

Interactions

In this chapter we consider the different types of magnetic interaction which can be important in allowing the magnetic moments in a solid to communicate with each other and potentially to produce long range order.

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4.1 Magnetic dipolar interaction

The first interaction which might be expected to play a rôle is the magnetic dipolar interaction. Two magnetic dipoles μ_1 and μ_2 separated by \mathbf{r} have an energy equal to

$$E = \frac{\mu_0}{4\pi r^3} \left[\mu_1 \cdot \mu_2 - \frac{3}{r^2} (\mu_1 \cdot \mathbf{r})(\mu_2 \cdot \mathbf{r}) \right] \quad (4.1)$$

which therefore depends on their separation and their degree of mutual alignment. We can easily estimate the order of magnitude of this effect for two moments each of $\mu \approx 1 \mu_B$ separated by $r \approx 1 \text{ \AA}$ to be approximately $\mu^2/4\pi r^3 \sim 10^{-23} \text{ J}$ which is equivalent to about 1 K in temperature.¹ Since many materials order at much higher temperatures (some around 1000 K), the magnetic dipolar interaction must be too weak to account for the ordering of most magnetic materials. Nevertheless, it can be important in the properties of those materials which order at milliKelvin temperatures.

¹See Fig. 3.8 for a handy conversion from energy to temperature.

4.2 Exchange interaction

Exchange interactions lie at the heart of the phenomenon of long range magnetic order. The exchange effect is subtle and not a little mysterious, since it seems surprising that one has to go to the bother of thinking about exchange operators and identical particles when all one is dealing with is a bar magnet and a pile of iron filings. But this, as so often with the subject of magnetism, is a demonstration of how quantum mechanics is at the root of many everyday phenomena. Exchange interactions are nothing more than electrostatic interactions, arising because charges of the same sign cost energy when they are close together and save energy when they are apart.

4.2.1 Origin of exchange

Consider a simple model with just two electrons which have spatial coordinates \mathbf{r}_1 and \mathbf{r}_2 respectively. The wave function for the joint state can be written as a product of single electron states, so that if the first electron is in state $\psi_a(\mathbf{r}_1)$

and the second electron is in state $\psi_b(\mathbf{r}_2)$, then the joint wave function is $\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)$. However this product state does not obey exchange symmetry, since if we exchange the two electrons we get $\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)$ which is not a multiple of what we started with. Therefore, the only states which we are allowed to make are symmetrized or antisymmetrized product states which behave properly under the operation of particle exchange. This was discussed in Section 1.3.4.

For electrons the overall wave function must be antisymmetric so the spin part of the wave function must either be an antisymmetric singlet state χ_S ($S = 0$) in the case of a symmetric spatial state or a symmetric triplet state χ_T ($S = 1$) in the case of an antisymmetric spatial state. Therefore we can write the wave function for the singlet case Ψ_S and the triplet case Ψ_T as

$$\begin{aligned}\Psi_S &= \frac{1}{\sqrt{2}}[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\chi_S \\ \Psi_T &= \frac{1}{\sqrt{2}}[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\chi_T,\end{aligned}\quad (4.2)$$

where both the spatial and spin parts of the wave function are included. The energies of the two possible states are

$$\begin{aligned}E_S &= \int \Psi_S^* \hat{\mathcal{H}} \Psi_S \, d\mathbf{r}_1 \, d\mathbf{r}_2 \\ E_T &= \int \Psi_T^* \hat{\mathcal{H}} \Psi_T \, d\mathbf{r}_1 \, d\mathbf{r}_2,\end{aligned}$$

with the assumption that the spin parts of the wave function χ_S and χ_T are normalized. The difference between the two energies is

$$E_S - E_T = 2 \int \psi_a^*(\mathbf{r}_1)\psi_b^*(\mathbf{r}_2)\hat{\mathcal{H}}\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) \, d\mathbf{r}_1 \, d\mathbf{r}_2. \quad (4.3)$$

Equation 1.70 shows how the difference between singlet and triplet states can be parametrized using $\mathbf{S}_1 \cdot \mathbf{S}_2$. For a singlet state $\mathbf{S}_1 \cdot \mathbf{S}_2 = -\frac{3}{4}$ while for a triplet state $\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{4}$. Hence the Hamiltonian can be written in the form of an 'effective Hamiltonian'

$$\hat{\mathcal{H}} = \frac{1}{4}(E_S + 3E_T) - (E_S - E_T)\mathbf{S}_1 \cdot \mathbf{S}_2. \quad (4.4)$$

This is the sum of a constant term and a term which depends on spin. The constant can be absorbed into other constant energy terms, but the second term is more interesting. The exchange constant (or exchange integral), J is defined by

$$J = \frac{E_S - E_T}{2} = \int \psi_a^*(\mathbf{r}_1)\psi_b^*(\mathbf{r}_2)\hat{\mathcal{H}}\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) \, d\mathbf{r}_1 \, d\mathbf{r}_2. \quad (4.5)$$

and hence the spin-dependent term in the effective Hamiltonian can be written

$$\hat{\mathcal{H}}^{\text{spin}} = -2J\mathbf{S}_1 \cdot \mathbf{S}_2. \quad (4.6)$$

If $J > 0$, $E_S > E_T$ and the triplet state $S = 1$ is favoured. If $J < 0$, $E_S < E_T$ and the singlet state $S = 0$ is favoured. This equation is relatively simple

Werner Heisenberg (1901–1976)

to derive for two electrons, but generalizing to a many-body system is far from trivial. Nevertheless, it was recognized in the early days of quantum mechanics that interactions such as that in eqn 4.6 probably apply between all neighbouring atoms. This motivates the Hamiltonian of the **Heisenberg model**:

$$\hat{\mathcal{H}} = - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (4.7)$$

where J_{ij} is the exchange constant between the i^{th} and j^{th} spins. The factor of 2 is omitted because the summation includes each pair of spins twice. Another way of writing eqn 4.7 is

$$\hat{\mathcal{H}} = -2 \sum_{i>j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (4.8)$$

Note that in some books, J is replaced by twice the value used here so that eqns 4.6–4.8 would become

$$\hat{\mathcal{H}}^{\text{spin}} = -J \mathbf{S}_1 \cdot \mathbf{S}_2, \quad (4.9)$$

$$\hat{\mathcal{H}} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (4.10)$$

$$\hat{\mathcal{H}} = - \sum_{i>j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (4.11)$$

where the $i > j$ avoids the ‘double-counting’ and hence the factor of two returns. Often it is possible to take J_{ij} to be equal to a constant J for nearest neighbour spins and to be 0 otherwise.

The calculation of the exchange integral can be complicated in general, but we here mention some general features. First, if the two electrons are on the same atom, the exchange integral is usually positive. This stabilizes the triplet state and ensures an antisymmetric spatial state which minimizes the Coulomb repulsion between the two electrons by keeping them apart. This is consistent with Hund’s first rule.

When the two electrons are on neighbouring atoms, the situation is very different. Any joint state will be a combination of a state centred on one atom and a state centred on the other. It is worth remembering that the energy of a particle in a one-dimensional box of length L is proportional to L^{-2} ; this is a kinetic energy and hence demonstrates that there is a large kinetic energy associated with being squeezed into a small box. The electrons therefore can save kinetic energy by forming bonds because this allows them to wander around both atoms rather than just one (i.e. wander in a ‘bigger box’). The correct states to consider are now not atomic orbitals but molecular orbitals (see Fig. 4.1). These can be **bonding** (spatially symmetric) or ‘**antibonding**’ (spatially antisymmetric), with the **antibonding** orbitals more energetically costly. This is because the antibonding orbital has a greater curvature and hence a larger kinetic energy. This favours singlet (antisymmetric) states and the exchange integral is therefore likely to be negative.

4.2.2 Direct exchange

If the electrons on neighbouring magnetic atoms interact via an exchange interaction, this is known as **direct exchange**. This is because the exchange interaction proceeds directly without the need for an intermediary. Though this seems the most obvious route for the exchange interaction to take, the reality in physical situations is rarely that simple.

Very often direct exchange cannot be an important mechanism in controlling the magnetic properties because there is insufficient direct overlap between neighbouring magnetic orbitals. For example, in rare earths the 4f electrons are strongly localized and lie very close to the nucleus, with little probability density extending significantly further than about a tenth of the interatomic

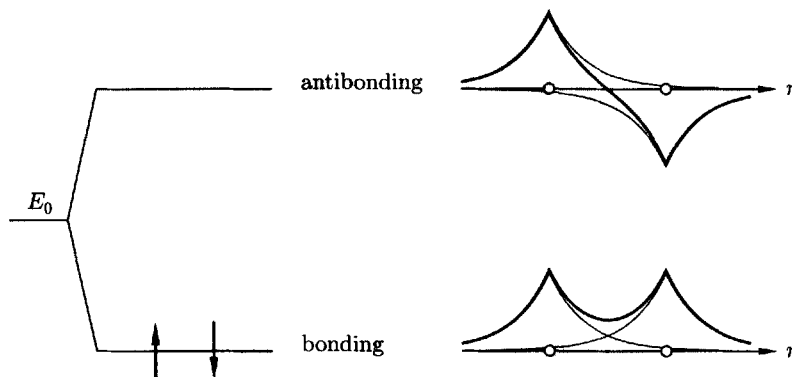


Fig. 4.1 Molecular orbitals for a diatomic molecule. The bonding orbital, which corresponds to the sum of the two atomic orbitals (symmetric under exchange, as far as the spatial part of the wave function is concerned), is of lower energy than the antibonding orbital, which corresponds to the difference of the two atomic orbitals (antisymmetric under exchange). This therefore favours a singlet ground state in which two electrons fill the bonding state and the antibonding state is empty. This diagram is appropriate for the hydrogen molecule H_2 which has a lower energy than that of two isolated H atoms (E_0). Note that the diatomic form of helium, He_2 , does not form because the four electrons from two He atoms would fill both the bonding and antibonding orbitals, corresponding to no net energy saving in comparison with two isolated He atoms.

spacing. This means that the direct exchange interaction is unlikely to be very effective in rare earths. Even in transition metals, such as Fe, Co and Ni, where the 3d orbitals extend further from the nucleus, it is extremely difficult to justify why direct exchange should lead to the observed magnetic properties. These materials are metals which means that the rôle of the conduction electrons should not be neglected, and a correct description needs to take account of both the localized and band character of the electrons.

Thus in many magnetic materials it is necessary to consider some kind of indirect exchange interaction.

4.2.3 Indirect exchange in ionic solids: superexchange

A number of ionic solids, including some oxides and fluorides, have magnetic ground states. For example, MnO (see Fig. 4.2) and MnF_2 are both antiferromagnets, though this observation appears at first sight rather surprising because there is no direct overlap between the electrons on Mn^{2+} ions in each system. The exchange interaction is normally very short-ranged so that the longer-ranged interaction that is operating in this case must be in some sense 'super'.

The exchange mechanism which is operative here is in fact known as **superexchange**. It can be defined as an indirect exchange interaction between non-neighbouring magnetic ions which is mediated by a non-magnetic ion which is placed in between the magnetic ions. It arises because there is a kinetic energy advantage for antiferromagnetism, which can be understood by reference to Fig. 4.3 which shows two transition metal ions separated by an oxygen ion. For simplicity we will assume that the magnetic moment on the transition metal ion is due to a single unpaired electron (more complicated cases can be dealt with in analogous ways). Hence if this system were perfectly ionic, each metal ion would have a single unpaired electron in a d orbital

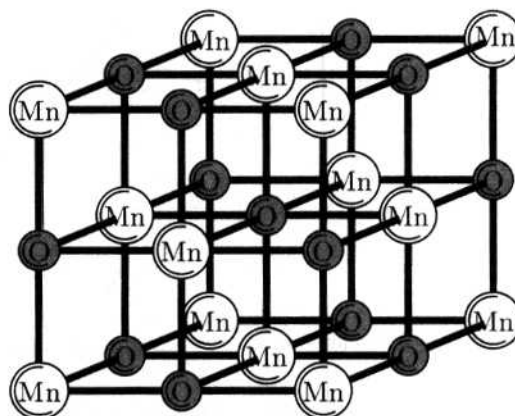
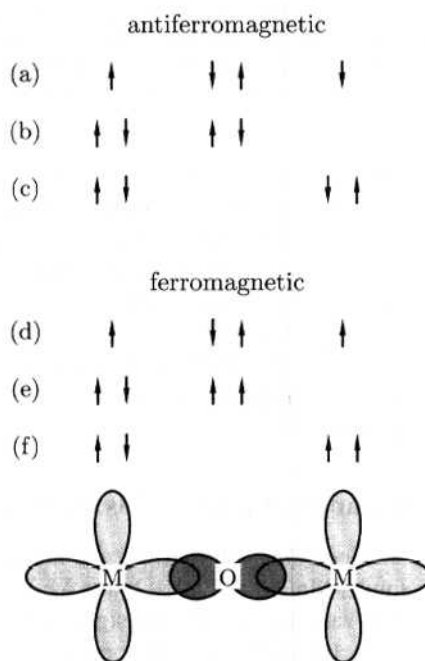


Fig. 4.2 The crystal structure of MnO. Nearest neighbour pairs of Mn^{2+} (manganese) ions are connected via O^{2-} (oxygen) ions.

Fig. 4.3 Superexchange in a magnetic oxide. The arrows show the spins of the four electrons and how they are distributed over the transition metal (M) and oxygen (O) atoms. M is assumed to have a single unpaired electron, making it magnetic. If the moments on the transition metal atoms are coupled antiferromagnetically (a, b, c), the ground state is (a) and this can mix with excited configurations like (b) and (c). The magnetic electrons can thus be delocalized over the M–O–M unit, thus lowering the kinetic energy. If the moments on the metal (M) atoms are coupled ferromagnetically (d, e, f), the ground state (d) cannot mix with excited configurations like (e) and (f) because these configurations are prevented by the exclusion principle. The ferromagnetic configuration therefore costs more energy.



and the oxygen would have two p electrons in its outermost occupied states. The figure demonstrates that antiferromagnetic coupling lowers the energy of the system by allowing these electrons to become delocalized over the whole structure, thus lowering the kinetic energy.

Because superexchange involves the oxygen orbitals as well as the metal atom, it is a second-order process and is derived from second-order perturbation theory. A general consequence of second-order perturbation theory is that the energy involved is approximately given by the square of the matrix element of the transition divided by the energy cost of making the excited state. Here the transition matrix element is controlled by a parameter called the hopping

integral t , which is proportional to the energy width of the conduction band (i.e. the bandwidth) in a simple tight-binding approach. The energy cost of making an excited state is given by the Coulomb energy U . Thus we have that $J \sim -t^2/U$. (In fourth-order it is possible to have an interaction of the form $\Delta E \propto -t^4(\mathbf{S}_1 \cdot \mathbf{S}_2)^2/U^3$ which is known as **biquadratic exchange**.)

The exchange integral consists of two parts. The first is a potential exchange term which represents the electron repulsion and favours ferromagnetic ground states, but is small when the ions are well separated. The second is a kinetic exchange term which dominates here and is the effect discussed above. It depends on the degree of overlap of orbitals and thus superexchange is strongly dependent upon the angle of the M–O–M bond. The figure has been drawn for one type of d orbital only, but the effect of other d orbitals which can overlap with the oxygen orbitals may also need to be added.

In some circumstances, superexchange can actually be ferromagnetic. For example, imagine a situation in which there is a coupling, through an oxygen ion, between an occupied e_g orbital on one magnetic ion and an unoccupied e_g orbital on another magnetic ion. There is an energetic advantage to the e_g electron hopping onto the unoccupied orbital, if when it arrives its spin is aligned with the spin of the t_{2g} electrons because of the Hund's rule coupling. Thus the superexchange could be ferromagnetic in this case, but this is weaker interaction and less common than the usual antiferromagnetic superexchange.

4.2.4 Indirect exchange in metals

In metals the exchange interaction between magnetic ions can be mediated by the conduction electrons. A localized magnetic moment spin-polarizes the conduction electrons and this polarization in turn couples to a neighbouring localized magnetic moment a distance r away. The exchange interaction is thus indirect because it does not involve direct coupling between magnetic moments. It is known as the **RKKY interaction** (or also as **itinerant exchange**). The name RKKY is used because of the initial letters of the surnames of the discoverers of the effect, Ruderman, Kittel, Kasuya and Yosida. The coupling takes the form of an r -dependent exchange interaction $J_{\text{RKKY}}(r)$ given by

$$J_{\text{RKKY}}(r) \propto \frac{\cos(2k_F r)}{r^3}. \quad (4.12)$$

at large r (assuming a spherical Fermi surface of radius k_F). The interaction is long range and has an oscillatory dependence on the distance between the magnetic moments. Hence depending on the separation it may be either ferromagnetic or antiferromagnetic. The coupling is oscillatory with wavelength π/k_F because of the sharpness of the Fermi surface. The RKKY interaction will be considered in more detail in chapter 7.

4.2.5 Double exchange

In some oxides, it is possible to have a ferromagnetic exchange interaction which occurs because the magnetic ion can show **mixed valency**, that is it can exist in more than one oxidation state. Examples of this include compounds containing the Mn ion which can exist in oxidation state 3 or 4, i.e. as Mn^{3+}

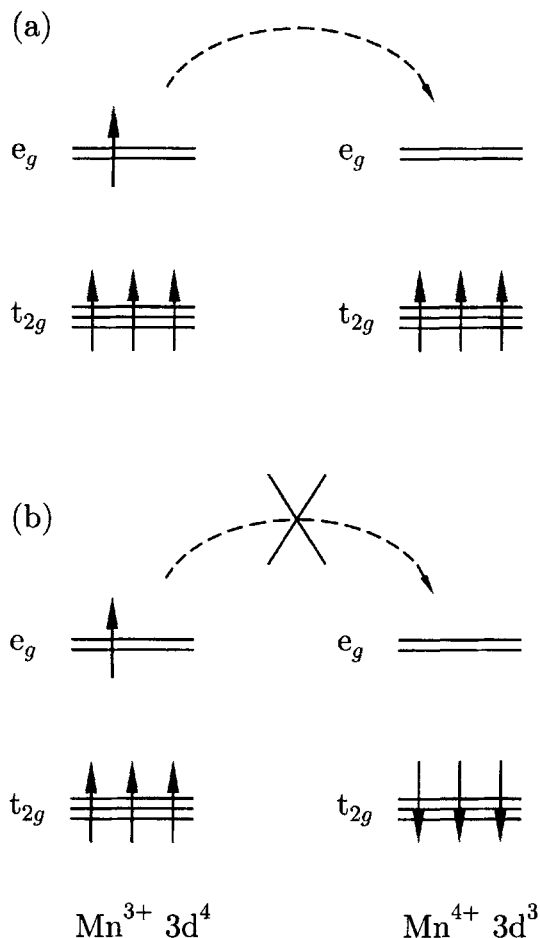


Fig. 4.4 Double exchange mechanism gives ferromagnetic coupling between Mn^{3+} and Mn^{4+} ions participating in electron transfer. The single-centre exchange interaction favours hopping if (a) neighbouring ions are ferromagnetically aligned and not if (b) neighbouring ions are antiferromagnetically aligned.

or Mn^{4+} . One such is the material $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ ($0 \leq x \leq 1$) which adopts a perovskite structure. Sr is divalent (it exists as Sr^{2+}) and La is trivalent (it exists as La^{3+}). This implies that a fraction x of the Mn ions are Mn^{4+} and $1 - x$ are Mn^{3+} . The end members of the series, with $x = 0$ and $x = 1$, are both antiferromagnetic insulators, as would be expected for an oxide material in which the magnetism is mediated by superexchange through the oxygen. LaMnO_3 contains only Mn^{3+} ions and Mn^{3+} is a Jahn–Teller ion. LaMnO_3 has A-type antiferromagnetic ordering (see Section 5.2). However when LaMnO_3 is doped with Sr up to a level of $x = 0.175$, the Jahn–Teller distortion vanishes and the system becomes ferromagnetic with a Curie temperature around room temperature, below which temperature the material becomes metallic.

The ferromagnetic alignment is due to the double exchange mechanism which can be understood with reference to Fig. 4.4. The e_g electron on a Mn^{3+} ion can hop to a neighbouring site only if there is a vacancy there of the same spin (since hopping proceeds without spin-flip of the hopping electron). If the neighbour is a Mn^{4+} which has no electrons in its e_g shell, this should present no problem. However, there is a strong single-centre (Hund's rule number 1) exchange interaction between the e_g electron and the three electrons in the

t_{2g} level which wants to keep them all aligned. Thus it is not energetically favourable for an e_g electron to hop to a neighbouring ion in which the t_{2g} spins will be antiparallel to the e_g electron (Fig. 4.4(b)). Ferromagnetic alignment of neighbouring ions is therefore required to maintain the high-spin arrangement on both the donating and receiving ion. Because the ability to hop gives a kinetic energy saving, allowing the hopping process shown in Fig. 4.4(a) reduces the overall energy. Thus the system ferromagnetically aligns to save energy. Moreover, the ferromagnetic alignment then allows the e_g electrons to hop through the crystal and the material becomes metallic. The issue of conductivity in double exchange ferromagnets will be further discussed in Section 8.9.5. Double exchange is, essentially, ferromagnetic superexchange in an extended system.²

Double exchange is also found in magnetite (Fe_3O_4) which contains an equal mixture of Fe^{2+} ($3d^6$) and Fe^{3+} ($3d^5$) ions on octahedral sites, together with the same number again of Fe^{3+} ions on tetrahedral sites. A double exchange interaction ferromagnetically aligns the Fe^{2+} and Fe^{3+} ions on the octahedral sites. The Fe^{3+} ions on the tetrahedral sites do not participate in this interaction and are coupled to the Fe^{3+} ions on the octahedral sites by an antiferromagnetic superexchange interaction. Thus the two sets of Fe^{3+} ions cancel out, leaving a net moment due to the Fe^{2+} ions alone. The measured magnetic moment per formula unit is very close to the expected $4 \mu_B$ due to just the Fe^{2+} ions.

²Ferromagnetic superexchange is normally applied to two isolated ions. The kinetic energy saved by ferromagnetic alignment corresponds to hopping into an excited state. Double exchange is applied to an extended system so the kinetic energy saved corresponds to a gain in electron bandwidth.

4.2.6 Anisotropic exchange interaction

It is also possible for the spin-orbit interaction to play a rôle in a similar manner to that of the oxygen atom in superexchange. Here the excited state is not connected with oxygen but is produced by the spin-orbit interaction in one of the magnetic ions. There is then an exchange interaction between the excited state of one ion and the ground state of the other ion. This is known as the anisotropic exchange interaction, or also as the Dzyaloshinsky-Moriya interaction. When acting between two spins \mathbf{S}_1 and \mathbf{S}_2 it leads to a term in the Hamiltonian, $\hat{\mathcal{H}}_{\text{DM}}$ equal to

$$\hat{\mathcal{H}}_{\text{DM}} = \mathbf{D} \cdot \mathbf{S}_1 \times \mathbf{S}_2. \quad (4.13)$$

The vector \mathbf{D} vanishes when the crystal field has an inversion symmetry with respect to the centre between the two magnetic ions. However, in general \mathbf{D} may not vanish and then will lie parallel or perpendicular to the line connecting the two spins, depending on the symmetry. The form of the interaction is such that it tries to force \mathbf{S}_1 and \mathbf{S}_2 to be at right angles in a plane perpendicular to the vector \mathbf{D} in such an orientation as to ensure that the energy is negative. Its effect is therefore very often to cant (i.e. slightly rotate) the spins by a small angle. It commonly occurs in antiferromagnets and then results in a small ferromagnetic component of the moments which is produced perpendicular to the spin-axis of the antiferromagnet. The effect is known as **weak ferromagnetism**. It is found in, for example, $\alpha\text{-Fe}_2\text{O}_3$, MnCO_3 and CoCO_3 .

4.2.7 Continuum approximation

In this section we return to the Heisenberg model given in eqn 4.7. For what follows later in the book it is useful to find an expression for this interaction in a continuum approximation in which the discrete nature of the lattice is ignored.

Let us first assume that J_{ij} can be taken to be equal to a constant, J , if i and j are nearest neighbours, and to be zero otherwise. Hence we write

$$\hat{\mathcal{H}} = - \sum_{\langle ij \rangle} J \mathbf{S}_i \cdot \mathbf{S}_j, \quad (4.14)$$

where the symbol $\langle ij \rangle$ below the \sum denotes a sum over nearest neighbours only. Let us consider classical spins, and assume that the angle between nearest neighbour spins is ϕ_{ij} and that it is very small, i.e. $\phi_{ij} \ll 1$ for all i and j . What we are essentially doing is assuming that the system shows ferromagnetism (see the next chapter) but the spins are not completely aligned.

With these assumptions, the energy of the system can be written as

$$E = -JS^2 \sum_{\langle ij \rangle} \cos \phi_{ij} = \text{constant} + \frac{JS^2}{2} \sum_{\langle ij \rangle} \phi_{ij}^2, \quad (4.15)$$

where the last equality is obtained using $\cos \phi_{ij} \approx 1 - \phi_{ij}^2/2$ for $\phi_{ij} \ll 1$. We will now ignore the constant term which just refers to the energy of the fully aligned state. We now define the reduced moment by $\mathbf{m} = \mathbf{M}/M_s$, where \mathbf{M} is the magnetization and M_s is the saturation magnetization. The unit vector \mathbf{m} therefore follows the direction of the spins and m_x , m_y and m_z can be thought of as the direction cosines of the spin at lattice point r_{ij} . Using the notation of Fig. 4.5, we can write

$$|\phi_{ij}| \approx |\mathbf{m}_i - \mathbf{m}_j| \approx |(\mathbf{r}_{ij} \cdot \nabla) \mathbf{m}|, \quad (4.16)$$

and so the energy can be written

$$E = JS^2 \sum_{\langle ij \rangle} [(\mathbf{r}_{ij} \cdot \nabla) \mathbf{m}]^2. \quad (4.17)$$

In the continuum limit, we ignore the discrete nature of the lattice and therefore write

$$E = A \int_V [(\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2] d^3r, \quad (4.18)$$

where A is given by

$$A = 2JS^2z/a, \quad (4.19)$$

a is the nearest neighbour distance and z is the number of sites in the unit cell ($z = 1$ for simple cubic, $z = 2$ for body-centred cubic (bcc) and $z = 4$ for face-centred cubic (fcc)).

This result can be seen from another perspective. If we assert that exchange arises from a non-uniform magnetization distribution, then if the non-uniformities are relatively smooth we can derive a result based on symmetry. The expression must be invariant with respect to spin rotations and also under change of sign of the magnetization components. Therefore we look for an expression of the lowest even orders of the derivatives of \mathbf{M} , consistent with the

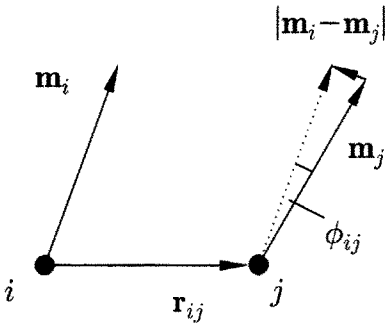


Fig. 4.5 The magnetic moments are represented by the reduced moments \mathbf{m}_i and \mathbf{m}_j at neighbouring sites i and j separated by a vector \mathbf{r}_{ij} . The angle between the moments is ϕ_{ij} . The reduced moments \mathbf{m}_i and \mathbf{m}_j are unit vectors by definition.

symmetry of the crystal. Since terms proportional to $\partial M_\alpha / \partial x_\beta$ would change sign if \mathbf{M} were reversed, we are left with terms quadratic in the gradient of the magnetization. The most general expression is

$$E = \sum_{\alpha\beta\gamma} C_{\alpha\beta} \frac{\partial M_\gamma}{\partial x_\alpha} \frac{\partial M_\gamma}{\partial x_\beta}, \quad (4.20)$$

where $C_{\alpha\beta}$ is a tensor with the symmetry of the crystal. In a cubic crystal, this reduces to

$$E = C \sum_{\alpha\gamma} \frac{\partial M_\gamma}{\partial x_\alpha} \frac{\partial M_\gamma}{\partial x_\alpha} = C [(\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2], \quad (4.21)$$

The expression in eqn 4.21 is sometimes written $C|\nabla\mathbf{M}|^2$ but note that you have to be a bit careful when taking the gradient of a vector.

which is equivalent to the result we have in eqn 4.18 above.

Further reading

- Further information on exchange interactions may be found in C. Herring in *Magnetism*, ed. G. Rado and H. Suhl, vol. 2B, p.1, Academic Press, New York 1966.
- A theoretical account of interactions in magnetic systems may be found in K. Yosida, *Theory of magnetism*, Springer 1996.
- Various exchange interactions in real systems are reviewed in P. A. Cox, *Transition metal oxides*, OUP 1995.
- A very thorough and helpful reference on exchange and exchange interactions is D. C. Mattis, *The theory of magnetism I*, Springer 1981.

Exercises

- (4.1) Show that two magnetic dipoles μ_1 and μ_2 separated by \mathbf{r} have a dipolar energy equal to

$$E = \frac{\mu_0}{4\pi r^3} \left[\mu_1 \cdot \mu_2 - \frac{3}{r^2} (\mu_1 \cdot \mathbf{r})(\mu_2 \cdot \mathbf{r}) \right]. \quad (4.22)$$

- (4.2) Calculate the magnitude of the magnetic field 1 Å and 10 Å from a proton in a direction (a) parallel and (b) perpendicular to the proton spin direction.

- (4.3) Estimate the ratio of the exchange and dipolar coupling of two adjacent Fe atoms in metallic Fe. (The exchange constant in Fe can be crudely estimated by setting it equal to $k_B T_C$ where T_C is the Curie temperature. For Fe, $T_C = 1043$ K.)

- (4.4) Provide a rough estimate of the size of the exchange constant in a magnetic oxide which is coupled by superexchange using the measured value of the electronic bandwidth (determined by inelastic neutron scattering) of

0.05 eV. Take the Coulomb energy to be ~ 1 eV. Hence estimate the antiferromagnetic ordering temperature.

- (4.5) Consider the case of two interacting spin- $\frac{1}{2}$ electrons. The good quantum numbers are $S = 0$ and 1 so that there is a triplet state and a singlet state which will be separated by an energy gap Δ . We define the sign of Δ so that when $\Delta > 0$ the singlet state ($S = 0$) is the lower state and when $\Delta < 0$ the triplet state is the lower state. These situations are shown in Fig. 4.6(a) and (b). Show that the susceptibility in this model is given by

$$\chi = \frac{2Ng\mu_B^2}{k_B T (3 + e^{\Delta/k_B T})}, \quad (4.23)$$

which is known as the Bleaney-Bowers equation. It is plotted in Fig. 4.6(c).