Chapter 2
Spin Models

Abstract Assuming only a basic knowledge of quantum mechanics, we develop the quantum mechanics of angular momentum, distinguishing between orbital and intrinsic angular momentum or spin. Suitable basis states are introduced, as are the fundamental operators which act upon these. We consider the situation of just two spins interacting via an exchange interaction. This leads us to introduce other spin operators and evaluate their commutators. We discuss what happens when there are large numbers of interacting spins. Finally we introduce the infinite linear (i.e. one-dimensional) chain of spin-1/2 atoms. Some preliminary classical results for this model are given as background for the full quantum treatment which will be studied in detail in the following chapters.

2.1 Spin Angular Momentum

In this section we give a brief summary of some of the important results about angular momentum [1] which are needed for a study of quantum spin systems.

There are two types of angular momentum which occur in nature. The first of these, in its classical form, is familiar from very early days and arises from motion, often circular, relative to some axis. This is called *orbital* angular momentum.

In quantum mechanics we usually first come across orbital angular momentum when we study the eigenstates of the Schrödinger equation (SE) for the hydrogen atom. The angular parts of these, using spherical polar coordinates, have the form

$$Y_{\ell,m}(\theta,\phi) \;=\; C_{\ell,m} P_{\ell}^{m}(\theta) e^{im\phi} \;,$$

where P_{ℓ}^{m} are polynomials in $\cos\theta$ and/or $\sin\theta$ of degree ℓ – the associated Legendre polynomials and $C_{\ell,m}$ is a normalisation constant.

These angular parts of the eigenstates of the time-independent SE have another significance. They are also eigenstates of the angular momentum operators. For a particle with momentum $\mathbf{p}$ and position vector $\mathbf{r}$ then the classical angular momentum relative to an axis through the origin and perpendicular to the plane of motion is $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, and in quantum mechanics the angular momentum operator has the same form

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$$\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$$

where ˆ denotes an operator. These operators have the commutators $\left[\hat{L}^x, \hat{L}^y\right] = i\hbar\hat{L}^z$ together with cyclic permutations.

Two of the most useful operators are $\hat{L}^z$ and $\hat{\mathbf{L}}^2 = (\hat{L}^x)^2 + (\hat{L}^y)^2 + (\hat{L}^z)^2$. This is because the $Y_{\ell,m}$ are eigenstates of both of these simultaneously. It is always possible to find states which are simultaneous eigenstates of two operators provided the operators commute and we can easily show that $[\hat{L}^z, \hat{\mathbf{L}}^2] = 0$. The corresponding eigenvalues are given by

$$\hat{L}^z Y_{\ell,m} = m\hbar Y_{\ell,m}; \qquad \hat{\mathbf{L}}^2 Y_{\ell,m} = \ell(\ell+1)\hbar^2 Y_{\ell,m}.$$

There are two other operators which have useful properties. These are defined as

$$\hat{L}^+ \equiv \hat{L}^x + i\hat{L}^y \quad \text{and} \quad \hat{L}^- \equiv \hat{L}^x - iL^y.$$

From these definitions it follows that

$$[\hat{L}^-, \hat{L}^+] = 2\hbar L^z$$

and it can also be shown that

$$\hat{L}^+ Y_{\ell,m} = 0 \quad \text{if } m = \ell.$$

However, if $m < \ell$ then

$$\hat{L}^z(\hat{L}^+ Y_{\ell,m}) = (m+1)\hbar(L^+ Y_{\ell,m}),$$
$$\hat{\mathbf{L}}^2(\hat{L}^+ Y_{\ell,m}) = \ell(\ell+1)\hbar^2(\hat{L}^+ Y_{\ell,m}).$$

This means that $L^+ Y_{\ell,m}$ is also an eigenstate of $\hat{L}^z$ and $\hat{\mathbf{L}}^2$. It has the same eigenvalue of $\hat{\mathbf{L}}^2$ as $Y_{\ell,m}$, but an eigenvalue of $\hat{L}^z$ which is increased by one unit of $\hbar$. Clearly $\hat{L}^+$ converts $Y_{\ell,m}$ into $Y_{\ell,m+1}$, to within a multiplicative constant, and it is called the *raising* operator. Similarly $\hat{L}^-$ converts $Y_{\ell,m}$ into $Y_{\ell,m-1}$ to within a multiplicative constant and is a *lowering* operator. That is $\hat{L}^+ Y_{\ell,m} = AY_{\ell,m+1}$ and $\hat{L}^- Y_{\ell,m} = BY_{\ell,m-1}$.

The second type sort of angular momentum which occurs in nature is the intrinsic spin of elementary particles. This is a fundamental property of a particle. It is often thought of as due to internal spinning of a particle, hence the name, but this is not correct since, for example, an electron has spin angular momentum but is believed to be a point particle with no internal structure.

The spin angular momentum has most of the properties of orbital angular momentum, but also some special properties. For the present we shall use $\hat{\mathbf{S}}$ for spin angular momentum instead of $\hat{\mathbf{L}}$. Again we can use the eigenstates of $\hat{S}^z$ and $\hat{\mathbf{S}}^2$ with the same quantum numbers ℓ and m such that

$$\begin{aligned}\hat{S}^z|\ell,m\rangle &= m\hbar|\ell,m\rangle \\ \hat{\mathbf{S}}^2|\ell,m\rangle &= \ell(\ell+1)\hbar^2|\ell,m\rangle\end{aligned}$$

Clearly the spin eigenstate $|\ell,m\rangle$ behaves here just like the orbital eigenstate $Y_{\ell,m}$, but there are two fundamental differences.

1. $|\ell,m\rangle$ does not have an explicit form in terms of θ and ϕ like $Y_{\ell,m}$.
2. ℓ may now be an integer, as before, *or* an integer $+\frac{1}{2}$, sometimes called a 'half-integer'.

The values of m still differ by unity and still take all values between $-\ell$ and $+\ell$ but if ℓ is an integer $+\frac{1}{2}$ then so are the m.

For example 1 If $\ell = \frac{3}{2}$ then the possible values of m are $-\frac{3}{2}$, $-\frac{1}{2}$, $\frac{1}{2}$, and $\frac{3}{2}$.

For example 2 If $\ell = \frac{1}{2}$ then m can be $-\frac{1}{2}$ or $\frac{1}{2}$.

We also have the operators $\hat{S}^+$ and $\hat{S}^-$ corresponding to $\hat{L}^+$ and $\hat{L}^-$ and with the same properties as before, namely

$$\hat{S}^+|\ell,m\rangle = 0 \quad \text{for} \quad m = \ell$$

while for $m < \ell$

$$\begin{aligned}\hat{S}^z(\hat{S}^+|\ell,m\rangle) &= (m+1)\hbar(\hat{S}^+|\ell,m\rangle) \\ \hat{\mathbf{S}}^2(\hat{S}^+|\ell,m\rangle) &= \ell(\ell+1)\hbar^2(S^+|\ell,m\rangle)\,.\end{aligned}$$

Again there are similar results for $\hat{S}^-|\ell,m\rangle$.

For the orbital angular momentum of an electron in a H-atom, states with different ℓ are possible, each of which has several possible values of m. For spin angular momentum the value of ℓ is *fixed* (it is a fundamental property of the particle) e.g. $\ell = \frac{1}{2}$ for electron $\ell = 1$ for some mesons etc. The only difference between eigenstates is the value of m.

In magnetic materials the magnetic moment of an atom may be due to a combination of spin and orbital angular momentum. The actual magnetic moment is a simple but non-trivial function of the two types, usually described in terms of the 'Landé g-factor' of the atom or ion which varies between 1 (for pure orbital angular momentum) and 2 (for pure spin angular momentum). However we shall always take the angular momentum to have a fixed value of ℓ (i.e. the 'magnitude') but allow m (i.e. the 'orientation') to vary. For this reason we usually refer to the angular momentum of a magnetic atom as a spin and use the symbol $\hat{\mathbf{S}}$, even when it is a combination of both types.

Single Spin-$\frac{1}{2}$

For a single spin-$\frac{1}{2}$ the value of ℓ is $\frac{1}{2}$. The value of m may be $+\frac{1}{2}$ or $-\frac{1}{2}$, so there are two eigenstates of $\hat{S}^z$:

$$|\ell,m\rangle \;=\; |\tfrac{1}{2},\tfrac{1}{2}\rangle \quad \text{or} \quad |\tfrac{1}{2},-\tfrac{1}{2}\rangle.$$

Alternative abbreviated notations for these which we use are

$$\begin{aligned} |\tfrac{1}{2},\tfrac{1}{2}\rangle &\equiv |\tfrac{1}{2}\rangle \equiv |+\rangle \\ |\tfrac{1}{2},-\tfrac{1}{2}\rangle &\equiv |-\tfrac{1}{2}\rangle \equiv |-\rangle\,. \end{aligned}$$

These two eigenstates form a complete set for a single spin $\frac{1}{2}$ so an arbitrary state may be written

$$\psi = \alpha|+\rangle + \beta|-\rangle.$$

The eigenstates are normalized and orthogonal:

$$\begin{aligned} \langle+|+\rangle = \langle-|-\rangle &= 1 \\ \langle+|-\rangle &= 0\,. \end{aligned}$$

From now on we shall omit the ˆ symbol on operators and also work in units in which $\hbar$ has the value 1. Hence

$$\begin{aligned} S^z|+\rangle &= \tfrac{1}{2}\hbar|+\rangle = \tfrac{1}{2}|+\rangle \\ S^z|-\rangle &= -\tfrac{1}{2}\hbar|-\rangle = -\tfrac{1}{2}|+\rangle \end{aligned}$$

Also

$$\begin{aligned} S^+|+\rangle &= 0 & S^-|-\rangle &= 0 \\ S^+|-\rangle &= |+\rangle & S^-|+\rangle &= |-\rangle \end{aligned}$$

Single Spin-1 This follows a similar pattern with $\ell = 1$ and $m = 1, 0, -1$. Again we use a simplified notation:

$$\begin{aligned} |1,1\rangle &\equiv |1\rangle \equiv |+\rangle \\ |1,0\rangle &\equiv |0\rangle \\ |1,-1\rangle &\equiv |-1\rangle \equiv |-\rangle \end{aligned}$$

and the effect of the spin operators is

$$\begin{aligned} S^+|-\rangle &= \sqrt{2}|0\rangle & S^+|0\rangle &= \sqrt{2}|+\rangle & S^+|+\rangle &= 0 \\ S^-|-\rangle &= 0 & S^-|0\rangle &= \sqrt{2}|-\rangle & S^-|+\rangle &= \sqrt{2}|0\rangle \\ S^z|-\rangle &= -|-\rangle & S^z|0\rangle &= 0 & S^z|+\rangle &= |+\rangle. \end{aligned}$$

There are similar results for higher spins.

2.2 Coupled Spins

When spins interact with each other new phenomena can arise such as large scale ferromagnetism or antiferromagnetism. If we study this behaviour using quantum mechanics then some results are very similar to what one would expect from a classical point of view. However, some results are quite different and this is what makes the study of interacting spin systems so fascinating.

The quantum treatment involves quite a lot of mathematics. In fact advanced treatments use some very sophisticated methods, but in this introductory text these will be kept to a minimum.

Much of our understanding comes from a study of exactly solvable models. These are rather specialised but because they can be solved exactly they can be studied in great depth. In 1D we shall consider in later chapters two models in particular:

1. the Heisenberg chain – studied using the 'Bethe Ansatz' and
2. the XY chain – studied using the 'Jordan-Wigner transformation'.

In the rest of this chapter we look at what happens when small numbers of spins interact with each other, in particular the similarities and differences between the classical and quantum mechanical cases. Simple results for much larger systems will be introduced, setting the stage for the more complicated infinite quantum systems discussed in later chapters.

2.3 Two Interacting Spin-$\frac{1}{2}$'s

Suppose we have just two atoms, each with spin-$\frac{1}{2}$, interacting with an isotropic exchange interaction J (Heisenberg Exchange). The Hamiltonian is

$$\mathcal{H} = J\,\mathbf{S}_1 \cdot \mathbf{S}_2 \tag{2.1}$$

Classically the energy of the system depends on the angle between the spins since

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = S_1 S_2 \cos\theta.$$

S_1 and S_2 are both $\frac{1}{2}$ so the energy is

$$E_{\text{class}} = \frac{1}{4}\,J\,\cos\theta,$$

and since $-1 \leq \cos\theta \leq 1$ all energies are possible between $+\frac{1}{4}J$ and $-\frac{1}{4}J$.

Quantum mechanically we need to find all the energy eigenstates of the system. First we write down a complete orthonormal set of states for the system. Then we write $\mathcal{H}$ as a matrix using this basis and finally diagonalise to find the eigenstates.

Using subscript 1 for the first spin, then a basis for the first spin consists of the two eigenstates of S_1^z, namely $|+\rangle_1$ and $|-\rangle_1$. Similarly $|+\rangle_2$ and $|-\rangle_2$ form a basis for the second spin. A basis for the pair is then

$$\{|++\rangle,\ \ |+-\rangle,\ \ |-+\rangle,\ \ |--\rangle\} \tag{2.2}$$

where $|++\rangle$ means $|+\rangle_1\,|+\rangle_2$ etc. Hence the matrix for $\mathcal{H}$ will be size 4 × 4.

It is useful to rewrite the Hamiltonian (2.1) as follows

$$\begin{aligned}\mathcal{H} &= J\,\mathbf{S}_1\cdot\mathbf{S}_2\\ &= J\,(S_1^zS_2^z + S_1^xS_2^x + S_1^yS_2^y)\\ &= J\left(S_1^zS_2^z + \frac{1}{2}S_1^+S_2^- + \frac{1}{2}S_1^-S_2^+\right)\end{aligned} \tag{2.3}$$

This is easily shown as follows:

$$\begin{aligned} S_1^+S_2^- &= (S_1^x + iS_1^y)(S_2^x - iS_2^y)\\ &= S_1^xS_2^x + S_1^yS_2^y + i(S_1^yS_2^x - S_1^xS_2^y)\\ \text{and}\;\; S_1^-S_2^+ &= S_1^xS_2^x + S_1^yS_2^y - i(S_1^yS_2^x - S_1^xS_2^y)\\ \text{so}\;\; S_1^+S_2^- + S_1^-S_2^+ &= 2(S_1^xS_2^x + S_1^yS_2^y). \end{aligned}$$

Now consider the effect of the Hamiltonian (2.3) operating on each member of the basis (2.2), noting the following points

1. All operators on *different* atoms commute e.g. $[S_1^x, S_2^y] = 0$.
2. S_1 operators act only on the first spin, and have no effect on the second

$$e.g. \quad S_1^+|--\rangle = |+-\rangle,$$

and likewise S_2 operators act only on the second spin.

First consider $S_1^zS_2^z$ operating on each basis state:

$$\begin{aligned} S_1^zS_2^z|++\rangle &= \frac{1}{2}\cdot\frac{1}{2}|++\rangle \quad = \quad \frac{1}{4}|++\rangle\\ S_1^zS_2^z|+-\rangle &= -\frac{1}{4}|+-\rangle\\ S_1^zS_2^z|-+\rangle &= -\frac{1}{4}|-+\rangle\\ S_1^zS_2^z|--\rangle &= +\frac{1}{4}|--\rangle. \end{aligned}$$

Now consider $S_1^+S_2^-$ and $S_1^-S_2^+$ operating on each basis state, noting that $S_1^+|++\rangle = 0$ since S_1^+ acts on $|+\rangle_1$ etc.:

$$\begin{aligned} S_1^+S_2^-|+-\rangle &= 0\\ S_1^+S_2^-|-+\rangle &= |+-\rangle\\ S_1^+S_2^-|--\rangle &= 0\\ S_1^-S_2^+|++\rangle &= 0\\ S_1^-S_2^+|+-\rangle &= |-+\rangle\\ S_1^-S_2^+|-+\rangle &= S_1^-S_2^+|--\rangle = 0 \end{aligned}$$

Using these together with (2.3) we get

$$\begin{aligned}
\mathcal{H}|++\rangle &= \frac{1}{4}J|++\rangle \\
\mathcal{H}|+-\rangle &= -\frac{1}{4}J|+-\rangle + \frac{1}{2}J|-+\rangle \\
\mathcal{H}|-+\rangle &= -\frac{1}{4}J|-+\rangle + \frac{1}{2}J|+-\rangle \\
\mathcal{H}|--\rangle &= \frac{1}{4}J|--\rangle,
\end{aligned}$$

which means that in matrix form, labelling the rows with the basis states

$$\mathcal{H} = J \begin{array}{cc} \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} & \begin{array}{c} |++\rangle \\ |+-\rangle \\ |-+\rangle \\ |--\rangle \end{array} \end{array}$$

The eigenvalues of this matrix are easily obtained (omitting J for clarity in the working)

$$\begin{vmatrix} \frac{1}{4} - E & 0 & 0 & 0 \\ 0 & -\frac{1}{4} - E & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} - E & 0 \\ 0 & 0 & 0 & \frac{1}{4} - E \end{vmatrix} = 0$$

$$\left(\frac{1}{4} - E\right)^2 \begin{vmatrix} -\frac{1}{4} - E & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{4} - E \end{vmatrix} = 0$$

$$\left(\frac{1}{4} - E\right)^2 \left[\left(\frac{1}{4} + E\right)^2 - \frac{1}{4}\right] = 0$$

$$\left(\frac{1}{4} - E\right)^2 \left[\left(\frac{1}{4} + E\right) + \frac{1}{2}\right]\left[\left(\frac{1}{4} + E\right) - \frac{1}{2}\right] = 0$$

giving $E = \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, -\frac{3}{4}$.

Thus, after restoring J, the eigenvalues are $E = \dfrac{J}{4}$ (3 times) and $-\dfrac{3J}{4}$. The first three of these form a triplet and the last one a singlet.

The maximum eigenvalue here, $\frac{J}{4}$, is the same as in the classical case, but the minimum eigenvalue, $-\frac{3J}{4}$, is much lower. This is clearly a new quantum effect.

Now let us consider the corresponding eigenstates. Since the three eigenvalues $\left(\frac{J}{4}\right)$ are degenerate the choice of corresponding eigenvectors is somewhat arbitrary. It is easy to verify that the following is a suitable orthonormal set.

$$\psi_1 \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \psi_2 \equiv \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \quad \psi_3 \equiv \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \psi_4 \equiv \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$$

the first three having eigenvalue $\frac{J}{4}$ and ψ_4 having eigenvalue $-\frac{3J}{4}$.

2.4 Commutators and Quantum Numbers

The commutation relations between the operators S^z, S^+ and S^- follow from those between S^x, S^y and S^z. From the definitions of $S^+ \equiv S^x + iS^y$ and $S^- \equiv S^x - iS^y$ we have

$$\begin{aligned} [S^z, S^+] &= [S^z, S^x] + i[S^z, S^y] \\ &= i\hbar S^y + i(-i\hbar S^x) \\ &= \hbar S^+ = S^+ \text{ (putting } \hbar = 1 \text{ again).} \end{aligned}$$

Similarly $[S^z, S^-] = -S^-$,
and $[S^-, S^+] = -i[S^y, S^x] + i[S^x, S^y] = -2S^z$.

For the interacting pair of spins the operator

$$S^z_T = S^z_1 + S^z_2$$

gives the z-component of total angular momentum of the pair.

Clearly $[S^z_T, S^z_1 S^z_2] = 0$ since only S^z_1 and S^z_2 are involved. Also

$$\begin{aligned} [S^z_T, S^+_1 S^-_2] &= [S^z_1, S^+_1 S^-_2] + [S^z_2, S^+_1 S^-_2] \\ &= [S^z_1, S^+_1]S^-_2 + S^+_1[S^z_2, S^-_2] \\ &= S^+_1 S^-_2 + S^+_1(-S^-_2) \quad = \quad 0, \end{aligned}$$

and similarly $[S^z_T, S^-_1 S^+_2] = 0$.

This means that S^z_T commutes with *each* term in Hamiltonian (2.3), so S^z_T is a good quantum number. In fact the basis states have the property

$$
\begin{aligned}
S_T^z|++\rangle &= \left(\frac{1}{2}+\frac{1}{2}\right)|++\rangle \;=\; |++\rangle\\
S_T^z|+-\rangle &= \left(\frac{1}{2}-\frac{1}{2}\right)|+-\rangle \;=\; 0\\
S_T^z|-+\rangle &= 0\\
S_T^z|--\rangle &= -|--\rangle
\end{aligned}
$$

so the eigenstates $\psi_1,\ \psi_2,\ \psi_3$ and ψ_4 have the properties that

$$S_T^z\psi_1 = \psi_1, \quad S_T^z\psi_2 = 0, \quad S_T^z\psi_3 = -\psi_3 \quad \text{and } S_T^z\psi_4 = 0.$$

ψ_2 and ψ_4 have eigenvalue 0 of S_T^z while ψ_1 has eigenvalue 1 and ψ_3 eigenvalue -1.

For Heisenberg exchange we also have one additional property. The Hamiltonian (2.3) is

$$\mathcal{H} = J\mathbf{S}_1 \cdot \mathbf{S}_2$$

which is obviously isotropic and does not distinguish between $x,\ y,\ z$. Since we know that $[S_T^z, \mathcal{H}] = 0$ it follows that $[S_T^x, \mathcal{H}] = 0$ and $[S_T^y, \mathcal{H}] = 0$ also.

If two operators commute it is possible to find states which are eigenstates of both simultaneously. Since $[S_T^x, S_T^z] \neq 0$ we can find states which are eigenstates of $\mathcal{H}$ and also of S_T^z as we have done and we could find (different) states which are eigenstates of $\mathcal{H}$ and also of S_T^x. However it is not possible to find states which are eigenstates of both S_T^x and S_T^z.

The total spin angular momentum is given by

$$
\begin{aligned}
\mathbf{S}_T &= \mathbf{S}_1 + \mathbf{S}_2\\
\text{so }\ \mathbf{S}_T^2 &= (\mathbf{S}_1 + \mathbf{S}_2)^2 = S_T^{x^2} + S_T^{y^2} + S_T^{z^2}.
\end{aligned}
$$

Since $\mathcal{H}$ commutes with all of S_T^x, S_T^y and S_T^z it follows that $[\mathbf{S}_T^2, \mathcal{H}] = 0$ also. The eigenstates $\{\psi_1, \psi_2, \psi_3, \psi_4\}$ are simultaneously eigenstates of $\mathcal{H}$, S_T^z and $\mathbf{S}_T^2$.

It may be easily verified that the corresponding eigenvalues of the operator $\mathbf{S}_T^2$ are given by

$$
\begin{aligned}
\mathbf{S}_T^2\psi_1 &= 2\psi_1\\
\mathbf{S}_T^2\psi_2 &= 2\psi_2\\
\mathbf{S}_T^2\psi_3 &= 2\psi_3\\
\mathbf{S}_T^2\psi_4 &= 0.
\end{aligned}
$$

Hence the three triplet states ψ_1, ψ_2, ψ_3 have total angular momentum quantum number $\ell = 1$, i.e. $\mathbf{S}_T^2\psi_1 = \ell(\ell+1)\psi_1$ with $\ell = 1$, while the singlet state ψ_4 has $\ell = 0$.

2.5 Physical Picture

A simple physical picture of this situation is as follows. Combining two spin-$\frac{1}{2}$ atoms, we can form either a 'spin-1' configuration or a 'spin-0' configuration. The 'spin-1' configuration can have 3 possible 'orientations', i.e. values of z component, giving

state	explicit form	'picture'	S_T	S_T^z	E	
ψ_1	$\vert{+}{+}\rangle$	$\uparrow\uparrow$	1	1	$J/4$	triplet
ψ_2	$\frac{1}{\sqrt{2}}(\vert{+}{-}\rangle + \vert{-}{+}\rangle)$	$\rightarrow\rightarrow$	1	0	$J/4$	
ψ_3	$\vert{-}{-}\rangle$	$\downarrow\downarrow$	1	-1	$J/4$	
ψ_4	$\frac{1}{\sqrt{2}}(\vert{+}{-}\rangle - \vert{-}{+}\rangle)$	$\uparrow\downarrow$	0	0	$-3J/4$	singlet

The three triplet states have the two spins parallel. This is called a *ferromagnetic* arrangement since the magnetic moments will also be parallel.

The singlet ψ_4 is a 'spin-0' configuration which has no 'orientation'. This state has antiparallel spins and is an *antiferromagnetic* arrangement.

It follows that if J is positive then the ground state is antiferromagnetic, but if J is negative then the ground state is ferromagnetic. This agrees with the classical picture, but the actual values of the energy are not the same as in the classical case.

2.6 Infinite Arrays of Spins

A magnetic crystal consists of a large number, N, of magnetic atoms in a regular array. Each atom has a 'spin' and associated magnetic moment. If the spins (and moments) are all aligned in the same direction we have a *ferromagnet* with a large net magnetic moment. Other possible configurations in the absence of a magnetic field are

disordered (random alignment) ⟶ paramagnet
alternating up and down ⟶ antiferromagnet

If a small magnetic field is applied to a paramagnet then the ordering will still be largely random but with a tendency to align in the opposite direction to the applied field.

The most important case in practice is the limit $N \to \infty$, called the *thermodynamic limit*. At any non-zero temperature, thermal fluctuations will tend to reduce the perfect alignment in a ferromagnet or antiferromagnet. However, there may still be a net alignment up to some critical temperature T_C above which the system is paramagnetic. This critical temperature is called the Curie temperature for a ferromagnet, and the Néel temperature, usually written as T_N, for an antiferromagnet (Fig. 2.1).

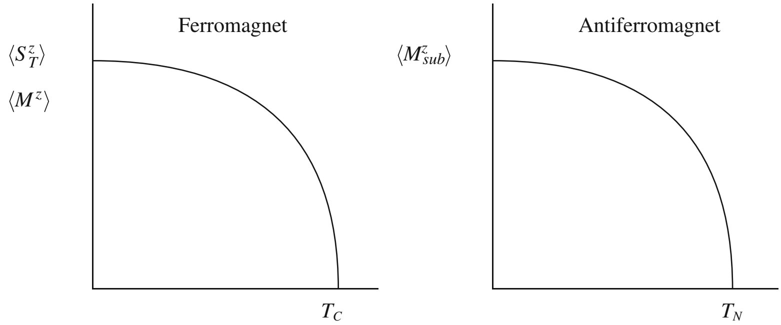


Fig. 2.1 Magnetisation of a ferromagnet and sublattice magnetisation of an antiferromagnet as a function of temperature. Note that the total magnetisation $\langle M^z \rangle$ is always zero for the antiferromagnet

In one dimension (1D) and two dimensions (2D) the critical temperature T_C or T_N is zero, i.e. $\langle M^z \rangle = 0$ or $\langle M^z_{\text{sub}} \rangle = 0$ for $T > 0$, where $M^z = g\beta S_T^z$ is the magnetisation, but at $T = 0$ we may still have ferromagnetic or antiferromagnetic ordering. In addition in 2D there occurs a more subtle type of ordering at non-zero temperatures known as the Kosterlitz–Thouless transition [2].

As we discussed earlier, the reason why atoms try to align parallel (or anti-parallel) is because of the interaction between them. Although this could be a magnetic dipole interaction, in practice it is usually an exchange interaction which is quantum mechanical in origin and derives from the electric Coulomb force between electrons and hence is much stronger than the magnetic dipole interaction.

Depending on the types of atom involved and the environment in which they exist the exchange interaction may have different forms. Examples are:

a. Heisenberg $J\,\mathbf{S}_1 \cdot \mathbf{S}_2$ (as before)
b. Ising $J S_1^z S_2^z$
c. Anisotropic (a combination of the above)

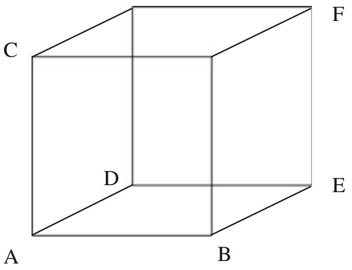
$$J[\Delta S_1^z S_2^z + (S_1^x S_2^x + S_1^y S_2^y)]$$

d. Biquadratic $J(\mathbf{S}_1 \cdot \mathbf{S}_2)^2$

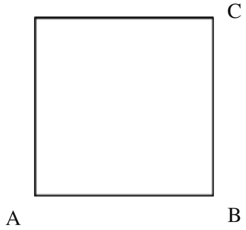
In addition there may be other terms in the Hamiltonian which are not interactions, but involve individual spins e.g. crystal field terms, typically of the form $A(S_1^z)^2$, or external magnetic field terms of the form HS_1^z.

A magnetic crystal consists of a large array with many (N) atoms. However, the exchange interaction is normally very short range. A simple approximation, but one that is accurate for many crystals, is to assume that only nearest-neighbours in the array interact. The simplest types of array are

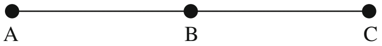
3D Simple cubic. A interacts with B, C and D but not with E or F.



2D Square. A interacts with B but not with C.



1D Chain. A interacts with B but not with C.



The differences between quantum mechanical and classical behaviour are most marked for low values of spin and for low dimensions. For these reasons, and also because it is the most tractable mathematically, we shall study first the 1D chain of spin-$\frac{1}{2}$ atoms interacting with nearest neighbour Heisenberg exchange.

2.7 1D Heisenberg Chain with $S = \frac{1}{2}$ and Nearest-Neighbour Interaction

Since this is a 1D system the ferromagnetic or antiferromagnetic ordering only occurs at zero temperature but as well as being simpler to handle than non-zero T it is arguably more interesting.

The details of how this chain is treated quantum mechanically is the subject of the next chapters. Here we simply set the stage by giving some simple classical results.

The mathematics is simplified if we use periodic boundary conditions. This means that the ends of the chain are joined so that the N'th atom is a nearest-neighbour of the first as well as of the $(N-1)$'th. Of course the chain is not actually curved to achieve this: it is purely a mathematical device which ensures that there are no ‘ends’ to worry about. In any case, we shall take the limit $N \to \infty$, so any curvature would tend to zero.

The Hamiltonian for the system is

$$\begin{aligned}\mathcal{H} &= J[\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \ldots + \mathbf{S}_N \cdot \mathbf{S}_1] \\ &= J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \quad \text{where } i + N \equiv i \end{aligned} \tag{2.4}$$

Since the interaction is nearest-neighbour only, the classical solution of (2.4) is very similar to the case of just two spins.

If $J < 0$ the lowest energy of a pair of spins occurs when they are aligned parallel, i.e. in the same direction. This can be achieved for every pair simultaneously if *all* the spins point in the same direction:

$$\cdots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \cdots$$

which is clearly a *ferromagnetic* arrangement. In this case the energy is $E = NJS^2 = \frac{1}{4}NJ$ which is negative.

If $J > 0$ the lowest energy of a pair is when they are antiparallel. Provided N is even this can be achieved for all pairs on the chain by alternating:

$$\cdots \underset{N-1}{\uparrow} \; \underset{N}{\downarrow} \; \underset{1}{\uparrow} \underset{2}{\downarrow} \underset{3}{\uparrow} \underset{4}{\downarrow} \uparrow \downarrow \cdots$$

which is an *anti*ferromagnetic arrangement. The energy is $E = -NJS^2 = -\frac{1}{4}NJ$.

Since each nearest-neighbour pair has its minimum energy configuration this arrangement minimises the overall energy and any other arrangement of the atoms would have higher energy.

Notice that rotation of *all* the spins by same amount does not affect the classical energy, i.e.

$$\ldots \nearrow \nearrow \nearrow \nearrow \nearrow \ldots \text{ or } \ldots \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \ldots$$

have the same energy as $\ldots \uparrow \uparrow \uparrow \uparrow \uparrow \ldots$ for the ferromagnetic arrangement. Similarly the antiferromagnetic arrangement can be rotated without changing the overall (classical) energy.

References

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