

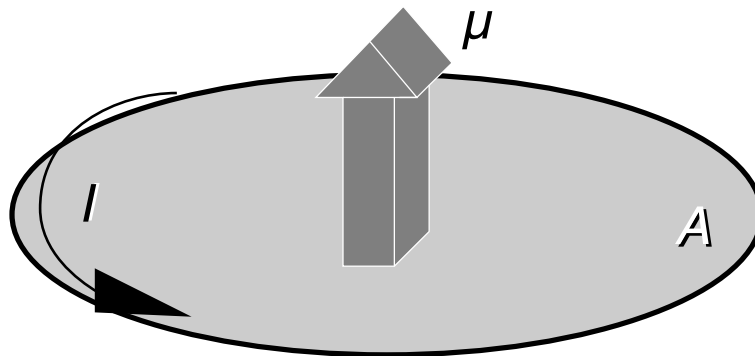
Chapter 2

Currents or Spins?

We bring up in the simplest possible terms some important concepts in magnetic phenomena, while seeking to dispel a few commonly held misconceptions. The topics broached here are treated more thoroughly in subsequent chapters.

2.1. Charge Currents or Spins?

An *insulator* with magnetic properties is a solid (or exceptionally, a liquid) in which the significant internal degrees of freedom are those of quantized atomic or ionic *spins*. A century ago, observation of macroscopic magnetic fields emanating from a solid would have been first-hand evidence of the presence of elementary Amperian charged current loops flowing within the material. Today, one turns to quantum mechanics for a correct explanation. For some insight into this change of perspective, consider the classical current loop illustrated below, in which a current I circulates around an area A .



The effective magnetic dipole strength is $\mu = IA/c$. In the limit $A \rightarrow 0$ and $I \rightarrow \infty$ with the product held constant, all the higher multipole fields vanish, as do the near-field corrections, leaving only the magnetic field of a point-dipole. The current associated with a charge e rotating at velocity \mathbf{v} around a circular track of radius a is $I = \frac{e|\mathbf{v}|}{2\pi a}$, hence the dipole moment is $\mu = I\pi a^2/c = \frac{e}{2mc}L$, where m is the mass, $e/2mc$ is the *classical gyromagnetic ratio* and L is the angular momentum $m|\mathbf{v}|a$.

At first thought, an array of Amperian current loops is indistinguishable from a similar array of permanent magnetic dipoles. It is tempting to construct a theory of ferromagnetism based on a distribution of currents within a solid. However, on further reflection this attribution becomes untenable. “Permanent” implies immutable, whereas array of current loops *must* and *will* wind themselves down to zero — given that in equilibrium, $|\mathbf{v}| \rightarrow 0$. The decay of magnetic moments can only be prevented if the individual angular momenta L are, somehow, *quantized* and $\neq 0$.

Indeed, while the concept of an Amperian current flow may be applicable to an induction coil or to an electromagnet, it does not address the source of magnetic fields in “permanent” magnetic materials, many of which are also electrical insulators. How could one justify a persistent *flow of current* in an *insulator*? Even if the material were doped and thereby acquired some free charges, one of the tenets of classical statistical mechanics is that *charge currents do not flow* spontaneously under conditions of *thermodynamic equilibrium*.¹

Therefore any first-principles explanation for the existence of elementary magnetic dipoles has to be sought elsewhere. There are only two plausible candidates: extrinsic, the electrons’ quantized orbital motions and intrinsic, their quantized spins.² Let us start with the latter.

The once radical notion that each electron carries an *intrinsic* half unit of the quantum of angular momentum \hbar was originally proposed by Goudsmit and Uhlenbeck³ for the most practical of reasons. An extra quantum number was required to reconcile observed atomic spectra and in particular, the number of electrons within a closed shell, to the symmetry principles of

¹ Bohr-Van Leuween’s theorem: originally formulated in the 1911 Ph.D. dissertation of Niels Bohr. See Sec. 1.6 for details.

² Spin is an *intrinsic* angular momentum; its magnitude is expressed in units of $\hbar = 1.054\,572\,66 \times 10^{-34}$ J sec.

³ G. E. Uhlenbeck and S. Goudsmit, *Naturwiss.* **33**, 953 (1925) and *Nature* **117**, 264 (1926).

the nascent quantum theory. This quantum number could only assume two values, $\pm\hbar/2$. A short time later, Dirac⁴ deduced this quantization from *spin*, a vector *operator* originating in the relativistic quantum mechanics of *fermions*.⁵ Still, electrons need not move at relativistic speeds to exhibit this extra degree of freedom.

According to Dirac's theory, spin angular momentum and a point magnetic dipole associated with it are localized at the instantaneous position of the electron. Thus they are inherent properties of the electron, regardless of whether the electron is attached to a particular atom or ion or whether it is free to move within the entire solid. The *total* "spin" of an atom or ion composed of many electrons has magnitude $S\hbar$, with $S = \frac{1}{2}, 1, \frac{3}{2}, \dots$, half-integer or integer values, fixed according to the number of participating electrons and the internal structure of the atom or ion, but rarely exceeding $\frac{7}{2}$, its value in some of the rare-earths.

Spin should be distinguished from *motional* angular momentum obtained by summing the orbital angular momenta of the individual particles (labeled i) within an atom or ion, $L\hbar = \sum_i r_i \times p_i$. The *orbital* quantum number L is also quantized but restricted to integer values $0, 1, 2, \dots$. Actually, it vanishes in the most magnetic of atoms or ions, those with half-filled shells! Moreover, when atoms are embedded in a solid or are made part of certain molecules, orbital rotations of their electrons are easily hindered. This frequently results in an effective $L = 0$, regardless of the original value of L in the atom. By contrast, the spin magnitudes are sturdier and are generally (albeit, not always) insensitive to their nonmagnetic surroundings.

Therefore, to the extent that any such generalization is permitted, it is correct to think of magnetic materials as being composed of high-spin "magnetic" atoms or ions only, drawn typically from the middle columns of the d - or f -transition series of the periodic table. *Nonmagnetic* ions that may be present in a magnetic material serve various functions: mechanical (to stabilize the material), electronic (affecting its electrical conductivity) or in some instances, providing the "glue" connecting nearby spins with one another (as the oxygen ligand ions do in "superexchange"). Other than in these passive ways, nonmagnetic ions or atoms are irrelevant in determining the magnetic properties of the medium. This now brings us to the question,

⁴ P. A. M. Dirac, *Proc. Roy. Soc.* **117A**, 610 (1928).

⁵ Particles satisfying Fermi-Dirac statistics and the Pauli principle, as discussed elsewhere in this book.

what are the various plausible, or even just possible, mechanisms by which the spins might interact and then cooperatively align themselves?

2.2. The Magnetic Dipole

Just as a stationary electron couples to electric fields through its intrinsic charge e , it couples to magnetic fields through the magnetic dipole associated with its spin. Such a spin S of electronic origin carries a magnetic moment of magnitude $\mu = g\mu_B S$, where $\mu_B = \frac{e\hbar}{2mc} = 9.274\,015\,4 \times 10^{-24}$ J/T is the “Bohr magneton,” a constant of nature. With $\hbar S$ the spin angular momentum, a spin’s gyromagnetic ratio as calculated from Dirac theory is $ge/2mc$ — similar to the classical value derived previously — except that $g = 2.002\,319\,304\dots$ (The “*Landé g factor*” $g \equiv 2$ in the Dirac theory, but there are small corrections due to quantum field-theoretic effects and possibly large corrections when the angular momentum $\neq 0$.) The factor 2 is in excellent agreement with observation and indicates that spin is not just a current loop shrunk to a point.⁶

Both the spin and its concomitant magnetic dipole transform like *three-dimensional vector* quantities. Each of the three components of such a vector is itself a quantum operator that fails to commute with the other two. (By changing the order in which they occur in a product such as $\mu_x\mu_y$ one changes the result to $\mu_y\mu_x \neq \mu_x\mu_y$.) According to the tenets of quantum mechanics *only one* component out of the three can be measured. It is often convenient to choose the z -axis for this preferred component, μ_z . This has an important consequence — and this is basically all that we need to know — that the magnetic dipole moment becomes quantized along this axis and is only permitted discrete projections along it. For spins S these are $\mu_z = g\mu_B S_z$, with S_z restricted to a set of $2S + 1$ “eigenvalues” $S, S - 1, \dots, -S$.⁷

In principle there are many ways to formulate the interactions among the spins. In Heisenberg-type models all three components of each vector spin are included in the interactions. The dynamics of Heisenberg-type models has proved rather difficult to solve and therefore a number of simpler

⁶ The value quoted here is for a free electron or to atoms with $L = 0$. In general g depends somewhat on the environment and may even have to be generalized to a tensor quantity.

⁷ If S is sufficiently large ($S \gg 1$) this equispaced discrete assignment correctly reduces to the continuous “correspondence limit” value $S \cos \theta$ with measure $d\theta \sin \theta$; however, in the extreme quantum limits of $S = 1/2$ and 1, which are in fact the most interesting, the discreteness *is* significant.

variants have been considered in the literature. In “XY models” (also known as “plane-rotator” models) just *two* components of the spin vectors appear in the Hamiltonian while the third is either discarded or arbitrarily set zero. The symmetry is profoundly modified by this truncation.

In the simplest model of all, the “Ising model” of magnetism⁸ or its various generalizations, a z -axis is fixed such that the only degree of freedom available to any given spin is to point “up” or “down” along this common axis. (The “transverse” components along the x - and y - axes and their concomitant magnetic moments are either omitted from the Hamiltonian or set to zero.) Whether physically justified or not, the Ising model has proved to be a wonderful mathematical tool and extraordinarily fruitful in the study of cooperative phenomena. Surprisingly, its most successful applications have been to *nonmagnetic* problems, ranging from the practical — such as the study of forest fires and epidemics, vacancies in solids and the ordering of binary alloys — to the most esoteric, with important applications in “critical phenomena” (phase transitions) and in pure mathematics.

In summary, a magnetic insulator containing “permanent” atomic or ionic spins *can* be fruitfully viewed as an array of N permanent magnetic dipoles $\boldsymbol{\mu}$. These could be aligned to form a maximum total magnetic moment $\mathbf{M} = N\boldsymbol{\mu}$ if the internal forces favor their alignment, or as small as $\mathcal{M} = |\mathbf{M}| = 0$ if the internal forces favor mutual cancellation of the individual magnetic moments. In determining from first principles which tendency carries the day, one must first decide on the nature of the mutual interactions between spins. We start by examining the most obvious, the dipole-dipole interactions, and find it surprisingly inimical to ferromagnetism in three dimensions (3D)!

2.3. The Magnetic Dipole-Dipole Interactions

This section examines the commonsense magnetostatic interactions.⁹ Each dipole generates a magnetic field able to exert a torque on the other dipoles. We expect that in the *stationary state of lowest energy* (i.e., the ground state), the *net* torque vanishes on each and every dipole. The magnetostatic

⁸ E. Ising, *Z. Phys.* **31**, 253 (1925).

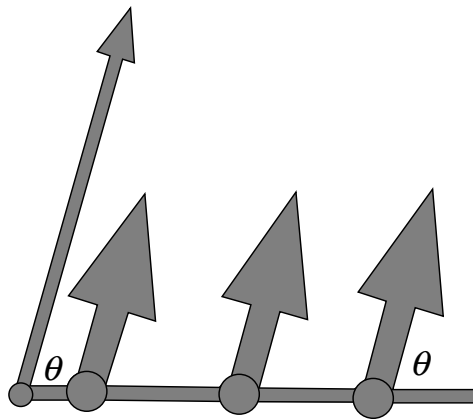
⁹ We find in this instance that common sense comes a cropper. In a subsequent paragraph we shall examine the *exchange* interactions between spins — the name given to a category of mechanisms as deeply rooted in the quantum theory as are the spins themselves — and it is there we find a plausible explanation for the cooperative behavior inherent in ferromagnetism and other significant magnetic phenomena.

interaction energy V of two dipoles at a distance R is a function of 4 variables:

$$V(R, \cos \theta_1, \cos \theta_2, \cos \theta_{1,2}) = \frac{1}{R^3} [\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - 3(\hat{R} \cdot \boldsymbol{\mu}_1)(\hat{R} \cdot \boldsymbol{\mu}_2)], \quad (2.1)$$

where $\mathbf{R} = (X, Y, Z)$, $\hat{R} = \mathbf{R}/R$ is a unit vector, and the dependence on direction cosines is obvious. According to (2.1) the interaction energy ranges from $-2|\boldsymbol{\mu}_1||\boldsymbol{\mu}_2|/R^3$ to $+2|\boldsymbol{\mu}_1||\boldsymbol{\mu}_2|/R^3$. To find the ferromagnetic ground state of N such dipoles, let us first orient them all parallel and adjust the orientation in such a manner that *each and every bond* V is optimized.

Consider a linear molecule of N dipoles, all oriented parallel to a common axis we shall define as the z -axis. The line along which they are strung lies at an arbitrary angle θ to the z -axis in the x - z plane, as shown below.



Then each 2-dipole bond is:

$$V(R_{ij}) = \frac{1}{R^3} [1 - 3 \cos^2 \theta] \mu_i \mu_j = J(R, \theta) S_i S_j. \quad (2.2)$$

Here $J(R, \theta) = \frac{1}{R^3} [1 - 3 \cos^2 \theta] (g\mu_B)^2$ increases with angle $|\theta|$ and decreases as $1/R^3$ with distance. In the state of least energy (the ground state), clearly $|\theta| = 0$ or π as shown below.

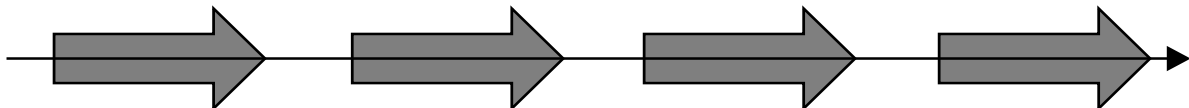


Fig. 2.1. The ground state of magnetic dipoles constrained to lie along a common molecular axis exhibits an anisotropic form of *ferromagnetism*.

The nearest-neighbor distance between magnetic ions, a_0 , the *magnetic lattice parameter*, can be as small as 2–3 Å, i.e. $2\text{--}3 \times 10^{-10}$ m in a dense magnetic salt. (In dilute magnetic substances it could be far greater.) The interaction parameter $J(m)$ of two spins at a distance ma_0 on this chain ($m = 1, 2, \dots$) is $J(m) = -2(g\mu_B)^2/(ma_0)^3$. Thus the total ground state energy of this configuration, the sum of V 's in (2.2),¹⁰ is:

$$\begin{aligned} E_0 &= -\frac{N}{2} \left\{ 2 \frac{(g\mu_B S)^2}{a_0^3} \right\} \left\{ \sum_{m=1}^{\infty} |m|^{-3} + \sum_{m=-\infty}^{-1} |m|^{-3} \right\} \\ &= -N \left\{ \frac{(g\mu_B S)^2}{a_0^3} \right\} \times 2\zeta(3), \end{aligned} \quad (2.3)$$

in which $\zeta(3) = 1.20206\dots$ is the Riemann zeta function. It is interesting to observe that the nearest-neighbor interactions at $m = \pm 1$ are responsible for $\frac{1}{1.202} = 83\%$ of the binding energy in this instance.¹¹ The *total* magnetic moment of N spins in this ground state has the maximum possible magnitude, μN . But to benefit from this (lowest) ground state energy (2.3), this ferromagnetic state has to be aligned at $\theta = 0$ or π , as in the illustration.

This is, in fact, what is observed in long thin bar magnets, such as magnetic needles or compass needles. So have we constructed a theory for magnetic needles of iron or steel? Let us examine this question more quantitatively. For a typical $a_0 = 2$ Å, Eq. (2.3) yields an energy *per site* $E_0/N = -(2S)^2 \times 2.5 \times 10^{-5}$ eV $\approx 0.3(2S)^2 k_B$ — too small by *any* measure!¹² Let us investigate the effects of finite temperature T .

Excited states of ferromagnets serve to lower the total magnetization; with increasing temperature they ultimately destroy it. For example, suppose we twisted all dipoles past the n^{th} by 180° so the first n have $\theta = 0$ and the remaining $N - n$ have $\theta = \pi$. The total energy exceeds the ground state (2.3) by a finite amount only, that we can estimate as $\Delta \approx 2|E_0/N| = 0.6(2S)^2 k_B$.

According to thermodynamics, the probability of one or more such breaks increases with temperature approximately as $N \exp -\Delta/kT$. Therefore once

¹⁰ Note: we include a factor 1/2 to avoid double-counting bonds. An alternative is to compute the total induced field energy $\frac{1}{8\pi} \int d^3r B^2(t)$ and add to it the interaction energy of the magnetic field with the dipoles.

¹¹ This suggests a great simplification in two- or three-dimensional arrays: for purposes of *estimating* energies, the dipole-dipole interactions can be treated as being effectively short-ranged and the sums restricted to nearest-neighbors.

¹² With $k_B T \approx 2.5 \times 10^{-2}$ eV at room temperature (300 K), the interaction energy *per site* for spins 1/2 thus corresponds to a mere 0.3 K.

T exceeds $\approx 0.6(2S)^2$ on the Kelvin scale, *there can be no long-range order*. In ordinary solids of iron, cobalt, chromium, manganese, and their oxides, $S = O(1)$, and this characteristic temperature is $O(1 \text{ or } 2 \text{ K})$ (one or two degrees Kelvin).

Hence we must look elsewhere if we are to understand the observed ferromagnetism of steel needles at room temperature (some 300 K). But supposing individual spins exceeded $S > 10$, could there be hope that dipolar room-temperature ferromagnetism exists? Indeed, such large spins *are* found in magnetic organic molecules. For example, the large, three-dimensional Fe8 molecule shown below (only the gridwork of Fe ions is shown: the organic framework is omitted) in which 6 iron atoms are parallel to an applied field and 2 are antiparallel, resulting in a total spin $S = 4 \times 5/2 = 10$. But here the physical *size* of such molecules ($a_0 \approx 10 \text{ to } 20 \text{ \AA}$) decreases the relevant V by a factor 10^{-2} to 10^{-3} and the dipolar forces turn out to be even smaller than before!

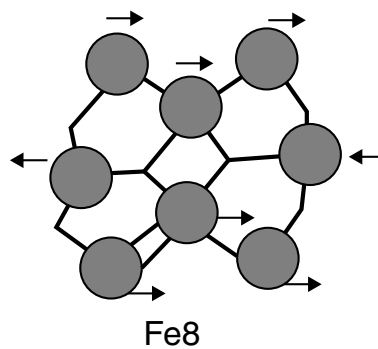


Fig. 2.2. [Schematic adapted from S. J. Blundell and F. L. Pratt, *Organic and Molecular Magnets*, *J. Phys.: Condens. Matter* **16**, R771–828 (2004).]

Next, consider $\theta = \pi/2$, spins pointing transverse to the chain. The energy of the ferromagnetic state becomes a maximum! Instead, we now find an *entirely different ground state* illustrated below. The optimum configuration for this orientation requires nearest-neighbor dipoles to be *antiparallel*: all even-numbered spins are “up” and odd-numbered spins “down,” or *vice versa*. In 3D such antiparallel configurations are known as *Néel states* and materials in which the Néel state is the ground state are “*antiferromagnets*.”¹³

¹³ Louis Néel was awarded the 1970 Nobel prize for this work from the 1930’s, in which he anticipated the existence of antiferromagnetism — found experimentally by H. Bizette, C. Squire and B. Tsai, *Comptes Rendus Acad. Sci.* **207**, 449 (1938) and ultimately confirmed using neutron scattering, by C. G. Schull and J. S. Smart, *Phys. Rev.* **76**, 1256 (1949).

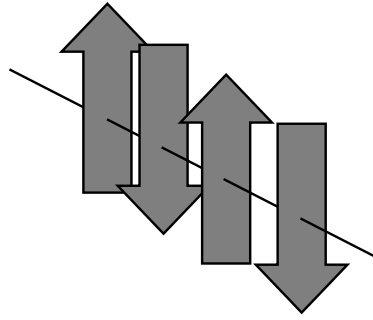


Fig. 2.3. Constrained \perp to the axis, linearly arrayed spins exhibit *antiferromagnetism*.

The total magnetic moment in the Néel state is zero. In the present example the energy is:

$$\begin{aligned}
 E_0 &= +\frac{N}{2} \left\{ \frac{(g\mu_B S)^2}{a_0^3} \right\} 2 \sum_{m=1}^{\infty} (-1)^m |m|^{-3} \\
 &= -N \left\{ \frac{(g\mu_B S)^2}{a_0^3} \right\} \times \frac{3}{4} \zeta(3). \tag{2.4}
 \end{aligned}$$

Although appropriately negative, the energy of this state (the Néel configuration) adds up to only $3/8$ of the preceding value. Even though this is not the minimum energy, there is no net torque on any one dipole and this state remains *stationary*, i.e. it is a *local* energy minimum.¹⁴ But whether this state is stable against *quantum* fluctuations remains to be seen. Generally, if there exists any channel for decay, the quantum states can and do “tunnel” into the more probable configurations of equal energy.

Next, extend the analysis to the simple cubic 3D lattice. Here the lattice sums are rather more difficult (but not impossible) to evaluate. However, we noted that dipolar interactions fall off quickly so that, judging from the preceding examples, if we just retained nearest-neighbor interactions the results should be accurate to within 20%.

Assume there is an ion on every point of a Cartesian grid $(n_x, n_y, n_z) \times a_0$ where the n_j are integers.

First consider the ferromagnetic state, in which the magnetic z -axis is parallel to one of the principal axes of the crystal and all spins are “up.” If at first we restrict the interactions to nearest-neighbors, a spin at grid

¹⁴ That is, if the spins were appropriately stimulated to surmount the energy barriers that keeps them antiparallel, they would ultimately re-align parallel to the direction of the chain and parallel to one another, as before, achieving a global minimum energy.

point (n_1, n_2, n_3) shares an attractive bond of strength $-2\left\{\frac{(g\mu_B S)^2}{a_0^3}\right\}$ with two neighbors at $(n_1, n_2, n_3 \pm 1)$, and a repulsive bond of strength $+\left\{\frac{(g\mu_B S)^2}{a_0^3}\right\}$ with each of four intraplanar neighbors, situated respectively at $(n_1 \pm 1, n_2, n_3)$ and $(n_1, n_2 \pm 1, n_3)$. *The sum total of nearest-neighbor interactions is zero.*

The same holds as well for the long-distance interactions in the ferromagnetic state. To see this, approximate lattice sums by three-dimensional integrals (as is justified at long distances). The angular average of $\cos^2 \theta$ over a unit sphere is $\frac{1}{3}$ and *each* interaction energy V in (2.1) vanishes on average. *Exact* lattice summation does not challenge this conclusion: the ferromagnetic state is indeed inherently unstable.

If, as we have seen, in an isotropic medium the dipole-dipole interaction *does not produce* a ferromagnetic ground state in 3D, then what does? And what *is* the ground state that results from purely dipole forces? One candidate for the lowest energy has each spin orientation “up” if $n_1 + n_2 =$ even integer, and “down” if $n_1 + n_2 =$ odd integer, independent of n_3 . This describes a Néel state within each x - y plane but assumes all x - y planes to be parallel (identical). (In the true 3D Néel state, the spins in the vertical direction would *also* be staggered, but then the energy is zero once again!) Retaining only nearest-neighbor bonds we estimate the ground state energy in this *columnar* state. Noting that each bond is shared by 2 sites we divide the sum by 2:

$$E_0 = -\frac{1}{2}8N \left\{ \frac{(g\mu_B S)^2}{a_0^3} \right\}, \quad (2.5)$$

with N the total number of sites. This configuration is clearly more favorable than either the Néel state or the ferromagnetic state. But is it sufficiently “sturdy” against small fluctuations or thermal excitations?

Choosing for the lattice parameter a typical value $a_0 \approx 2 \text{ \AA}$, E_0/N as calculated above yields $O(1k_B)$ *per site*.¹⁵ For $S = \frac{1}{2}$, at all temperatures exceeding 1 K, thermal fluctuations allow the dipoles to re-orient, destroying any remnant ground state correlations. Such crude estimates rule out magnetostatics as a credible mechanism for *any* of the cooperative forms of magnetism at any temperature $T > O(1)$.

¹⁵ For $S = \frac{1}{2}$. (For spins $S = \frac{7}{2}$, such configurations might be worth investigating at very low temperatures.) Here and throughout, $k_B = 1.380\,658 \times 10^{-23}$ Joules/K is Boltzmann’s constant.

Still, magnetic dipolar forces do play a role in modifying the properties of magnetic materials, in domain formation, and in the *shape-dependent anisotropy* of permanent magnets. We shall take this topic up again in the next Section.

2.4. The Exchange Interactions

Exchange “forces” are not forces in the usual sense. The energy splitting between quantized parallel and antiparallel spin configurations must be computed by some independent means and parametrized by a *scalar* “exchange constant” J . In the simplest instances where this splitting can be calculated explicitly, it is the result of a concatenation of two effects: the Pauli exclusion principle (affecting only electrons of parallel spin), and their two-body electrostatic repulsion. Although here we can anticipate the consequences of such a mechanism, details are more conveniently postponed to a later chapter.

There are two principal categories of exchange interactions: the *intra*-atomic interactions which favor spin alignment and are responsible for the operation of Hund’s rules in unfilled atomic shells, and the *inter*-atomic interactions which govern relative spin alignment in neighboring ions or atoms. Both are canonically expressed through similar *scalar* two-body interaction Hamiltonians of the form

$$H_{ij} = J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (2.6)$$

where the $J_{ij}(R_{ij})$ are typically independent of the *orientation* of \mathbf{R}_{ij} relative to any fixed axis. Both this isotropy and the strength of the J_{ij} (which typically range upward of $O(10^3 \text{ K})$) distinguish the exchange interactions from the dipolar. However, the sign of J_{ij} is not always negative, favoring parallel spins. In many instances it is positive and favors antiparallel spins, or it may even oscillate with distance R_{ij} , as is the case in metals.

For the sake of argument let us assume that the spins occupy fixed points on a regular lattice and that those $J(R_{ij})$ which are not zero (e.g., the nearest-neighbor interactions) are *all negative*. Under this assumption it is possible to prove rigorously that the ground state, *in any geometry and in any dimension, is ferromagnetic*.

The proof is immediate: if all the spins are parallel $\mathbf{S}_i \cdot \mathbf{S}_j = S^2$. If the J ’s are all nonpositive, the energy $\sum_{(ij)} J(R_{ij}) S^2$ has mathematically the *lowest possible value*, i.e. it is the ground state. The total spin is then $S_T = NS$

and it is macroscopic. Its $2S_T + 1$ quantized projections along any arbitrary z -axis range from $-NS$ to $+NS$; all projections have the same energy.

In his 1942 Ph.D. thesis at M.I.T., J. M. Luttinger pointed out the following amusing generalization. Suppose the discrete Fourier transform of $J(R_{ij})$, $\sum_{(ij)} J(R_{ij})e^{iq \cdot R_{ij}} = j(q)$, has a minimum at some point q_0 then among the ground state configurations one must include the spiral configuration $S_i = S(\cos q_0 \cdot R_i, \sin q_0 \cdot R_i, 0)$. The ferromagnetic state is the limiting case of this spiral at $q_0 = 0$. If there exist several values of q_0 that minimize $j(q)$, then more complicated phases may be manifest. For example, if $J(R)$ is positive and restricted to nearest-neighbors on a simple cubic lattice, the Néel state is the ground state (as the reader should be able to show). Ideally, the total magnetization $M = Ng\mu_B S$ in the ferromagnetic ground state (a vector quantity), is free to point in *any* direction in a “magnetically soft” material. Because the magnetostatic energy vanishes in the ferromagnetic



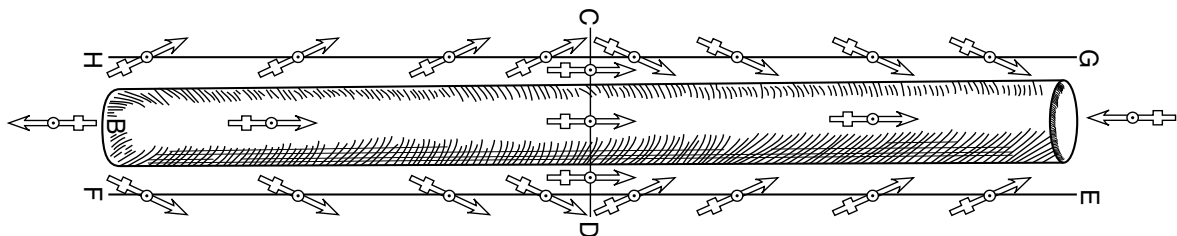
Fig. 2.4. Domains on the Surface of Cobalt.

Different shadings reveal different axes of magnetization. Width of individual domains ranges from 10^4 Å to 10^5 Å.

configuration, commonsense dictates that magnetostatics should not enter into the ferromagnetic states nor into their dynamic excitation spectrum.

But it does! We recall that in a cubic medium the magnetostatic energy *can* be lowered for configurations in which the dipoles are antiparallel to one another. This small but not insignificant reduction in magnetostatic energy is achieved through the formation of *magnetic domains*. Spins within a given domain are aligned ferromagnetically along a given local z -axis, but as the z -axes of nearest-neighbor domains are not co-linear all flux lines close in the optimal state and the *net* magnetization of the ferromagnet actually vanishes. A number of domains are visible in the Fig. 2.4, a microphotograph of the surface of a generic cobalt crystal.

A notable exception to spontaneous domain formation is the long, thin, essentially one-dimensional, cylinder or needle. Preceding considerations have made it plausible that if the exchange interactions are negative, individual dipoles align along the long axis of the cylinder, thereby optimizing *both* exchange *and* magnetostatic energies in the ground state. In fact this shape for permanent bar magnets, with north and south poles lying at opposite ends of a long bar, “works” and has been traditional since ancient times. The picture below, purporting to show the lines of force around a cylindrical magnet, is taken from William Gilbert’s *De Magnete*, a lengthy and learned monograph first published in London in 1600, arguably the first printed textbook in any branch of modern physics, discussed earlier in Sec. 1.2.



2.5. Metals and Their Alloys

Magnetism in metals poses a number of special challenges. If the electrons transport their spins by appreciable distances a description based on localized spins is patently inappropriate.

In ordinary nonmagnetic metals the kinetic energy of motion is minimized when half the electrons have spin “up” and the other half spin “down.” An external magnetic field pointing “up” promotes an excess of “up” over “down” electrons; a magnetization of magnitude $M = g\mu_B(N_\uparrow - N_\downarrow)$ ensues.

The gain (lowering) in energy $-B \cdot M$ occurs at a cost $+\frac{X}{2}(N_{\uparrow} - N_{\downarrow})^2$ in total kinetic energy. X , a parameter characteristic of the metal and independent of T , has dimension of energy — i.e., $X \propto 1/\rho_{\text{F}}$, where ρ_{F} is defined as the “density of states” ($\rho_{\text{F}}de =$ number of distinct electronic energy levels between e_{F} and $e_{\text{F}} + de$). Minimizing the total energy *w.r.* to $(N_{\uparrow} - N_{\downarrow})$ yields $M = (g\mu_{\text{B}})^2 B/X$. We call this property, that the total energy is lowered in a magnetic field, a *paramagnetic* response. The *paramagnetic susceptibility* of the metal, defined as the ratio of M to B , is a positive quantity which, in metals, is proportional to ρ_{F} .

A ferromagnet such as iron builds up its *spontaneous* magnetization *via* internal atomic “exchange” forces that mimic the action of an external field. However, the precise mechanism that produces the exchange interaction is not entirely straightforward. Some magnetic metals and alloys have been dubbed “half-magnets,” as it appears that the majority spin-up electrons are immobile while the minority of spin down electrons are itinerant! We discuss this paradoxical situation in due course.

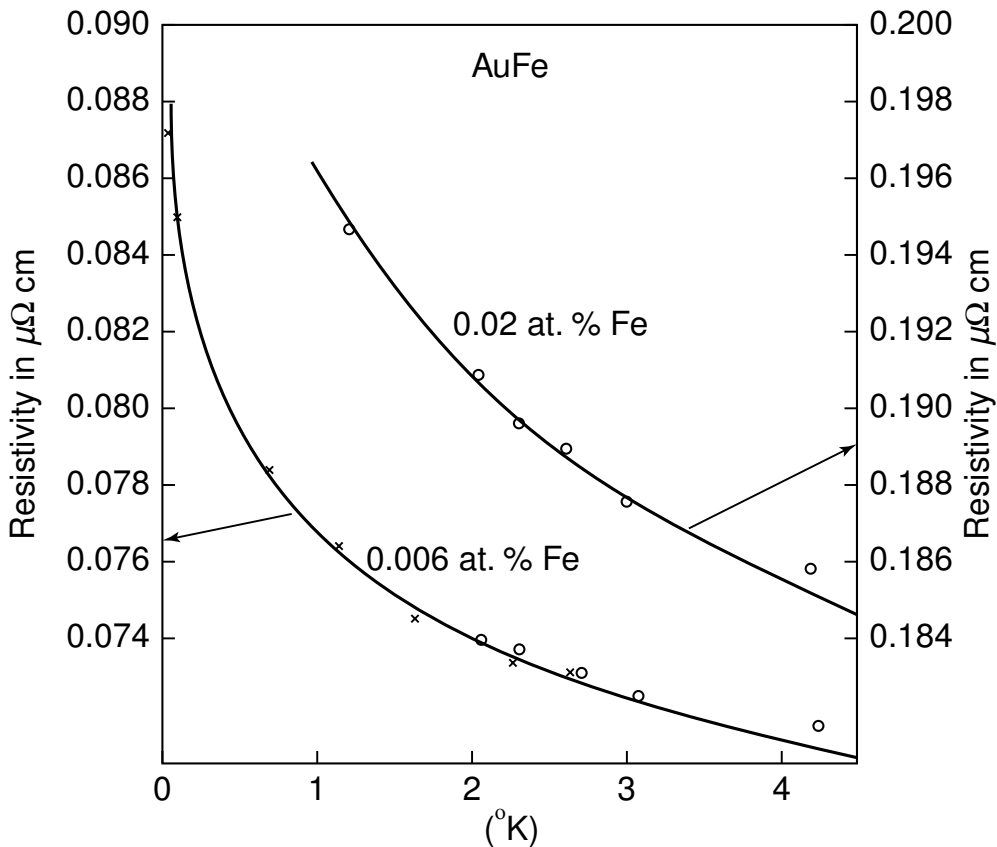


Fig. 2.5. Resistivity of dilute Fe alloys, as function of T .

Surprisingly, even a *single* magnetic impurity affects the properties of a nonmagnetic metal, as was first observed in extremely dilute alloys of manganese (Mn) or iron (Fe) in the nonmagnetic metals copper (Cu) and gold (Au). In the preceding figure we show the experimentally observed¹⁶ excess electrical resistance of nonmagnetic gold, after it is doped by iron impurities to concentrations of 0.02 and 0.006 atomic %. The excess resistivity that appears at low T is the so-called “Kondo effect,” a condensation of conduction electrons’ spins to screen the localized moment, *a phenomenon that becomes the more remarkable the greater the dilution and the lower the temperature.*

The Kondo effect could only be understood on the basis of many-body theory and therefore it challenged theorists for two decades starting from the mid-1960’s. Together with the study of screening in Coulomb interactions among electrons in metals and of arcane phenomena associated with superconductivity, the study of the Kondo effect helped drive theoretical and experimental research along unprecedented directions during this period. In fact, the Kondo effect did not yield center stage of magnetic studies until the mid-1980’s, when first the *quantum Hall effect*, followed by *high-temperature superconductivity*, then *giant-* (and even *colossal-*) *magnetoresistance*, entered the scene.

At the same time that the mysteries surrounding the dilute Kondo effect were being unraveled the study of more concentrated magnetic alloys revealed equally puzzling features.

At magnetic concentrations exceeding $O(1\%)$, the magnetic impurity atoms interact with one another, with nontrivial interaction energy. If they are disposed at random, a new phase — the “spin glass” — appears. The mechanism for their interaction is most interesting. Each individual magnetic impurity polarizes the metallic medium in its immediate vicinity. The response of these electrons is not monotonic, but exhibits “Friedel oscillations.” That is, when measured or calculated as a function of distance R from a magnetic impurity, the polarization of the electron gas behaves asymptotically approximately as,

$$\sigma(R) \approx J_{\text{eff}} \frac{\cos(2k_{\text{F}}R + \varphi)}{R^3} \quad (2.7)$$

with J_{eff} a lumped constant, φ a phase shift, and k_{F} the characteristic wave-vector at the Fermi surface of the metal (inversely proportional to the de

¹⁶ Adapted from work by D. K. C. MacDonald, W. B. Pearson and I. M. Templeton.

Broglie wavelength of a conduction electron at the Fermi surface). The interaction of a spin S_j at a distance R_j from a spin S_0 at the origin takes the form $\sigma(R_j)S_j \cdot S_0$, where σ can be of either sign: positive (antiferromagnetic) or negative (ferromagnetic) depending on the phase $2k_F R_j + \varphi$.

The formula (2.7) is not applicable at small distances nor does it take into account the Kondo effect mentioned previously. Nevertheless it signals that in a dilute alloy in which the nearest-neighbor R is random, the spin-spin interaction has a frozen-in *random* sign. There results a cooperative spin “glass” in which the spins *can* become fixed at low temperatures, after assuming one of possibly many metastable random configurations mandated by the set of frozen-in random bonds. Observed properties shared by all spin glasses include: electrical resistivity dependent on magnetic ordering, hysteresis upon warming and cooling, and a specific heat linear in T at low temperature. When a spin glass is cooled in an external magnetic field B and the field is subsequently removed, the remnant magnetization depends on the sign and magnitude of B . Spin glasses in their low-temperature phases are in apparent violation of Nernst’s theorem.¹⁷

2.6. Superconductivity

Arguably the most remarkable discovery of the recent decades occurred in 1987 when perovskites containing planes of the antiferromagnetic oxide CuO_2 were found to exhibit *superconductivity* at temperatures $O(100\text{ K})$ after appropriate doping. A race is now on to find new materials that superconduct at or above room temperature. Were this pursuit successful it would, of course, extend the reign of quantum physics to room temperature while enabling the implementation of dramatically new technologies — creating an industrial “quantum” revolution with unimaginable consequences.

The search for a convincing theoretical explanation of high-temperature superconductivity (HTS) has finally narrowed to some mechanisms virtually identical to those that govern ordinary magnetic materials. There is agreement on general structural and electronic features, but not on what are the precise mechanisms (superexchange?) nor even on the primordial role of the oxide CuO_2 (is it unique in its properties?) in promoting the *pairing* of electrons into Cooper pairs.

¹⁷ Also known as the “third law of thermodynamics,” it asserts that the ground state of all substances is essentially unique, therefore entropy vanishes in the limit as $T \rightarrow 0$.

For example, suppose we postulated the emission of a magnon by a mobile electron and its subsequent re-absorption by a second, correlated electron of opposite spin. Is this similar to the “retarded phonon-exchange mechanism” that causes pairing the classic low- T_c superconductors, or is it more akin to quantum electrodynamics, in which the virtual exchange of photons by two equally charged objects results in an effective Coulomb *repulsion*, *not* attraction? At the present time there exist many conflicting opinions and theories for this most vital phenomenon but none has gained general acceptance nor confirmation.

2.7. The Need to Study Spin Angular Momentum

In many aspects of condensed matter physics and in some emerging fields such as “spintronics,” magnetic phenomena play a prominent role — but one that cannot even be assessed without an accurate understanding of the underlying electron physics. In developing an adequate theoretical framework for what turns out to be a complex many-body problem we shall first turn to small systems that can be solved in closed form (including familiar examples taken from atomic and molecular physics), for clues. In so doing, it will be necessary to reëxamine what is meant by angular momentum, spin, etc., using the language of quantum mechanics. The following chapter deals with this topic. Chapter 4 surveys some uses to which spin polarized electrons may be put.