PHYS 342/555
Condensed Matter in a Nutshell

Instructor: Dr. Pengcheng Dai

Professor of Physics

The University of Tennessee

(Room 407A, Nielsen, 974-1509)

(Office hours: TR 1:10PM-2:00 PM)

Lecture room 314 Nielsen
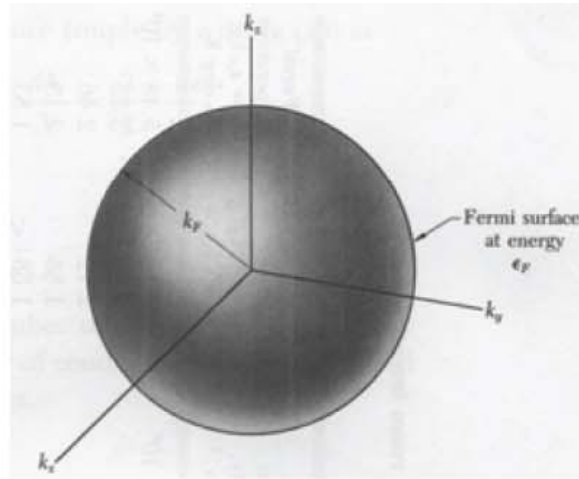
Chapter 14. Review problems

Lecture in pdf format will be available at:

http://www.phys.utk.edu

Fermi surfaces and metals

The Fermi surface is the surface of constant energy ε_F in $\vec{k}$ space. The electrical properties of the metal are determined by the shape of the Fermi surface.

Fermi surface, at energy ϵ_F

Since the energy of a one-electron level is directly proportional to k^2, when N is enormous the occupied region will be indistinguishable from a sphere. The radius of this sphere is called k_F (F for Fermi), and its volume Ω is $4\pi k_F^3 / 3$. The # of allowed $\vec{k}$ within the sphere is:

$\left(\dfrac{4\pi k_F^3}{3}\right)\left(\dfrac{V}{8\pi^3}\right) = \dfrac{k_F^3}{6\pi^2}V$. Since each allowed k-value leads to two
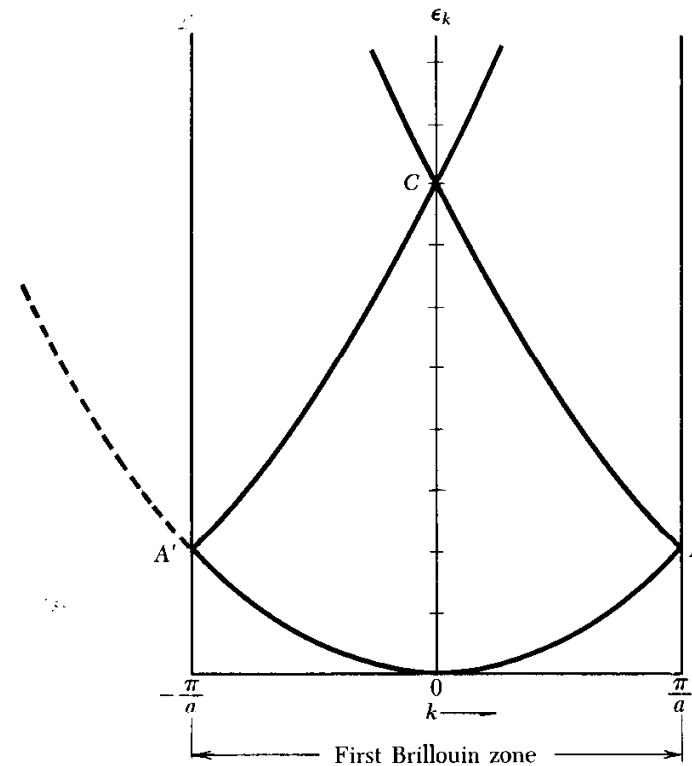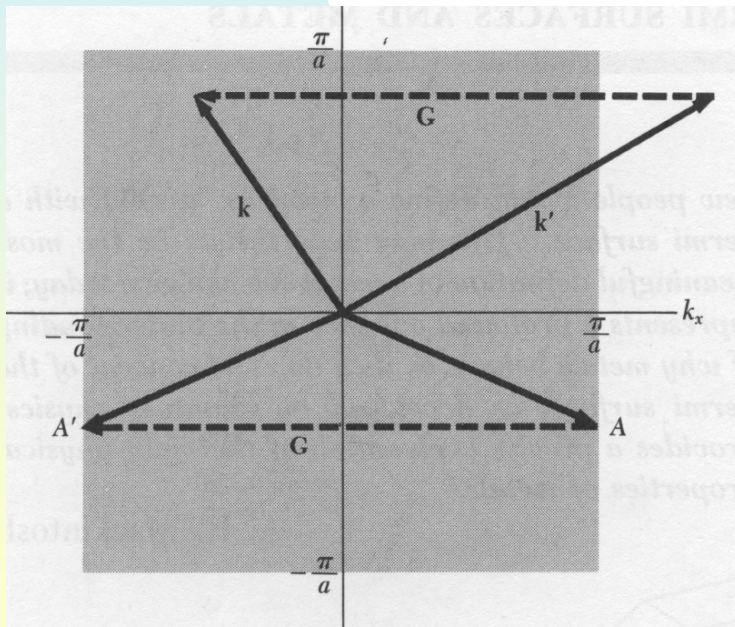
one-electron levels, we must have $N = 2\dfrac{k_F^3}{6\pi^2}V = \dfrac{k_F^3}{3\pi^2}V$.

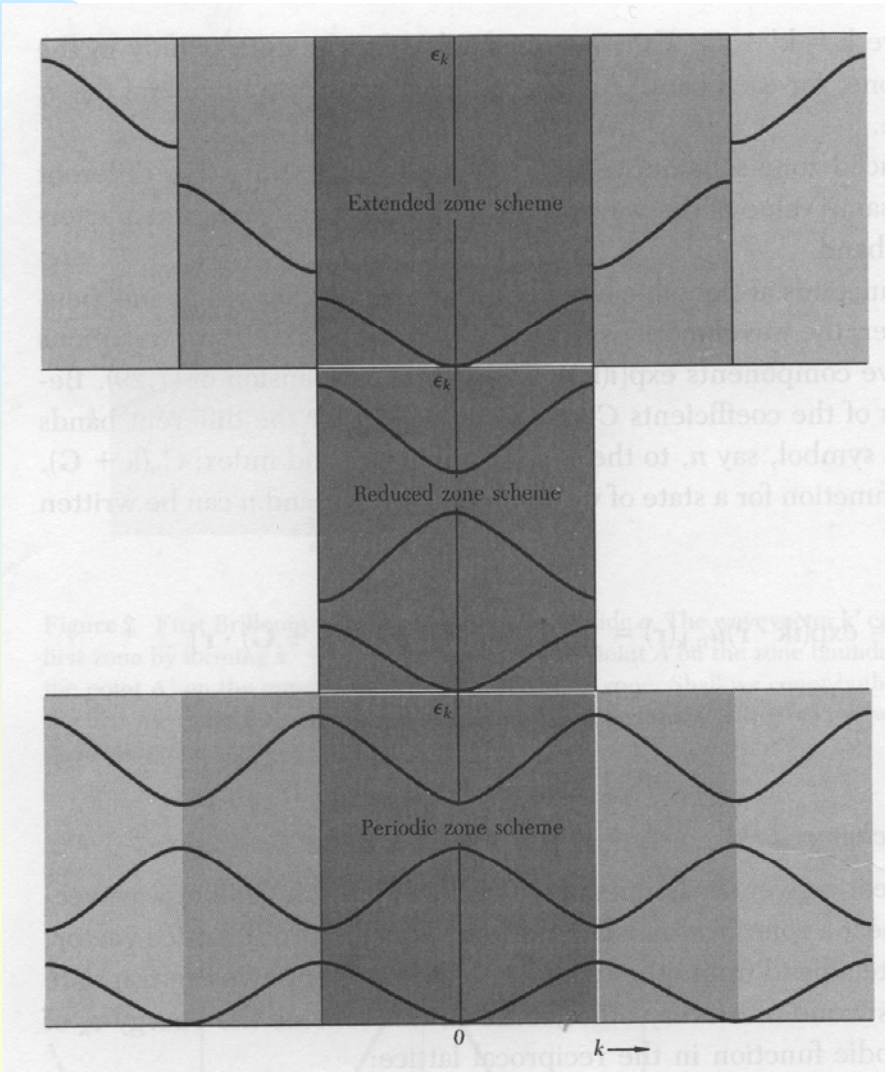If electron density is $n = N/V$, then we have $n = k_F^3 / 3\pi^2$.

Reduced zone scheme

For a Bloch function written as $\psi_{k'}(\vec{r}) = e^{i\vec{k}'\cdot\vec{r}} u_{k'}(\vec{r})$, with $\vec{k}'$ outside the first Brillouin zone, we have $\vec{k} = \vec{k}' + \vec{G}$.

$$\psi_{k'}(\vec{r}) = e^{i\vec{k}'\cdot\vec{r}} u_{k'}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\left(e^{-i\vec{G}\cdot\vec{r}} u_{k'}(\vec{r})\right) \equiv e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r}) = \psi_k(\vec{r})$$

Periodic zone scheme

Extended zone scheme

Reduced zone scheme

Periodic zone scheme

The energy ε_k of a band is periodic function in reciprocal lattice: $\varepsilon_{\vec{k}} = \varepsilon_{\vec{k}+\vec{G}}$. This is known as the periodic zone scheme. In a simple cubic lattice, the dispersion has form:

$$\varepsilon_k = -\alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a).$$

1. Consider an electron gas of density n_0 in three dimensions that is completely ferro-magnetic: all electron spins point in the same direction. Derive:

(a) The Fermi wave vector in terms of n_0.

(b) The parameter r_s as the radius in atomic units that encloses one unit of charge.

(c) The average kinetic energy per electron.

1. Figure 5.7 shows the first three Brillouin zones of a square lattice.
   a) Show that the area of the third zone is equal to that of the first. Do this by appropriately displacing the various fragments of the third zone until the first zone is covered completely.
   b) Draw the fourth zone, and similarly show that its area is equal to that of the first zone.
2. Draw the first three zones for a two-dimensional rectangular lattice for which the ratio of the lattice vectors $a/b = 2$. Show that the areas of the second and third zones are each equal to the area of the first.
3. Convince yourself that the shapes of the first Brillouin zones for the fcc and bcc lattices are those in Fig. 5.8.
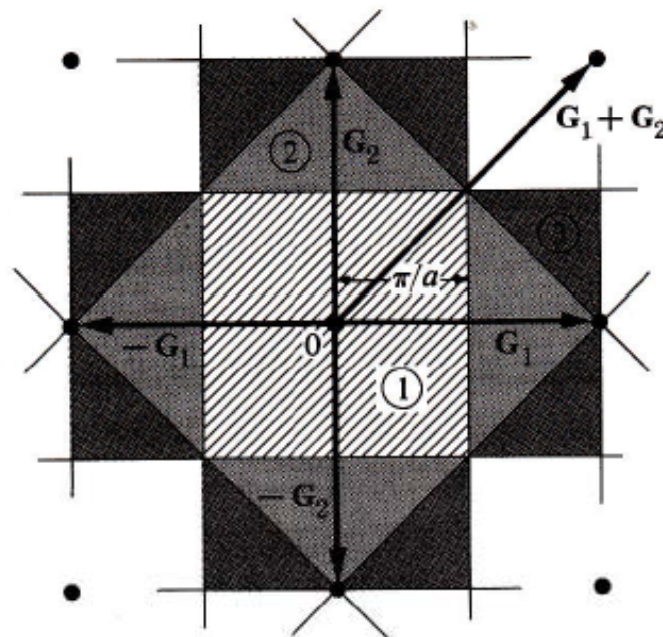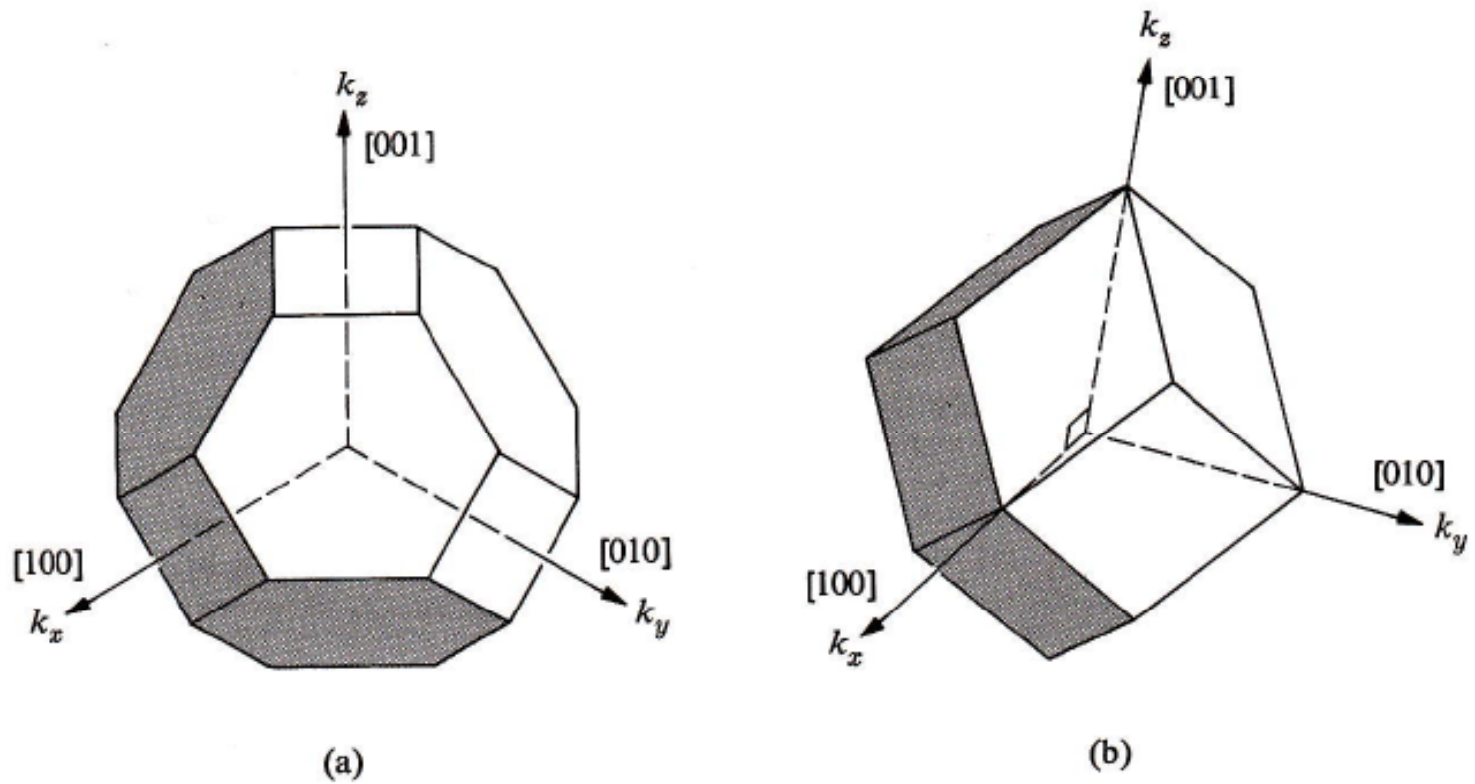
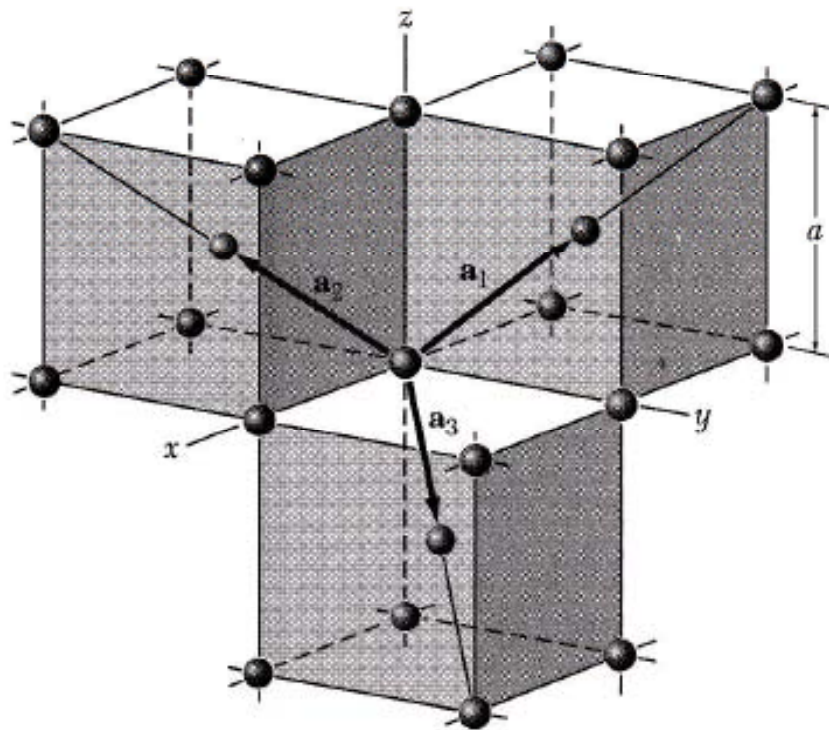**Fig. 5.8** The first Brillouin zone for (a) an fcc lattice, and (b) a bcc lattice.

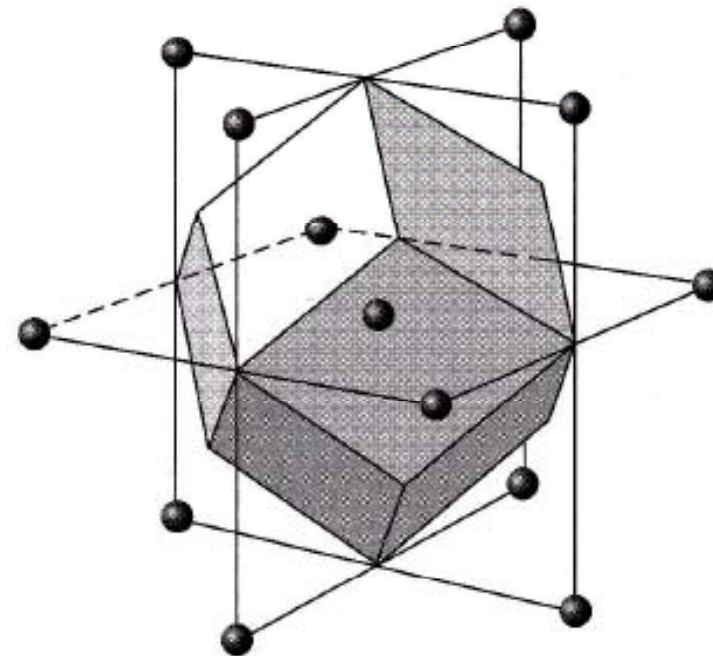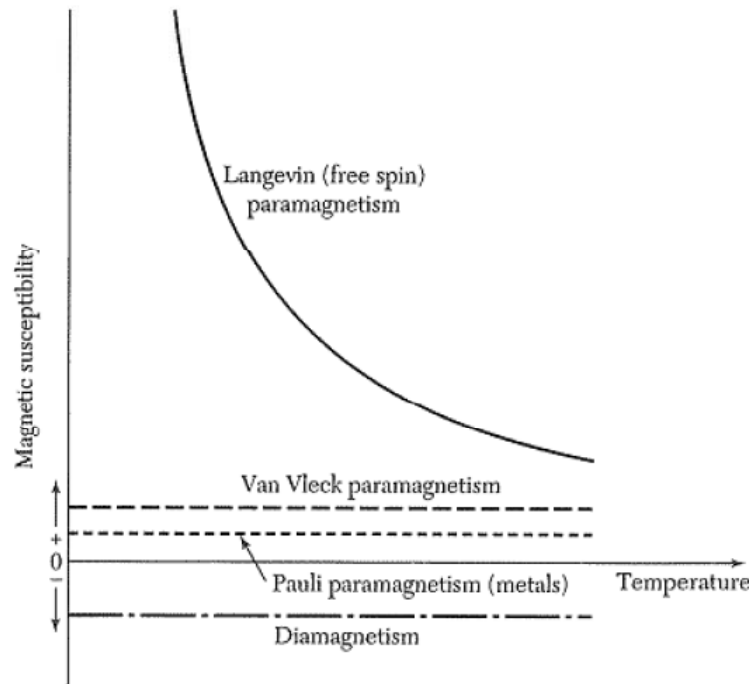**Figure 12** Primitive basis vectors of the body-centered cubic lattice.

Figure 13 First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombic dodecahedron.

Bohr-van Leeuwen Theorem

$\langle M \rangle = \langle \gamma L \rangle = 0$ according to classical statistics.

→ magnetism obeys quantum statistics.

Main contribution for free atoms:

- spins of electrons   paramagnetism
- orbital angular momenta of electrons
- Induced orbital moments   diamagnetism

(figure: Magnetic susceptibility vs Temperature)

- Langevin (free spin) paramagnetism
- Van Vleck paramagnetism
- Pauli paramagnetism (metals)
- Diamagnetism

Electronic structure	Moment
H: 1s	$M \sim S$
He: $1s^2$	$M = 0$
unfilled shell	$M \neq 0$
All filled shells	$M = 0$

Magnetization $M \equiv$ magnetic moment per unit volume

Magnetic subsceptibility per unit volume $\chi = \dfrac{M}{H}$ In vacuum, $H = B$.

χ_M = molar subsceptibility

σ = specific subsceptibility

nuclear moments ~ 10^{-3} electronic moments

2-10

Langevin diamagnetism equation

The diamagnetic susceptibility per unit volume is,

$$\chi = -\frac{NZe^2}{6mc^2}\langle r^2 \rangle;$$

where N is the number of atoms per unit volume, $\langle r^2 \rangle$ is the mean square distance of the electrons from the nucleus, Z is number of electrons in each nuclei.

	He	Ne	Ar	Kr	Xe
χ_M in CGS in 10^{-6} cm^3/mole:	−1.9	−7.2	−19.4	−28.0	−43.0

Larmor Precession

$$A = \frac{1}{c} \int d^3x' \frac{\mathbf{J}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

Magnetic (dipole) moment:
$$\mathbf{m} \equiv \frac{1}{2c} \int d^3x' \, \mathbf{x}' \times \mathbf{J}(\mathbf{x}') \qquad\qquad \mathbf{A} = \frac{\mathbf{m} \times \mathbf{x}}{r^3}$$

For a current loop:
$$\mathbf{J} \, d^3x = I \, d\mathbf{l} \qquad\qquad \mathbf{m} = \frac{1}{2c} \oint \mathbf{x} \times I \, d\mathbf{l} = \frac{I}{c} \, Area$$

For a charge moving in a loop:
$$\mathbf{J}(\mathbf{x}) = q \, \mathbf{v} \, \delta(\mathbf{x} - \mathbf{x}_q) \qquad (\text{charge at } \mathbf{x}_q)$$

$$\mathbf{m} = \frac{1}{2c} \int d^3x' \, \mathbf{x}' \times q \, \mathbf{v} \delta(\mathbf{x}' - \mathbf{x}_q) = \frac{q}{2c} \mathbf{x}_q \times \mathbf{v} = \frac{q}{2mc} \mathbf{L} = \gamma \, \mathbf{L}$$

Caution: we'll set **L** to η **L** in the quantum version

Classical gyromagnetic ratio
$$\gamma = \frac{q}{2mc} \qquad\qquad \mu_B = \frac{e\hbar}{2mc}$$

Torque on **m** in magnetic field:
$$\Gamma = \frac{d\mathbf{L}}{dt} = \mathbf{m} \times \mathbf{B} = \gamma \, \mathbf{L} \times \mathbf{B}$$

→ **L** precesses about **B** with the Larmor frequency
$$\omega_L = \gamma B = \frac{qB}{2mc}$$

Lorentz force:
$$m \frac{d\mathbf{v}}{dt} = \frac{q}{c} \mathbf{v} \times \mathbf{B} \qquad \rightarrow \text{cyclotron frequency} \qquad \omega_c = \frac{qB}{mc} = 2\omega_L$$

Paramagnetism

Electronic paramagnetism:

1. Atoms, molecules, and lattice defects possessing an odd number of electrons.

2. Free atoms and ions with a partly filled inner shell: transition elements; ions isoelectronic with transition elements; rare earth and actinide elements.

3. A few compounds with an even number of electrons, including molecular oxygen and organic biradicals.

4. Metals.

Quantum Theory of Paramagnetism

Magnetic moment of free atom or ion: $\boldsymbol{\mu} = \gamma \hbar \mathbf{J} = -g \mu_B \mathbf{J}$ $\mathbf{J} = \mathbf{L} + \mathbf{S}$

Caution: **J** here is dimensionless.

γ = gyromagnetic ratio.
g – g factor.

$g \mu_B \equiv -\gamma \hbar$

μ_B = Bohr magneton.

$\mu_B = \dfrac{e \hbar}{2 m c}$ ~ spin magnetic moment of free electron

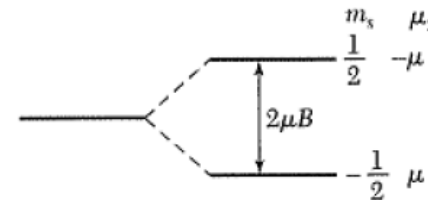For electrons $g = 2.0023$

For free atoms, $g = 1 + \dfrac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$

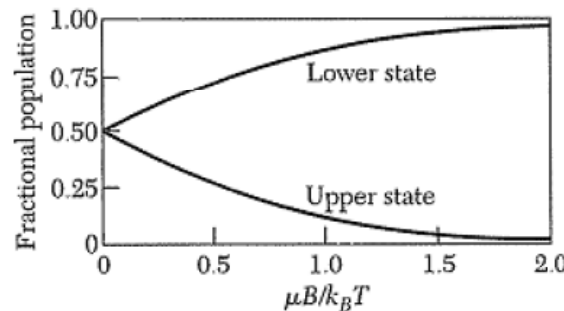$U = -\boldsymbol{\mu} \cdot \mathbf{B} = m_J \, g \, \mu_B \, B$ $m_J = -J, -J+1, \cdots, J-1, J$

For a free electron, $L = 0$, $S = \frac{1}{2}$, $g = 2$,
$\rightarrow$ $m_J = \pm \frac{1}{2}$, $U = \pm \mu_B B$.

Anomalous Zeeman effect

m_s μ_z
$\frac{1}{2}$ $-\mu$
$2\mu B$
$-\frac{1}{2}$ μ

$\dfrac{N_-}{N} = \dfrac{e^{-\beta \mu B}}{e^{\beta \mu B} + e^{-\beta \mu B}}$

$\dfrac{N_+}{N} = \dfrac{e^{\beta \mu B}}{e^{\beta \mu B} + e^{-\beta \mu B}}$

Hund's Rules

For filled shells, spin orbit couplings do not change order of levels.

Hund's rule (L-S coupling scheme):
Outer shell electrons of an atom in its ground state should assume
1. Maximum value of S allowed by exclusion principle.
2. Maximum value of L compatible with (1).
3. $J = |L-S|$ for less than half-filled shells.
   $J = L+S$ for more than half-filled shells.

Causes:
1. Parallel spins have lower Coulomb energy.
2. e's meet less frequently if orbiting in same direction (parallel Ls).
3. Spin orbit coupling lowers energy for $L \cdot S < 0$.

Mn^{2+}: $3d^5$ (1) $\rightarrow$ $S = 5/2$ exclusion principle $\rightarrow$ $L = 2+1+0-1-2 = 0$

Ce^{3+}: $4f^1$ $L = 3$, $S = \frac{1}{2}$ (3) $\rightarrow$ $J = |3-\frac{1}{2}| = 5/2$ $^2F_{5/2}$

Pr^{3+}: $4f^2$ (1) $\rightarrow$ $S = 1$ (2) $\rightarrow$ $L = 3+2 = 5$ (3) $\rightarrow$ $J = |5-1| = 4$ $^3H_4$

1. Use Hund's rule to deduce the order of atomic filling for d-orbitals ($\ell = 2$).

4. **Heat capacity from internal degrees of freedom.** (a) Consider a two-level system with an energy splitting $k_B\Delta$ between upper and lower states; the splitting may arise from a magnetic field or in other ways. Show that the heat capacity per system is

$$C = \left(\frac{\partial U}{\partial T}\right)_\Delta = k_B \frac{(\Delta/T)^2 \, e^{\Delta/T}}{(1 + e^{\Delta/T})^2} \, .$$

The function is plotted in Fig. 11. Peaks of this type in the heat capacity are often known as **Schottky anomalies**. The maximum heat capacity is quite high, but for $T \ll \Delta$ and for $T \gg \Delta$ the heat capacity is low. (b) Show that for $T \gg \Delta$ we have $C \cong k_B(\Delta/2T)^2 + \dots$. The hyperfine interaction between nuclear and electronic magnetic moments in paramagnetic salts (and in systems having electron spin order) causes splittings with $\Delta \approx 1$ to 100 mK. These splittings are often detected experimentally by the presence of a term in $1/T^2$ in the heat capacity in the region $T \gg \Delta$. Nuclear electric quadrupole interactions with crystal fields also cause splittings, as in Fig. 12.
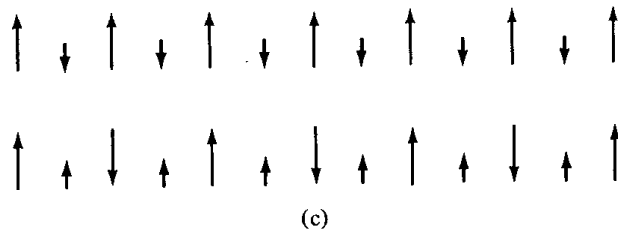
Chapter 12 Ferromagnetism and Antiferromagnetism

(a)

(b)

(c)
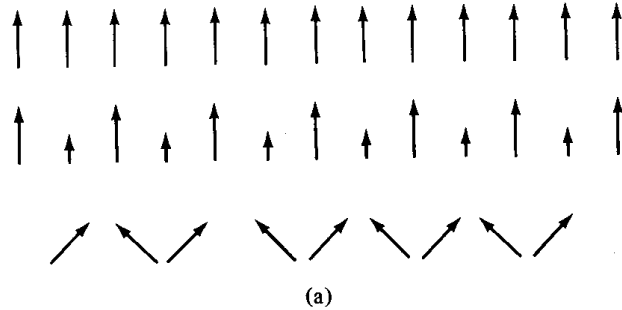
A ferromagnet has a spontaneous magnetic moment in zero applied magnetic field.
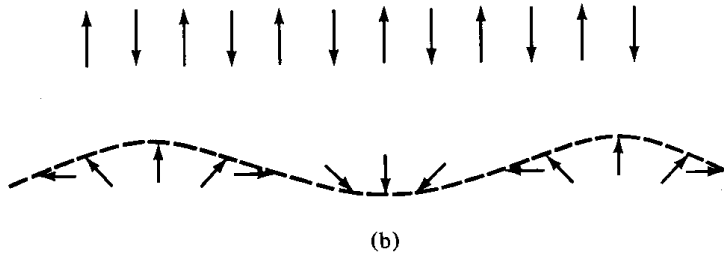
Antiferromagnet

Ferrimagnetic ordering

Assume the exchange coupling between spin $\vec{S}_i$ and $\vec{S}_j$ is J, Heisenberg model has the energy of the system,

$$U = -2J\vec{S}_i \cdot \vec{S}_j$$

Since U is the scalar product of the vector spin operators $\vec{S}_i$ and $\vec{S}_j$, it will favor parallel spins if J is positive and antiparallel if J is negative. For a system with many spins, the total spin Hamiltonian is simply that for the two-spin case, summed over all pairs of ions:

$$H^{spin} = -\sum_{p=1}^{N} 2J\vec{S}_p \cdot \vec{S}_{p+1} \qquad \text{If}$$

1. All magnetic ions are far enough apart that the overlap of their electronic wave functions is very small.

2. When the angular momentum of each ion contains an orbital as well as a spin part, the coupling in the spin Hamiltonian may depend on the absolute as well as the relative spin orientations.

The approximate connection between the exchange integral J and the Curie temperature T_C. For the atom under consideration has z nearest neighbors, each connected with the central atom by the exchange coupling J. For more distance neighbors we take J as zero

$$J = \frac{3k_B T_C}{2zS(S+1)}.$$
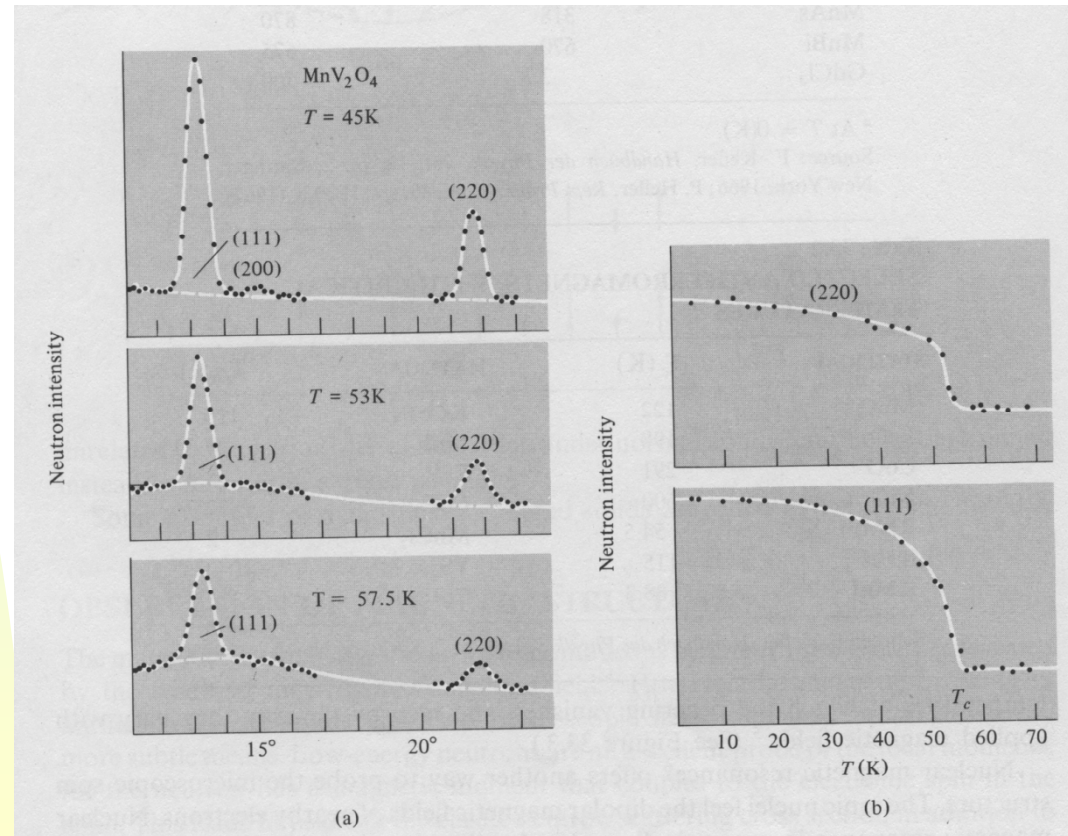
Magnons

A magnon is a quantized spin wave. Consider N spins each of magnitude S on a line or a ring, with nearest neighbor spins coupled by the Heisenerg interaction:

$$U = -2J \sum_{p=1}^{N} \vec{S}_p \cdot \vec{S}_{p+1}.$$

If $\vec{S}_p$ are classical vectors, then in the ground state $\vec{S}_p \cdot \vec{S}_{p+1} = S^2$ and the exchange energy of the system is $U_0 = -2NJS^2$.

For an excited state with one particular spin reversed, the total energy increased by $8JS^2$, so that $U_1 = U_0 + 8JS^2$.

For the pth spin, we have $-2J\vec{S}_p \cdot (\vec{S}_{p-1} + \vec{S}_{p+1})$.

Assuming traveling wave solutions of the form

$$S_p^x = u \exp[i(pka - \omega t)]; \quad S_p^y = v \exp[i(pka - \omega t)].$$

$$-i\omega u = (2JS/\hbar)[2 - (e^{-ika} + e^{ika})]v = (4JS/\hbar)(1 - \cos ka)v;$$

$$-i\omega v = -(2JS/\hbar)[2 - (e^{-ika} + e^{ika})]u = -(4JS/\hbar)(1 - \cos ka)u;$$

$$\begin{vmatrix} i\omega & (4JS/\hbar)(1 - \cos ka) \\ -(4JS/\hbar)(1 - \cos ka) & i\omega \end{vmatrix} = 0$$

Therefore $\hbar\omega = 4JS(1 - \cos ka).$

At low momentum transfer and long wave lengths, we have

$$(1 - \cos ka) \approx \frac{1}{2}(ka)^2$$

$$\hbar\omega \approx (2JSa^2)k^2.$$

Antiferromagnetic Magnons

We obtain the dispersion relation of magnons in a one-dimensional anti-ferromagnet by making the appropriate substitutions in the treatment (16)–(22) of the ferromagnetic line. Let spins with even indices $2p$ compose sublattice A, that with spins up ($S^z = S$); and let spins with odd indices $2p + 1$ compose sublattice B, that with spins down ($S^z = -S$).

We consider only nearest-neighbor interactions, with J negative. Then (18) written for A becomes, with a careful look at (17),

$$dS^x_{2p}/dt = (2JS/\hbar)(-2S^y_{2p} - S^y_{2p-1} - S^y_{2p+1}) ;$$ (45a)

$$dS^y_{2p}/dt = -(2JS/\hbar)(-2S^x_{2p} - S^x_{2p-1} - S^x_{2p+1}) .$$ (45b)

The corresponding equations for a spin on B are

$$dS^x_{2p+1}/dt = (2JS/\hbar)(2S^y_{2p+1} + S^y_{2p} + S^y_{2p+2}) ;$$ (46a)

$$dS^y_{2p+1}/dt = -(2JS/\hbar)(2S^x_{2p+1} + S^x_{2p} + S^x_{2p+2}) .$$ (46b)

We form $S^+ = S^x + iS^y$; then

$$dS^+_{2p}/dt = (2iJS/\hbar)(2S^+_{2p} + S^+_{2p-1} + S^+_{2p+1}) ;$$ (47)

$$dS^+_{2p+1}/dt = -(2iJS/\hbar)(2S^+_{2p+1} + S^+_{2p} + S^+_{2p+2}) .$$ (48)
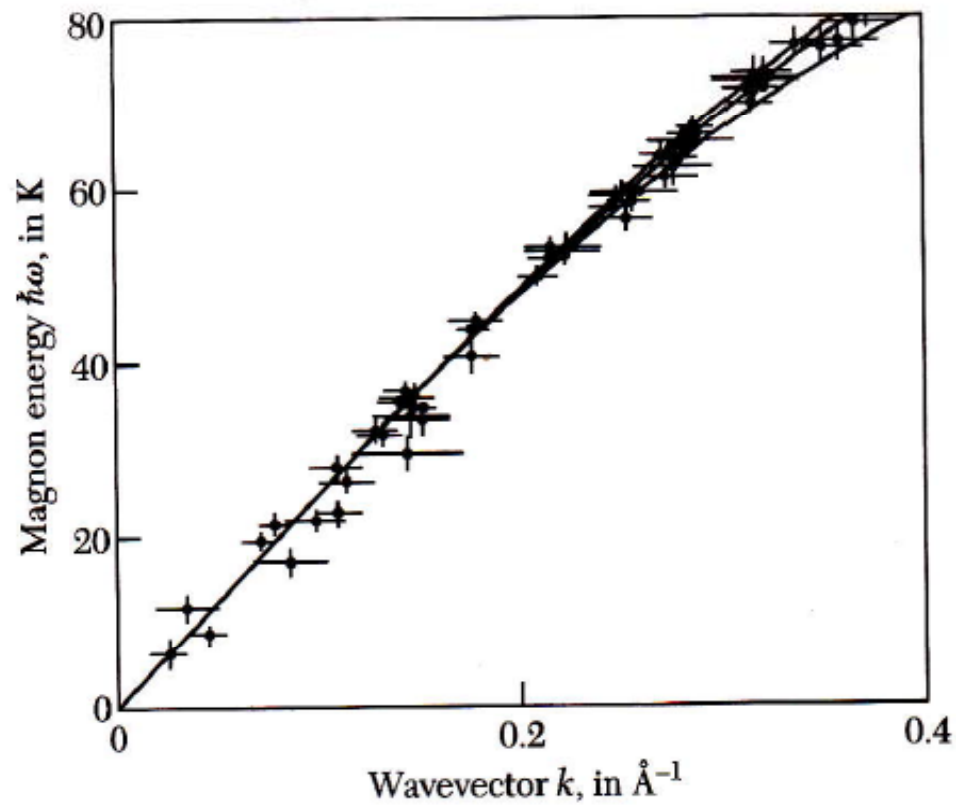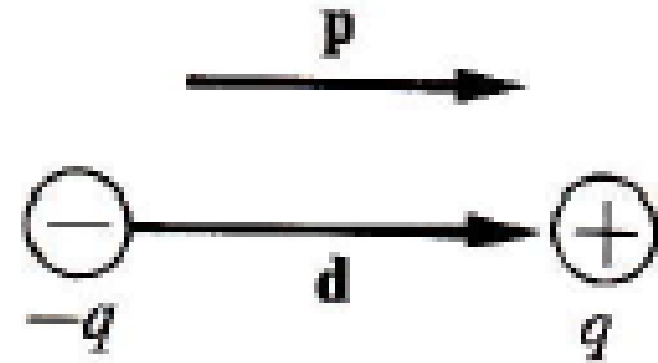
Figure 23 Magnon dispersion relation in the simple cubic antiferromagnet $RbMnF_3$ as determined at 4.2 K by inelastic neutron scattering. (After C. G. Windsor and R. W. H. Stevenson.)

Chapter 13: Dielectrics and ferroelectrics

Polarization

$$\mathscr{E} = \frac{1}{4\pi\epsilon_0} \frac{3(\mathbf{p} \cdot \mathbf{r})\,\mathbf{r} - r^2\mathbf{p}}{r^5},$$

Since the polarization of a medium—i.e., the alignment of the molecular moment—is produced by the field, it is plausible to assume that the molecular moment is proportional to the field. Thus we write

$$\mathbf{p} = \alpha \mathscr{E}, \tag{8.15}$$

where the constant α is called the *polarizability* of the molecule. The expression (8.15) is expected to hold good, except in circumstances in which the field becomes very large, in which case other terms must be added to (8.15) to form what is, in effect, a Taylor-series expansion of $\mathbf{p}$ in terms of $\mathscr{E}$. Equation (8.15) may be regarded as the first term in this expansion. (Higher-order terms lead to nonlinear effects.)

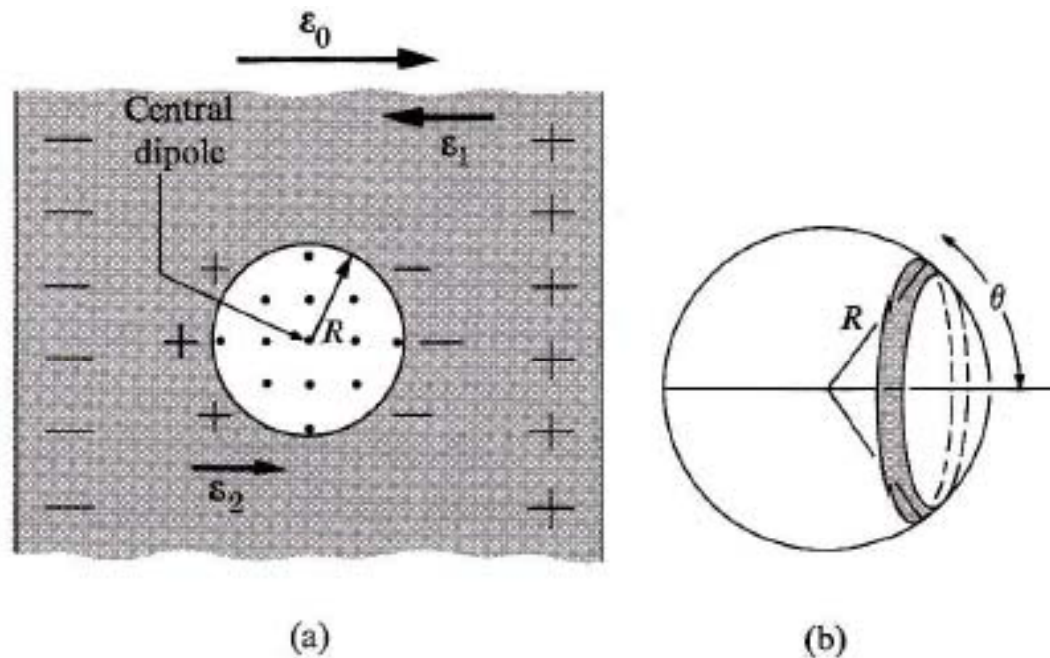The polarization $\mathbf{P}$ can now be written as

$$\mathbf{P} = N\alpha\mathscr{E}, \tag{8.16}$$

which, when substituted into (8.6), yields

$$\mathbf{D} = \epsilon_0\mathscr{E} + N\alpha\mathscr{E} = \epsilon_0\left(1 + \frac{N\alpha}{\epsilon_0}\right)\mathscr{E}. \tag{8.17}$$

Comparing this result with (8.9), one finds

$$\epsilon_r = 1 + (N\alpha/\epsilon_0), \tag{8.18}$$

(a)　　　　　　　　　　　　　　　(b)

concerned (Fig. 8.5). The interaction of our dipole with the other dipoles lying inside the cavity is, however, to be treated microscopically, which is necessary since the discrete nature of the medium very close to the dipoles should be taken into account. The local field, acting on the central dipole, is thus given by the sum

$$\mathscr{E}_{loc} = \mathscr{E}_0 + \mathscr{E}_1 + \mathscr{E}_2 + \mathscr{E}_3, \qquad (8.24)$$

where $\mathscr{E}_0$ is the external field, $\mathscr{E}_1$ the field due to the polarization charges lying at the external surfaces of the sample, $\mathscr{E}_2$ the field due to the polarization charges lying on the surface of the Lorentz sphere, and $\mathscr{E}_3$ the field due to other dipoles lying within the sphere. Note that the part of the medium between the sphere and the external surface does not contribute anything since, in effect, the volume polarization charges compensate each other, resulting in a zero net charge in this region.

Dielectric constant and polarizability

The dielectric constant ε of an isotropic medium relative to vacuum is defined as

$$\varepsilon \equiv \frac{E + 4\pi P}{E} = 1 + 4\pi\chi$$

The polarizability α of an atom is defined in terms of the local electric field at the atom:

$$p = \alpha E_{local}$$

The polarization of a crystal is then

$$P = \sum_j N_j p_j = \sum_j N_j \alpha_j E_{local}(j).$$

The total polarizability can be separated into three parts:

1. electronic: arises from the displacement of the electron shell relative to a nucleus.

2. ionic: comes from the displacement of a charged ion with respect to other ions.

3. dipolar: from molecules with a permanent electric dipole moment that can change orientation in an applied electric field.

Show that the polarizability of a conducting metallic sphere of radius a is $\alpha = a^3$.
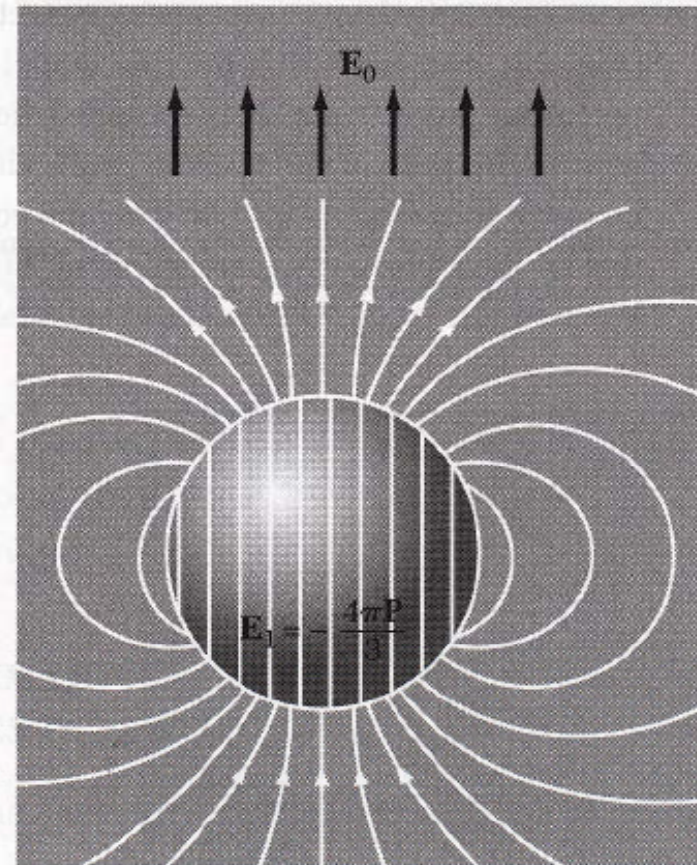

Figure 26 The total field inside a conducting sphere is zero. If a field $\mathbf{E}_0$ is applied externally, then the field $\mathbf{E}_1$ due to surface charges on the sphere must just cancel $\mathbf{E}_0$, so that $\mathbf{E}_0 + \mathbf{E}_1 = 0$ within the sphere. But $\mathbf{E}_1$ can be simulated by the depolarization field $-4\pi\mathbf{P}/3$ of a uniformly polarized sphere of polarization $\mathbf{P}$. Relate $\mathbf{P}$ to $\mathbf{E}_0$ and calculate the dipole moment $\mathbf{p}$ of the sphere. In SI the depolarization field is $-\mathbf{P}/3\epsilon_0$.
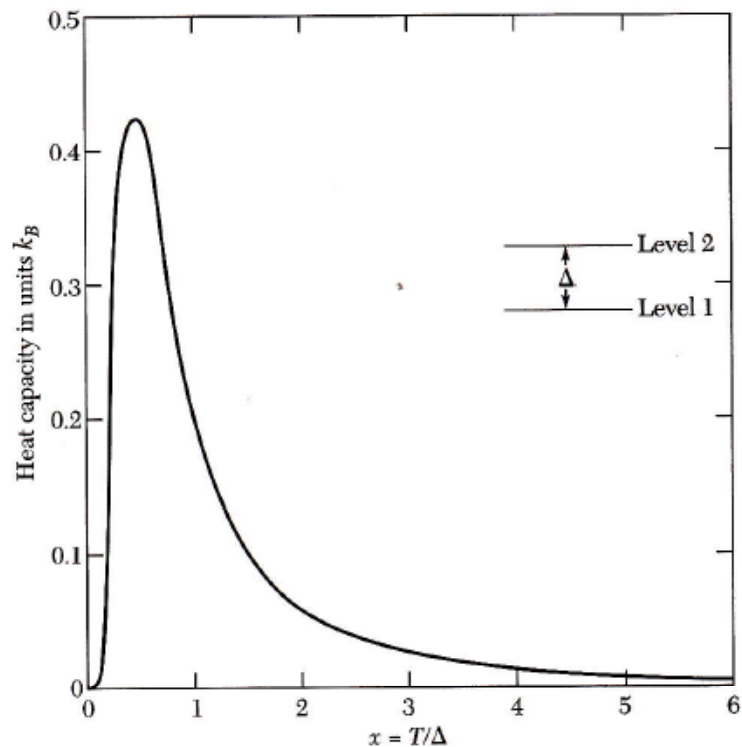
Figure 11 Heat capacity of a two-level system as a function of T/Δ, where Δ is the level splitting. The Schottky anomaly in the heat capacity is a very useful tool for determining energy level splittings of ions in rare-earth and transition-group metals, compounds, and alloys.
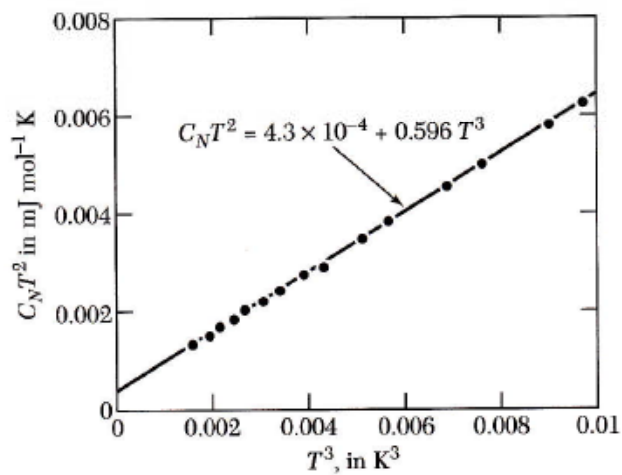

$$C_N T^2 = 4.3 \times 10^{-4} + 0.596\, T^3$$

Figure 12 The normal-state heat capacity of gallium at $T < 0.21$ K. The nuclear quadrupole ($C \propto T^{-2}$) and conduction electron ($C \propto T$) contributions dominate the heat capacity at very low temperatures. (After N. E. Phillips.)