Mean field theory

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Abstract

The magnetic property of systems is one of the fundamental properties in solid state physics. Using SQUID (superconducting quantum interference device) magnetometer, in recent years one can easily and exactly measure the magnetization and magnetic susceptibility of many systems (one-, two-, and three-dimensional magnets) as a function of temperature and magnetic field. The authors have been studying on the magnetic phase transitions of low dimensional systems (in particular quasi two-dimensional systems and spin glass systems) for many years. This lecture note was written based on our experience. So we think that this note may be useful to graduate students and undergraduate students who want to study the magnetism experimentally.

Here we consider the critical behaviors of a simple ferromagnetic system which undergoes a ferromagnetic phase transition (the second order) at the Curie temperature T_c. The spontaneous magnetization as an order parameter, starts to appear below T_c. The magnetic susceptibility diverges as the temperature approaches T_c from both sides. These critical behaviors are explained in terms of a mean-field theory. The Curie-Weiss law, the temperature dependence of the spontaneous magnetization, and the mean-field exponents of the magnetization and magnetic susceptibility are discussed using this mean-field theory.

The mean-field theory begins with the van der Waals equation of state (van der Waals 1873) for the liquid-gas transition and the Weiss (1906) molecular field theory for ferromagnetism. The mean-field theory is an example of approximate solution. Onsager's theory of the Ising model is an example of an exact solution. While the mean-field theory often seems too crude, the exact solutions are too complicated. A peculiar feature of critical phenomena is that there is very little one can do to improve the mean-field theory substantially without solving the problem exactly. This makes the theory of critical phenomena a very difficult field. The major disadvantage of the mean-field theory is that the effect of fluctuations is ignored. It turns out to be difficult to understand and to analyze mathematically the effect of fluctuations (S.K. Ma[1]).

Content

10. Critical behavior of the second-order phase transitions
11. Conclusion

1. Magnetization for the spin 1/2 system[1-6]

We discuss the magnetization for spin 1/2. The system consists of many spins (N_A; Avogadro number). There is no interaction between any two spins. The magnetic moment of spin ($S = 1/2$) is given by

$$\hat{\mu}_z = -2\mu_B \hat{S}_z / \hbar = -\mu_B \hat{\sigma}_z ,$$

where $\hat{\sigma}_z$ is a Pauli spin operator along the z axis. Then the spin Hamiltonian (Zeeman energy) is described by

$$\hat{H} = -\hat{\mu}_z B = \mu_B \hat{\sigma}_z B , \qquad (1)$$

in the presence of a magnetic field B along the z axis, where the Bohr magneton μ_B is given by

$$\mu_B = \frac{e\hbar}{2mc} \quad (e>0).$$

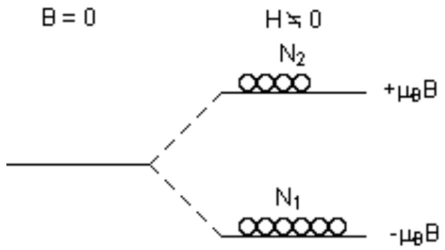


Fig.1 Zeeman splitting of the degenerate state under the application of magnetic field B.

The doublet state (degenerate) is split into two states:

1. lower energy level ($-\mu_B B$): state $\left|-\right\rangle$; μ_B (magnetic moment)
2. upper energy state ($\mu_B B$): state $\left|+\right\rangle$; - μ_B (magnetic moment)

The probability of finding the system in the lower state

$$\frac{N_1}{N_A} = \frac{e^x}{e^x + e^{-x}}$$

where $x = \mu_B B/(k_B T)$. The probability of finding the system in the upper state is

$$\frac{N_2}{N_A} = \frac{e^{-x}}{e^x + e^{-x}}$$

The total magnetization M is

$$M = \mu_B (N_1 - N_2) = N_A \mu_B \left(\frac{e^x - e^{-x}}{e^x + e^{-x}} \right) = N_A \mu_B \tanh x \,. \tag{2}$$

For x<<1, tanh(x) ≈ x. Then we have

$$M = N_A \mu_B \left(\frac{\mu_B B}{k_B T} \right) = \frac{N_A \mu_B{}^2}{k_B T} B \,. \tag{3}$$

The magnetic susceptibility (molar) is defined as

$$\chi_M = \frac{M}{B} = \frac{N_A \mu_B{}^2}{k_B T} = \frac{N_A \mu_B{}^2}{3 k_B T} g^2 S(S+1) \,. \tag{4}$$

where g is a Landé g-factor and $g = 2$ for $S = 1/2$. We introduce the effective magnetic moment P_{eff};

$$P_{eff} = g\sqrt{S(S+1)} \,. \tag{5}$$

Then the susceptibility obeys a Curie law

$$\chi_M = \frac{C_M}{T} \,. \tag{6}$$

where C_{M} is the Curie constant and is defined by

$$C_M = \frac{N_A \mu_B{}^2}{3 k_B} P_{eff}{}^2 = 0.125049\ P_{\mathrm{eff}}^2 \approx P_{\mathrm{eff}}^2/8. \tag{7}$$

For x»1, tanh(x) ≈ 1. Then we have a saturation magnetization

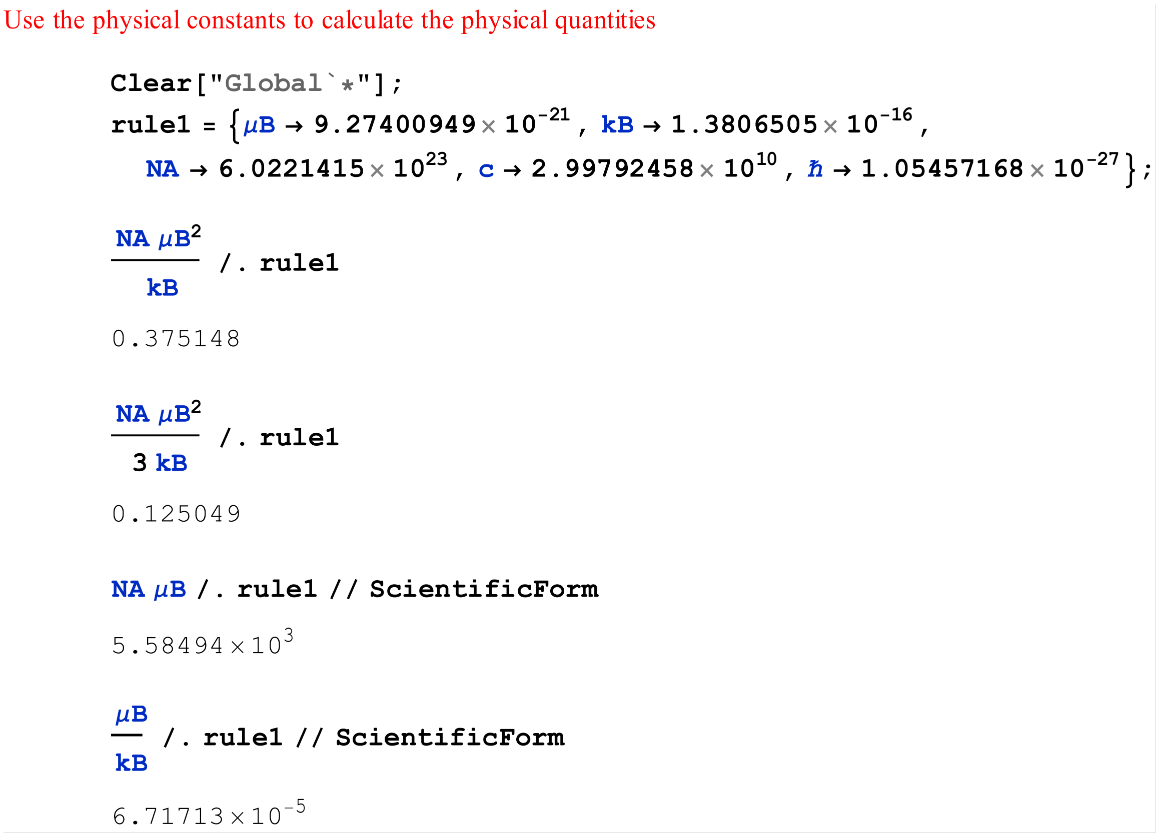
$$M_s = N_A \mu_B g S = N_A \mu_B = 5.58494 \times 10^3 \text{ emu}. \tag{8}$$

Note that

μ_B = 9.2740094910 × 10^{-21} emu.

1 emu = erg/Gauss.

((Mathematica))



Use the physical constants to calculate the physical quantities

```
Clear["Global`*"];
rule1 = {μB → 9.27400949 × 10^-21 , kB → 1.3806505 × 10^-16 ,
   NA → 6.0221415 × 10^23 , c → 2.99792458 × 10^10 , ℏ → 1.05457168 × 10^-27};

NA μB^2
─────── /. rule1
  kB

0.375148

NA μB^2
─────── /. rule1
 3 kB

0.125049

NA μB /. rule1 // ScientificForm

5.58494 × 10^3

μB
── /. rule1 // ScientificForm
kB

6.71713 × 10^-5
```

2. Brillouin function[4]

We discuss the magnetization in general cases (J). In this case, the magnetic moment is given by

$$\hat{\mu}_z = -g_J \mu_B \hat{J}_z \, , \tag{9}$$

where $\hat{J}_z$ is the (dimensionless) angular momentum ($J_z = J, J\text{-}1, \ldots, \text{-}J$), and g_J is a Landé g-factor. Then the spin Hamiltonian (Zeeman energy) is described by

$$\hat{H} = -\hat{\mu}_z B = -(-g_J \mu_B \hat{J}_z) B = g_J \mu_B \hat{J}_z B \, , \tag{10}$$

in the presence of a magnetic field B. Under the magnetic field, the degenerate ground state is split into ($2J$+1) states. The energy level and the magnetic moment for each state are given by

$$\varepsilon(J_Z) = g\mu_B B J_z \text{ and } \mu(J_z) = -g_J \mu_B J_z \, , \tag{11}$$

respectively. The magnetization M at T is given by

$$\begin{aligned}
M &= N_A\langle \mu(J_z)\rangle \\
&= -N_A g_J \mu_B \langle J_z\rangle \qquad , \qquad\qquad (12) \\
&= N_A g_J \mu_B \frac{\sum\limits_{J_z=-J}^{J}(-J_z)e^{-\beta\varepsilon(J_z)}}{\sum\limits_{J_z=-J}^{J} e^{-\beta\varepsilon(J_z)}}
\end{aligned}$$

where $\beta = 1/(k_B T)$. For simplicity we put

$$x = \frac{g_J \mu_B J B}{k_B T}. \qquad (13)$$

Then we have

$$\begin{aligned}
M &= N_A g_J \mu_B \frac{\sum\limits_{J_z=-J}^{J}(-J_z)e^{-\frac{x}{J}J_z}}{\sum\limits_{J_z=-J}^{J} e^{-\frac{x}{J}J_z}} \qquad , \qquad\qquad (14) \\
&= N_A g_J \mu_B J \frac{d}{dx}\ln\Big(\sum_{J_z=-J}^{J} e^{-\frac{x}{J}J_z}\Big) = N_A g_J \mu_B J B_J(x)
\end{aligned}$$

where $B_J(x)$ is the Brillouin function and is defined by

$$B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{1}{2J}x\right). \qquad (15)$$

((Mathematica))

Derivation of Brillouin function

```
Clear["Global`*"];
f1 = Sum[ Exp[-x/J Jz], {Jz, -J, J}] //
   ExpToTrig // TrigFactor;

h1 = D[Log[f1], x] // Simplify
```

$$\frac{-\mathrm{Coth}\left[\frac{x}{2\,J}\right] + (1 + 2\,J)\,\mathrm{Coth}\left[x + \frac{x}{2\,J}\right]}{2\,J}$$

Property of $B_J(x)$

(i) $\lim_{J\to\infty} B_J(x) = L(x) = \coth x - \frac{1}{x}$; $L(x)$ is a Langevin function. (16)

(ii) $\lim_{x\to 0} B_J(x) = \frac{J+1}{3J}x$. (17)

(iii) $\lim_{x\to\infty} B_J(x) = 1$. (18)

For x<<1,

$$M = N_A g_J \mu_B J B_J(x) = \frac{N_A g_J{}^2 \mu_B{}^2}{3k_B T} J(J+1)B. \qquad (19)$$

The susceptibility (molar) is given by

$$\chi = \frac{M}{B} = \frac{N_A \mu_B{}^2}{3k_B T} g_J{}^2 J(J+1) = \frac{C_M}{T}, \qquad (20)$$

where C_M is the Curie constant and is defined by

$$C_M = \frac{N_A \mu_B{}^2}{3k_B} g_J{}^2 J(J+1) = \frac{N_A \mu_B{}^2}{3k_B} P_{eff}{}^2 \approx \frac{1}{8} P_{eff}{}^2, \qquad (21)$$

and P_{eff} is the effective magnetic moment (dimensionless);

$$P_{eff} = g_J\sqrt{J(J+1)}.$$

For $x\to\infty$, we have a saturation magnetization M_s,

$$M_s = N_A g_J \mu_B J. \qquad (22)$$

((**Note**))

The Curie law gives direct evidence that the ground state is degenerate in the absence of an external magnetic field.

((**Note**))

Conventionally we use emu for the unit of the susceptibility, in stead of emu/Oe. emu=erg/Oe = erg/Gauss. erg = Gauss cm^3.

3. Calculation of *M* vs *B/T*[4]

The Landé *g*-factor g_J is defined by

$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}, \tag{23}$$

where *L* and *S* are orbital and spin angular momentum, respectively. We define the magnetization per unit atom as

$$\widetilde{M} = \frac{M}{N_A \mu_B} = g_J J B_J(x), \tag{24}$$

where

$$x = \frac{g_J \mu_B J B}{k_B T}$$

For the iron group ions (Cr^{3+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, …), the orbital angular momentum is *quenched*. In this case the magnetization is given by Eq.(24) with $J = S$. Although g_J is equal to 2 theoretically, for convenience we use the notation $g_J = g$. The value of *g* is not equal to 2 in real systems.

((**Note**)) $S = 5/2$ for Mn^{2+} with $(3d)^5$ electron configuration, $S = 1$ for Ni^{2+} with $(3d)^8$ electron configuration, and $S = 1/2$ for Cu^{2+} with $(3d)^9$ electron configuration (see Hund rule[4]).

((Mathematica))

Property of the Brillouin function

```
Clear["Global`*"];
```

$$\text{BJ}[x\_] := \left(\frac{2\,J+1}{2\,J}\ \text{Coth}\left[\frac{2\,J\,+\,1}{2\,J}\ x\right] - \frac{1}{2\,J}\ \text{Coth}\left[\frac{1}{2\,J}\ x\right]\right);$$

```
Series[BJ[x], {x, 0, 7}] // FullSimplify // Normal
```

$$\frac{(1+J)\ x}{3\ J} - \frac{(1+J)\ (1+2\ J\ (1+J))\ x^{3}}{90\ J^{3}} + \frac{\left(-1+(1+2\ J)^{6}\right)\ x^{5}}{30\,240\ J^{6}} - \frac{\left(-1+(1+2\ J)^{8}\right)\ x^{7}}{1\,209\,600\ J^{8}}$$

```
Limit[BJ[x], J → ∞] // Simplify
```

$$-\frac{1}{x} + \text{Coth}[x]$$

```
Limit[BJ[x], x → 0]
```

$$0$$

Magnetic moment M0 = M/(NA μB) per unit magnetic atom

$$\mathrm{M0} = \mathrm{g}\,\mathrm{J}\,\mathrm{BJ}\left[\frac{\mathrm{g}\,\mu\mathrm{B}\,\mathrm{J}\,\mathrm{B}}{\mathrm{kB}\,\mathrm{T}}\right]$$

$$\mathrm{g}\,\mathrm{J}\left(-\frac{\mathrm{Coth}\left[\frac{\mathrm{B}\,\mathrm{g}\,\mu\mathrm{B}}{2\,\mathrm{kB}\,\mathrm{T}}\right]}{2\,\mathrm{J}}+\frac{(1+2\,\mathrm{J})\,\mathrm{Coth}\left[\frac{\mathrm{B}\,\mathrm{g}\,(1+2\,\mathrm{J})\,\mu\mathrm{B}}{2\,\mathrm{kB}\,\mathrm{T}}\right]}{2\,\mathrm{J}}\right)$$

We assume the case of the quenching of the orbital angular momentum, g = 2, J = S

```
rule1 = {g → 2,  J → S, B → 10^3 B1, μB → 9.27400949 × 10^-21 ,
   kB → 1.3806505 × 10^-16 , NA → 6.0221415 × 10^23};
```

y = B (kOe)/T (K)

```
M1 = M0 /. rule1 /. B1 → T y;

p1 = Plot[Evaluate[Table[M1, {S, 1 / 2,  4, 1 / 2}]],
   {y, 0, 40}, AxesLabel → {"B(kOe)/T(K)", "M/(NA  μB)" },
   Prolog → AbsoluteThickness[2.5], PlotPoints → 100,
   PlotStyle → Table[{Hue[0.1 i], Thick}, {i, 0, 8}],
   Background → GrayLevel[0.7]];
p2 = Plot[Evaluate[Table[2 S, {S, 1 / 2,  4, 1 / 2}]],
   {y, 0, 40}, AxesLabel → {"B(kOe)/T(K)", "M/(NA  μB)" },
   PlotPoints → 100,
   PlotStyle → Table[{Hue[0.1 i], Thick}, {i, 0, 8}],
   Background → GrayLevel[0.7]];
Show[p1, p2]
```

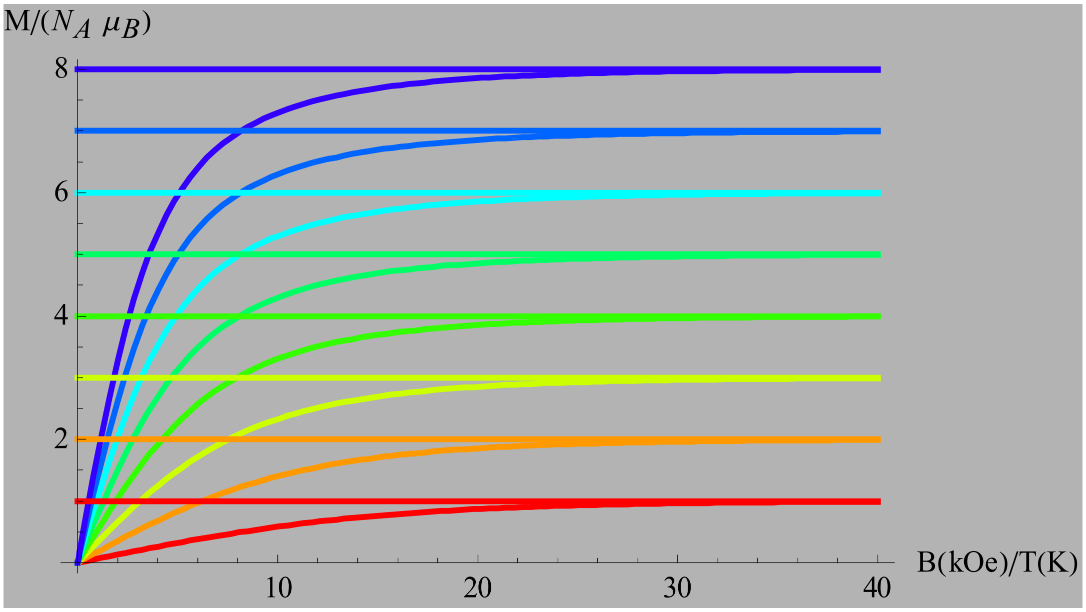


Fig.2 Magnetic moment per spin ($M/N_A\mu_B$) as a function of B(kOe)/T(K) for spin S = 1/2, 1, 3/2, 2, 5/2, 3, 7/2, and 4. g = 2. J = S. The straight lines parallel to the x axis denotes the saturation magnetization.

4. Langevin function $L(x)$

((Mathematica))

Langevin function

```
                                       1
Clear["Global`*"]; L[x_] := Coth[x] - - ; Series[L[x], {x, 0, 10}] // Normal
                                       x
```

```
x   x^3   2 x^5   x^7    2 x^9
- - --- + ----- - ---- + ------
3   45    945     4725   93 555
```

```
Plot[{L[x], x / 3}, {x, 0, 4}, AxesLabel → {"x", "L(x)" }, PlotPoints → 100,
 PlotStyle → Table[{Hue[0.5 i], Thick}, {i, 0, 1}], Background → LightGray]
```

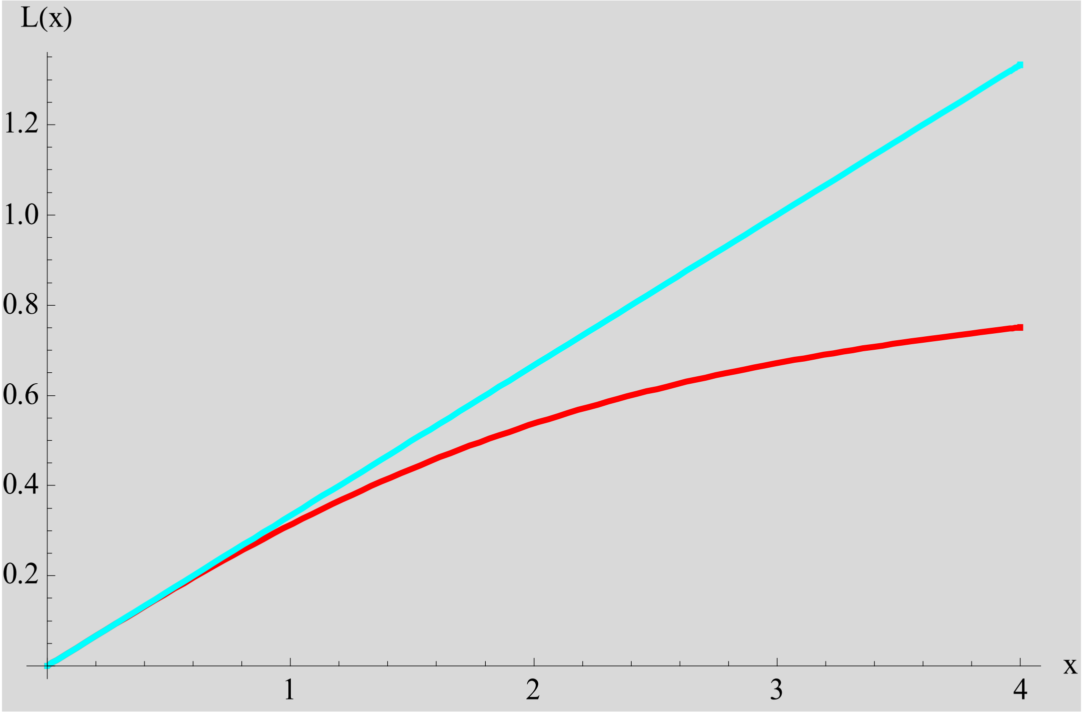


Fig.3 Plot of the Langevin function $y = L(x)$ and $y = x/3$ as a function of x.

5. Mean-field theory[1-6]

We consider a ferromagnet. All magnetic moments are ordered along the same direction below a Curie temperature T_c, forming a spontaneous magnetization even in zero applied magnetic field. In the mean-field theory, it is assume that each magnetic atom experiences a exchange field B_E proportional to the magnetization M,

$$B_E = AM \; . \tag{25}$$

Now we consider the magnetization of the ferromagnet for $T>T_c$ in the presence of an external magnetic field B. The magnetization M is described by

$$M = \frac{C_M}{T}(B + B_E) \, , \tag{26}$$

where C_M is the Curie constant. Then we obtain the magnetic susceptibility χ

$$\chi = \frac{M}{B} = \frac{C_M}{T - C_M A} = \frac{C_M}{T - \Theta} \, , \tag{27}$$

where $\Theta = C_M A$ is the Curie-Weiss temperature. Note that Θ is equal to T_c in the mean-field theory. When $\Theta>0$, $\tilde{J}$ is ferromagnetic. When $\Theta<0$, $\tilde{J}$ is antiferromagnetic.

6. Origin of exchange interaction[4]

The exchange field gives an approximate representation of the quantum-mechanical exchange interaction

$$E_{ex} = -2\tilde{J}\sum_{i<j}\mathbf{S}_i \cdot \mathbf{S}_j\ , \qquad (28)$$

where the sum is over nearest neighbor pairs. $\tilde{J}$ is the exchange interaction and is related to the overlap of the charge distribution of spins *i*, *j*. This equation is called the Heisenberg model. The interaction related to the *i*-th spin is given by

$$E_{ex}| = -2\tilde{J}z < \mathbf{S} > \cdot \mathbf{S}_i = -(-g\mu_B\mathbf{S}_i)\cdot\mathbf{B}(i)\,, \qquad (29)$$

where *z* is the number of nearest-neighbor spins and ***B***(*i*) is the exchange field seen by the *i*-th spin,

$$\mathbf{B}(i) = -\frac{2\tilde{J}z}{g\mu_B} < \mathbf{S} > . \qquad (30))$$

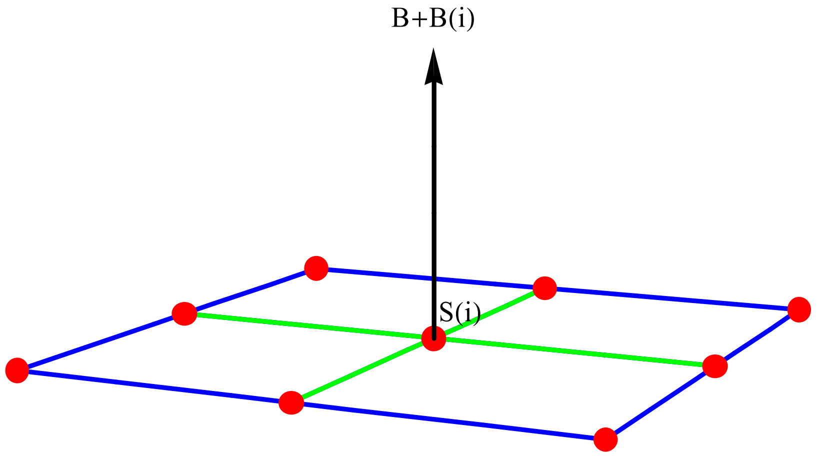


Fig. Mean field ***B***(i) applied the spin ***S***$_i$ (at the center in this Fig), arising from the exchange interaction with the surrounding spins (in this case, *z* = 4). ***B*** is the applied magnetic field.

The magnetization ***M*** is given by

$$\boldsymbol{M} = -g\mu_B N_A < \boldsymbol{S} > . \qquad (31)$$

Then the exchange field is

$$\boldsymbol{B}(i) = -\frac{2\tilde{J}z}{g\mu_B}\frac{\boldsymbol{M}}{(-g\mu_B N_A)} = \frac{2z\tilde{J}}{g^2{\mu_B}^2 N_A}\boldsymbol{M} = A\boldsymbol{M}\ , \qquad (32)$$

which means that

$$A = \frac{2z\widetilde{J}}{g^2\mu_B{}^2 N_A}\,. \tag{33}$$

In the presence of a mean field, the molar magnetization can be described by

$$M = \frac{C_M}{T}[B + AM]$$

where C_M is the Curie constant and is given by

$$C_M = \frac{N_A g^2 \mu_B{}^2 S(S+1)}{3k_B}$$

From this equation M can be derived as

$$M = \frac{C_M}{T - CA} B$$

The corresponding susceptibility is

$$\chi_M = \frac{M}{B} = \frac{C_M}{T - C_M A} = \frac{C_M}{T - \Theta}$$

The Curie-Weiss temperature Θ is given by

$$\Theta = C_M A = \frac{N_A g^2 \mu_B{}^2 S(S+1)}{3k_B} \frac{2z\widetilde{J}}{g^2 \mu_B{}^2 N_A} = \frac{2z\widetilde{J}}{3k_B} S(S+1)\,. \tag{34}$$

Note that Θ is positive for ferromagnetic exchange interaction ($\widetilde{J}$ >0) and Θ is negative for antiferromagnetic interaction ($\widetilde{J}$ >0). From this equation $\widetilde{J}$ is expressed in terms of Θ as

$$\widetilde{J} = \frac{3k_B\Theta}{2zS(S+1)}\,. \tag{35}$$

From this expression, one can evaluate the value of exchange interaction between the nearest neighbor interactions.

7. Real system: stage-2 $CrCl_3$ GIC[7]

Here we show some typical example of DC magnetic susceptibility for stage-2 $CrCl_3$ graphite intercalation compound (GIC). See the paper [M. Suzuki and I.S. Suzuki, Phys.

Rev. B **57**, 10674-83 (1998). Magnetic phase transitions of $CrCl_3$ graphite intercalation compound] for more detail.

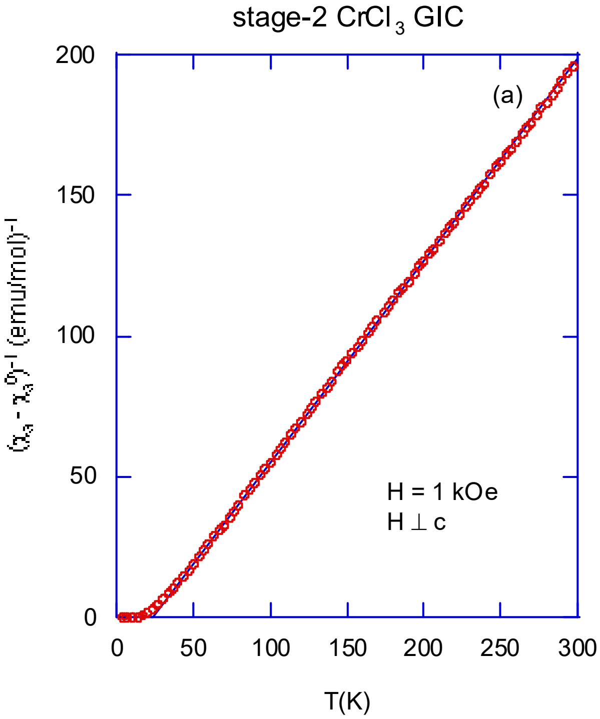


Fig.4(a) The reciprocal susceptibility as a function of T for stage-2 $CrCl_3$ GIC. $B//c$ plane (perpendicular to the c axis). $B = 1$ kOe. The straight line denotes the Curie-Weiss law.

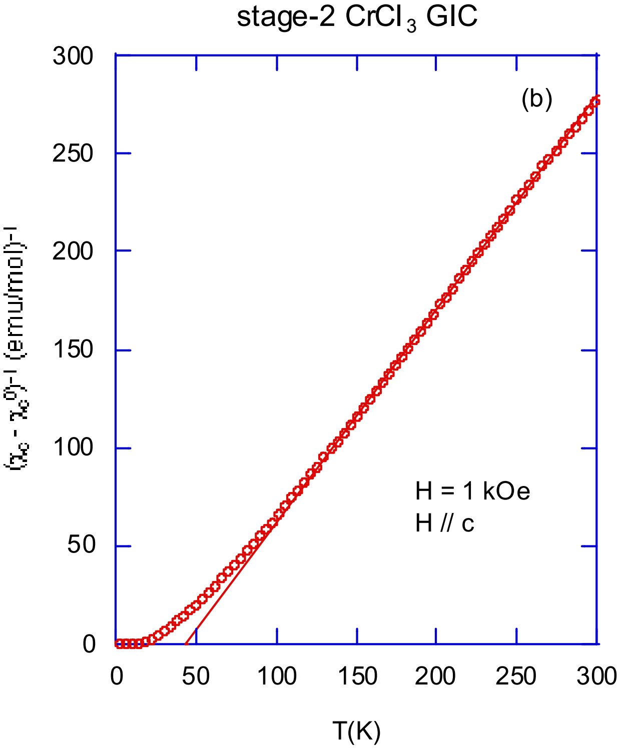


Fig.4(b) The reciprocal susceptibility as a function of T for stage-2 $CrCl_3$ GIC. $B//c$ (parallel to the c axis). B = 1 kOe. The straight line denotes the Curie-Weiss law.

The stage-2 $CrCl_3$ GIC is a two-dimensional (2D) Heisenberg ferromagnet with small XY anisotropy and very weak antiferromagnetic interplanar exchange interaction. This compound undergoes magnetic phase transitions at T_{c1} = 11.5K, T_{c2} = 10.3 – 10.5 K, T_{c3} = 8.67 – 9.70 K, and T_g = 5.7 – 7 K. Below T_{c1} a 2D ferromagnetic long-range order with spin component along the c axis appears, forming an axial ferromagnetic phase. Below T_{c2} a 2D ferromagnetic long-range order of spin component perpendicular to the c axis appears, forming an oblique phase. Below T_{c3} there appears a 3D antiferromagnetic order accompanying spin-glass-like behavior. Below T_g the system enters into a reentrant spin glass phase arising from the competition between a ferromagnetic Cr^{3+}-Cr^{3+} interaction and possible antiferromagnetic Cr^{2+}-Cr^{2+} interaction. The role of Cr^{2+} with Ising symmetry may be crucial for the axial ferromagnetic and oblique phases.

We find that the DC magnetic susceptibility along the c plane obeys a Curie-Weiss law in the temperature range $50 \leq T \leq 300$ K. The least squares fit of the data to

$$\chi_M = \frac{C_M}{T - \Theta} + \chi_M{}^0$$

yields the Curie-Weiss temperature Θ_a = 24.05±0.05 K and the Curie constant C_a = 1.388 ± 0.002 emu K/mol, where $\chi_M{}^0$ is a temperature-independent susceptibility. Figure 4(a) shows the reciprocal susceptibility $(\chi_a - \chi_0)^{-1}$ as a function of temperature. The deviation of data from a straight line (exhibiting the Curie-Weiss law) becomes appreciable below 30 K, implying the growth of short-range spin order. The effective magnetic moment $P_{\mathrm{eff}}^{(a)}$ is calculated from C_a as $P_{\mathrm{eff}}^{(a)} = (3.332 \pm 0.005)\ \mu_B$, which is relatively smaller than 3.87 μ_B for the complete quenching of orbital angular momentum: $P_{\mathrm{eff}} = 2[S(S+1)]$ with $S = 3/2$. The positive Θ_a indicates that the intraplanar exchange interaction is ferromagnetic. The intraplanar exchange interaction is estimated as $\tilde{J} = 3.21 \pm 0.01$ K from the relation

$$\Theta = 2z\tilde{J}S(S+1)/3$$

with $z = 3$.

We find that the DC magnetic susceptibility along the c axis obeys a Curie-Weiss law in the temperature range $150 \leq T \leq 300$ K. The least squares fit of the data to the Curie-Weiss law yields the Curie-Weiss temperature $\Theta_c = 43.94 \pm 0.67$ K and the Curie constant $C_c = 0.916 \pm 0.008$ emu K/mol. Figure 4(b) shows the reciprocal susceptibility $(\chi_c - \chi_0)^{-1}$ as a function of temperature. The effective magnetic moment $P_{\mathrm{eff}}^{(c)}$ is calculated from C_c as $P_{\mathrm{eff}}^{(c)} = (2.71 \pm 0.12)\ \mu_B$, which is much smaller than 3.87 μ_B. The intraplanar exchange interaction is estimated as $\tilde{J} = 5.86 \pm 0.09$ K. We have a ratio $T_c/\Theta = 0.26$, which is much smaller than 1.

((**Note**)) Molecular field

$$\begin{aligned} B &= \frac{2zJ}{g^2 {\mu_B}^2 N_A} M \\ &= \frac{2zJ}{g^2 {\mu_B}^2 N_A} N_A g \mu_B S \\ &= \frac{2zJ}{g\mu_B} S \end{aligned}$$

where

$$\frac{k_B}{\mu_B} = 1.4887 \ \text{[T/K]}$$

So we have

$$B = B \approx 14.3\,\mathrm{T} \qquad \text{for stage 2 CrCl}_3 \text{ GIC}$$

From the magnetic susceptibility measurements of many kinds of the 1D, 2D and 3D magnetic systems, one can reach the following conclusions.

(i) In the mean field theory, Θ is equal to T_c.

(ii) The Curie-Weiss temperature Θ is higher than T_c in real system. $T_c/\Theta<1$ for the 3D systems.

(iii) T_c/Θ monotonically decreases with decreasing the dimension of the system. $T_c/\Theta \ll 1$ for the 1D systems.

8. Temperature dependence of the spontaneous magnetization[2,3]

What is the temperature dependence of the spontaneous magnetization M below T_c for the ferromagnet? We use the Brillouin expression for the magnetization given by Eq.(24) with $g_J = g$ and $J = S$,

$$y = \frac{M}{N_A g\mu_B S} = B_S(x), \tag{36}$$

where x is expressed by

$$x = \frac{g\mu_B S}{k_B T} B_E = \frac{g\mu_B S}{k_B T} AM = \frac{2zJS}{k_B T g\mu_B N_A} M \,. \tag{37}$$

The parameter y is also rewritten as

$$y = \frac{M}{N_A g\mu_B S} = \frac{k_B T}{2zJS^2} x = \frac{T}{T_c}\frac{S+1}{3S} x \,. \tag{38}$$

Then we have two equations,

$$y = B_S(x), \text{ and } y = \frac{T}{3T_c}\frac{S+1}{S} x, \tag{39}$$

when T/T_c is changed as a parameter.

We now discuss the simplest case ($S = 1/2$). We have

$$y = \tanh(x), \text{ and } y = tx, \tag{40}$$

where t is a reduced temperature, $t = T/T_c$. Here we solve

$$y=\tanh(y/t), \tag{41}$$

using the ContourPlot in the Mathematica. Note that y is the normalized magnetization. It takes a maximum (= 1) at $t = 0$.

((Mathematica))

```
Clear["Global`*"]; y1 = Tanh[x]; y2 = t x;
p1 = Plot[y1, {x, 0, 3}, AxesLabel → {"x", "y" }, PlotPoints → 100,
  PlotStyle → {Hue[0], Thick}, Background → LightGray];
p2 = Plot[Evaluate[Table[y2, {t, 0.2, 2, 0.2}]], {x, 0, 3},
  AxesLabel → {"x", "y" }, PlotPoints → 100,
  PlotStyle → Table[{Hue[0.1 i], Thick}, {i, 0, 10}],
  Background → LightGray];
g1 = Graphics[{Text[Style["t=0.2", Black, 12], {2.8, 0.6}],
   Text[Style["t=0.4", Black, 12], {2.8, 1.2}],
   Text[Style["t=0.6", Black, 12], {2.1, 1.2}],
   Text[Style["t=0.8", Black, 12], {1.5, 1.2}],
   Text[Style["t=1", Black, 12], {1.2, 1.2}],
   Text[Style["t=1.2", Black, 12], {0.89, 1}]}];
Show[p1, p2, g1, PlotRange → {{0, 3}, {0, 1.2}}]
```

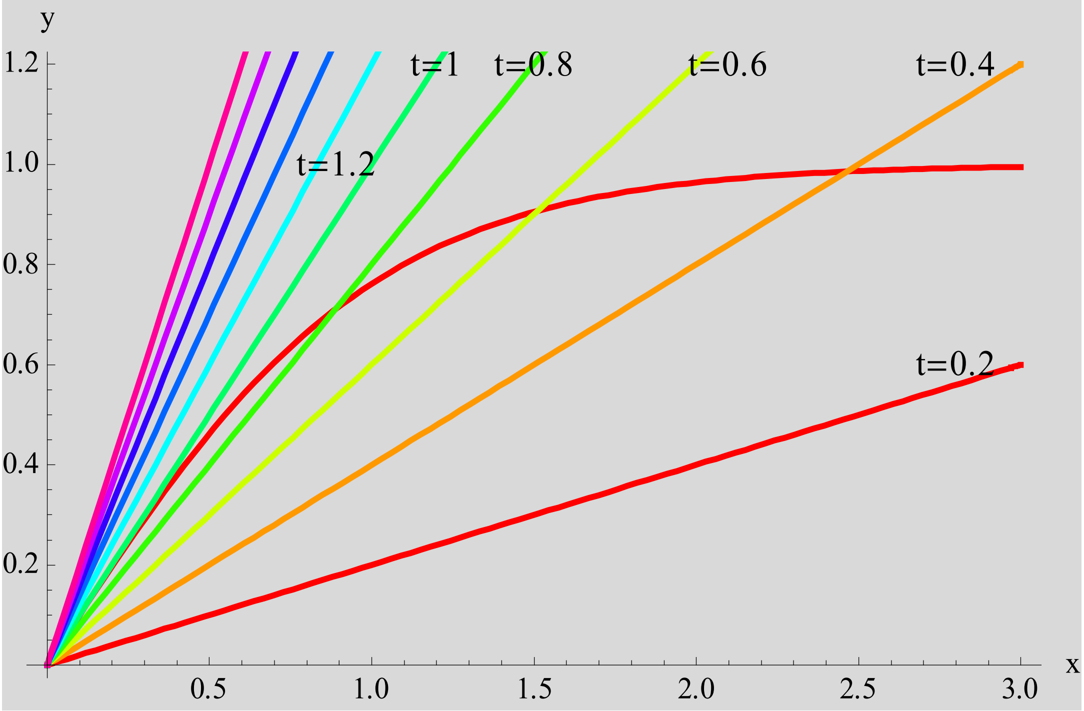


Fig.5 Plot of y = tanh(x) and $y = tx$ (the stratight lines with different t) as a function of x. $t = T/T_c$. Graphically the solution of x and y for the fixed T is obtained from the intersection of these two curves.

((**Mathematica**))

Critical behavior of ferromagnetic phase transtion

```
Clear["Global`*"];
f1 = ContourPlot[Evaluate[Tanh[x/t] - x == 0], {t, 0.5, 1.1}, {x, 0, 1.1},
  ContourStyle → {Hue[0], Thick}, AxesLabel → {"t", "x"} , PlotPoints → 200,
  Background → LightGray];
g1 = Graphics[{Text[Style["t=T/Tc", Black, 12], {1.05, 0.02}],
   Text[Style["y", Black, 12], {0.52, 1.05}]}];
Show[f1, g1]
```

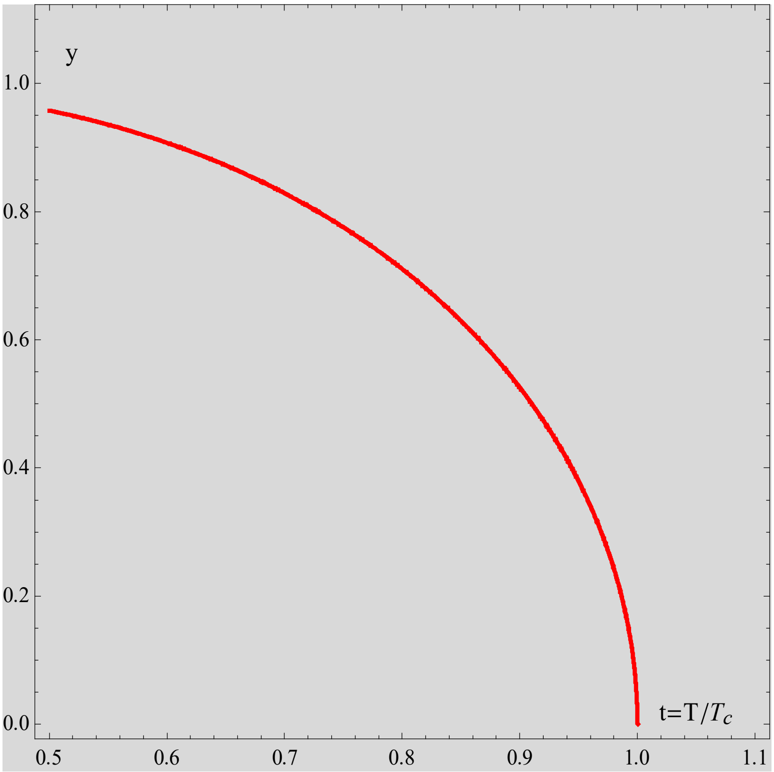


Fig.6 Spontaneous magnetization y as a function of t. The value of y is obtained from the equation $y = \tanh(y/t)$. $t = T/T_c$. $y = 1$ at $t = 0$.

8 Mean-field exponent[2,3]

A. Spontaneous magnetization exponent

We start with $y=\tanh(y/t)$ ($B = 0$) for $S = 1/2$. When y is very small, we can expand Eq.(41) around $y = 0$, we have

$$y = \frac{y}{t} - \frac{y^3}{3t^3}\text{, or } 1 = \frac{1}{t} - \frac{y^2}{3t^3}, \qquad (42)$$

or

$$y^2 = 3t^2(1-t) \approx 3(1-t)\text{ ,or } y \approx \sqrt{3}(1-t)^{1/2}. \tag{43}$$

Thus the critical exponent β of the magnetization is equal to 1/2 (mean-field exponent). M is equal to

$$M = N_A \mu_B \sqrt{3}(1 - T/T_c)^{1/2}. \tag{44}$$

B. Magnetic susceptibility exponent

In the presence of B, B_E is replaced by $B_E + B$ in Eq.(37)

$$x = \frac{g\mu_B S}{k_B T}(B + B_E) = \frac{g\mu_B SB}{k_B T} + \frac{3S}{S+1}\frac{y}{t}, \tag{45}$$

For $S = 1/2$ and $g = 2$,

$$x = \frac{\mu_B B}{k_B T} + \frac{y}{t}. \tag{46}$$

Then we have

$$y = \tanh\left(\frac{y}{t} + \frac{\mu_B B}{k_B T}\right). \tag{47}$$

After the series expansion of this equation around $y = 0$ and $B = 0$, we take a derivative of the equation with respect to B. The magnetic susceptibility χ is defined by

$$\chi = \frac{\partial M}{\partial B} = N_A \mu_B \frac{\partial y}{\partial B}. \tag{48}$$

For $T > T_c$

$$\chi = \frac{\partial M}{\partial B} = N_A \mu_B \frac{\partial y}{\partial B}\bigg|_{y=0} = \frac{N_A {\mu_B}^2}{k_B}(T - T_c)^{-1}, \tag{49}$$

For $T < T_c$

$$\chi = \frac{\partial M}{\partial B} = N_A \mu_B \frac{\partial y}{\partial B}\bigg|_{y=\sqrt{3(1-t)}} = \frac{N_A {\mu_B}^2}{2k_B}(T_c - T)^{-1} \tag{50}$$

Then the critical exponent of the magnetic susceptibility γ is equal to 1 (the mean-field exponent).

((Mathematica))

Molecular field exponents

Spontaneous magnetization

```
eq1 = Series[Tanh[y / t], {y, 0, 3}] // Normal
```

$$\frac{y}{t} - \frac{y^3}{3\,t^3}$$

```
eq2 = y - eq1;

eq3 = Solve[eq2 == 0, y]
```

$$\left\{\{y \to 0\},\ \left\{y \to -\sqrt{3}\ \sqrt{t^2 - t^3}\right\},\ \left\{y \to \sqrt{3}\ \sqrt{t^2 - t^3}\right\}\right\}$$

```
y0 = y /. eq3[[3]] // Simplify;
```

Therefore $y0 = \sqrt{3}\ \sqrt{1 - t}$ near $t = 1$

Magnetic susceptibility exponent

```
eq4 = Series[Tanh[y/t + μB B/(kB T)], {B, 0, 3}] // Normal;

eq5 = Series[eq4, {y, 0, 3}] // Normal;

eq6 = y - eq5; eq7 = eq6 /. y → z[B];
eq8 = Solve[D[eq7 == 0, B], z'[B]];
eq9 = z'[B] /. eq8[[1]] /. B → 0
```

$$\frac{3\,kB^2\,t^3\,T^2\,\mu B - 3\,kB^2\,t\,T^2\,\mu B\,z[0]^2}{-3\,kB^3\,t^2\,T^3 + 3\,kB^3\,t^3\,T^3 + 3\,kB^3\,T^3\,z[0]^2}$$

```
χup = NA μB eq9 /. {z[0] → 0} // Simplify // Factor
```

$$\frac{NA\,t\,\mu B^2}{kB\,(-1 + t)\,T}$$

```
χdw = NA μB eq9 /. {z[0] → √3 √(1 - t)} // Simplify // Factor
```

$$\frac{NA\,t\,\left(-3 + 3\,t + t^2\right)\,\mu B^2}{kB\,(-1 + t)\,\left(-3 + t^2\right)\,T}$$

9. Critical behavior of the second-order phase transitions[1,3,5]

When the external magnetic field B vanishes, the magnetization M below T_c is a decreasing function of T and vanishes at T_c. In the vicinity of T_c the power law behavior

$$M \approx (1 - T / T_c)^{\beta}, \qquad (51)$$

is a common feature, where β is called a critical exponent of the magnetization. $\beta = 1/2$ for the mean-field theory.

As T approaches T_c, the magnetic susceptibility is seen to diverge. The divergence is characterized by the exponents γ and γ'

$$\chi \approx (T / T_c - 1)^{-\gamma} \text{ for } T>T_c, \qquad (52)$$

$$\chi \approx (1 - T / T_c)^{-\gamma'} \text{ for } T<T_c. \qquad (53)$$

where $\gamma = \gamma'$; $\gamma = 1$ for the mean-field theory.

The specific heat at $B = 0$ is observed to have a singularity at T_c. the singularity is characterized by the exponents α and α'.

$$C \approx (T / T_c - 1)^{-\alpha} \text{ for } T>T_c, \qquad (54)$$

$$C \approx (1 - T / T_c)^{-\alpha'} \text{ for } T<T_c. \qquad (55)$$

where $\alpha = \alpha'$.

The renormalization group introduced by Wilson[8] in the early 1970s provided a method for calculating exponents and established that they should depend on the spatial dimension d, the symmetry of the order parameter ($n = 1$ for the Ising, $n = 2$ for XY, and $n = 3$ for Heisenberg), and the symmetry and range of interactions. Thus there are universality classes, and all transitions in the same universality class have the same critical exponents.

For the 2D Ising system, the critical exponents are given by $\alpha = 0$, $\beta = 0.125$, $\gamma = 1.75$, $\nu = 1$, $\delta = 15$, and $\eta = 0.25$, where α, ν, δ, and η are critical exponents of specific heat, correlation length, magnetization vs B at $T = T_c$, and the Fisher-Burford exponent of the correlation function, respectively.

10. Conclusion

We have discussed the mean-field theory of ferromagnetic system. The mean field of this theory is not appropriate for low dimensional systems where the spin fluctuation effect is not neglected. The mean-field theory is replaced by the Onsager's exact solution on the 2D Ising system and the renormalization group method for general systems. Nevertheless, the mean-field theory is still useful in our understanding the concept of critical behavior qualitatively.

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APPENDIX Evaluation of Weiss field

(Walter Lewin, MIT 8.02 Physics II: Electricity and Magnetism Spring 2002)
Evaluation of Weiss field

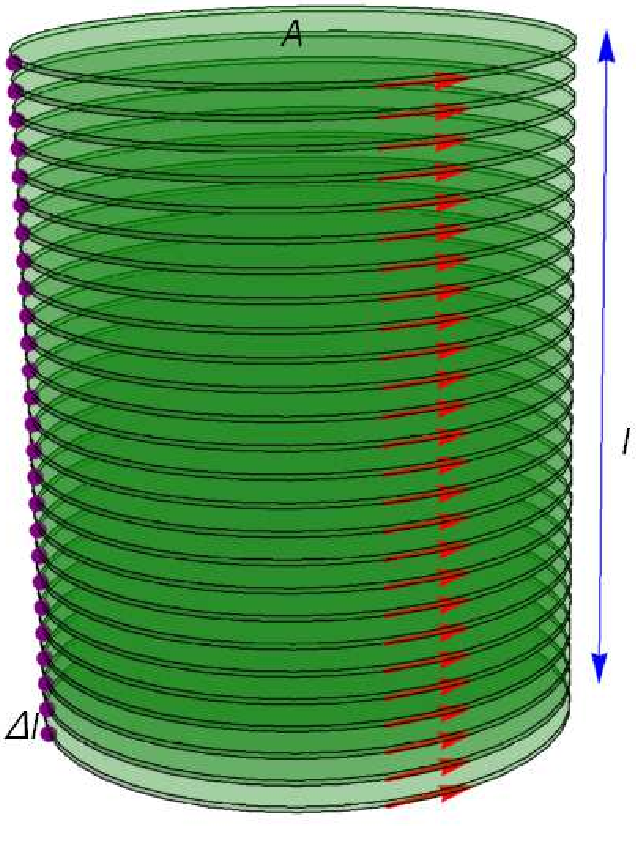

Fig. Solenoid coil. $\Delta l = a$. $A = a^2$, where a is a lattice constant of simple cubic.

We assume that the system has a simple cubic lattice with a lattice constant a. We now evaluate the magnitude of the Weiss field for this system. To this end, we assume that the number of atoms per unit volume is given by

$$n_0 = \frac{1}{a^3}.$$

where each atom has one electron, then the number density of electrons is

$$n = n_0 = \frac{1}{a^3}$$

We consider the cylinder of area A and length l. The electron system consists of current (I) circulating around the axis of the cylinder. When the separation between adjacent currents is $\Delta l\ (= a)$ and the total number of windings is N_1, we get the relation

$$N_1 = \frac{l}{\Delta l} = \frac{l}{a}$$

The magnetic field generated by the coils (carrying current I)

$$B = \mu_0 I \frac{N_1}{l} = \mu_0 (IA) \frac{N_1}{Al} = \mu_0 (IA) \frac{1}{Aa} = \mu_0 (IA) \frac{1}{a^3} = \mu_0 (IA) n \qquad \text{(SI units)}$$

We assume that the area A is given by $A = a^2$. Note that the magnetic moment is given by

$$IA = k\mu_B,$$

where k is on the order of unity and μ_B is the Bohr magneton. Then the Weiss magnetic field is obtained as

$$B = \mu_0 (k\mu_B) n$$

When $k = 2$ and $a = 3$ Å, the magnitude of B is evaluated as

$$B \approx 0.86 \text{ T}.$$

since

$$n = 3.70 \text{ x } 10^{28} \text{ m}^{-3}$$