# Antiferromagnets in magnetic field

**Masatsugu Sei Suzuki**
**Department of Physics, SUNY at Binghamton**

**(Date: May 21, 2012)**

**Louis Eugène Félix Néel** (22 November 1904 – 17 November 2000) was a French physicist born in Lyon. He studied at the Lycée du Parc in Lyon and was accepted at the École Normale Supérieure in Paris. He obtained the degree of Doctor of Science at the University of Strasbourg. He was corecipient (with the Swedish astrophysicist Hannes Alfvén) of the Nobel Prize for Physics in 1970 for his pioneering studies of the magnetic properties of solids. His contributions to solid state physics have found numerous useful applications, particularly in the development of improved computer memory units. About 1930 he suggested that a new form of magnetic behavior might exist; called antiferromagnetism, as opposed to ferromagnetism. Above a certain temperature (the Néel temperature) this behaviour stops. Néel pointed out (1947) that materials could also exist showing ferrimagnetism. Néel has also given an explanation of the weak magnetism of certain rocks, making possible the study of the history of Earth's magnetic field.

http://en.wikipedia.org/wiki/Louis_N%C3%A9el

---

Here we discuss the molecular field theory of antiferromagnet. We show that the experimental results of $MnF_2$ (typical 3D antiferromagnet) can be well explained in terms of this molecular field theory.

## 1. Molecular field in antiferromagnet

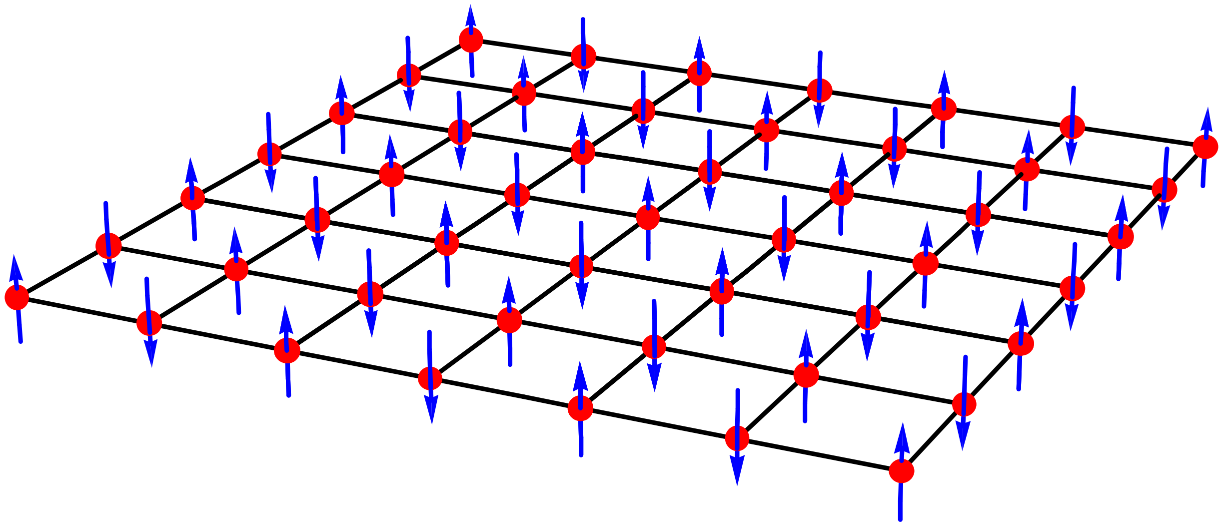


**Fig.** 2D Ising antiferromagnet on the square lattice, forming two sublattices.

The mean exchange fields acting on the sublattices 1 and 2 may be written as

$$\mathbf{H}_m(1) = -A\mathbf{M}_2 + B\mathbf{M}_1,$$

$$\mathbf{H}_m(2) = -A\mathbf{M}_1 + B\mathbf{M}_2,$$

($A$>0 and $B$>0)

Spins in the sublattice 1 are parallel to each other. Spins in the sublattice 2 are antiparallel to those in the sublattice 1.

$\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ are the sublattice magnetization.

$$\mathbf{M}_1 = -\mathbf{M}_2,$$

for $\boldsymbol{H} = 0$.

The net magnetization: $\mathbf{M}_{net} = \mathbf{M}_1 + \mathbf{M}_2$.

The staggered magnetizarion $\mathbf{M}_{stag} = \mathbf{M}_1 - \mathbf{M}_2$.

For $\boldsymbol{H} = 0$,

$$\mathbf{M}_{stag} = 2\mathbf{M}_1 ,$$

with

$$\mathbf{M}_1 = -\mathbf{M}_2 .$$

## 2. Néel temperature ($T_N$)

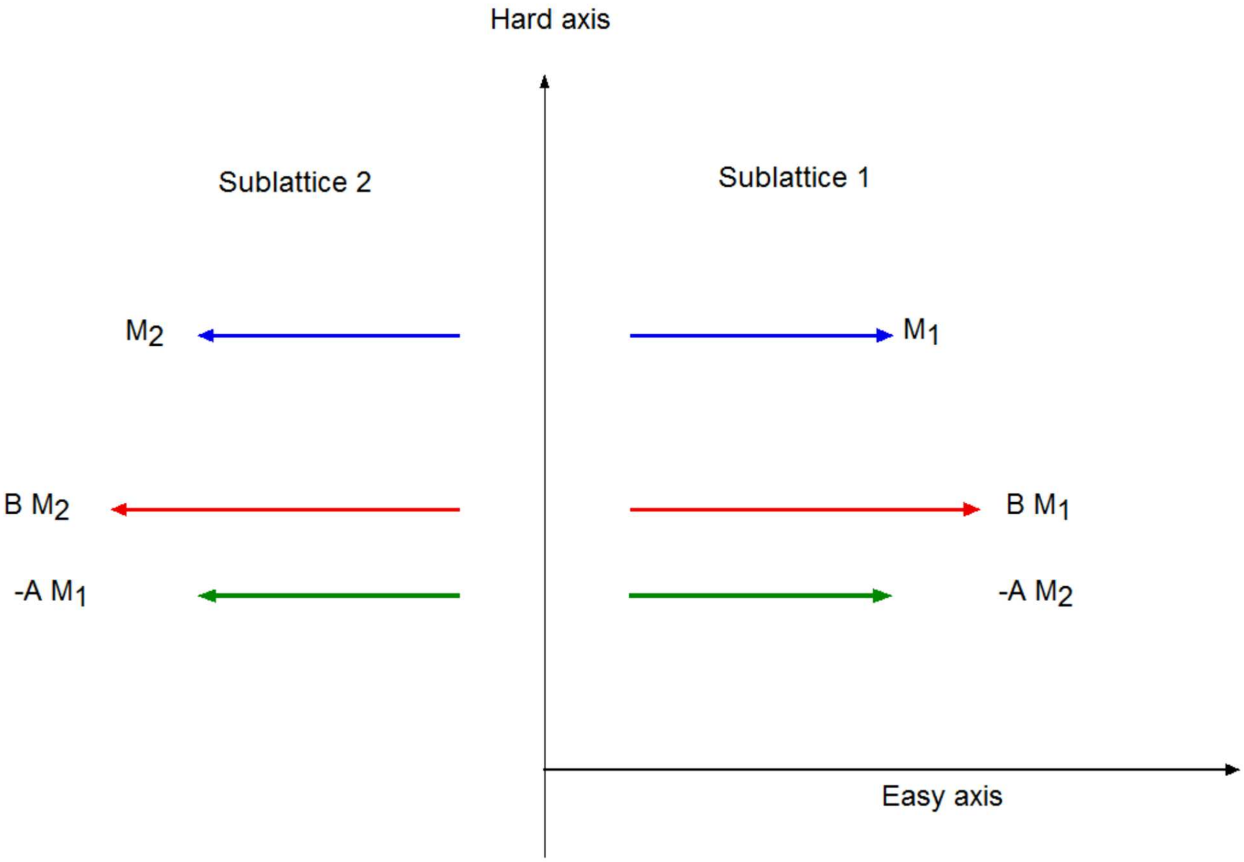
When $\boldsymbol{H} = 0$, the effective fields are given by

$$\mathbf{H}_m(1) = -A\mathbf{M}_2 + B\mathbf{M}_1 = (A+B)\mathbf{M}_1 ,$$

$$\boldsymbol{H}_m(2) = -A\boldsymbol{M}_1 + B\boldsymbol{M}_2 = (A+B)\boldsymbol{M}_2 .$$

where

$$\boldsymbol{M}_2 = -\boldsymbol{M}_1$$



The sublattice magnetization is

$$M_1 = \frac{N}{2} g\mu_B S B_s(x),$$

with

$$x = \frac{g\mu_B S}{k_B T}(A+B)M_1 .$$

We put $y$ as

$$y = \frac{M_1}{\frac{N}{2} g\mu_B} = \frac{2M_1}{Ng\mu_B} = SB_s(x) .$$

The value of $y$ can be rewritten as

$$y = \frac{2k_B T x}{Ng^2 {\mu_B}^2 S(A+B)} .$$

When $T$ is a fixed parameter, the intersection of the curve

$$y = SB_s(x),$$

and a straight line, leads to the value of $y$ at the fixed temperature $T$ below the Néel temperature $T_N$.

## 3. Determination of Néel temperature $T_N$.

We use the property of Brillouin function such that

$$\lim_{x\to 0} SB_s(x) = \frac{1}{3}(S+1)x .$$

At $T = T_N$, the tangential line of $y = SB_s(x)$ at $x = 0$ is given by

$$y = \frac{1}{3}(S+1)x .$$

This line should coincide with the straight line given by

$$y = \frac{2k_B T_N x}{N g^2 \mu_B{}^2 S(A+B)}.$$

Then the value of $T_N$ is obtained as

$$T_N = \frac{N g^2 \mu_B{}^2}{3k_B} S(S+1)\left(\frac{A+B}{2}\right).$$

## 4. Temperature dependence of the sublattice magnetization

$$y = \frac{tx(S+1)}{3},$$

where $t$ is a reduced temperature,

$$t = \frac{T}{T_N},$$

$$B_S(x) = \frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}x\right) - \frac{1}{2S}\coth\left(\frac{1}{2S}x\right).$$

The solution of the equation

$$y = SB_S\left(\frac{3y}{t(S+1)}\right),$$

leads to the temperature dependence of the sublattice magnetization.

((**Mathematica**))
Here we use the ContourPlot, in order to get the value of $y$ as a function of $t$.

$$y = SB_S\left(\frac{3y}{t(S+1)}\right)$$

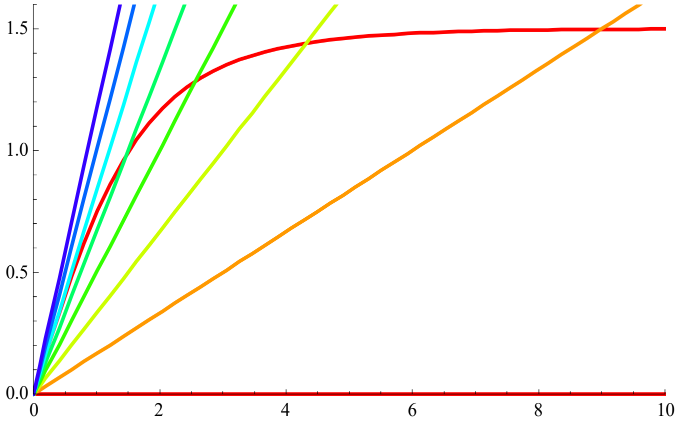


Fig. $S = 3/2$.

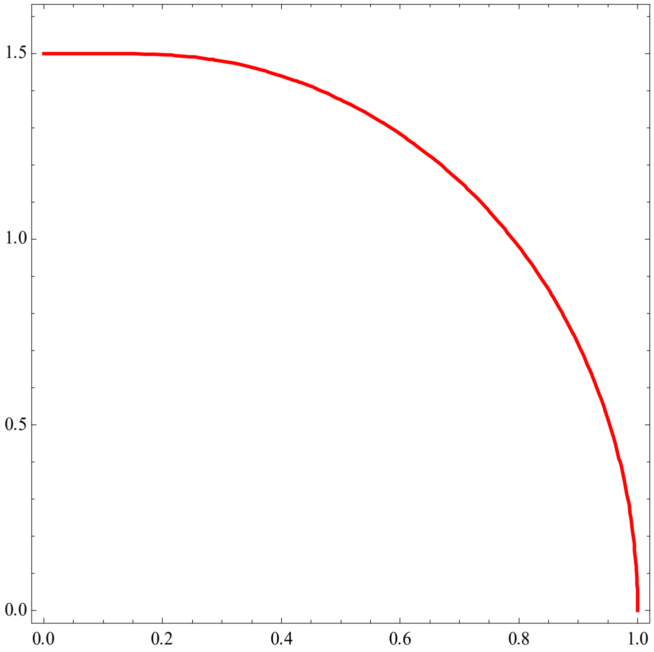
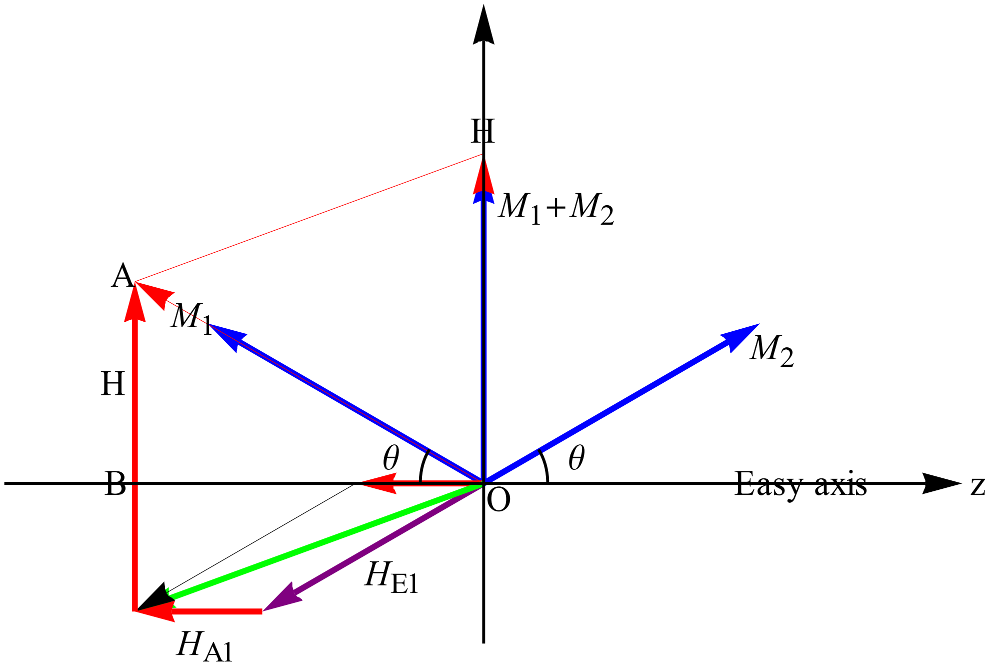


**Fig.** Magnetization $y$ vs reduced temperature $t$ for $S = 3/2$. The ContourPlot of the Mathematica is used for the curve.

## 5. Perpendicular susceptibility $\chi_\perp$

We consider the case when the magnetic field is applied along the hard axis.



The field acting on the sublattice 1 is given by

$$\mathbf{H}_m(1) = (\mathbf{H} - A\mathbf{M}_2 + \mathbf{H}_{A1}) + B\mathbf{M}_1 = (\mathbf{H} + \mathbf{H}_{E1} + \mathbf{H}_{A1}) + B\mathbf{M}_1$$

which should be parallel to the sublattice magnetization 1, $\boldsymbol{M}_1$. In other words, the field $(\mathbf{H} + \mathbf{H}_{E1} + \mathbf{H}_{A1})$ should be parallel to $\boldsymbol{M}_1$ since the field $B\boldsymbol{M}_1$ is already parallel to $\boldsymbol{M}_1$;

$$(\mathbf{H} + \mathbf{H}_{E1} + \mathbf{H}_{A1}) \times \mathbf{M}_1 = 0\,.$$

The field acting on the sublattice 2 is given by

$$\mathbf{H}_m(2) = (\mathbf{H} - A\mathbf{M}_1 + \mathbf{H}_{A2}) + B\mathbf{M}_2 = (\mathbf{H} + \mathbf{H}_{E2} + \mathbf{H}_{A2}) + B\mathbf{M}_2$$

which should be parallel to the sublattice magnetization 2, $\boldsymbol{M}_2$. In other words, the field $(\mathbf{H} + \mathbf{H}_{E2} + \mathbf{H}_{A2})$ should be parallel to $\boldsymbol{M}_2$ since the field $B\boldsymbol{M}_2$ is already parallel to $\boldsymbol{M}_2$.

$$(\mathbf{H} + \mathbf{H}_{E2} + \mathbf{H}_{A2}) \times \mathbf{M}_2 = 0$$

Note that

$$\mathbf{H}_{E2} = -A\mathbf{M}_1\,, \qquad \mathbf{H}_{E1} = -A\mathbf{M}_2\,,$$

and ***H***A1 and ***H***A2 are directed along the easy axis (either parallel or antiparallel).

The perpendicular susceptibility is defined by

$$\chi_\perp = \frac{2M_1 \sin\theta}{H},$$

$$H_{A1} = \frac{K}{M_1^2} M_{1z} = \frac{K}{M_1^2} M_1 \cos\theta = \frac{K}{M_1}\cos\theta = H_A \cos\theta .$$

From the condition

$$(\mathbf{H} + \mathbf{H}_{E1} + \mathbf{H}_{A1}) \times \mathbf{M}_1 = 0 .$$

(here for simplicity, we make use of the geometry of the above figure), we have

$$\tan\theta = \frac{\overline{AB}}{\overline{OB}} = \frac{H - H_{E1}\sin\theta}{H_{E1}\cos\theta + H_{A1}} = \tan\theta = \frac{\sin\theta}{\cos\theta},$$

or

$$H\cos\theta = 2H_{E1}\cos\theta\sin\theta + H_{A1}\sin\theta = (2H_{E1}\cos\theta + H_{A1})\sin\theta ,$$

or

$$\sin\theta = \frac{H\cos\theta}{2H_{E1}\cos\theta + H_{A1}} = \frac{H\cos\theta}{2H_{E1}\cos\theta + H_A\cos\theta} = \frac{H}{2H_{E1} + H_A} .$$

Then we get

$$\chi_\perp = \frac{2M_1}{H}\sin\theta = \frac{2M_1}{H}\frac{H}{2H_{E1} + H_A} = \frac{2M_1}{2H_{E1} + H_A} = \frac{1}{\frac{H_{E1}}{M_1} + \frac{H_A}{2M_1}} = \frac{1}{A + \frac{K}{2M_1^2}}$$

When $K \approx 0$,

$$\chi_\perp = \frac{1}{A} = \frac{N(g\mu_B)^2}{4zJ}.$$

The total magnetization is given by the condition, $\sin\theta = 1$.

$$\sin\theta = \frac{H}{2H_{E1} + H_A} = 1,$$

or

$$H_s = 2H_{E1} + H_A. \qquad \text{(Saturation field).}$$

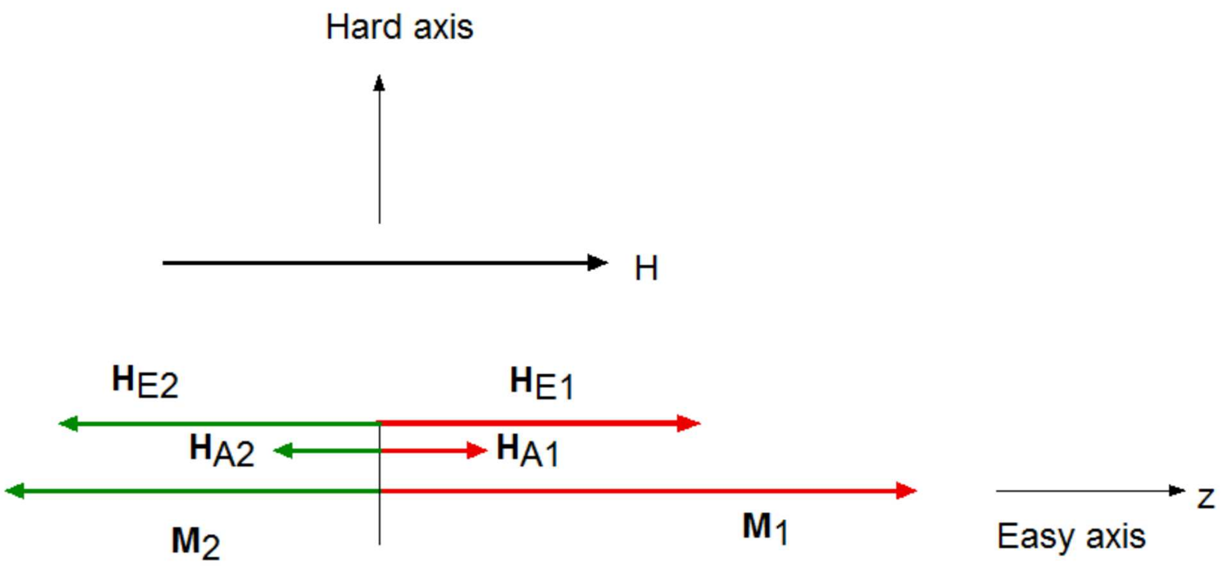
---

((**Mathematica**))

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

H1 = {0, H0, 0}; M2 = {M0 Cos[θ], M0 Sin[θ], 0};
M1 = {-M0 Cos[θ], M0 Sin[θ], 0}; HA1 = {-HA0 Cos[θ], 0, 0};
F1 = H1 - A M2 + HA1 + B M1;
eq1 = Cross[F1, M1];

eq2 = Solve[eq1[[3]] == 0, Sin[θ]] // Simplify

                    H0
{{Sin[θ] → ─────────────── }}
              HA0 + 2 A M0

     2 M0 Sin[θ]
X = ───────────── /. eq2[[1]]
         H0

     2 M0
─────────────
 HA0 + 2 A M0
```

---

## 6. Parallel susceptibility $\chi_{//}$



$$\mathbf{M}_1 + \mathbf{M}_2 = \delta M$$

The field acting on the sublattice 1 is given by

$$\begin{aligned}\mathbf{H}_m(1) &= \mathbf{H} - A\mathbf{M}_2 + B\mathbf{M}_1 + \mathbf{H}_{A1} \\ &= \mathbf{H} - A\mathbf{M}_2 + B\mathbf{M}_1\end{aligned}$$

The field acting on the sublattice 2 is given by

$$\begin{aligned}\mathbf{H}_m(2) &= \mathbf{H} - A\mathbf{M}_1 + B\mathbf{M}_2 + \mathbf{H}_{A2} \\ &\approx \mathbf{H} - A\mathbf{M}_1 + B\mathbf{M}_2\end{aligned}$$

For simplicity, we assume that $\boldsymbol{H}_{\mathrm{A1}}$ and $\boldsymbol{H}_{\mathrm{A2}}$ are negligibly small. We also suppose that

$$\mathbf{M}_1 = (M_0 + \frac{\delta M}{2})\mathbf{e}_z, \quad \mathbf{M}_2 = (M_0 - \frac{\delta M}{2})(-\mathbf{e}_z).$$

Then we get

$$\mathbf{H}_m(1) = [H + A(M_0 - \frac{\delta M}{2}) + B(M_0 + \frac{\delta M}{2})]\mathbf{e}_z$$
$$= [H + (A+B)M_0 - (A-B)\frac{\delta M}{2}]\mathbf{e}_z$$

$$\mathbf{H}_m(2) = [H - A(M_0 + \frac{\delta M}{2}) - B(M_0 - \frac{\delta M}{2})]\mathbf{e}_z$$
$$= [H - (A+B)M_0 - (A-B)\frac{\delta M}{2}]\mathbf{e}_z$$

or

$$\mathbf{H}_m(2) = [-H + (A+B)M_0 + (A-B)\frac{\delta M}{2}](-\mathbf{e}_z)\,.$$

Then

$$M_0 + \frac{\delta M}{2} = \frac{N}{2} g\mu_B S B_S(x_1)\,,$$

$$M_0 - \frac{\delta M}{2} = \frac{N}{2} g\mu_B S B_S(x_2)\,,$$

where

$$x_1 = \frac{g\mu_B S}{k_B T}[H + (A+B)M_0 - (A-B)\frac{\delta M}{2}]$$
$$= x_0 + \frac{g\mu_B S}{k_B T}[H - (A-B)\frac{\delta M}{2}]$$

$$x_2 = \frac{g\mu_B S}{k_B T}[-H + (A+B)M_0 + (A-B)\frac{\delta M}{2}]$$
$$= x_0 + \frac{g\mu_B S}{k_B T}[-H + (A-B)\frac{\delta M}{2}]$$

and

$$x_0 = \frac{g\mu_B S}{k_B T}(A+B)M_0\,.$$

The net magnetization is

$$\delta M = \frac{N}{2} g\mu_B S[B_S(x_1) - B_S(x_2)].$$

We use the Taylor expansion,

$$B_S(x_1) = B_S(x_0) + B_S'(x_0)(x_1 - x_0),$$

$$B_S(x_2) = B_S(x_0) + B_S'(x_0)(x_2 - x_0),$$

and

$$B_S(x_1) - B_S(x_2) = B_S'(x_0)(x_1 - x_2).$$

Thus we have

$$\delta M = \frac{N}{2} g\mu_B S B_S'(x_0)(x_1 - x_2).$$

Noting that

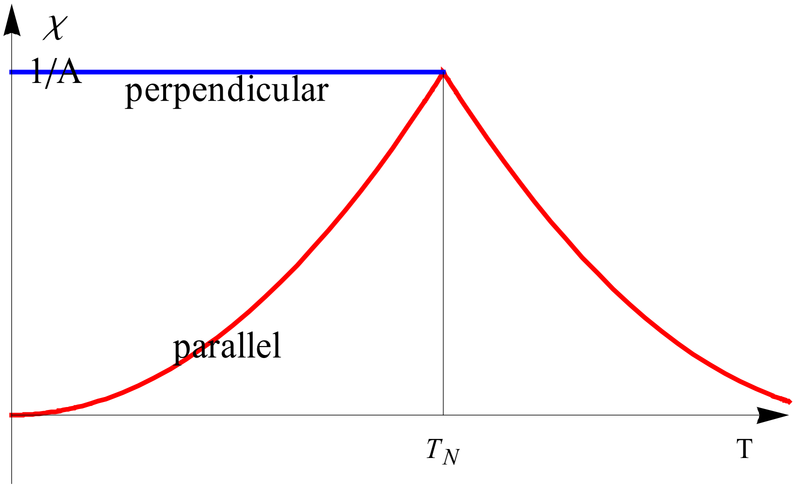
$$x_1 - x_2 = \frac{2g\mu_B S}{k_B T}[H - (A-B)\frac{\delta M}{2}],$$

we get

$$\delta M = \frac{Ng^2{\mu_B}^2 S^2}{k_B T} B_S'(x_0)[H - (A-B)\frac{\delta M}{2}].$$

The parallel susceptibility is

$$\chi_{//} = \frac{\delta M}{H} = \frac{\dfrac{Ng^2{\mu_B}^2 S^2}{k_B} B_S'(x_0)}{T + \dfrac{Ng^2{\mu_B}^2 S^2}{k_B} B_S'(x_0)\left(\dfrac{A-B}{2}\right)}.$$



(i) At $T = 0$ K, $x_0 \to \infty$. $B_S'(x_0) = 0$

$$\chi_{//} = 0$$

(ii) At $T = T_N$

$$B_S'(x_0) = B_S'(0) = \frac{S+1}{3S}$$

because of $M_0 = 0$.

Using the value of $T_N$ (obtained from the previous section)

$$T_N = \frac{Ng^2\mu_B{}^2 S(S+1)}{3k_B}\left(\frac{A+B}{2}\right)$$

we have

$$\chi_{//} = \frac{\dfrac{Ng^2\mu_B{}^2S^2}{k_B}B_S'(x_0)}{T_N + \dfrac{Ng^2\mu_B{}^2S^2}{k_B}B_S'(x_0)\left(\dfrac{A-B}{2}\right)} = \frac{1}{\left(\dfrac{A+B}{2}\right)+\left(\dfrac{A+B}{2}\right)} = \frac{1}{A}$$

$\chi_{//}$ monotonically increases from 0 to $1/A$ with increasing $T$.

(iii) $T > T_N$

$$\delta M = \frac{N}{2} g\mu_B S[B_S(x_1) - B_S(x_2)],$$

where

$$x_1 = \frac{g\mu_B S}{k_B T}[H - (A - B)\frac{\delta M}{2}],$$

$$x_2 = -\frac{g\mu_B S}{k_B T}[H - (A - B)\frac{\delta M}{2}],$$

where

$$x_0 = \frac{g\mu_B S}{k_B T}(A + B)M_0 \to 0 .$$

Then we have

$$\delta M = \frac{N}{2} g\mu_B S[B_S(x_1) - B_S(-x_1)] = Ng\mu_B SB_S(x_1),$$

since $B_S(-x_1) = B_S(x_1)$ (odd function of *H*). Since

$$B_S(x_1) = \frac{S+1}{3S} x_1 ,$$

the above equation can be rewritten as

$$\delta M = Ng\mu_B SB_S(x_1) \approx Ng\mu_B S\frac{S+1}{3S} x_1 = \frac{Ng^2 \mu_B{}^2}{3k_B T} S(S+1)[H - (A - B)\frac{\delta M}{2}] .$$

Then the susceptibility for $T > T_N$ is

$$\chi = \frac{\delta M}{H} = \frac{\dfrac{Ng^2 \mu_B{}^2 S(S+1)}{3k_B}}{T + \dfrac{Ng^2 \mu_B{}^2 S(S+1)}{3k_B}(\dfrac{A-B}{2})} .$$

(Curie-Weiss type susceptibility)

The susceptibility obeys the Curie-Weiss law

$$\Theta_N = \frac{Ng^2{\mu_B}^2 S(S+1)}{3k_B}(\frac{A-B}{2}),$$

$$C = \frac{Ng^2{\mu_B}^2}{3k_B}S(S+1),$$

$$\chi = \frac{C}{T+\Theta_N}.$$

The expression of $\Theta_N$ is different from that of $T_N$.

$$T_N = \frac{Ng^2{\mu_B}^2 S(S+1)}{3k_B}\left(\frac{A+B}{2}\right),$$

$$\Theta_N = \frac{Ng^2{\mu_B}^2 S(S+1)}{3k_B}(\frac{A-B}{2}).$$

## 7. Simple expression of $\Theta_N$

For simplicity we assume that $B = 0$.

$$E_{ex}|_1 = 2zJ < \mathbf{S}_2 > \cdot \mathbf{S}_1 = -(-g\mu_B \mathbf{S}_1)\cdot \mathbf{H}_m(1)$$

or

$$\mathbf{H}_m(1) = \frac{2zJ}{g\mu_B} < \mathbf{S}_2 >$$

The magnetization

$$\mathbf{M}_2 = -g\mu_B \frac{N}{2} < \mathbf{S}_2 >$$

Then the exchange field is

$$\mathbf{H}_m(1) = \frac{2zJ}{g\mu_B}\frac{\mathbf{M}_2}{-g\mu_B\frac{N}{2}} = -\frac{4zJ}{g^2\mu_B{}^2N}\mathbf{M}_2 = -A\mathbf{M}_2$$

where

$$A = \frac{4zJ}{g^2\mu_B{}^2N}.$$

Using this expression of $A$, $\Theta_N$ is expressed by

$$\Theta_N = \frac{2zJS(S+1)}{3k_B}.$$

---

Table

| System | $T_N$(K) | $\Theta_N$ (K) |
|---|---|---|
| $FeCl_2$ | 24 | 48 K |
| $CoCl_2$ | 25 | 38.1 |
| $NiCl_2$ | 50 | 68.2 |
| $MnF_2$ | 67 | 82 |
| MnO | 116 | 610 |

((Note)) In the molecular field, $T_N/\Theta_N = 1$.

## 8. Magnetic properties of $MnF_2$

$MnF_2$ is one of the most thoroughly investigated antiferromagnetic compounds. $MnF_2$ has a simple tetragonal crystal structure with the $Mn^{2+}$ ions (S = 5/2) forming a body-centered lattice. Below $T_N$, the Mn spins at the body-center and corner sites align antiferromagnetically with the weak anisotropy, due to dipole-dipole interactions orienting the spins along the c axis.

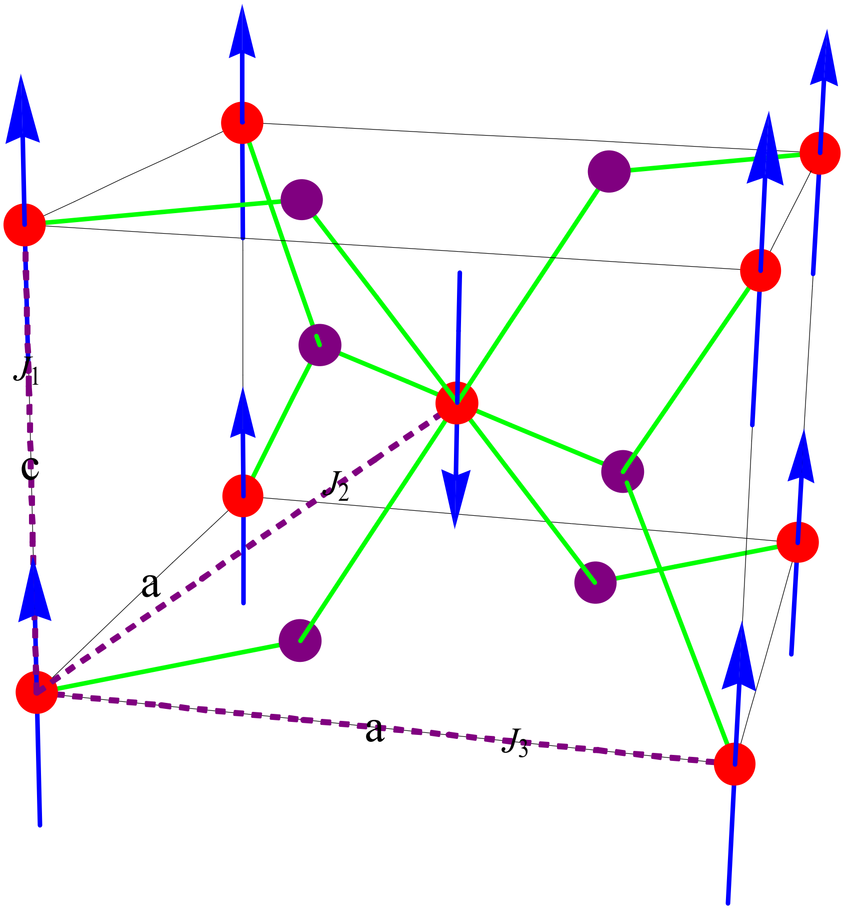


**Fig.** Antiferromagnetic structure of $MnF_2$ [$TiO_2$ (rutile) type structure] below $T_N$. $a = b = 4.8734$ Å and $c = 3.3099$ Å.. The exchange interactions in $MnF_2$ are also shown. $J_2$ is the main exchange interaction between the nearest neighbor $Mn^{2+}$ spins in $MnF_2$ and is antiferromagnetic. $S = 5/2$. There are two Mn atoms and 4 F atoms in the conventional unit cell ($a$ x $b$ x $c$). The position vectors of Mn atoms are (000) and (0.5, 0.5, 0.5). The position vectors of F atoms are (0.5, 0.5, 0.5), (0.305, 0.305,0), (0.305, 0.305,1),(0.695, 0.695, 0), (0.695, 0.695,1), (0.805, 0.195, 0.5), and (0.195, 0.805, 0.5).

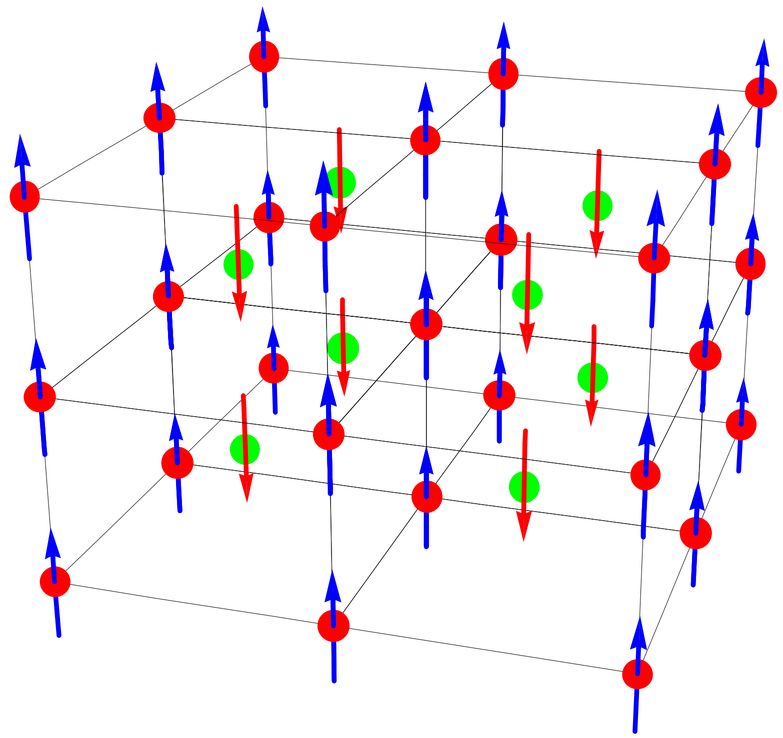


**Fig.** Sublattices A (red) and B (green) in $MnF_2$

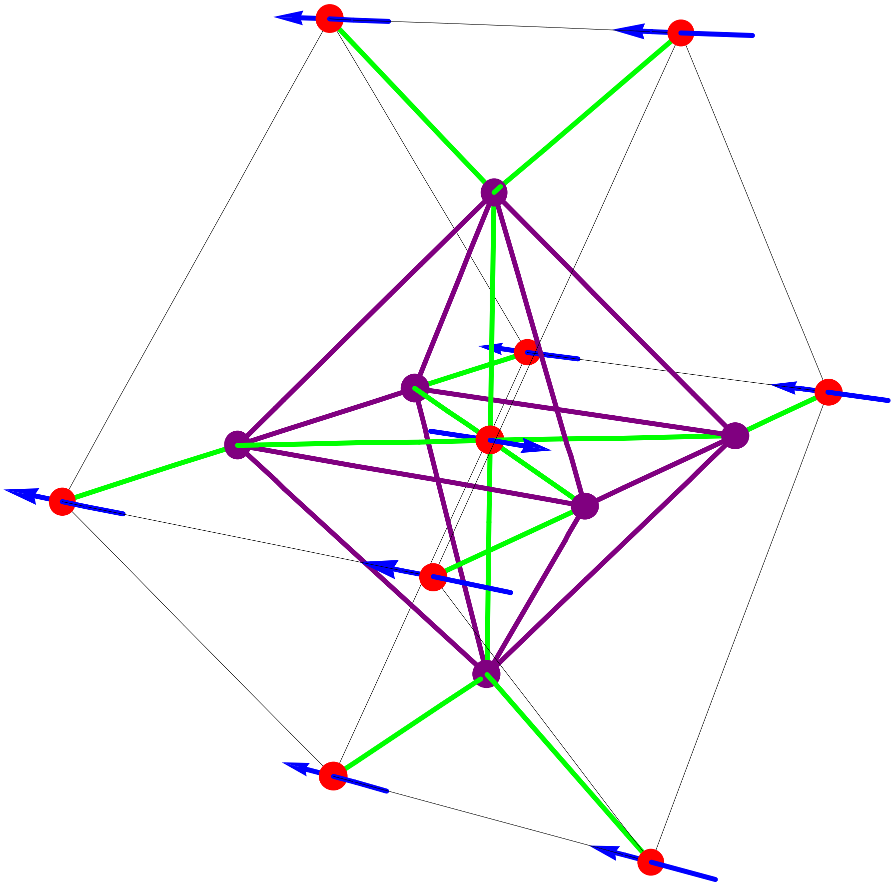


**Fig.** Structure of $MnF_2$. Mn (red) and F (purple). The direction of spins is the *c* axis (the z axis). The *x* and *y* axes are also shown. These axes are parallel to the straight lines connecting Mn atoms.

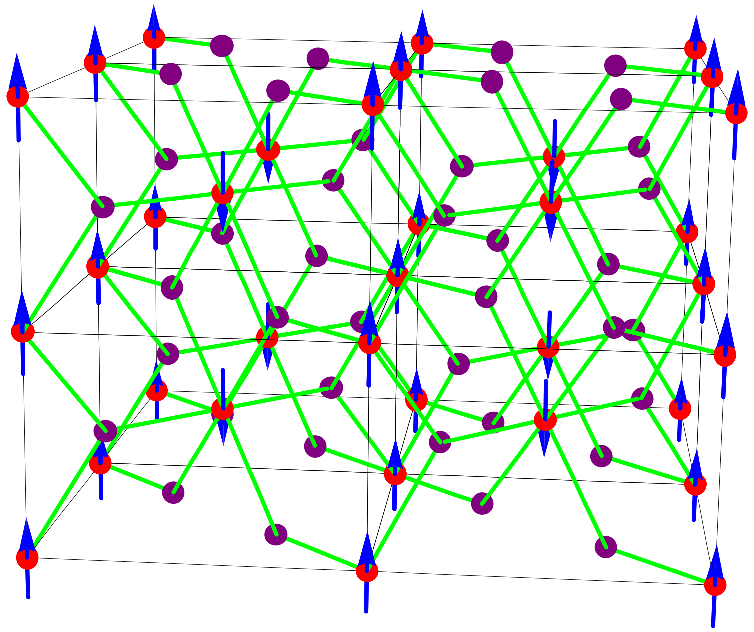


**Fig.** Structure of $MnF_2$. This figure is drawn using the Mathematica (Graphics3D).

The exchange interactions $J_1$, $J_2$, and $J_3$ are given by

$J_1$ = 0.028 meV =0.324926 K
$J_2$ =-0.152 meV = 1.76388 K (between the nearest neighbor $Mn^{2+}$ spins)
$J_3$ = -0.004 meV = -0.046418 K

((Note)) 1 meV = 11.6045 K.

The important parameters of $MnF_2$ are given as follows.

$T_N$ = 67.459 K (Néel temperature)
$H_{SF}$ = 92 kOe at 4.2 K (Spin flop magnetic field, which will be discussed later)
$H_E$ = 525.19 kOe (exchange field)

The exchange field is defined by

$$H_E = \frac{2zJ_2S}{g\mu_B} = 525.190 \text{ kOe}.$$

where $J_2$ (<0) is the antiferromagnetic interaction between $Mn^{2+}$ spins in $MnF_2$. The anisotropy field $H_A$ can be calculated from the relation (which will be discussed later) as

$$H_A = \frac{{H_{SF}}^2}{2H_E} = 8.234 \text{ kOe}.$$

The perpendicular susceptibility at $T = 0$ K an be evaluated

$$\chi_\perp = \frac{1}{A} = \frac{g^2 {\mu_B}^2 N_A}{4z|J_2|} = 0.0266873 \text{ (emu/Mn mol)},$$

where $z$ is the number of the nearest neighbor Mn atoms, $z = 8$. This value of $\chi_\perp$ is in very good agreement with the experimental value

$$\chi_M = 250\times 10^{-6}(emu/g)92.934855(g/mol) = 0.0232337 \text{ emu/mol at } T_N.$$

The exchange field is evaluated as

$$H_E = \frac{2z|J_2|S}{g\mu_B} = 525.190 \text{ kOe}.$$

(i) According to Keffer (F. Keffer, Phys. Rev.B **87**, 608 (1952). "Anisotropy in the antiferromagnetic $MnF_2$.", the single ion anisotropy of $MnF_2$ is given by

$$D = -0.012 \text{ cm}^{-1} = -0.0172653 \text{ K}.$$

Then the anisotropy field is evaluated as

$$H_A = \frac{2DS}{g\mu_B} = 642.584 \text{ Oe}.$$

where

$$H_A = \frac{NDS^2}{\frac{1}{2}g\mu_B NS} = \frac{2DS}{g\mu_B}.$$

(ii) Using the experimental value of $H_A$ (= 8.234 kOe), the value of $D$ is calculated as

$$D = -\frac{g\mu_B H_A}{2S}$$ =- 0.221 K.

This value of $D$ is rather different from that reported by Keffer. The negative value of $D$ indicates that the spin symmetry of $MnF_2$ is Ising. In other words, the easy direction of spins is the *c* axis (*z* axis). Note that the single ion anisotropy $D$ is given by

$$D = \frac{\lambda}{2}(g_c - g_a).$$

where $\lambda$ is the spin orbit coupling constant, $g_c$ and $g_a$ are the g-factors along the *c* axis and the *a* axis.

---

## 9. Dipole-dipole interaction in $MnF_2$

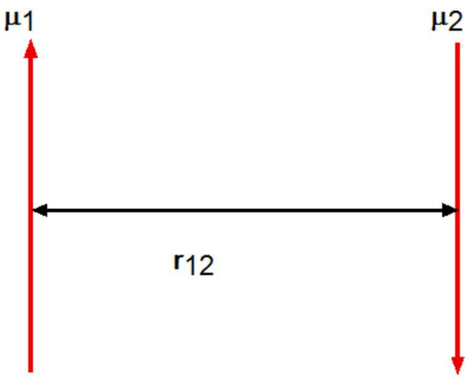
The magnetic dipolar interaction is given by

$$H_{dipole} = \frac{(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2) r_{12}^2 - 3(\boldsymbol{\mu}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\mu}_2 \cdot \mathbf{r}_{12})}{r_{12}^5}$$

with

$$\boldsymbol{\mu}_1 = -g\mu_B \mathbf{S}_1, \qquad \boldsymbol{\mu}_2 = -g\mu_B \mathbf{S}_2$$

(i)



$$H_{dipole} = \frac{(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2) r_{12}{}^2}{r_{12}{}^5} = \frac{\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2}{r_{12}{}^3} = -\frac{\mu_1 \mu_2}{a^3}$$

where *a* is the lattice constant. This means that the antiferromagnetic spin configuration is favorable in energy.

(ii)

$$H_{dipole} = \frac{\mu_1 \mu_2 r_{12}{}^2 - 3\mu_1 \mu_2 r_{12}{}^2}{r_{12}{}^5} = \frac{-2\mu_1 \mu_2{}^2}{a^3}$$

This means that the ferromagnet spin configuration is favorable in energy. For $MnF_2$, we calculate the magnitude of the dipole interaction;

$$\xi = \frac{2\mu_1 \mu_2}{a^3} = \frac{2g^2 \mu_B{}^2 S^2}{a^3}$$

When $S = 5/2$, g = 2 and $a = a_0$ (in the units of Å),

$$\xi = \frac{2.68408}{a_0{}^3}\ [\text{meV}]$$

or

$$\xi = \frac{31.1474}{a_0^{\ 3}}\,[\mathrm{K}].$$

where $a = a_0$ (in the units of Å). From Fig. (below), the dipole interaction is of the order of 0.5 K when $a$ = 4 Å.

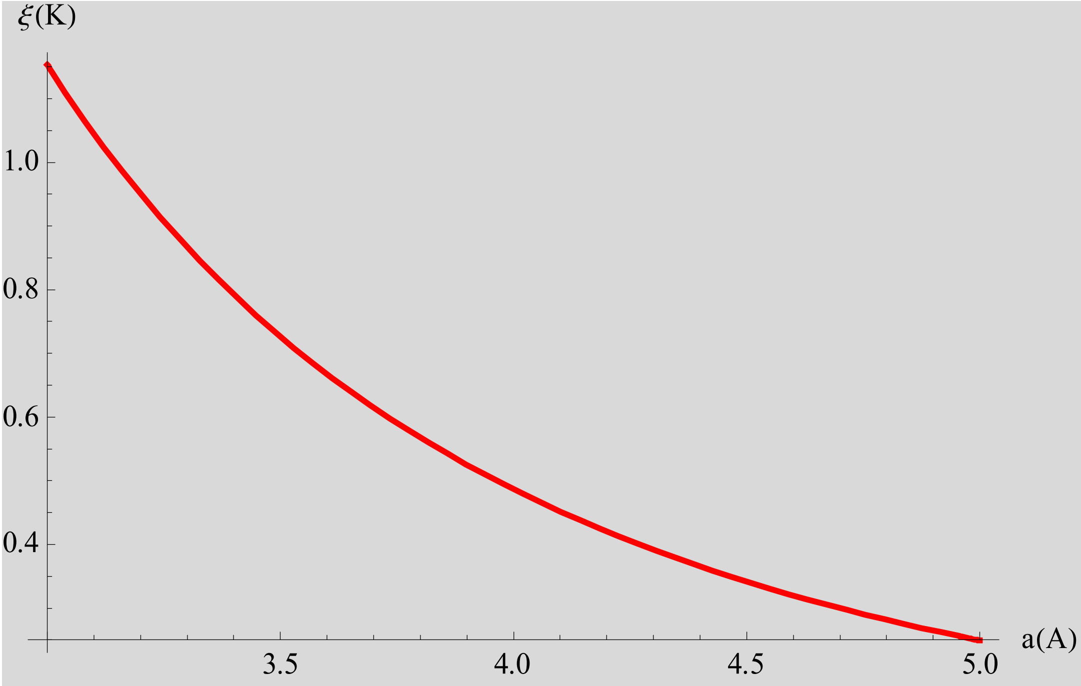


**Fig.** dipole-dipole interaction as a function of the lattice constant *a*.

## 10. Comment on the anisotropy field in $MnF_2$ (L.J. de Jongh and A.R. Miedema)

The (uniaxial ) anisotropy may be calculated from the spin-wave gap as measured by zero-field, zero-temperature AFMR by Johnson and Nethercot (1959). They found $\omega/\gamma = (9.33 \pm 0.05)\mathrm{x}10^4$ Oe, in excellent agreement with the value $(9.3 \pm 0.2)$ x $10^4$ Oe obtained by Jacobs (1961) for the spin-flop field. With the aid of the formula $(\omega/\gamma)^2 = 2H_EH_A - H_A^2$ and the above-mentioned value for the antiferromagnetic exchange, one deduces $H_A$ = 8220 Oe ($H_A$=$H_E$ = 1:6 $10^{-2}$), which should be accurate within 2%. It turns out that the anisotropy is for the most part of dipolar origin. Keffer (1952) calculated the dipolar contribution to be 8300 Oe. Correction for zero-point reduction (2.4%) reduces this to 8100 Oe. The remaining part of about 100 Oe, due to crystal-field effects, is considerably smaller than Keffer's estimate of 500 Oe, yet it is about twice as large as that reported for $K_2MnF_4$ (Folen 1972).

(from

L.J. de Jongh and A.R. Miedema, Adv. Phys. **23**, 947-1170 (1974). "Experiments on simple magnetic model systems.").

((Note))

$H_A$ = 8220 Oe →0.5521 K

$H_A$ = 8300 Oe →0.5575 K

## 11. Magnetic susceptibility of MnF$_2$

According to the spin wave thoery of antiferromagnet [R. Kubo, Phys. Rev. B **87**, 568 (1952)], the parallel susceptibility is expressed by

$$\chi_{//} \approx \chi_{\perp}(\frac{T}{T_N})^2 .$$

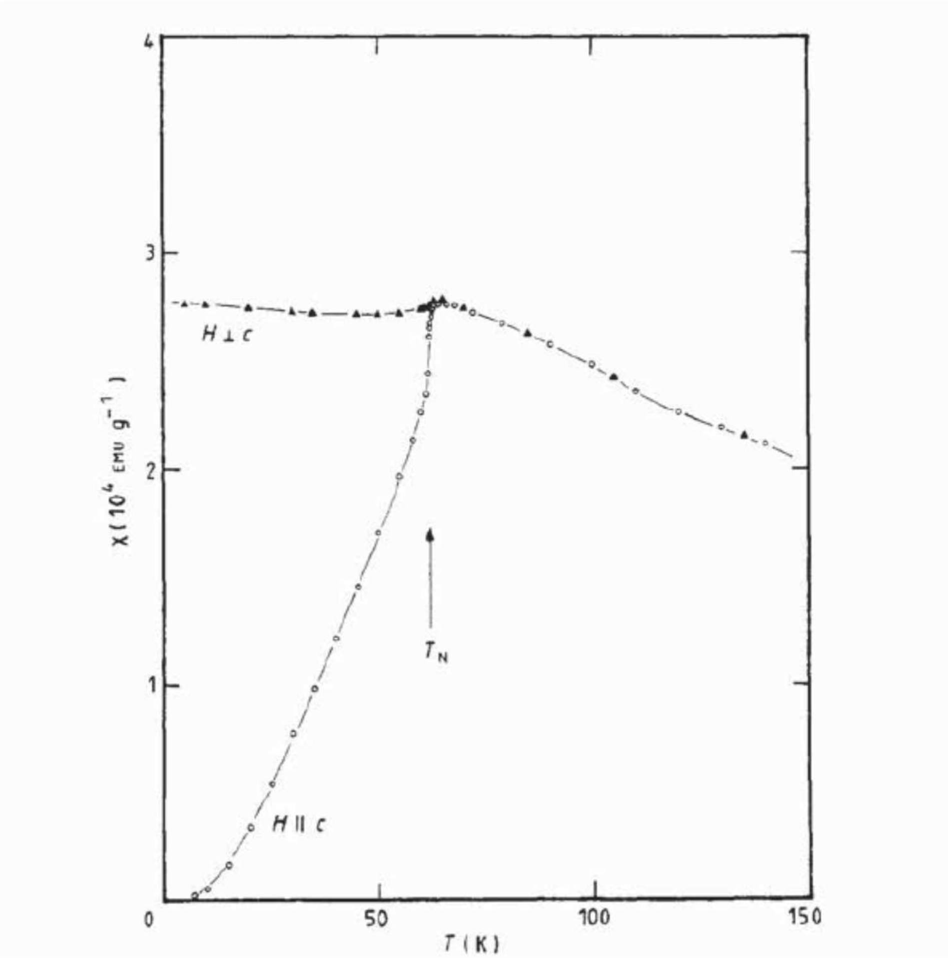


**Fig.** Parallel ($//c$) and perpendicular ($\perp c$) susceptibility of MnF$_2$ as a function of temperature. [H. Ikeda and K. Kikuta, J. Phys. C Solid State Physics, **16**, L445, 1983].

M(molar mass) = 92.934855 g/mol. $\chi_M (emu/mol) = M(g/mol)\chi_g (emu/g)$.

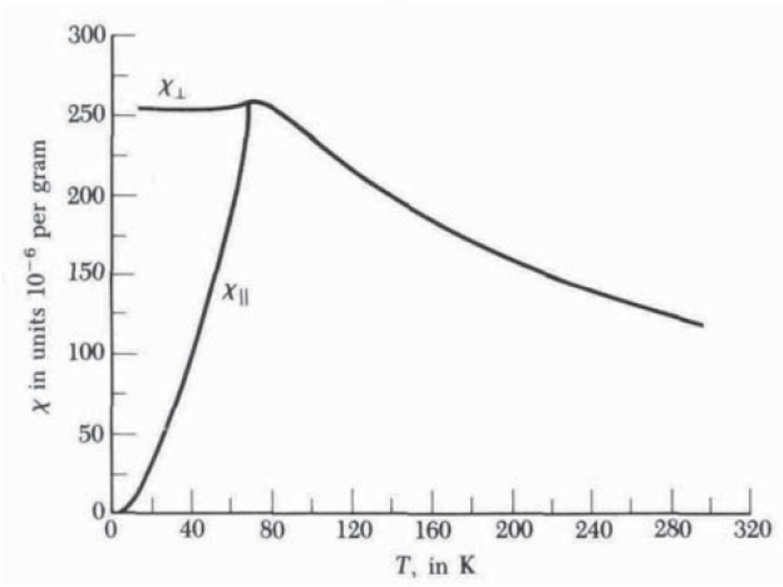


**Fig.** Susceptibility of MnF$_2$ (from Phys.927, Prof. Tsymbal, University of Nebraska, Lincoln)
http://physics.unl.edu/~tsymbal/teaching/SSP-927/Section%2016_Magnetic_Properties_2.pdf

((**Note**))
The saturation magnetization of MnF$_2$ is

$$N_A g \mu_B S = 27924.7 \text{ emu/Mn mol.}$$

for $S = 5/2$.

---

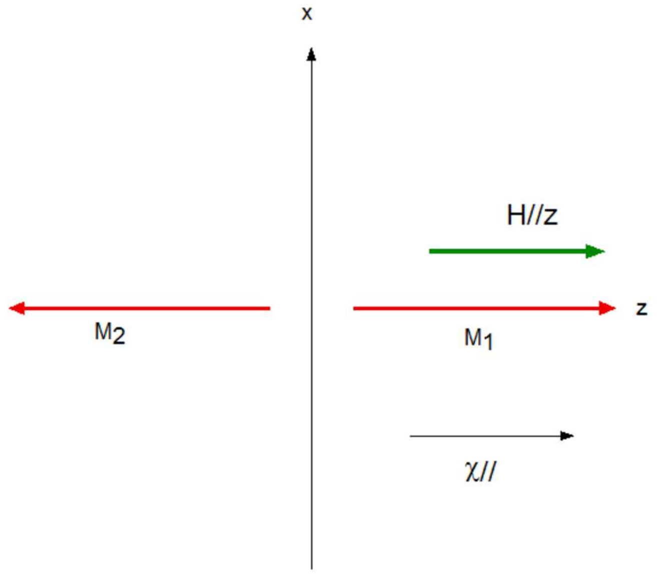
## 12. Magnetization of antiferromagnet

We define the anisotropy of antiferromagnet $F_A$ as

$$F_A = -\frac{K}{2}(\alpha_{1z}{}^2 + \alpha_{2z}{}^2) \qquad (K>0).$$

where $\alpha_{1z}$ and $\alpha_{2z}$ are the directional cosine.

### (a) The case when *H* is applied along the *z* axis (easy axis, weak field)

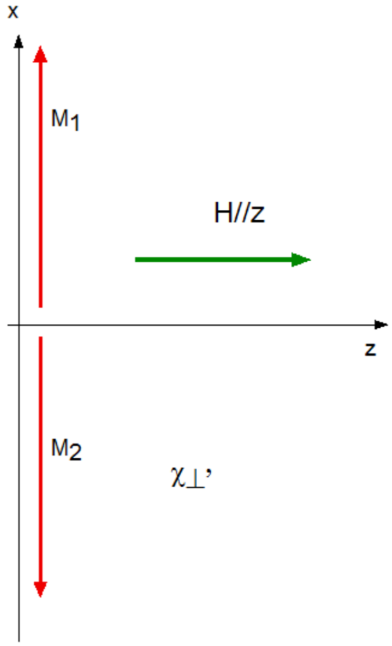


The magnetic field is applied along the *z* axis. The free energy of this system is

$$\Delta F_{//} = -\frac{1}{2}\chi_{//}H^2 - K\ ,$$

where $\chi_{//}$ is the susceptibility along the *z* axis.

### (b) The case when *H* is applied along the *z* axis (stronger field)



The free energy of this system is

$$\Delta F_{\perp} = -\frac{1}{2}\chi_{\perp}' H^2,$$

where $\chi_{\perp}'$ is the susceptibility along the *z* axis when $M_1$ and $M_2$ are parallel to the *x* axis.

When $\Delta F_{//} \geq \Delta F_{\perp}$, the case (b) is favorable compared to the case (a). This condition can be rewritten as

$$-\frac{1}{2}\chi_{//} H^2 - K \geq -\frac{1}{2}\chi_{\perp}' H^2,$$

or

$$(\chi_{\perp}' - \chi_{//}) H^2 \geq 2K .$$

For $H \geq H_f = \sqrt{\dfrac{2K}{\chi_{\perp}' - \chi_{//}}}$,

the spins rotates from the *z*-axis to the *x*-axis (***spin flipping transition***).

At $T = 0$ K,

$$\chi_{//} = 0, \qquad \text{and} \qquad \chi_{\perp}' \approx \frac{1}{A}.$$

Then we have

$$H_f = \sqrt{2KA} = \sqrt{2\frac{K}{M_1}AM_1} = \sqrt{2H_E H_A}.$$

Note that

$$A = \frac{4zJ}{g^2 {\mu_B}^2 N}, \qquad M_1 = \frac{N}{2} g\mu_B S.$$

Then the fields $H_E$ and $H_A$ are given by

$$H_E = AM_1 = \frac{4zJ}{g^2 {\mu_B}^2 N}\frac{N}{2} g\mu_B S = \frac{2zJS}{g\mu_B}$$

$$H_A = \frac{K}{M_1}$$

where $M_1$ is the sublattice magnetization. Usually we assume the single ion anisotropy

$$-DS^2$$

as an anisotropy;

$$K = DS^2$$

The anisotropy field is expressed by

$$H_A = \frac{N_A DS^2}{M_1} = \frac{2N_A DS^2}{N_A g\mu_B S} = \frac{2DS}{g\mu_B}$$

## 13. More general case

At $T = 0$ K,

$$\chi_{//} = 0, \qquad \text{and} \qquad \chi_{\perp}' = \frac{1}{A - \frac{K}{2M_1^2}} \qquad \text{(Kanamori, exercise 6-3)}$$

Then the spin-flop field is

$$H_f = \sqrt{\frac{2K}{\chi_{\perp}'}} = \sqrt{2K(A - \frac{K}{2M_1^2})} = \sqrt{\frac{K}{M_1}(2AM_1 - \frac{K}{M_1})} = \sqrt{H_A(2H_E - H_A)}$$

## 14. Saturation field

$$\chi_{\perp}' H_s = 2M_1$$

Then $H_s$ is expressed by

$$H_s = \frac{2M_1}{\chi_{\perp}'} = 2M_1(A - \frac{K}{2M_1^2}) = 2M_1 A - \frac{K}{M_1} = 2H_E - H_A$$

## 15. Condition of the spin flop transition

$$\begin{aligned} H_s^2 - H_f^2 &= (2H_E - H_A)^2 - H_A(2H_E - H_A) \\ &= 2(2H_E - H_A)(H_E - H_A) \end{aligned}$$

If $H_E > H_A$, we have

$$H_s > H_f$$

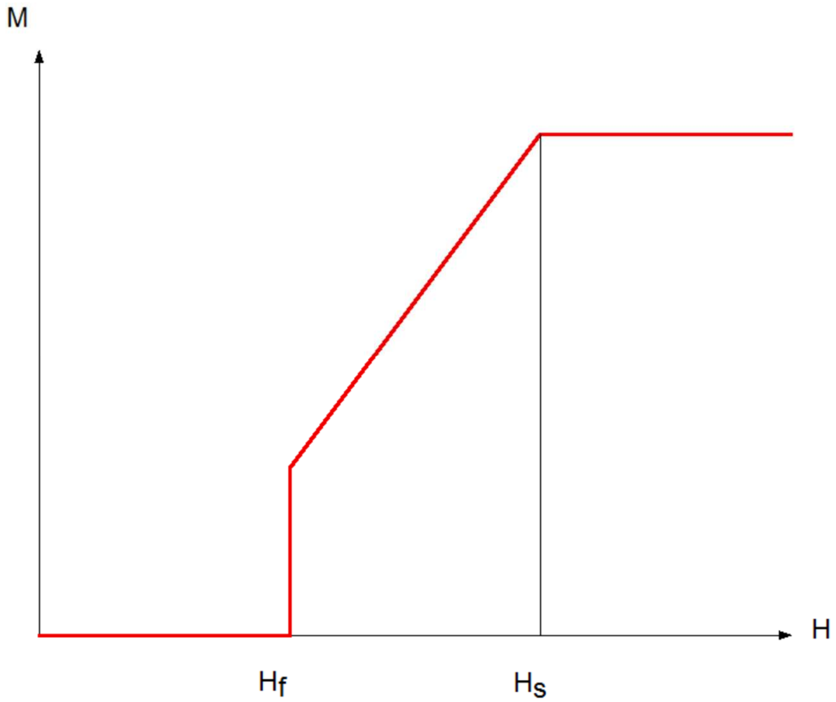


**Fig.** Magnetization curve during the spin-flop behavior in the presence of external magnetic field. $H_f$ is the spin-flop field and $H_s$ is the saturation field.

## 16. Néel temperature derivation

When $H = 0$, $\delta M = 0$. Then

$$\mathbf{H}_m(1) = (A+B)M_0\mathbf{e}_z$$

$$M_0 = \frac{N}{2} g\mu_B S B_S(x_1)$$

where

$$x = \frac{g\mu_B S}{k_B T}(A+B)M_0$$

$$y = \frac{M_0}{\frac{N}{2} g\mu_B} = SB_S(x)$$

The value of y can be written as

$$y = \frac{2M_0}{Ng\mu_B} = \frac{2k_B Tx}{Ng^2\mu_B{}^2 S(A+B)}$$

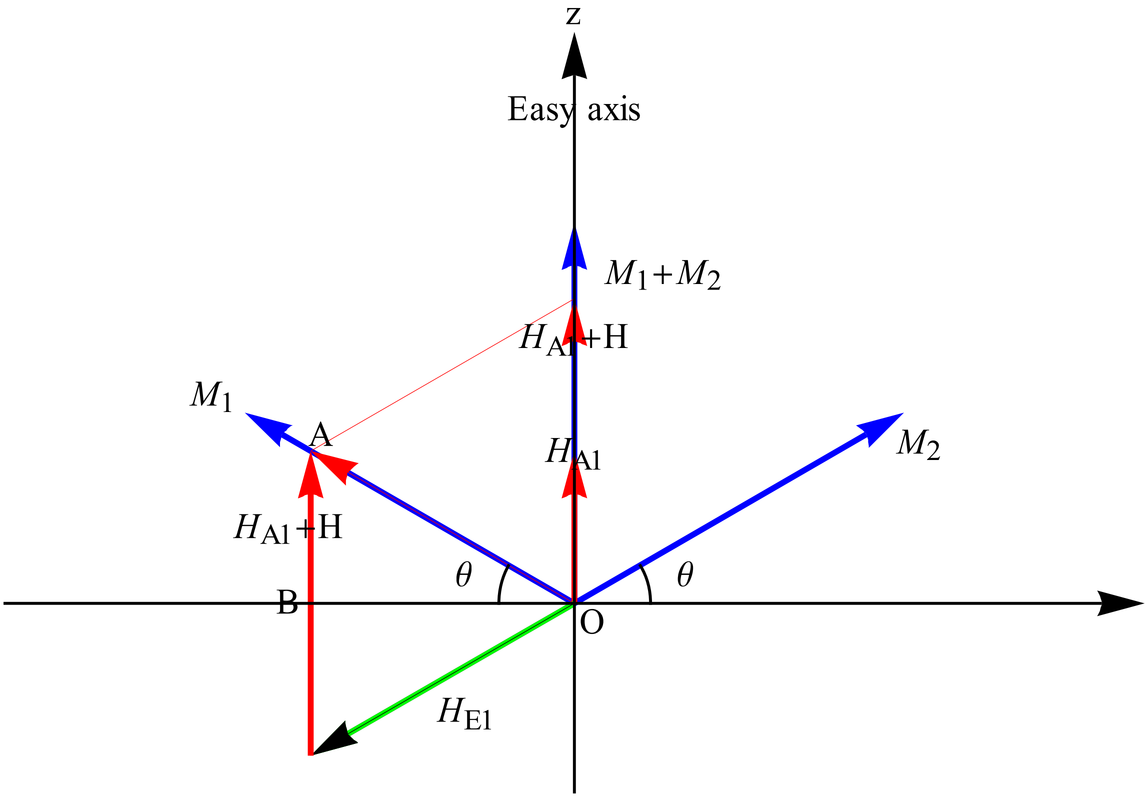
At $T = T_N$, $y = \frac{1}{3}(S+1)x$

$$\boxed{T_N = \frac{Ng^2\mu_B{}^2 S(S+1)}{3k_B}\left(\frac{A+B}{2}\right)}$$

---

**17.**

We consider the case when the magnetic field is applied along the easy axis ($z$ axis) . What is the magnetic susceptibility along the $z$ axis.



In the above figure, we get

$$M_{1z} = M_1 \sin\theta, \qquad M_{2z} = M_2 \sin\theta$$

$$H_{A1} = \frac{K}{M_1^{\ 2}} M_{1z} = \frac{K}{M_1^{\ 2}} M_1 \sin\theta = \frac{K}{M_1}\sin\theta$$

$$H_{A2} = \frac{K}{M_2^{\ 2}} M_{2z} = \frac{K}{M_2^{\ 2}} M_2 \sin\theta = \frac{K}{M_2}\sin\theta$$

where

$$M_1 = M_2 . \qquad \mathbf{H}_{E1} = -A\mathbf{M}_2 , \qquad \mathbf{H}_{E2} = -A\mathbf{M}_1 .$$

The susceptibility along the easy axis is

$$\chi_\perp ' = \frac{M_{1z} + M_{2z}}{H} = \frac{2M_1 \sin\theta}{H} .$$

In the above figure, we have the relation

$$\tan\theta = \frac{\overline{AB}}{\overline{OB}} = \frac{H + H_{A1} - H_{E1}\sin\theta}{H_{E1}\cos\theta} ,$$

or

$$2H_{E1}\sin\theta = H + H_{A1} = H + H_A \sin\theta ,$$

or

since

$$H_{A1} = \frac{K}{M_1}\sin\theta = \frac{K}{M}\sin\theta = H_A \sin\theta ,$$

and

$$H_A = \frac{K}{M} .$$

Thus we have

$$2H_E \sin\theta = H + H_A \sin\theta, \qquad \sin\theta = \frac{H}{2H_E - H_A}$$

where

$$H_{E1} = H_E = AM$$

Then we get

$$\chi_\perp' = \frac{2M_1 \sin\theta}{H} = \frac{M}{H_E - \frac{H_A}{2}} = \frac{M}{AM - \frac{K}{2M}} = \frac{1}{A - \frac{K}{2M^2}}$$

The saturation field is given by

$$\sin\theta = \frac{H}{2H_E - H_A} = 1, \qquad H_c = 2H_E - H_A$$

## 18. The physical principles of magnetism

A.H. Morrish (John Wiley & Sons, New York, 1965)

If, on the application of *H*, the sublattice magtnetization remains collinear with the easy direction, the change in free energy per unit volume is

$$\Delta F_T = -\frac{1}{2}\chi_{//} H^2.$$

Suppose, however, the sublattice magnetization lie perpendicular to the easy direction. If K ≈ 0, this change in free energy is

$$\Delta F_T = -\frac{1}{2}\chi_\perp H^2.$$

Now, for an antiferromagnetic material, $\chi_\perp > \chi_{//}$ for $T<T_N$. Therefore, under these conditions, the perpendicular orientation would be the ground state.

For $K = 0$, $\Delta F_T = K - \frac{1}{2}\chi_\perp H^2$ for the perpendicular orientation: the parallel orientation is in the state of the lowest energy provided $H$ is not too large. At a critical field $H_f$, defined by the equation

$$-\frac{1}{2}\chi_{//} H^2 = K - \frac{1}{2}\chi_\perp H^2$$

or

$$H = \sqrt{\frac{2K}{\chi_\perp - \chi_{//}}}$$

the energy of the two states are equal. Hence, for $H<H_f$, the sublattice magnetization will be parallel to the easy direction, whereas for $H>H_f$, they will be perpendicular. The change from the parallel to the perpendicular orientation is usually called spin flopping.

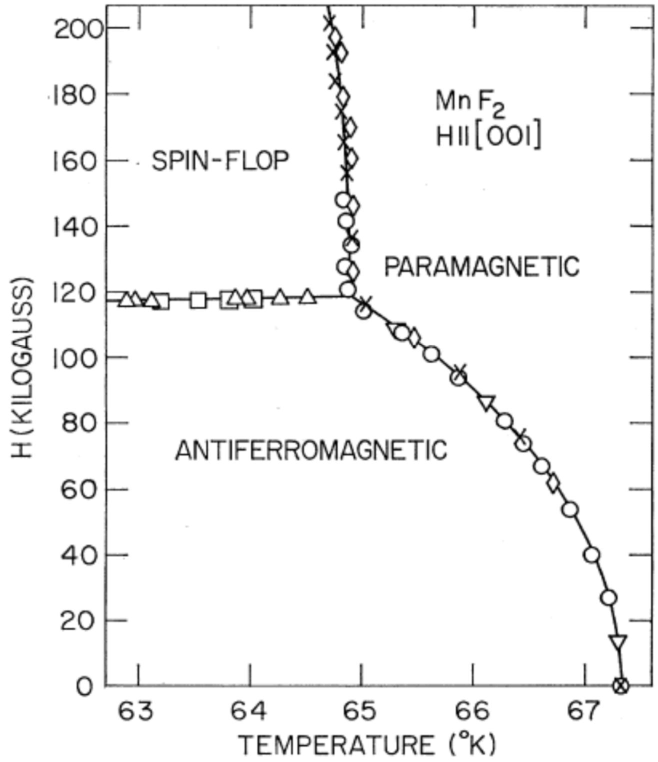
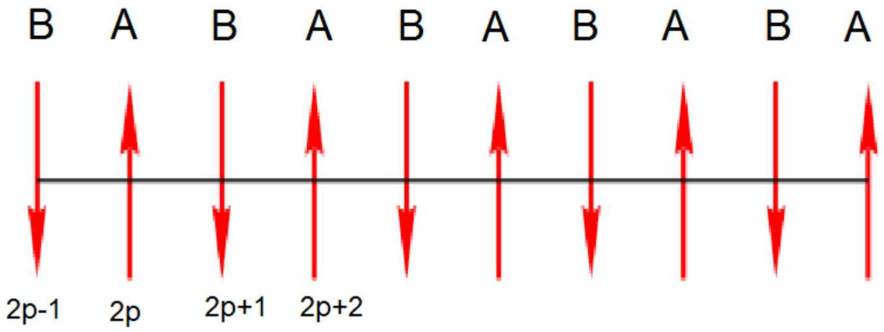


**Fig.** Magnetic phase diagram of $MnF_2$ between 63 and 67.5 K and with *H*//*c* axis (easy axis) [Y. Shapira and S. Foner, Phys. Rev. B **1**, 3083 (1969)).

## 19. Spin wave in the antiferromagnet



Let spins with even indices -2*p* compose sublattice A, that with spin up ($S_{2p}{}^{z} = S$)., and let spins with odd indices 2*p*+1 compose sublattice B, that with spin down ($S_{2p+1}{}^{z} = -S$). We consider only nearest-neighbor interactions with *J*. For spins on the sublattice A (*J*>0),

$$\frac{dS_{2p}{}^{x}}{dt} = \frac{2JS}{\hbar}[2S_{2p}{}^{y} + (S_{2p-1}{}^{y} + S_{2p+1}{}^{y})]$$

$$\frac{dS_{2p}{}^{y}}{dt} = -\frac{2JS}{\hbar}[2S_{2p}{}^{x} + (S_{2p-1}{}^{x} + S_{2p+1}{}^{x})]$$

The corresponding equations for a spin on the sublattice B,

$$\frac{dS_{2p+1}{}^{x}}{dt} = -\frac{2JS}{\hbar}[2S_{2p+1}{}^{y} + (S_{2p}{}^{y} + S_{2p+2}{}^{y})]$$

$$\frac{dS_{2p+1}{}^{y}}{dt} = \frac{2JS}{\hbar}[2S_{2p+1}{}^{x} + (S_{2p}{}^{x} + S_{2p+2}{}^{x})]$$

We define anew parameter,

$$S^{+} = S^{x} + iS^{x}$$

Then we get

$$\frac{dS_{2p}{}^{+}}{dt} = -\frac{2iJS}{\hbar}[2S_{2p}{}^{+} + (S_{2p-1}{}^{+} + S_{2p+1}{}^{+})]$$

$$\frac{dS_{2p+1}{}^{+}}{dt} = \frac{2iJS}{\hbar}[2S_{2p+1}{}^{+} + (S_{2p}{}^{+} + S_{2p+2}{}^{+})]$$

We look for solutions of the form

$$S_{2p}{}^{+} = u\exp[i(pka - \omega t)$$

$$S_{2p+1}{}^{+} = v\exp[i(pka - \omega t)$$

with

$$\omega_{ex} = \frac{4JS}{\hbar}$$

Then

$$\omega u = \frac{1}{2}\omega_{ex}(2u + ve^{-ika} + ve^{ika}) = \omega_{ex}[u + v\cos(ka)]$$

$$-\omega v = \frac{1}{2}\omega_{ex}(2v + ue^{-ika} + ue^{ika}) = \omega_{ex}[v + u\cos(ka)]$$

or

$$\begin{pmatrix} \omega_{ex} - \omega & \omega_{ex}\cos(ka) \\ \omega_{ex}\cos(ka) & \omega_{ex} + \omega \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

These have nontrivial solution if

$$\begin{vmatrix} \omega_{ex} - \omega & \omega_{ex}\cos(ka) \\ \omega_{ex}\cos(ka) & \omega_{ex} + \omega \end{vmatrix} = 0$$

Then we have

$$\omega = \omega_{ex}\left|\sin(ka)\right|$$

For *ka*<<1,

$$\omega = \omega_{ex}|ka|$$

This dispersion relation is different from that of ferromagnet.

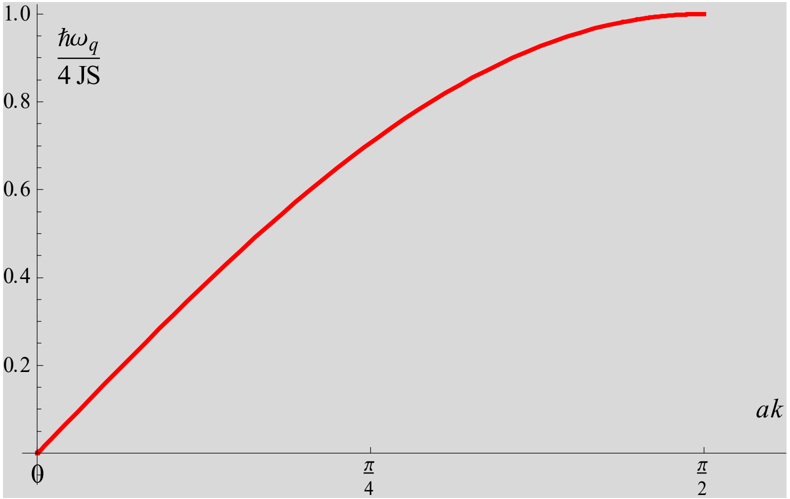


Fig. The dispersion relation of magnon for the 1D antiferromagnetic chain. a is the lattice constant. The size of the magnetic unit cell is twice larger than the lattice spacing.

## 20. Quantization of spin waves (antiferromagnet)

We use the Holstein-Primakoff method.

(a) $S_j^z \approx S$ (+ sublattice)

$$S_j^z = S - a_j^* a_j, \qquad S_j^+ = \sqrt{2S}a_j, \qquad S_j^- = \sqrt{2S}a_j^*$$

(b) $S_l^z \approx -S$ (-sublattice)

$$S_l^z = -S + b_l^* b_l, \qquad S_l^+ = \sqrt{2S}b_l^*, \qquad S_l^- = \sqrt{2S}b_j$$

Hamiltonian

$$H = 2|J|\sum_{<j,l>}\mathbf{S}_j\cdot\mathbf{S}_l - g\mu_B H_A(\sum_j S_j^z - \sum_l S_l^z)$$
$$= -Nz|J|S^2 + 2|J|S\sum_{<j,l>}[(n_j + n_l) + a_j^* b_\ell^* + a_j b_l] - Ng\mu_B S H_A(\sum_j n_j + \sum_l n_l)$$

where *z* is the number of the nearest-neighbor pairs. Only the exchange interaction between spins in different sublattices is not equal to zero. We have

$$a_j = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{q}} a_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}_j}$$

and

$$b_l = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{q}} b_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}_j}$$

where *N*/2 is the number of spins in the sublattice. Then *H* can be rewritten as

$$H = -Nz|J|S^2 + 2|J|Sz\sum_{\mathbf{q}}[(a_{\mathbf{q}}^{*}a_{\mathbf{q}} + b_{\mathbf{q}}^{*}b_{\mathbf{q}}) + \gamma(\mathbf{q})(a_{\mathbf{q}}^{*}b_{\mathbf{q}}^{*} + a_{\mathbf{q}}b_{\mathbf{q}})]$$
$$- Ng\mu_B SH_A + g\mu_B SH_A \sum_{q}(a_{\mathbf{q}}^{*}a_{\mathbf{q}} + b_{\mathbf{q}}^{*}b_{\mathbf{q}})$$

where

$$\gamma(\mathbf{q}) = \frac{1}{z}\sum_{\boldsymbol{\rho}} e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}$$

***q*** is the vector connecting between nearest neighbor spins. We have a transformation (Bogolyubov transformation)

$$A_{\mathbf{q}} = \cosh\theta_{\mathbf{q}} a_q + \sinh\theta_{\mathbf{q}} b_q^{*}, \qquad B_{\mathbf{q}} = \cosh\theta_{\mathbf{q}} b_q + \sinh\theta_{\mathbf{q}} a_q^{*}$$

or

$$a_{\mathbf{q}} = \cosh\theta_{\mathbf{q}} A_q - \sinh\theta_{\mathbf{q}} B_q^{*}, \qquad b_{\mathbf{q}} = \cosh\theta_{\mathbf{q}} B_q - \sinh\theta_{\mathbf{q}} A_q^{*}$$

When we choose

$$\tanh 2\theta_{\mathbf{q}} = \frac{\gamma(\mathbf{q})}{1+\alpha}$$

with

$$\alpha = \frac{g\mu_B H_A}{2|J|zS}$$

we have $H$ as

$$H = -Nz|J|S^2 - 2|J|Sz\sum_{\mathbf{q}}[1+\alpha-\sqrt{(1+\alpha)^2-[\gamma(\mathbf{q})]^2}]$$
$$+\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}(A_{\mathbf{q}}{}^{*}A_{\mathbf{q}}+B_{\mathbf{q}}{}^{*}B_{\mathbf{q}})$$

where the first term $-Nz|J|S^2$ is the ground state of the classical spin system, the second term is the lowering of the energy due to the zero-point oscillation of spins, the third term is the excitation of magnons,

$$\hbar\omega_{\mathbf{q}} = 2|J|zS\sqrt{(1+\alpha)^2-[\gamma(\mathbf{q})]^2}$$

In the presence of an external magnetic field

$$\hbar\omega_{\mathbf{q}} = 2|J|zS\sqrt{(1+\alpha)^2-[\gamma(\mathbf{q})]^2} \pm g\mu_B H$$

## 21. Energy of ground state

In the ground state

$$A_{\mathbf{q}}{}^{*}A_{\mathbf{q}} = B_{\mathbf{q}}{}^{*}B_{\mathbf{q}} = 0\,.$$

the energy of the ground state is given by

$$E_G = -Nz|J|S^2 - 2|J|Sz\sum_{\mathbf{q}}[1+\alpha-\sqrt{(1+\alpha)^2-[\gamma(\mathbf{q})]^2}],$$

which is lower than the classical energy (corresponding to the first term). This means that the Neel state does not correspond to the ground state.

We consider the case when $\alpha = 0$ ($H_A = 0$, and $H = 0$).

$$E_G = -Nz|J|S^2 - 2|J|Sz\sum_{\mathbf{q}}[1-\sqrt{1-[\gamma(\mathbf{q})]^2}]$$

**(a) 1D chain**

$$\gamma(q) = \cos(qa)$$

$$E_G = -2N|J|S^2(1 + \frac{0.363}{S})$$

$E_G$ is lower than the eneygy of the classical Néel state ($= -2N|J|S^2$).

**(b) 2D square lattice**

$$\gamma(q) = \frac{1}{2}[\cos(q_x a) + \cos(q_y a)]$$

$$E_G = -4N|J|S^2(1 + \frac{0.158}{S})$$

(c) 3D cubic

$$E_G = -6N|J|S^2(1 + \frac{0.0938}{S})$$

## 22. $\hbar\omega_{\mathbf{q}}$ at $q = 0$

$\hbar\omega_{\mathbf{q}}$ is given by

$$\hbar\omega_{\mathbf{q}} = 2|J|zS\sqrt{(1+\alpha)^2 - [\gamma(\mathbf{q})]^2}\ .$$

At $q = 0$, $\gamma(\mathbf{q}) = 1$. Then we have

$$\hbar\omega_{\mathbf{q}}|_{\mathbf{q}=0} = 2|J|zS\sqrt{(1+\alpha)^2 - 1} = g\mu_B\sqrt{H_A(2H_E + H_A)} \approx g\mu_B\sqrt{2H_A H_E}$$

for $H_E >> H_A$, where

$$H_E = \frac{2|J|zS}{g\mu_B}, \qquad H_A = \frac{2DS}{g\mu_B}.$$

The spin flop field is defined by

$$H_f \approx \sqrt{2H_A H_E} \ .$$

Then we have

$$\hbar\omega_{\mathbf{q}}\,|_{\mathbf{q}=0} = g\mu_B H_f \,.$$

## 23. The magnetization due to the excitation of magnons

The total number of magnons excited at a temperature $T$ is

$$\sum_q \left\langle n_{\mathbf{q}} \right\rangle = \int d\omega D(\omega) < n(\omega) > ,$$

where $D(\omega)$ is the number of magnon modes per unit frequency range.

$$D(\omega)d\omega = \frac{V}{(2\pi)^3} 4\pi q^2 dq = \frac{V}{(2\pi)^3} 4\pi q^2 \frac{dq}{d\omega} d\omega .$$

We use the magnon dispersion relation,

$$\omega_q = \omega = \frac{4JS}{\hbar} aq \ ,$$

$$\frac{d\omega}{dq} = \frac{4JSa}{\hbar} .$$

Then the density of states is given by

$$D(\omega) = \frac{V}{2\pi^2}\left(\frac{\hbar}{4JSa}\right)^3 \omega^2 .$$

The integral is taken over the allowed range of $\boldsymbol{q}$, which is the first Brillouin zone. At $T = 0$ K, we may carry the integral between 0 and $\infty$, because $<n(\omega)> \rightarrow\infty$ exponentially as $\omega\rightarrow\infty$.

$$\sum_q \langle n_{\mathbf{q}} \rangle = \frac{V}{2\pi^2}\left(\frac{\hbar}{4JSa}\right)^3 \int_0^\infty \frac{\omega^2 d\omega}{e^{\beta\hbar\omega}-1}$$

$$= \frac{V}{2\pi^2}\left(\frac{\hbar}{4JSa}\right)^3 \left(\frac{k_B T}{\hbar}\right)^3 \int_0^\infty \frac{x^2 dx}{e^x - 1}$$

$$= \frac{V}{2\pi^2 a^3}\left(\frac{k_B T}{4JS}\right)^3 \int_0^\infty \frac{x^2 dx}{e^x - 1}$$

Since $V = Na^3$ and

$$\int_0^\infty \frac{x^2 dx}{e^x - 1} = 2.40411$$

The deviation of the sublattice magnetization is proportional to

$$\sum_q \langle n_{\mathbf{q}} \rangle = \frac{N}{2\pi^2}\left(\frac{k_B T}{4JS}\right)^3 2.40411$$

which is proportional to $T^3$.

## 24. Heat capacity due to the excitation of magnons

The heat capacity is given by

$$C = \frac{dE}{dT} = \frac{\hbar^2}{k_B T^2}\int d\omega D(\omega)\frac{\omega^2}{(e^{\beta\hbar\omega}-1)(1-e^{-\beta\hbar\omega})}$$

where $\beta = 1/(k_B T)$,

$$E = \sum_q \hbar\omega_q \langle n_q \rangle = \int d\omega D(\omega)\hbar\omega \frac{1}{e^{\beta\hbar\omega}-1}$$

$$\frac{d}{dT}\frac{1}{e^{\beta\hbar\omega}-1} = \frac{\hbar\omega}{k_B T^2}\frac{1}{(e^{\beta\hbar\omega}-1)(1-e^{-\beta\hbar\omega})}$$

Then we get

$$
\begin{aligned}
C &= \frac{\hbar^2}{k_B T^2}\frac{V}{2\pi^2}\left(\frac{\hbar}{4JSa}\right)^3 \int d\omega \frac{\omega^4}{(e^{\beta\hbar\omega}-1)(1-e^{-\beta\hbar\omega})} \\
&= \frac{\hbar^2}{k_B T^2}\frac{V}{2\pi^2}\left(\frac{\hbar}{4JSa}\right)^3 \left(\frac{k_B T}{\hbar}\right)^5 \int_0^\infty dx \frac{x^4}{(e^x-1)(1-e^{-x})} \\
&= k_B \frac{N}{2\pi^2}\left(\frac{k_B T}{4JS}\right)^3 \int_0^\infty dx \frac{x^4}{(e^x-1)(1-e^{-x})}
\end{aligned}
$$

Here we note that

$$
\int_0^\infty \frac{x^4 dx}{(e^x-1)(1-e^{-x})} = 25.9758
$$

and $V = Na^3$. Then we have

$$
C = k_B \frac{N}{2\pi^2}\left(\frac{k_B T}{4JS}\right)^3 25.9758 = k_B N \left(\frac{k_B T}{4JS}\right)^3 1.31595
$$

The heat capacity is proportional to $T^3$.

## 25. Antiferromagnetic resonance of $MnF_2$ at $H = 0$

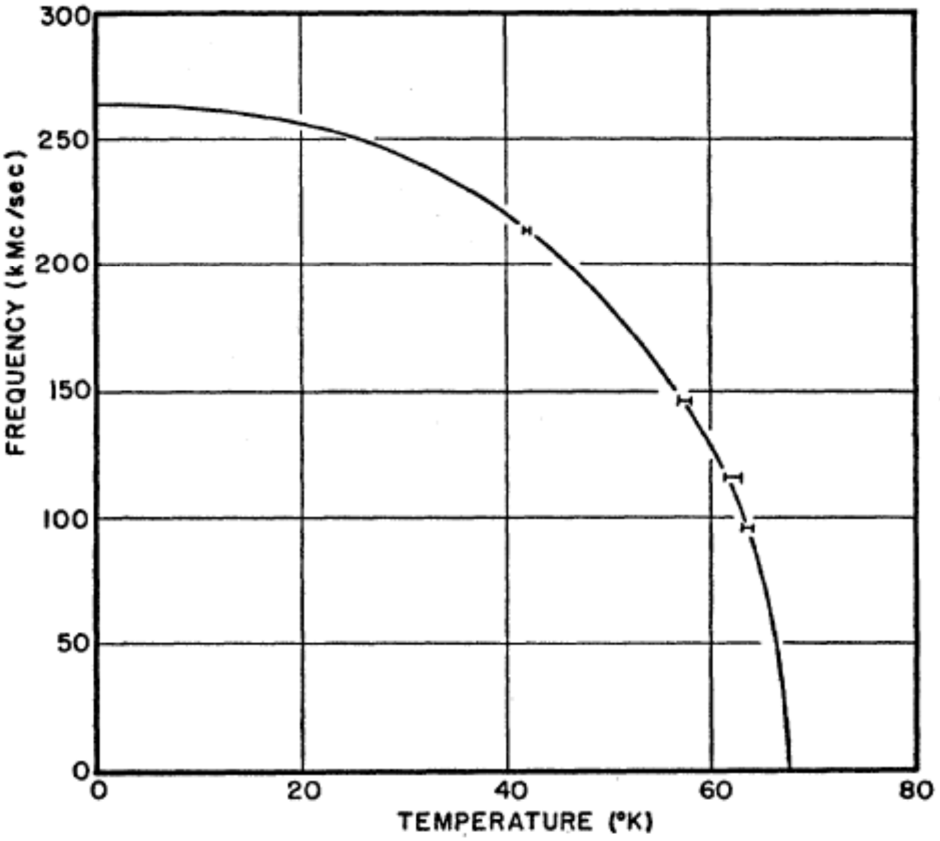


**Fig.** Temperatures at which antiferroamgnetic resonance occurs in $MnF_2$ at H = 0 for various frequencies [F.M. Johnson and A.H. Nethercot, Jr. Phys. Rev. **104**, 847 (1957). "Antiferromagnetic resonance in $MnF_2$."

In $MnF_2$,

$$g\mu_B H_f = 1.07664 \text{ meV} = 260.33 \text{ k MHz} = 0.26033 \text{ GHz}$$

This value is in good agreement with the result observed by Johnson and Nethercot, Jr..

## 26. Magnetic neutron scattering of $MnF_2$

The magnetic Bragg peaks appear at

$$h + k + l = \text{odd},$$

where the reciprocal lattice vectors are denoted by

$$\mathbf{Q} = \mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*.$$

with

$$a^* = \frac{2\pi}{a}, \qquad b^* = \frac{2\pi}{a}, \qquad b^* = \frac{2\pi}{c},$$

since the magnetic structure factor is proportional to

$$S_G = 1 - \exp[-i\pi(h+k+l)]$$

The nuclear Bragg peaks appear at

$$h+k+l = \text{even},$$

since the nuclear structure factor is proportional to

$$S_G = 1 + \exp[-i\pi(h+k+l)].$$

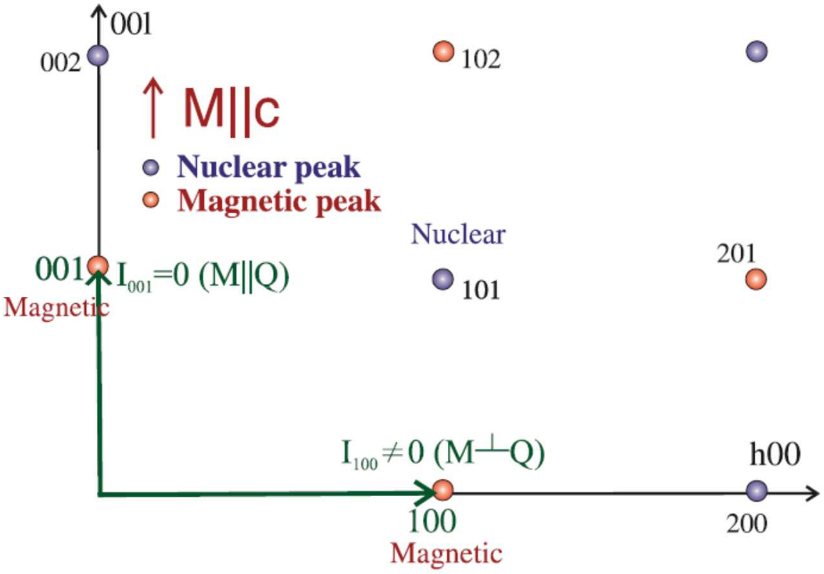


**Fig.** The (*h k l*) scattering plane of $MnF_2$ with k = 0. The nuclear Bragg reflections ($h+k+l$ = even) are shown with blue circles. The magnetic Bragg peaks ($h+k+l$ = odd) are shown with red circles. The magnetic moment is parallel to the c axis. No magnetic scattering is observed at (001) magnetic Bragg position (Yamani et al., 2010).

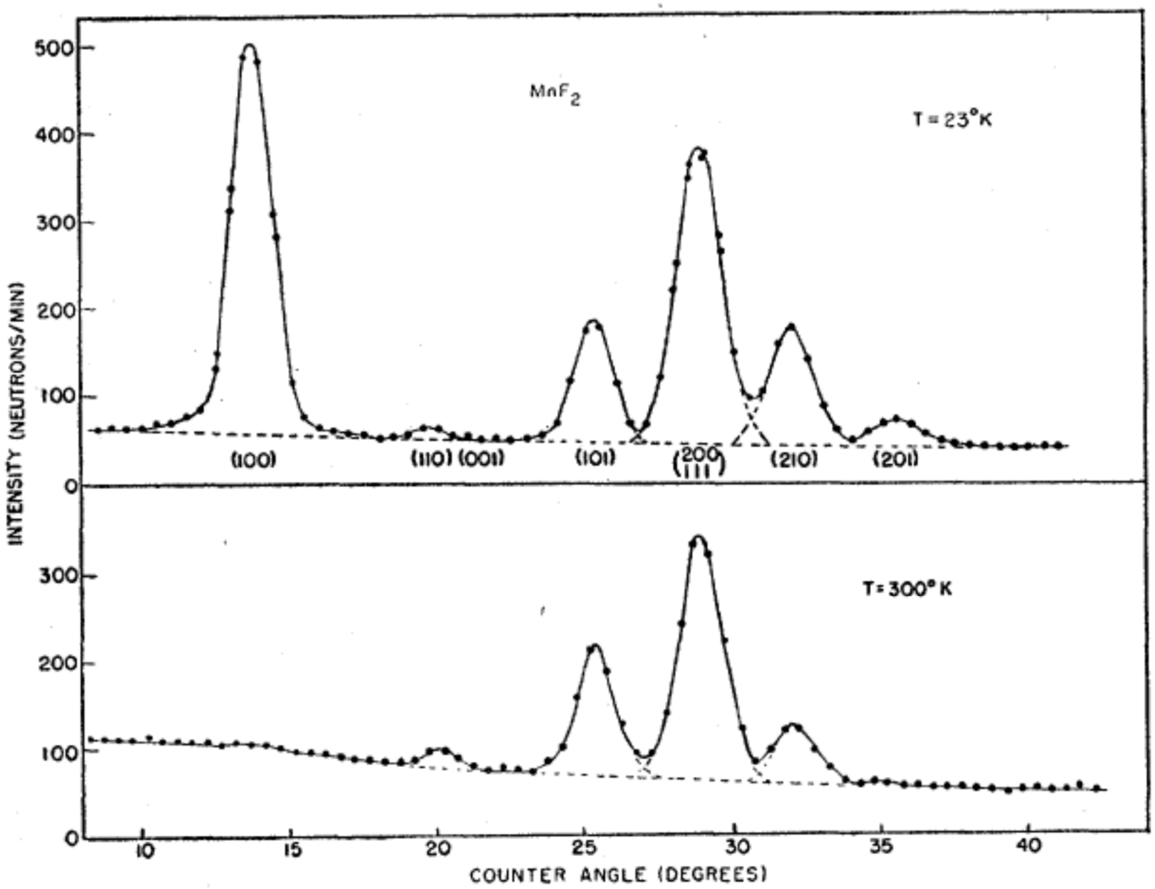


**Fig.** Neutron diffraction patters for $MnF_2$ in the paramagnetic state (295 K) and in the antiferromagnetic state (23 K). The unit cells for antiferromagnetic and nuclear scattering are of the same size. (Erickson, 1953). The powdered sample are used.

## 27. Critical behavior of $MnF_2$

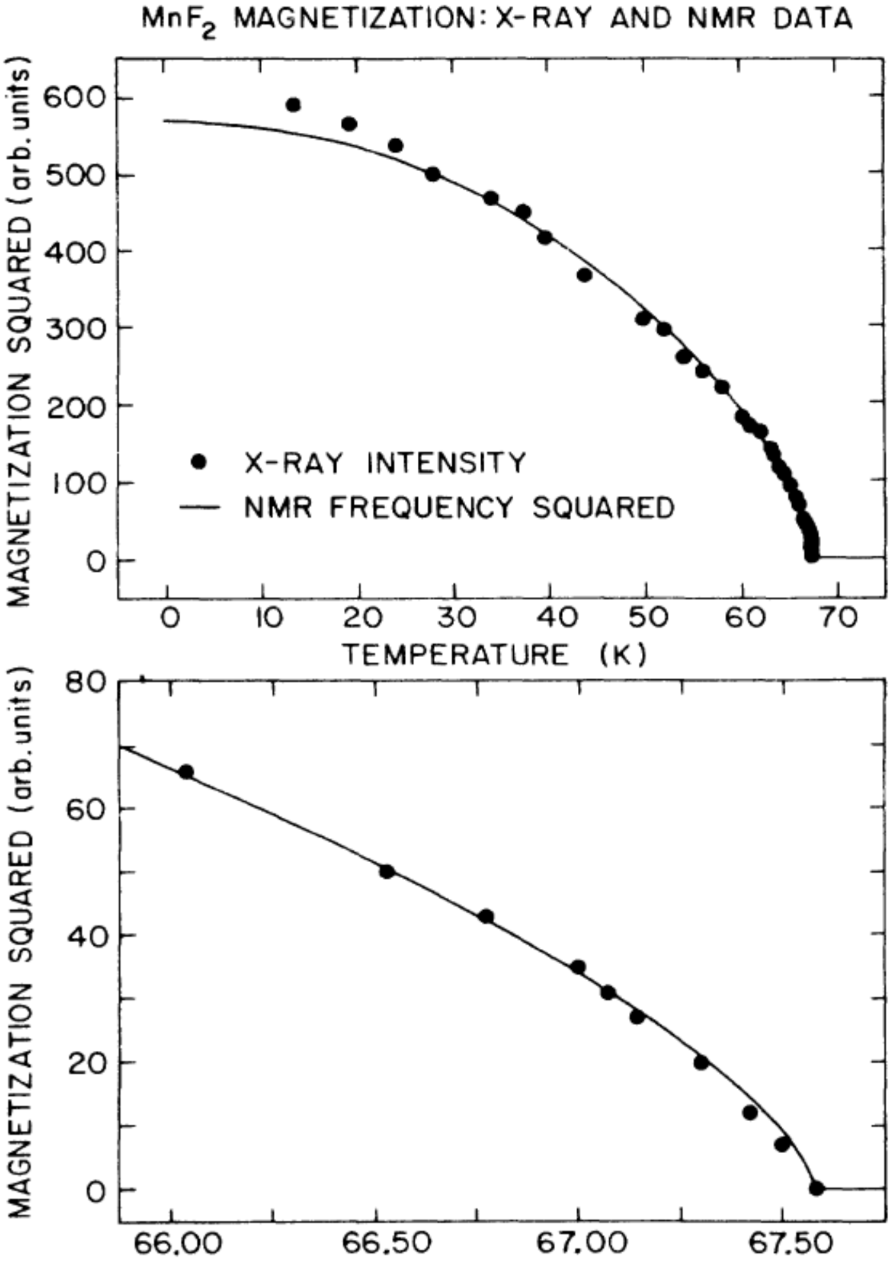


**Fig.** Peak intensity at the magnetic (300) Bragg point as a function of temperature. MnF$_2$. The solid lines represent the square of the magnetic order parameter as measured by NMR.[A.I. Goldman et al. Phys. Rev. B **36**, 5609 (1987)].

The critical exponents are obtained as

$$\gamma = 1.25 \pm 0.007, \qquad \nu = 0.643 \pm 0.003,$$

$\eta = 0.056 \pm 0.008$ .

## REFERENCES

1. F. Keffer, Phys. Rev.B **87**, 608 (1952). "Anisotropy in the antiferromagnetic $MnF_2$."
2. R. Kubo, Phys. Rev. **87**, 568 (1952). "The spin-wave theory of antiferromagnets."
3. R.A. Erickson, Phys. Rev. B **90**, 779 (1953). "Neutron diffraction studies of antiferromagnetism in manganous fluoride and some isomorphous compounds."
4. F.M. Johnson and A.H. Nethercot, Jr. Phys. Rev. **104**, 847 (1957). "Antiferromagnetic resonance in $MnF_2$."
5. P. Heller, Phys. Rev. **146**, 403 (1966). "Nuclear magnetic resonance studies of critical phenomena in MnF2. I. Time-average properties."
6. O. Nikotin, P.A. Lindgard, and O.W. Dietrich, J. Phys. C Solid State Physics **2**, 1168 (1969). "Magnon dispersion relation and exchange interactions in $MnF_2$."
7. O.W. Dietrich, J. Phys. C (Solid State Physics) **2**, 2022 (1969) "Critical magnetic fluctuations in $MnF_2$.
8. Y. Shapira and S. Foner, Phys. Rev. B **1**, 3083 (1970). "Magnetic phase diagram of $MnF_2$ from ultrasonic and differential magnetization measurements."
9. M.P. Schulhof, P. Heller, P. Nathans, and A. Linz, Phys. Rev.B **1**, 2304 (1970). "Critical magnetic scattering in manganese fluoride."
10. H. Ikeda and K. Kikuta, J. Phys. C Solid State Physics, **16**, L445 (1983).
11. A.I. Goldman, K. Mohanty, G. Shirane, P.M. Horn, R.L. Greene, C.J. Peters, T.R. Thurston, and R.J. Birgeneau, Phys. Rev. B **36**, 5609 (1987). "Magnetic x-ray scattering measurements on $MnF_2$."
12. Z. Yamani, Z. Tun, and D.H. Ryan, Can. J. Phys. **88**, 771 (2010). Tutorial/article didactique, Neutron scattering study of the classical antiferromagnet $MnF_2$; perfect hands-on neutron scattering teaching course.
13.

---

## APPENDIX

Property of the Brillouin function

$$B_S(x) = \frac{2S+1}{2S}\coth(\frac{2S+1}{2S}x) - \frac{1}{2S}\coth(\frac{1}{2S}x),$$

or

$$SB_S(x) = \frac{2S+1}{2}\coth(\frac{2S+1}{2S}x) - \frac{1}{2}\coth(\frac{1}{2S}x).$$

The series expansion around $x = 0$:

$$SB_S(x) = \frac{1}{3}(1+S)x - \frac{(1+S)[1+2S(1+S)]}{90S^2}x^3 + \frac{[(1+2S)^6 - 1]}{30240S^5}x^5 + \ldots$$

(i)

$$\lim_{S\to\infty} B_S(x) = \coth x - \frac{1}{x}. \qquad \text{(Langevin function)}$$

(ii)

$$\lim_{x\to 0} B_S(x) = \frac{S+1}{3S}x, \qquad \lim_{x\to 0} B_S'(x) = \frac{S+1}{3S}.$$

(iii)

$$\lim_{x\to\infty} B_S(x) = 1, \qquad \lim_{x\to\infty} B_S'(x) = 0.$$