The equation which gives the stable points is

$$\frac{\partial \mathscr{F}}{\partial M} = 0 = 2aM + 4bM^3 = 2M(2bM^2 + a), \tag{5.15}$$

which is in the same form as in eq. (5.6), thus is the same equation. This is sometimes called "magnetic equation of state." As in Fig. 5.2, the system is paramagnetic for (a) $a \geq 0$, and ferromagnetic for (b) $a < 0$. We now find that a is a parameter: i) which determines $\mathscr{F}(M)$; ii) which has no anomaly at zero, the transition point of M. Therefore a is a "relevant" parameter for the transition (in a sense, a parameter that drives the transition). a must vary in the first order for thermodynamic parameters like temperature, pressure, etc. Figure 5.2(c) shows such continuous change in $\mathscr{F}(M)$ with the variation of a, and the appearance of stable points other than $M = 0$ at the transition point $a = 0$. This indicates that we are considering a second order phase transition, which does not have latent heat at the ferromagnetic transition. If we take temperature T as the relevant parameter of the transition, a should be in the first order of T. As the expression of a, which is zero at the transition point and in the first order in T, we can write $a = k(T_C - T)/T_C$. Then a finite solution of M_0 for eq. (5.15) is given by

$$M_0 = \sqrt{-\frac{a}{2b}} = \sqrt{\frac{k(T_C - T)}{2bT_C}}. \tag{5.16}$$

5.2.2 Spontaneous symmetry breaking

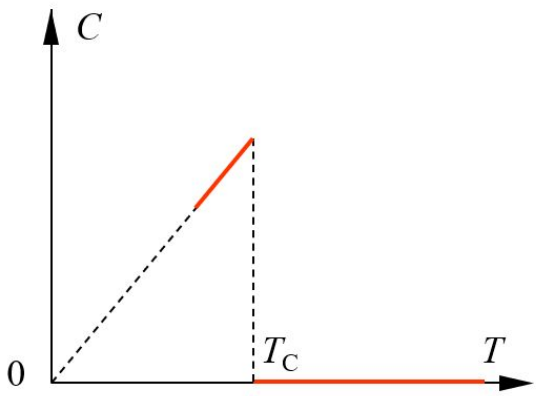
In the region $T \leq T_C$, $\mathscr{F}(\pm M_0)$ are the thermodynamically stable solutions, in which $\langle M \rangle = M_0$ or $-M_0$. These correspond to the **spontaneous magnetization** of ferromagnets, which was introduced in the first lecture [*1]. For the expansion of eq. (5.14), we have used the symmetry of free energy (5.13) deduced from the symmetry of Hamiltonian (5.1) for the symmetry operation $\forall i : \boldsymbol{S}_i \to -\boldsymbol{S}_i$. In the region $T < T_C$, $M = 0$ is unstable and one of stable solutions $\pm M_0$ is realized. Due to (5.13), the symmetry operation does not change the free energy, but now M is the parameter determining the state of the system. That means the operation changes the state. The situation is summarized that the symmetry of realized state is broken while that of the system (Hamiltonian) is kept. Such a phenomenon is called **spontaneous symmetry breaking**. The concept was introduced by Yoichiro Nambu[5, 6, 7] from the analogy of the BCS theory (and the Bogoliubov theory) for superconductivity and the mechanism for the appearance of particle mass. It is one of the basic concepts in physics, has been widely applied to a variety of phenomena under active research. There are many textbooks including the one for general public written by Nambu himself[8, 9, 10, 11].

The continuous spatial symmetry in the original system with random direction of spins is broken in the state with spontaneous magnetization M_0, in which the spins are in order pointing a single point in space. The parameter that appears at the critical point and represents the order of the state is called **order parameter**.

5.3 Critical exponent

$\mathscr{F}$ in the presence of spontaneous magnetization M_0 is given as a function of temperature as

$$\mathscr{F}(T) = \mathscr{F}_0 + aM_0^2 + bM_0^4 = \mathscr{F}_0 - \frac{a^2}{4b} = \mathscr{F}_0 - \frac{k^2(T_C - T)^2}{4bT_C^2}. \tag{5.17}$$



Then in $T \leq T_C$, the specific heat C is given by

$$C = -T\frac{\partial^2 \mathscr{F}}{\partial T^2} = \frac{k^2 T}{2bT_C^2}. \tag{5.18}$$

On the other hand in $T \geq T_C$, $C = 0$ because $M_0 = 0$ and $\mathscr{F}(T) = \mathscr{F}_0$. Then the specific heat has a jump of

$$\Delta C = \frac{k^2}{2bT_C}, \tag{5.19}$$

at $T = T_C$ which is illustrated in the left.

Now when a small magnetic field is introduced, in the lowest order approximation, we can replace the term of external

[*1] As also introduced in the lecture, in practice, with zero-field cooling from above the Curie temperature, we cannot observe macroscopic spontaneous magnetization due to the formation of magnetic domains, which build up magnetic circuit and confine the magnetic flux inside.

field in Hamiltonian (5.1) with $-BM$, where M is the magnetization. That is we add the first order term as

$$\mathscr{F}(M) = \mathscr{F}_0 + aM^2 + bM^4 - BM. \tag{5.20}$$

Then from

$$\frac{\partial \mathscr{F}}{\partial M} = 0 = 2aM + 4bM^3 - B, \tag{5.21}$$

we get $M^3 \propto B$ just at the critical point $T = T_\mathrm{C}$ because $a = 0$.

So far we have obtained the expressions for magnetization M, susceptibility χ and specific heat C in the forms of

$$M \propto \begin{cases} B^{1/\delta} & (T = T_\mathrm{C}), \\ (T_\mathrm{C} - T)^\beta & (T < T_\mathrm{C}), \end{cases} \tag{5.22a}$$

$$\chi \propto \begin{cases} (T - T_\mathrm{C})^{-\gamma} & (T > T_\mathrm{C}), \\ (T_\mathrm{C} - T)^{-\gamma'} & (T < T_\mathrm{C}), \end{cases} \tag{5.22b}$$

$$C \propto \begin{cases} (T - T_\mathrm{C})^{-\alpha} & (T > T_\mathrm{C}), \\ (T_\mathrm{C} - T)^{-\alpha'} & (T < T_\mathrm{C}). \end{cases} \tag{5.22c}$$

As above, we pick up a relevant parameter, which drives a phase transition in the system, and consider the shift from the critical value. The power indices of the "shift" in the functional expressions of physical quantities are called **critical exponents**. This is particularly important concept in the second order phase transitions. The above symbols α, β, γ, δ, $\cdots$ are habitually used in the field of magnetism and statistical physics. There is an anomaly of jump for the specific heat in eq. (5.22c), we apply the forms of critical exponent separately for $T < T_\mathrm{C}$ and for $T_\mathrm{C} < T$. In both cases the main term is a constant in the expression of $T - T_\mathrm{C}$, hence $\alpha = \alpha' = 0$.

The critical exponents depend on symmetry, dimension, range of interaction, way of approximation, etc. of the model. On the other hand, the variations in the system parameters do not change the exponents. The property is expressed as the critical exponents have **universality**. Further, we can classify the theoretical models (including approximations) of phase transitions with the set of the values of critical exponents. This classification called **universality class**, depends, as we saw in the introduction of the GL theory, often symmetry of the system. The universality class is also determined by general properties of the system such as the spatial dimension, the range of interaction. The next table summarizes the values of critical exponents in the mean field theory.

Critical exponent	α	β	γ	δ
Mean field approximation	0	1/2	1	3

Though we have introduced the concept of universality class, the model examined is only the mean field theory of Heisenberg model. We would like to have a short look at the other models.

5.4 Theoretical models of ferromagnet (localized spins)

The theoretical models of magnetic materials are the big stage for statistical physics. In the above we consider the Heisenberg model as ferromagnetic insulators. In the Heisenberg model, the spin variable has three components $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$. In the **XY model**, the spin components are limited to two, that is $\boldsymbol{S}_i = (S_i^x, S_i^y)$. In the **Ising model**, the spin has a single component. In the Heisenberg model and the XY model, the spin degree of freedom takes a continuous value while in the Ising model it is quantized to the two values.

5.4.1 XY model

First we pick up a direction for "angle zero," then because the spins in this model are in the two-dimensional plane, we can assign an angle ϕ_i for each site i measured from the angle zero. Then the angle between the spins at sites i and j is $\phi_i - \phi_j$. Accordingly the Hamiltonian of the XY model can be written as

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j). \tag{5.23}$$

In the two dimensional XY model, there is no long range order due to the Mermin-Wagner theorem though it has another type of phase transition, in which the order parameter decreases not with exponential damping but with power of distance damping. The transition is called Berezinskii-Kosterlitz-Thouless (BKT) transition[12]. The BKT transition is caused by excitations called vortices, in which the spins form rotation structures. They have two possible directions of rotation, and we distinguish them with the naming vortex and anti-vortex. An attractive force works between a vortex and an anti-vortex, which form a vortex pair bound state. The bound states are more stable than free unbound vortices. In the low temperature phase all vortices are bound into pairs. With increasing temperature the number of vortex pairs increases and at the transition point free unbound vortices appear due to the weakening of attractive force by screening. This can be taken as a two-dimensional melting transition.

It is easier to realize the XY model (5.23) in superconducting Josephson networks than in spin systems[13]. A Josephson network is an arrangement of superconducting islands and junctions connecting them. They can be prepared by e.g., lithography, or growth of granular films. We can write the phase of superconducting order parameter on each plaquette (island) i as ϕ_i[*2]. Then the summation of Josephson energy is written in the form of (5.23). Also two-dimensional vortices mentioned above appear in a thin film of superfluid on a plate (the film flow effect). Hence observation of the BKT transition has been reported in such systems.

5.4.2 Ising model

The name of the Ising model comes from Ernst Ising, who showed the solution of this model in the case of nearest neighbor interaction[14]. It can be expressed by the Hamiltonian:

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i, \tag{5.24}$$

where i, j are indices of the lattice. S_i is the Ising spin on i, which takes values ± 1. In the second term μB is written as h for simplicity. The Ising model may be the most known model of magnetic materials. The model is so simple, and overall, not only the solution by Ernst Ising for one-dimensional model, but also the rigorous solution of two-dimensional model in the absence of magnetic field[15] are the base of study for various physics in this system.

The critical exponents of these models are listed in the following table[16]. What is written using the decimal point is the value obtained by the computation with the Monte Carlo method.

Model (Universality class)	α	β	γ	δ
2D Ising	0	1/8	7/4	15
3D Ising	0.115	0.324	1.239	4.82
3D XY	−0.01	0.34	1.32	4.9
3D Heisenberg	−0.11	0.36	1.39	4.9
Mean field approximation	0	1/2	1	3

*2 This quantity is not gauge invariant, not an observable. However the phase difference appears in the Hamiltonian is a gauge invariant observable.

5.5 Anti-ferromagnetic Heisenberg model

Next we consider the case when the interaction is anti-ferromagnetic ($J < 0$) in the Heisenberg model:

$$\mathscr{H} = -2J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \mu \sum_i \boldsymbol{B} \cdot \boldsymbol{S}_i. \tag{5.1}$$

We consider a two dimensional square lattice with nearest neighbor interaction. When the system is in the anti-ferromagnetic order, the classical ground state of two-dimensional square lattice Heisenberg model is a Néel ordering state, in which the neighboring spins are in anti-parallel order. We divide the entire crystal lattice into A and B sublattices, and consider a state in which the spins are parallel in each lattice. In the treatment of ferromagnetic Heisenberg model, we first applied an external magnetic field to give direction to the isotropic space[*3]. In the anti-ferromagnetic case, we take a similar method. This time as in the right panel of Fig. 5.3, we need to prepare the field that changes the direction alternatively with site[17]. Anyway the alternative field will be set to zero in the ordered state. We consider the starting state as the moments are alternatively aligned with the alternative field with oblique angle due to the external magnetic field as illustrated in the right panel of Fig. 5.3.

Let $\boldsymbol{B}_\mathrm{u}$ be the external constant field, $\pm\boldsymbol{B}_\mathrm{s}$ be the site-alternative field. The fields on the two kinds of sites are

$$\left.\begin{aligned} \boldsymbol{B}_\mathrm{A} &= \boldsymbol{B}_\mathrm{u} + \boldsymbol{B}_\mathrm{s}, \\ \boldsymbol{B}_\mathrm{B} &= \boldsymbol{B}_\mathrm{u} - \boldsymbol{B}_\mathrm{s}. \end{aligned}\right\} \tag{5.25}$$

The effective Hamiltonian of the molecular field approximation is

$$\mathscr{H}_\mathrm{eff}(i) = -2J \sum_\delta \langle \boldsymbol{S}_{i+\delta} \rangle \cdot \boldsymbol{S}_i - \mu \boldsymbol{B}_\mathrm{A} \cdot \boldsymbol{S}_i \quad (i \in \mathrm{A}), \tag{5.26a}$$

$$\mathscr{H}_\mathrm{eff}(j) = -2J \sum_\delta \langle \boldsymbol{S}_{j+\delta} \rangle \cdot \boldsymbol{S}_j - \mu \boldsymbol{B}_\mathrm{B} \cdot \boldsymbol{S}_j \quad (j \in \mathrm{B}). \tag{5.26b}$$

The averaged magnetic moments at the two sites are

$$\left.\begin{aligned} \boldsymbol{M}_\mathrm{A} &= \mu \langle \boldsymbol{S}_i \rangle = \boldsymbol{M}_\mathrm{u} + \boldsymbol{M}_\mathrm{s} \\ \boldsymbol{M}_\mathrm{B} &= \mu \langle \boldsymbol{S}_j \rangle = \boldsymbol{M}_\mathrm{u} - \boldsymbol{M}_\mathrm{s} \end{aligned}\right\}. \tag{5.27}$$

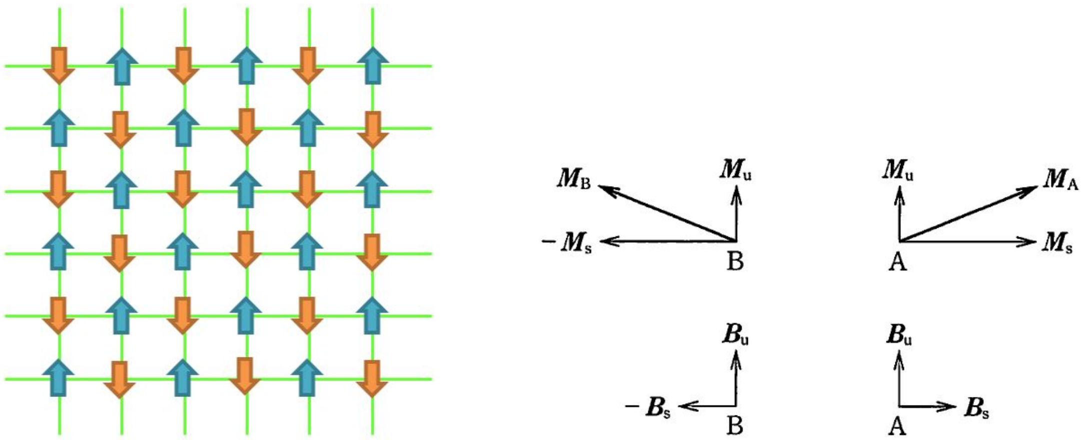


Fig. 5.3 Left: Illustration of Néel anti-ferromagnetic order. Right: Drawing of “seeds field” to set the spins around the anti-ferromagnetic order. From [17].

*3 In theories, without such “seeds” field, the system continues to take the unstable solution.

We here define the Brillouin "vector" function as

$$\vec{B}_S(\boldsymbol{x}) = B_S(x)\frac{\boldsymbol{x}}{x}. \tag{5.28}$$

Then the self-consistent equation is written as [*4],

$$\boldsymbol{M}_\mathrm{u} + \boldsymbol{M}_\mathrm{s} = \mu S \vec{B}_S \left\{ \frac{\mu S}{k_\mathrm{B}T} \left[\boldsymbol{B}_\mathrm{u} + \boldsymbol{B}_\mathrm{s} + \frac{2\alpha_z J}{\mu^2}(\boldsymbol{M}_\mathrm{u} - \boldsymbol{M}_\mathrm{s}) \right] \right\}. \tag{5.29}$$

Above the critical temperature $T > T_\mathrm{N}$, from $\vec{B}_S(\boldsymbol{x}) \sim (S+1)\boldsymbol{x}/3S$, we write

$$\boldsymbol{M}_\mathrm{u} + \boldsymbol{M}_\mathrm{s} = \chi_0 \left[\boldsymbol{B}_\mathrm{u} + \boldsymbol{B}_\mathrm{s} + \frac{2\alpha_z J}{\mu^2}(\boldsymbol{M}_\mathrm{u} - \boldsymbol{M}_\mathrm{s}) \right]. \tag{5.30}$$

The definition of χ_0 is in eq. (5.6).

Then **uniform susceptibility** χ_u, and **sublattice susceptibility** χ_s are given by

$$\chi_\mathrm{u} = \lim_{B_\mathrm{u}\to 0} \frac{M_\mathrm{u}}{B_\mathrm{u}} = \chi_0 \left(1 - \frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1}, \tag{5.31a}$$

$$\chi_\mathrm{s} = \lim_{B_\mathrm{s}\to 0} \frac{M_\mathrm{s}}{B_\mathrm{s}} = \chi_0 \left(1 + \frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1}. \tag{5.31b}$$

Because $J < 0$, χ_u does not diverge. On the other hand χ_s diverges at **Néel temperature**

$$k_\mathrm{B}T_\mathrm{N} = \frac{2}{3}S(S+1)\alpha_z|J|. \tag{5.32}$$

Hence with $\boldsymbol{B}_\mathrm{s} \to 0$, we have **sublattice spontaneous magnetization** $\boldsymbol{M}_\mathrm{s}$.

From the expansion around the spontaneous magnetization $\boldsymbol{M}_\mathrm{s}$,

$$\boldsymbol{M}_\mathrm{u} + \boldsymbol{M}_\mathrm{s} = \mu S \left[\vec{B}_S \left(\frac{\mu S}{k_\mathrm{B}T} \frac{-2\alpha_z J}{\mu^2} \boldsymbol{M}_\mathrm{s} \right) + \frac{d}{dM_\mathrm{s}} B_S \left(\frac{\mu S}{k_\mathrm{B}T} \frac{-2\alpha_z J}{\mu^2} \boldsymbol{M}_\mathrm{s} \right) \left(-\boldsymbol{M}_\mathrm{u} - \frac{\mu^2}{2\alpha_z J}\boldsymbol{B}_\mathrm{u} \right) \right]. \tag{5.33}$$

From the first term in the rhs, we obtain the self-consistent equation for M_s as

$$M_\mathrm{s} = \mu S B_S \left(\frac{\mu S}{k_\mathrm{B}T} \frac{-2\alpha_z J}{\mu^2} M_\mathrm{s} \right). \tag{5.34}$$

By taking derivative of both sides with M_s we know

$$1 = \mu S \frac{d}{dM_\mathrm{s}} B_S \left(\frac{\mu S}{k_\mathrm{B}T} \frac{-2\alpha_z J}{\mu^2} M_\mathrm{s} \right).$$

Then from the second term in the rhs of eq. (5.33), we obtain

$$\boldsymbol{M}_\mathrm{u} = -\boldsymbol{M}_\mathrm{u} - \frac{\mu^2}{2\alpha_z J}\boldsymbol{B}_\mathrm{u}. \tag{5.35}$$

And from $\boldsymbol{M}_\mathrm{u} = -\mu^2 \boldsymbol{B}_\mathrm{u}/4\alpha_z J$, the uniform susceptibility is obtained as

$$\chi_\mathrm{u} = \lim_{B_\mathrm{u}\to 0} \frac{M_\mathrm{u}}{B_\mathrm{u}} = -\frac{\mu^2}{-4\alpha_z J}. \tag{5.36}$$

The above results are illustrated in Fig. 5.4.

[*4] $\alpha_z = 4$ in the present case

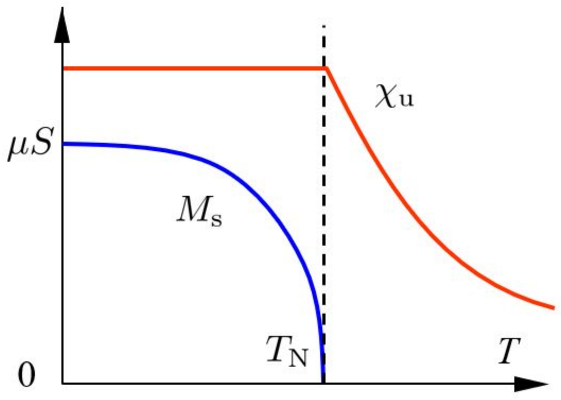


Fig. 5.4 Illustration of (uniform) susceptibility and sub-lattice spontaneous magnetization in anti-ferromagnetic Heisenberg model.

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