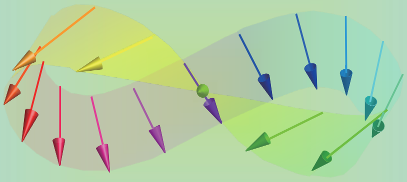
Nanoelectronics

11



Atsufumi Hirohata

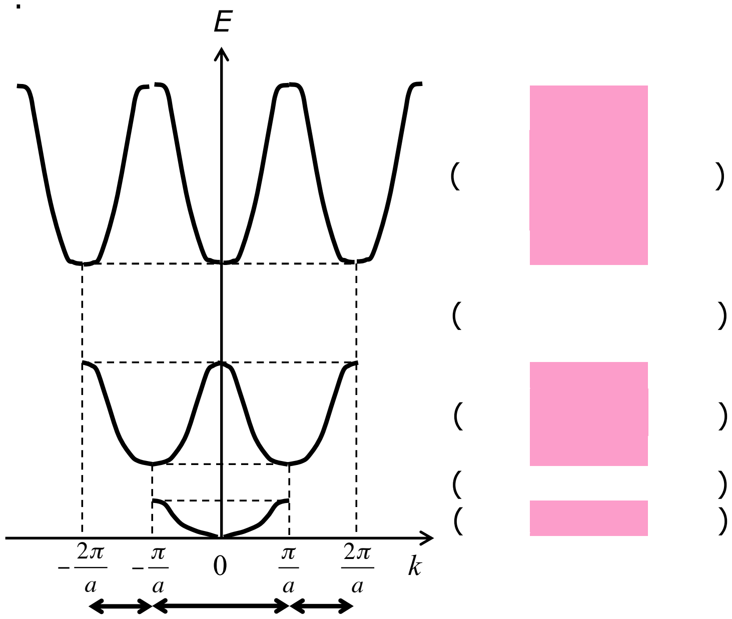
Department of Electronic Engineering

THE UNIVERSITY of York

12:00 Thursday, 23/February/2023 (SLB 101)

Quick Review over the Last Lecture

Harmonic oscillator :



( )

Contents of Nanoelectonics

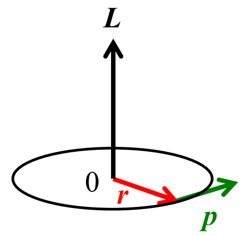
11 Magnetic spin

- Origin of magnetism
- Spin / orbital moment
- Paramagnetism
- Ferromagnetism
- Antiferromagnetism

Origin of Magnetism

Angular momentum $\boldsymbol{L}$ is defined with using momentum $\boldsymbol{p}$:

$\boldsymbol{L} =$



z component is calculated to be $L_z = xp_y - yp_x$

In order to convert L_z into an operator, $p \to \frac{\hbar}{i}\frac{\partial}{\partial q}$

$$\mathbf{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

By changing into a polar coordinate system, $\mathbf{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial \varphi}$

Similarly,

$$\mathbf{L}_x = -\frac{\hbar}{i}\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right),\ \mathbf{L}_y = -\frac{\hbar}{i}\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

Therefore,

$$\mathbf{L}^2 = \mathbf{L}_x{}^2 + \mathbf{L}_y{}^2 + \mathbf{L}_z{}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial^2\varphi}\right]$$

In quantum mechanics, observation of state $\psi = R\Theta\Phi$ is written as

$$\mathbf{L}^2\psi = -\hbar^2\left[\frac{1}{\Theta\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{m_l{}^2}{\sin^2\theta}\right]R\Theta\Phi = \hbar^2 K(R\Theta\Phi) = l(l+1)\hbar^2\psi$$

Origin of Magnetism (Cont'd)

Thus, the eigenvalue for L^2 is

$$\boldsymbol{L}^2 = l(l+1)\hbar^2 \quad \therefore |\boldsymbol{L}| = \sqrt{l(l+1)}\hbar \quad (l = 1,\ 2,\ 3,\ \ldots)$$

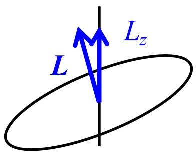
→ azimuthal quantum number (defines the magnitude of $\boldsymbol{L}$)

Similarly, for L_z,

$$L_z = m_l\hbar \quad (m_l = 0,\ \pm1,\ \pm2,\ \ldots)$$

→ magnetic quantum number (defines the magnitude of L_z)

For a simple electron rotation,



→ Orientation of $\boldsymbol{L}$:

In addition, principal quantum number :

defines electron shells

n = 1 ( ), 2 ( ), 3 ( ), ...

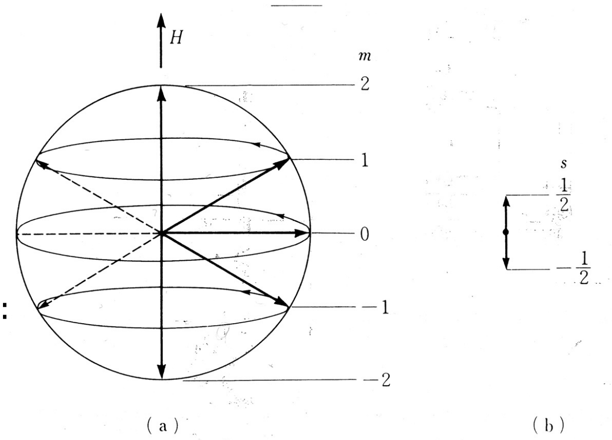


Fig. 3.3. Spatial quantization for orbital (a) and spin (b) angular momenta.

* S. Chikazumi, *Physics of Ferromagnetism* (Oxford University Press, Oxford, 1997).

Orbital Moments

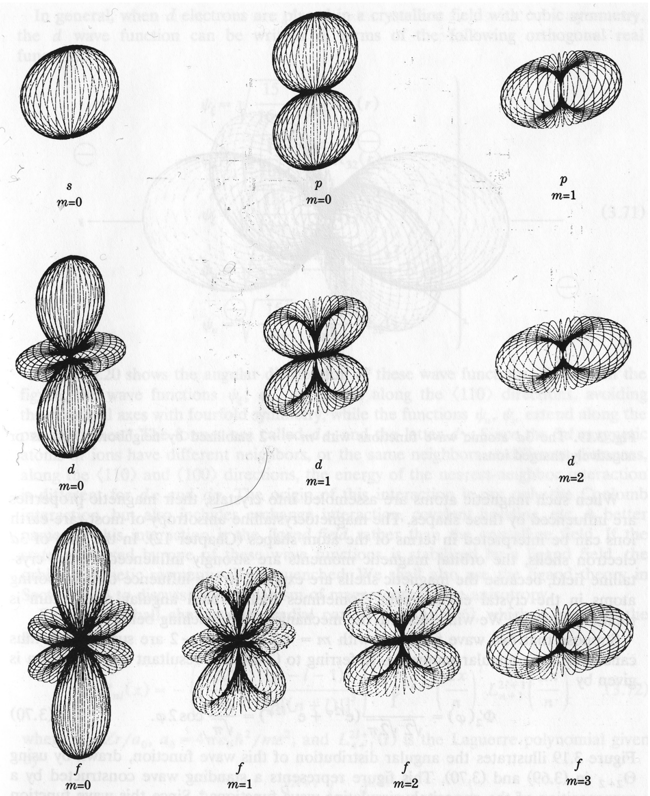


Fig. 3.18. Angular distribution of atomic wave functions with various orbital and magnetic quantum numbers.

Orbital motion of electron :

generates magnetic moment

$\boldsymbol{m} = -\mu_B \boldsymbol{L}/\hbar$

$\rightarrow \mu_B$: (1.165×10^{-29} Wb·m)

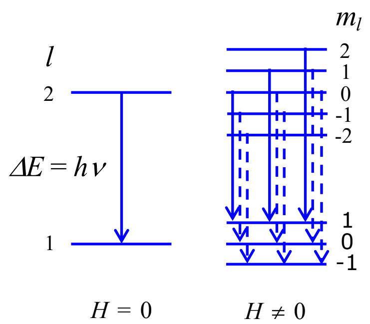
* S. Chikazumi, *Physics of Ferromagnetism* (Oxford University Press, Oxford, 1997).

Spin Moment and Magnetic Moment

Zeeman splitting :

For H atom, energy levels are split under H

dependent upon m_l.



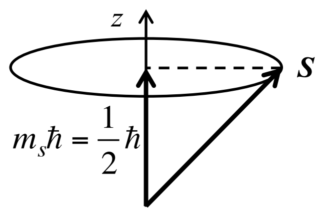
Spin momentum :

$$\begin{cases} \boldsymbol{L} \quad l \quad m_l = l, l-1, \ldots, 0, \ldots, -l \quad (2l+1) \\ \boldsymbol{S} \quad s \quad m_s = s, -s \quad \left(s = \frac{1}{2}\right) \quad 2 \end{cases}$$

$$\therefore |\boldsymbol{S}| = \sqrt{s(s+1)}\hbar = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\hbar$$

$\therefore \boldsymbol{m} =$

$\rightarrow g = 1$ ($\boldsymbol{J}$:), 2 ($\boldsymbol{J}$:)



Summation of angular momenta :

Russel-Saunders model $\boldsymbol{J} =$ +

Magnetic moment :

$$\boldsymbol{M} = \boldsymbol{M}_{\text{orb}} + \boldsymbol{M}_{\text{spin}} = -\mu_B(\boldsymbol{L} + 2\boldsymbol{S})/\hbar = -g\mu_B \boldsymbol{J}/\hbar$$

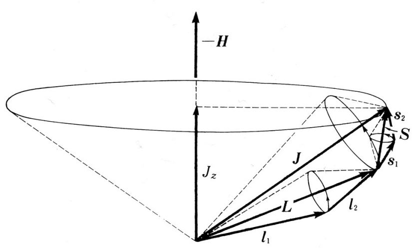
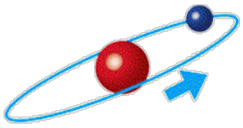
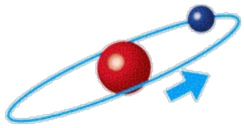


Fig. 3.7. Russell–Saunders coupling.

* S. Chikazumi, *Physics of Ferromagnetism* (Oxford University Press, Oxford, 1997).

Magnetic Moment





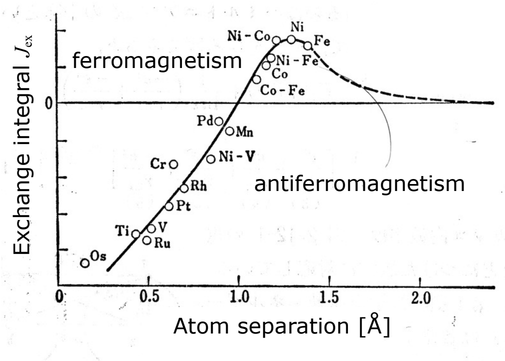
Exchange Energy and Magnetism

Exchange interaction between spins :

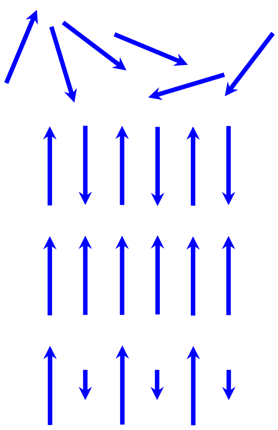
$$E_{\mathrm{ex}} = -2J_{\mathrm{ex}}\boldsymbol{S}_i\boldsymbol{S}_j$$

$\rightarrow E_{\mathrm{ex}}$: minimum for / configurations

$\rightarrow J_{\mathrm{ex}}$:



Dipole moment arrangement :

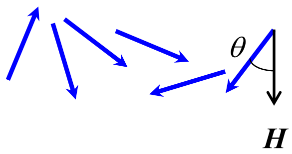


* K. Ota, *Fundamental Magnetic Engineering I* (Kyoritsu, Tokyo, 1973).

Paramagnetism

Applying a magnetic field $\boldsymbol{H}$, potential energy of a magnetic moment with θ is

$$U = -\boldsymbol{m}\boldsymbol{H} = -mH\cos\theta \qquad \rightarrow \boldsymbol{m} \text{ rotates to decrease } U.$$



Assuming the numbers of moments with θ is n and energy increase with $\theta + d\theta$ is $+\,dU$,

$$\frac{dn}{n} \propto \frac{1}{T}(-dU) \quad \therefore \ln n \propto \frac{-U}{T} + \text{const.} \quad \therefore \ln n = \frac{-U}{k_B T} + \ln n_0$$

$$\therefore n = n_0 \exp\left(\frac{-U}{k_B T}\right) \quad \rightarrow \quad \text{distribution}$$

Sum of the moments along z direction is between $-J$ and $+J$

$$M = \sum m_z n = \sum -g\mu_B M_J n_0 \exp\left(\frac{-U}{k_B T}\right) \qquad (M_J : z \text{ component of } \boldsymbol{M})$$

Here, $N = \sum n = \sum n_0 \exp\left(\frac{-U}{k_B T}\right) \quad \therefore n_0 = N \Big/ \sum \exp\left(\frac{-U}{k_B T}\right)$

$$\therefore M = \frac{N\sum g\mu_B(-M_J)\exp\left(\frac{-U}{k_B T}\right)}{\sum \exp\left(\frac{-U}{k_B T}\right)} = Ng\mu_B \frac{\sum b\exp(by)}{\sum \exp(by)} \qquad \left(b \equiv -M_J,\ y \equiv \frac{g\mu_B H}{k_B T}\right)$$

Paramagnetism (Cont'd)

Now, $\sum \exp(by) = e^{-Jy} + e^{-(J-1)y} + \cdots + e^{Jy} = e^{-Jy} + e^{-Jy}e^{y} + \cdots + e^{Jy} = \dfrac{e^{-Jy} - e^{Jy}e^{y}}{1 - e^{y}}$

$$\therefore e^{-y/2}\sum \exp(by) = \frac{e^{-y/2}\left(e^{-Jy} - e^{Jy}e^{y}\right)}{e^{-y/2}\left(1 - e^{y}\right)} = \frac{e^{-Jy}e^{-y/2} - e^{Jy}e^{y/2}}{e^{-y/2} - e^{y/2}}$$

Using $\sinh a = \dfrac{1}{2}\left(e^{a} - e^{-a}\right)$ $\qquad \therefore \sum e^{by} = \dfrac{e^{\left(J+\frac{1}{2}\right)y} - e^{-\left(J+\frac{1}{2}\right)y}}{e^{y/2} - e^{-y/2}} = \dfrac{\sinh\left(J+\frac{1}{2}\right)y}{\sinh\frac{y}{2}}$

Using $\dfrac{d}{dy}\left(\ln\sum e^{by}\right) = \dfrac{\sum be^{by}}{\sum e^{by}}$

$$\frac{d}{dy}\left(\ln\sum e^{by}\right) = \frac{d}{dy}\left[\ln\frac{\sinh\left(J+\frac{1}{2}\right)y}{\sinh\frac{y}{2}}\right] = \frac{d}{dy}\left[\ln\sinh\left(J+\frac{1}{2}\right)y - \ln\sinh\frac{y}{2}\right]$$

$$= \frac{1}{\sinh\left(J+\frac{1}{2}\right)y}\cosh\left(J+\frac{1}{2}\right)y \cdot \left(J+\frac{1}{2}\right)y - \frac{1}{\sinh\frac{y}{2}}\cosh\frac{y}{2}\cdot\frac{1}{2}$$

$$= \left(J+\frac{1}{2}\right)\coth\left(J+\frac{1}{2}\right)y - \frac{1}{2}\coth\frac{y}{2}$$

$$= \left(\frac{2J+1}{2}\right)\coth\left(\frac{2J+1}{2}\right)a - \frac{1}{2}\coth\frac{a}{2J} \qquad (a \equiv Jy)$$

Therefore,

$$M = Ng\mu_B J\left[\left(\frac{2J+1}{2J}\right)\coth\left(\frac{2J+1}{2J}\right)a - \frac{1}{2J}\coth\frac{a}{2J}\right] = Ng\mu_B J B_J(a) \qquad \left(a = \frac{g\mu_B JH}{k_B T}\right)$$

$\rightarrow B_J(a)$: Brillouin function

For $a \rightarrow \infty$ ($H \rightarrow \infty$ or $T \rightarrow 0$),

$$B_J(a) = 1 - \frac{1}{J}e^{-a/J} - \cdots \rightarrow 1$$

For $J \rightarrow 0$, $M \rightarrow 0$

For $J \rightarrow \infty$ (classical model),

$$\frac{2J+1}{2J} \rightarrow 1$$

$$\frac{1}{2J}\coth\frac{a}{2J} = \frac{1}{2J}\left(\cosh\frac{a}{2J}\Big/\sinh\frac{a}{2J}\right) \rightarrow \frac{1}{2J}\left(1\Big/\frac{a}{2J}\right) = \frac{1}{a}$$

$$\therefore B_\infty(a) = \coth a - \frac{1}{a} \equiv L(a)$$

$\rightarrow L(a)$: Langevin function

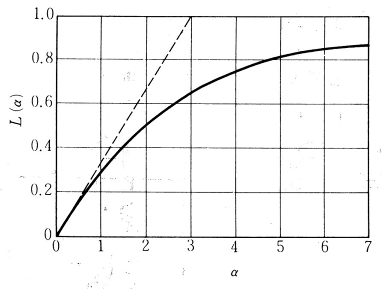


Fig. 5.9. Langevin function.

* S. Chikazumi, *Physics of Ferromagnetism* (Oxford University Press, Oxford, 1997).

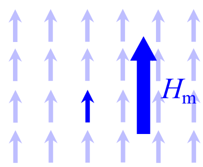
Ferromagnetism

Weiss molecular field : $H_m = wM$ (w : molecular field coefficient, M : magnetisation)

In paramagnetism theory, $M = Ng\mu_B J B_J(a)$, $a = \dfrac{g\mu_B JH}{k_B T}$

Substituting H with $H + wM$, and replacing a with x,

$$M = Ng\mu_B J B_J(x),\ x = \frac{g\mu_B J}{k_B T}(H + wM)$$



Spontaneous magnetisation at $H = 0$ is obtained as $k_B T = g\mu_B JwM$

Using M_0 at $T = 0$,

$$\begin{cases} \dfrac{M}{M_0} = B_J(x) \\ \dfrac{M}{M_0} = \dfrac{k_B Tx}{Ng^2\mu_B^2 J^2 w} \end{cases}$$

For $x << 1$, $B_J(x) \approx \dfrac{J+1}{3J}x$

Assuming $T = \Theta$ satisfies the above equations,

$$\frac{M}{M_0} = \frac{J+1}{3J}x = \frac{k_B\Theta}{Ng^2\mu_B^2 J^2 w}x$$

$$\therefore \Theta = \frac{Ng^2\mu_B^2 J(J+1)w}{3k_B} = \frac{Nm^2}{3k_B}w$$

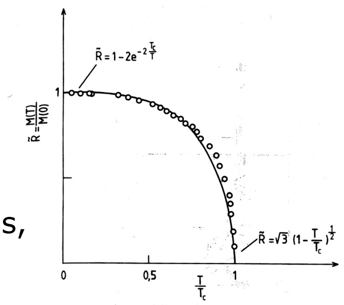


Fig. 8.7. Magnetization of a ferromagnet below the Curie temperature T_c. Experimental values for nickel from [8.4, 8.5]

Θ (T_C) : Curie temperature

* H. Ibach and H. Lüth, *Solid-State Physics* (Springer, Berlin, 2003).

Ferromagnetism (Cont'd)

For $x << 1$, $\quad B_J(x) \approx \dfrac{J+1}{3J}x$

$$M = Ng\mu_B J B_J(x) = Ng\mu_B\ (J+1)\frac{x}{3}$$

$$= Ng^2{\mu_B}^2 J(J+1)\frac{1}{3k_B T}(H + wM)$$

$$\therefore M = C\frac{1}{T}(H + wM) \qquad \left(C \equiv Ng^2{\mu_B}^2 J(J+1)/3k_B = Nm^2/3k_B\right)$$

$$\therefore M = C\frac{H}{T - Cw}$$

Therefore, susceptibility χ is

$$\chi = \frac{M}{H} = \frac{C}{T - Cw} = \frac{C}{T - \Theta}$$

(C : Curie constant)

$\rightarrow$ law

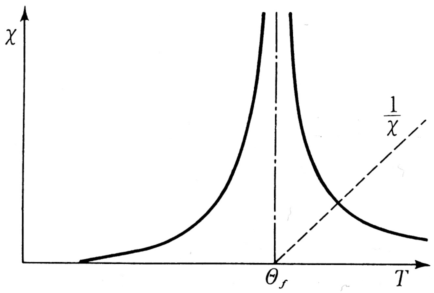


Fig. 6.4. Divergence of magnetic susceptibility in the vicinity of the Curie point.

** S. Chikazumi, *Physics of Ferromagnetism* (Oxford University Press, Oxford, 1997).

Spin Density of States

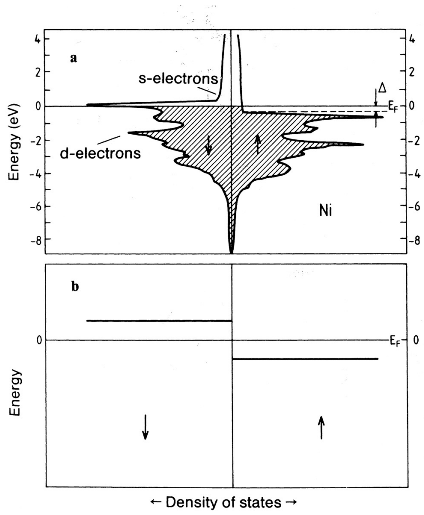
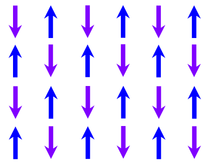


Fig. 8.6. (**a**) Calculated density of states of nickel (after [8.3]). The exchange splitting is calculated to be 0.6 eV. From photoelectron spectroscopy a value of about 0.3 eV is obtained. However the values cannot be directly compared, because a photoemitted electron leaves a hole behind, so that the solid remains in an excited state. The distance Δ between the upper edge of the d-band of majority spin electrons and the Fermi energy is known as the Stoner gap. In the bandstructure picture, this is the minimum energy for a spin flip process (the s-electrons are not considered in this treatment). (**b**) A model density of states to describe the thermal behavior of a ferromagnet

* H. Ibach and H. Lüth, *Solid-State Physics* (Springer, Berlin, 2003).

By applying the Weiss field onto independent A and B sites (for $x << 1$),

$$\begin{cases} M_\mathrm{A} = \frac{1}{2} N g \mu_\mathrm{B} J B_J(x_\mathrm{A}) = \frac{Nm^2}{6k_\mathrm{B}T} H_\mathrm{A} = \frac{C}{2T} H_\mathrm{A} \\ M_\mathrm{B} = \frac{1}{2} N g \mu_\mathrm{B} J B_J(x_\mathrm{B}) = \frac{Nm^2}{6k_\mathrm{B}T} H_\mathrm{B} = \frac{C}{2T} H_\mathrm{B} \end{cases}$$



Therefore, total magnetisation is

$$M = M_\mathrm{A} + M_\mathrm{B} = \frac{C}{2T}\left[\left(H - wM_\mathrm{A} - w'M_\mathrm{B}\right) + \left(H - w'M_\mathrm{A} - wM_\mathrm{B}\right)\right] = \frac{C}{2T}\left[2H + \left(w + w'\right)M\right]$$

$$\therefore \chi = \frac{M}{H} = \frac{C}{T + \frac{C}{2}\left(w + w'\right)} = \frac{C}{T + \Theta}$$

$\rightarrow$ temperature (T_N)

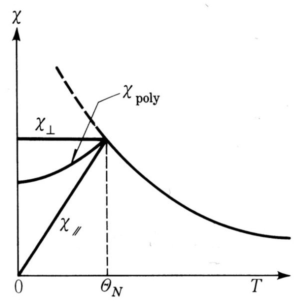


Fig. 7.7. Temperature dependence of magnetic susceptibility of antiferromagnetic materials. (Symbols are the same as Fig. 7.6.)

* S. Chikazumi, *Physics of Ferromagnetism* (Oxford University Press, Oxford, 1997).