Chapter 3
Quantum Treatment of the Spin-$\frac{1}{2}$ Chain

Abstract For the spin-1/2 linear chain the simplest state is the fully aligned state, which is the ground state if the interaction is ferromagnetic. The ground state energy is easily calculated. The elementary excitations are states in which the spin of one atom is reversed, although the actual states are linear combinations of many of these states. Again the energies can be calculated exactly. For antiferromagnetic coupling these states, along with the aligned state, are still eigenstates albeit of much higher in energy than the actual ground state. Much information can also be obtained from a detailed study of the states with two reversals. Using these results it is possible to gradually increase the number of such reversals and still obtain exact eigenstates. This is the fundamental idea of the Bethe Ansatz, which is described in detail. When exactly half the atoms are reversed then the true antiferromagnetic ground state is obtained.

3.1 General Remarks

In the previous chapter we obtained some results using a classical treatment of the spin chain with the Hamiltonian Eq. (2.4). In this chapter we give a quantum mechanical treatment and obtain many more results, some of which have classical analogues which were not given there.

As a first step we construct a basis for the N spin-$\frac{1}{2}$ atoms. For a single atom a basis consists of the two states $\{|+\rangle, |-\rangle\}$. For the complete chain a basis would be all states of form

$$|\underset{1}{+}\underset{2}{+}\underset{3}{-}\underset{4}{-}\underset{5}{+}--+----++\ldots\rangle$$

where the spin of each atom may be $+$ or $-$. Clearly the number of states in the basis is 2^N which is very large. We can now proceed to find the eigenstates of Eq. (2.4) using this basis.

First rewrite Eq. (2.4) as

$$\mathcal{H} = J\sum_{i=1}^{N}\left[S_i^z S_{i+1}^z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)\right]. \tag{3.1}$$

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As before, we define the total z component as

$$S_T^z = \sum_j S_j^z .$$

Now clearly $[S_T^z, S_i^z S_{i+1}^z] = 0$ since only S^z operators are involved.

$$\begin{aligned}
\text{Also}\qquad [S_T^z, S_i^+ S_{i+1}^-] =&\ S_i^+ [S_T^z, S_{i+1}^-] + [S_T^z, S_i^+] S_{i+1}^- \\
=&\ S_i^+ [S_{i+1}^z, S_{i+1}^-] + [S_i^z, S_i^+] S_{i+1}^- \\
=&\ S_i^+ (-S_{i+1}^-) + S_i^+ S_{i+1}^- \ = \ 0
\end{aligned}$$

and similarly $[S_T^z, S_i^- S_{i+1}^+] = 0$. Hence S_T^z commutes with each term in $\mathcal{H}$ so

$$[S_T^z, \mathcal{H}] = 0 .$$

This result is the same as in the two spin case and again we can choose the eigenstates of $\mathcal{H}$ to be eigenstates of S_T^z also.

Also, just as in the two spin case, because the Heisenberg exchange interaction is isotropic, it follows that if we define S_T^x and S_T^y similarly, each of these will also commute with $\mathcal{H}$. (This will not be true for other types of interaction.) Therefore the square of the total angular momentum (or spin)

$$\mathbf{S}_T^2 \equiv S_T^{x^2} + S_T^{y^2} + S_T^{z^2}$$

also commutes with $\mathcal{H}$. For example $[\mathbf{S}_T^2, \mathcal{H}] = 0$.

Hence for the Heisenberg Hamiltonian we can choose the eigenstates of $\mathcal{H}$ to be simultaneously eigenstates of $\mathbf{S}_T^2$ and any one of S_T^z, S_T^x or S_T^y. They cannot be eigenstates of all four operators since none of S_T^z, S_T^x or S_T^y commutes with each other. In practice we always choose them to be simultaneous eigenstates of $\mathbf{S}_T^2$ and S_T^z.

3.2 Aligned State

There is only one state in the basis with $S_T^z = N\frac{1}{2}$ namely the aligned state

$$|A\rangle \ \equiv \ |+++\cdots+++\rangle$$

which has all spins up. It follows that this must be an eigenstate of $\mathcal{H}$. ($\mathcal{H}$ commutes with S_T^z so there is no coupling to states with different S_T^z). In fact we can see this clearly by calculating

$$\mathcal{H}|A\rangle = J\sum_i \left[S_i^z S_{i+1}^z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)\right]|A\rangle \tag{3.2}$$

First note that $S_i^z|A\rangle = \frac{1}{2}|A\rangle$ since the ith atom is $|+\rangle$, and so $S_i^z S_{i+1}^z|A\rangle = \frac{1}{4}|A\rangle$.

Also $S_i^+|A\rangle = 0$ since the ith atom is in the state $|+\rangle$ and $S_{i+1}^+|A\rangle = 0$ since the $(i+1)$th atom is also in the state $|+\rangle$. Therefore, $S_i^+ S_{i+1}^-|A\rangle = 0$ and $S_i^- S_{i+1}^+|A\rangle = 0$. Thus,

$$\mathcal{H}|A\rangle = J\sum_i \left[\frac{1}{4}|A\rangle + 0|A\rangle\right] = \frac{JN}{4}|A\rangle.$$

This proves that the aligned state $|A\rangle$ is an eigenstate of $\mathcal{H}$ with eigenvalue $\frac{NJ}{4}$. It is useful to define $E_A \equiv \frac{NJ}{4}$, the energy eigenvalue of the aligned state.

If J is negative this is the actual ground state, and since all the atoms are parallel (‘up’) it is ferromagnetic. The eigenvalue E_A is the ground state energy of the system and it is exactly the same as in the classical case. It is important to notice that the ground state is highly degenerate. The same arguments show that the state with all atoms ‘down’ is also an eigenstate with eigenvalue E_A. In fact there is an eigenstate with this eigenvalue for *every* value of S_T^z, and this corresponds to the rotation without change of energy that we saw in the classical case.

If J is positive then $|A\rangle$ is actually the state of highest energy. It is still a valid eigenstate but obviously not the ground state. In fact as we shall see later the ground state is very complicated but is truly antiferromagnetic.

3.3 Single Deviation States

Now consider states with $S_T^z = \frac{N}{2} - 1$, i.e. one deviation from the aligned state. In the basis there are N states with a single spin in the $|-\rangle$ state. These are

$$\begin{aligned} |-++++\ldots++\rangle &\equiv |1\rangle \\ |+-+++\ldots++\rangle &\equiv |2\rangle \\ |++-++\ldots++\rangle &\equiv |3\rangle \quad \text{etc.} \end{aligned}$$

When we change a spin from $|+\rangle$ to $|-\rangle$ the value of S^z for that spin changes from $+\frac{1}{2}$ to $-\frac{1}{2}$, so the change is -1. Hence each of the above states has $S_T^z = \frac{N}{2} - 1$. There are no other states in the basis with this value of S_T^z.

Consider one of these states

$$|j\rangle \equiv |+++\ldots+\underset{\substack{\uparrow \\ j\text{th site}}}{-}+\ldots++\rangle$$

and act upon it by terms in $\mathcal{H}$ given by Eq. (3.1).

$$\begin{aligned} S_i^z S_{i+1}^z |j\rangle &= \frac{1}{4}|j\rangle \quad \text{if } j \neq i,\ i+1 \\ &= -\frac{1}{4}|j\rangle \quad \text{if } j = i,\ i+1\,. \end{aligned}$$

In $\sum_i S_i^z S_{i+1}^z$ there are two terms in which $i = j$ or $i+1 = j$, all the others ($N-2$ of these) satisfy the first condition. Hence

$$\sum_i S_i^z S_{i+1}^z |j\rangle \;=\; \left[(N-2)\frac{1}{4} + 2\left(-\frac{1}{4}\right)\right]|j\rangle \;=\; \left(\frac{N}{4} - 1\right)|j\rangle.$$

Now consider the effect of operator $S_i^+ S_{i+1}^-$ on $|j\rangle$.

$$S_i^+ S_{i+1}^- |j\rangle \;=\; 0 \quad \text{unless } i = j \quad \text{since only the } j\text{th spin is ‘down’}$$

If $i = j$ then

$$\begin{aligned} S_j^+ S_{j+1}^- |j\rangle &= S_j^+ S_{j+1}^- |++\ldots+\underset{j}{-}+\ldots+\rangle \\ &= S_{j+1}^- |++\ldots+\underset{j}{+}+\ldots+\rangle \\ &= |++\ldots++\underset{j+1}{-}\ldots+\rangle = |j+1\rangle. \end{aligned}$$

Therefore $\sum_i S_i^+ S_{i+1}^- |j\rangle \;=\; |j+1\rangle$.

Similarly

$$\sum_i S_i^- S_{i+1}^+ |j\rangle = |j-1\rangle. \quad \text{(Coming from the term with } i+1 = j\text{)}$$

Hence, using Eq. (3.1)

$$\begin{aligned} \mathcal{H}|j\rangle &= J\left[\left(\frac{N}{4} - 1\right)|j\rangle + \frac{1}{2}|j-1\rangle + \frac{1}{2}|j+1\rangle\right] \\ &= E_A|j\rangle + J\left[\frac{1}{2}|j-1\rangle + \frac{1}{2}|j+1\rangle - |j\rangle\right]. \end{aligned} \tag{3.3}$$

A true eigenstate state of $\mathcal{H}$ is constructed as a linear combination of the $|j\rangle$ by putting

$$\psi = \sum_j f_j |j\rangle \tag{3.4}$$

where the f_j are coefficients. The Schrödinger equation is

$$\mathcal{H}\psi = E\psi$$

and therefore

$$\sum_j f_j \mathcal{H}|j\rangle = E \sum_j f_j |j\rangle$$

$$\sum_j f_j E_A |j\rangle + \sum_j f_j J \left[\frac{1}{2}|j-1\rangle + \frac{1}{2}|j+1\rangle - |j\rangle\right] = E \sum_j f_j |j\rangle.$$

Now operate on the left by $\langle \ell|$. Since the basis is orthonormal

$$\langle \ell | j\rangle = \delta_{\ell j} \quad \text{etc.}$$

and therefore

$$J\left[\frac{1}{2} f_{\ell+1} + \frac{1}{2} f_{\ell-1} - f_\ell\right] \;=\; (E - E_A) f_\ell \;=\; \varepsilon f_\ell, \tag{3.5}$$

where $\varepsilon \;=\; E - E_A$ is the energy difference between this state and the aligned state.

This is a simple difference equation for the f_ℓ. The solutions have the form of plane waves

$$f_\ell = c_k e^{ik\ell} \qquad (c_k \text{ constant}) \tag{3.6}$$

as can be seen by substituting in Eq. (3.5):

$$J\left[\frac{1}{2} c_k e^{ik(\ell+1)} + \frac{1}{2} c_k e^{ik(\ell-1)} - c_k e^{ik\ell}\right] = \varepsilon_k c_k e^{ik\ell}$$

where ε_k is the value of ε associated with k. Dividing by $c_k e^{ik\ell}$

$$J\left[\frac{1}{2} e^{ik} + \frac{1}{2} e^{-ik} - 1\right] \;=\; \varepsilon_k$$

$$\text{and so} \qquad \varepsilon_k \;=\; J(\cos k - 1). \tag{3.7}$$

Clearly we have solutions of (3.5) with the form (3.6) for any value of k. However, site $\ell + N$ is the same as site ℓ because of the periodic boundary conditions, and therefore

$$f_{\ell+N} = f_\ell.$$

Using (3.6) $c_k e^{ik(\ell+N)} = c_k e^{ik\ell}$
so $e^{ikN} = 1 = e^{i2\pi\lambda}$ where λ is an integer.
It follows that k is given by

$$k = \lambda \frac{2\pi}{N} \quad \text{with} \quad 0 \le \lambda \le N-1\,.$$

There are N different eigenstates of this form corresponding to the N possible values of λ.

In summary we have found that eigenstates with $S_T^z = \frac{N}{2} - 1$ (i.e. with 1 net deviation from the aligned state) have the form

$$\psi_k = c_k \sum_\ell e^{ik\ell} |\ell\rangle \quad \text{where} \quad k = \lambda \frac{2\pi}{N}$$

with λ an integer, and the corresponding eigenvalue is $\varepsilon_k = J(\cos k - 1)$. c_k is an arbitrary constant. Normalising the eigenstates by putting $\langle \psi_k | \psi_k \rangle = 1$ gives $c_k = \dfrac{1}{\sqrt{N}}$.

If J is negative then the ground state is the aligned ferromagnetic state and these states are the *elementary excitations* and are called 'spin-waves' or 'magnons'. The excitation energy ε_k is given by

$$\varepsilon_k = -J(1 - \cos k)$$

and since J is negative

$$\varepsilon_k = |J|(1 - \cos k) \quad \text{which is shown in Fig. 3.1}$$

The parameter k is often called a wave-vector even though in 1D it is a 'one-component vector', effectively a scalar.

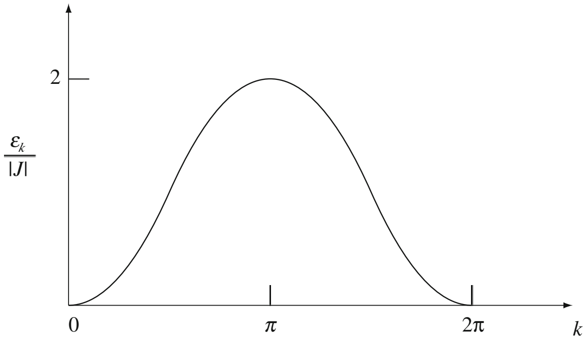

Fig. 3.1 Spectrum of elementary excitations (spin waves) of the 1D spin-$\frac{1}{2}$ chain with ferromagnetic isotropic nearest-neighbour Heisenberg exchange

3.4 Two Deviation States

Now consider states with $S^z_T = \frac{N}{2} - 2$, i.e. two deviations from the aligned state. As we shall see the eigenstates have the form of two spin waves which interact with each other. Sometimes the interaction is small and the energies of the spin waves are only slightly perturbed from those of free spin waves, together with small shifts in the k-vectors. In other cases the interaction is strong leading to a new type of state known as a bound state.

In the basis there are $\frac{N(N-1)}{2}$ states with two '−' spins. For example

$$|\underset{1}{-}\underset{2}{-}++++\cdots+\rangle \equiv |12\rangle$$

$$|\cdots+\underset{j_1}{-}+++\cdots+\underset{j_2}{-}+\ldots\rangle \equiv |j_1 j_2\rangle$$

Clearly $|j_1 j_2\rangle \equiv |j_2 j_1\rangle$ so to avoid overcounting we insist that $j_2 > j_1$. Note $j_2 \neq j_1$ since if we try to lower S^z for a spin-$\frac{1}{2}$ which is already in a '−' state we get 0 :

$$S^-_{j_1}|+\rangle = |-\rangle$$
$$(S^-_{j_1})^2|+\rangle = S^-_{j_1}|-\rangle = 0.$$

Now act on the basis states with the terms in $\mathcal{H}$.
Firstly consider $S^z_i S^z_{i+1}|j_1 j_2\rangle$:

a. $S^z_i S^z_{i+1}|j_1 j_2\rangle = \frac{1}{4}|j_1 j_2\rangle$ provided $j_1 \neq i, i+1$ and $j_2 \neq i, i+1$, i.e. neither of i nor $i+1$ is '−'.

b. $S^z_i S^z_{i+1}|j_1 j_2\rangle = -\frac{1}{4}|j_1 j_2\rangle$ if $i = j_1$ and $i+1 \neq j_2$ or if $i \neq j_1$ and $i+1 = j_2$, i.e. one of $i, i+1$ is '−' but not both.

c. $S^z_i S^z_{i+1}|j_1 j_2\rangle = \frac{1}{4}|j_1 j_2\rangle$ if $i = j_1$ and $i+1 = j_2$, i.e. both i and $i+1$ are '−'.

There are thus two distinct cases after summing over i :

(a) j_1, j_2 adjacent i.e. $j_2 = j_1 + 1$ e.g. $|++\cdots+--+\ldots\rangle$ then

$$\sum_i S^z_i S^z_{i+1}|j_1 j_1+1\rangle$$
$$= \left[(N-3)\frac{1}{4} + 2\left(-\frac{1}{4}\right) + 1\left(\frac{1}{4}\right)\right]|j_1 j_1+1\rangle$$

where the first term comes from the case with $i, i+1$ both '+', the second from the case with one '+' and the other '−' and the third term from the case with both '−'. Hence

$$\sum_i S_i^z S_{i+1}^z |j_1 j_1+1\rangle \;=\; \left(\frac{N}{4}-1\right)|j_1 j_1+1\rangle.$$

(b) j_2 not adjacent to j_1 $|++-++\cdots++-++\rangle$

$$\sum_i S_i^z S_{i+1}^z |j_1 j_2\rangle$$
$$= \left[(N-4)\frac{1}{4}+4\left(-\frac{1}{4}\right)\right]|j_1 j_2\rangle \;=\; \left(\frac{N}{4}-2\right)|j_1 j_2\rangle.$$

Now consider

$$S_i^+ S_{i+1}^- |j_1 j_2\rangle$$

This will be 0 unless $i = j_1$ or j_2. It will also be 0 if $i+1 = j_1$ or j_2.

Again after summing over i there are two distinct cases:

(a) j_1, j_2 adjacent

$$\sum_i S_i^+ S_{i+1}^- |j_1 j_1+1\rangle \;=\; |j_1 j_1+2\rangle,$$

only one term in the sum giving a non-zero result.

(b) j_1, j_2 not adjacent

$$\sum_i S_i^+ S_{i+1}^- |j_1 j_2\rangle \;=\; |j_1+1, j_2\rangle + |j_1 j_2+1\rangle,$$

thus two terms giving non-zero results.

Similarly

$$\begin{aligned}\sum_i S_i^- S_{i+1}^+ |j_1 j_2\rangle &= |j_1-1, j_1+1\rangle \quad \text{if } j_2 = j_1+1\\ &= |j_1-1, j_2\rangle + |j_1, j_2-1\rangle \quad \text{otherwise.}\end{aligned}$$

Hence, if $j_2 \neq j_1 + 1$ (and $j_1 \neq 1,\ j_2 \neq N$, due to periodic boundary conditions) then

$$\begin{aligned}\mathcal{H}|j_1 j_2\rangle = J\Big(\frac{N}{4} - 2\Big)|j_1 j_2\rangle \\ +\frac{J}{2}\Big(|j_1 - 1, j_2\rangle + |j_1 + 1, j_2\rangle + |j_1, j_2 - 1\rangle + |j_1, j_2 + 1\rangle\Big),\end{aligned}$$

while, if $j_2 = j_1 + 1$ (or $j_1 = 1$ and $j_2 = N$, again due to periodic boundary conditions) then

$$\mathcal{H}|j_1 j_1 + 1\rangle = J\Big(\frac{N}{4} - 1\Big)|j_1 j_1 + 1\rangle + \frac{J}{2}\Big(|j_1 - 1, j_1 + 1\rangle + |j_1, j_1 + 2\rangle\Big).$$

The actual eigenstate is a linear combination of the form

$$\psi = \sum_{j_1 j_2} f_{j_1 j_2}|j_1 j_2\rangle \qquad j_2 > j_1\,,$$

so the Schrödinger equation $\mathcal{H}\psi = E\psi$ gives

$$\sum_{j_1=1}^{N-1}\sum_{j_2=j_1+1}^{N} f_{j_1 j_2}\mathcal{H}|j_1 j_2\rangle \;=\; \sum_{j_1}\sum_{j_2} f_{j_1 j_2}E|j_1 j_2\rangle.$$

Multiplying on the left by $\langle \ell_1 \ell_2|$ and using

$$\begin{aligned}\langle \ell_1 \ell_2 | j_1 j_2\rangle &= \delta_{\ell_1 j_1}\delta_{\ell_2 j_2} \\ \langle \ell_1 \ell_2 | j_1 - 1\, j_2\rangle &= \delta_{\ell_1 j_1 - 1}\delta_{\ell_2 j_2} \qquad \text{etc.}\end{aligned}$$

gives eventually two equations

$$(E_A - E - 2J)f_{\ell_1\ell_2} + \frac{J}{2}\Big(f_{\ell_1-1\ell_2} + f_{\ell_1+1\ell_2} + f_{\ell_1\ell_2-1} + f_{\ell_1\ell_2+1}\Big) \;=\; 0 \qquad (3.8)$$

provided $\ell_2 \neq \ell_1 + 1$, and

$$(E_A - E - J)f_{\ell_1\ell_1+1} + \frac{J}{2}\Big(f_{\ell_1-1\ell_1+1} + f_{\ell_1\ell_1+2}\Big) \;=\; 0\,. \qquad (3.9)$$

Equation (3.9) acts as a sort of ‘boundary condition’ to (3.8). It differs from (3.8) in that there are only two ‘incorrect’ bonds (i.e. of the form $+-$ or $-+$ rather than $++$) instead of four giving J instead of $2J$ in the first term. Furthermore, terms where the lowering operator acts twice at the same site are missing, as these cannot occur for spin$-\frac{1}{2}$.

Again these are difference equations and we can easily find a solution of (3.8) of the form

$$f_{\ell_1,\ell_2} = e^{ik_1\ell_1}e^{ik_2\ell_2} \tag{3.10}$$

Proof After substituting (3.10) into (3.8) and then dividing by $e^{ik_1\ell_1}e^{ik_2\ell_2}$ we get

$$(-\varepsilon - 2J) + \frac{J}{2}\Big(e^{-ik_1} + e^{ik_1} + e^{-ik_2} + e^{ik_2}\Big) = 0$$

where $\varepsilon \equiv E - E_A$. Therefore

$$\varepsilon = J(\cos k_1 + \cos k_2 - 2) \tag{3.11}$$

Provided this is satisfied then f_{ℓ_1,ℓ_2} as given is a solution. Note that this solution has an energy ε which consists of sum of two energies of same form as for a single deviation state $\varepsilon_k = J(\cos k - 1)$. However, as we shall see, the values of k_1, k_2 are not the same as the values which occur in ε_k.

We must still satisfy the 'boundary condition' Eq. (3.9). For a given value of ε given by (3.11), then clearly both

$$f_{\ell_1,\ell_2} = e^{ik_1\ell_1}e^{ik_2\ell_2}$$

and

$$f'_{\ell_1,\ell_2} = e^{ik_2\ell_1}e^{ik_1\ell_2}$$

satisfy (3.8). The most general solution of (3.8) is thus

$$f_{\ell_1,\ell_2} = c_1 e^{ik_1\ell_1}e^{ik_2\ell_2} + c_2 e^{ik_2\ell_1}e^{ik_1\ell_2}. \tag{3.12}$$

Only the ratio of c_1 and c_2 is important as the absolute values can be determined by normalisation. Put $\frac{c_1}{c_2} = e^{i\phi}$ (we allow ϕ to be complex so there is no loss of generality here) and then write

$$f_{\ell_1,\ell_2} = C\Big(e^{ik_1\ell_1}e^{ik_2\ell_2}e^{i\phi/2} + e^{ik_1\ell_2}e^{ik_2\ell_1}e^{-i\phi/2}\Big) \tag{3.13}$$

where C is an overall normalisation constant.

Substituting this into (3.9), then, after dividing by $Ce^{ik_1\ell_1}e^{ik_2\ell_1}e^{-i\phi/2}$, we get

$$(-\varepsilon - J)\Big(e^{ik_2}e^{i\phi} + e^{ik_1}\Big) + \frac{J}{2}\Big(e^{-ik_1}e^{ik_2}e^{i\phi} + e^{-ik_2}e^{ik_1} + e^{i2k_2}e^{i\phi} + e^{i2k_1}\Big) = 0.$$

It is convenient to introduce $x_1 = e^{ik_1}$, $x_2 = e^{ik_2}$, and $y = e^{i\phi}$ so that

$$(-\varepsilon - J)(x_2 y + x_1) + \frac{J}{2}\left(x_2^2 y + x_1^2 + x_1^{-1} x_2 y + x_1 x_2^{-1}\right) \; = \; 0\,. \qquad (3.14)$$

Now use the earlier result that

$$\begin{aligned} \varepsilon \;&=\; J(\cos k_1 + \cos k_2 - 2) \\ \text{so} \quad -\varepsilon - J \;&=\; J(1 - \cos k_1 - \cos k_2) \\ &=\; J\left(1 - \frac{x_1}{2} - \frac{x_1^{-1}}{2} - \frac{x_2}{2} - \frac{x_2^{-1}}{2}\right). \end{aligned}$$

Substituting into (3.14) and cancelling J gives

$$Py + Q \;=\; 0 \qquad (3.15)$$

where

$$\begin{aligned} P &= \left(1 - \frac{x_1}{2} - \frac{x_1^{-1}}{2} - \frac{x_2}{2} - \frac{x_2^{-1}}{2}\right) x_2 + \frac{1}{2} x_2^2 + \frac{1}{2} x_1^{-1} x_2 \\ &= x_2 - \frac{x_1 x_2}{2} - \frac{1}{2}. \end{aligned}$$

Q is the same except that $x_1 \leftrightarrow x_2$,

$$\text{so} \quad Q \;=\; x_1 - \frac{x_1 x_2}{2} - \frac{1}{2}.$$

From (3.15) $\quad y \;=\; -\dfrac{Q}{P}$

$$\text{so} \quad \frac{y+1}{y-1} \;=\; \frac{\left(-\frac{Q}{P} + 1\right)}{\left(-\frac{Q}{P} - 1\right)} \;=\; \frac{Q-P}{Q+P}.$$

$$\begin{aligned} \text{Now} \quad Q - P &= x_1 - x_2 \\ \text{and} \quad Q + P &= x_1 + x_2 - x_1 x_2 - 1 \end{aligned}$$

which can be rewritten as :

$$Q - P \;=\; x_1 - x_2 \;=\; \frac{1}{2}\Big[(1 - x_2)(1 + x_1) - (1 - x_1)(1 + x_2)\Big]$$

and

$$Q + P \;=\; x_1 + x_2 - x_1 x_2 - 1 \;=\; -(1 - x_1)(1 - x_2).$$

Therefore

$$\begin{aligned}\frac{y+1}{y-1} &= \frac{1}{2}\left[\frac{(1-x_2)(1+x_1)-(1-x_1)(1+x_2)}{-(1-x_1)(1-x_2)}\right]\\ 2\left(\frac{y+1}{y-1}\right) &= \left(\frac{x_1+1}{x_1-1}\right)-\left(\frac{x_2+1}{x_2-1}\right).\end{aligned}$$

Now note that $i\left(\frac{x_1+1}{x_1-1}\right) = i\left(\frac{e^{ik_1}+1}{e^{ik_1}-1}\right) = \cot\frac{k_1}{2}$.

Similarly $i\left(\frac{x_2+1}{x_2-1}\right) = \cot\frac{k_2}{2}$ and $i\left(\frac{y+1}{y-1}\right) = \cot\frac{\phi}{2}$,

so that finally

$$2\cot\frac{\phi}{2} = \cot\frac{k_1}{2} - \cot\frac{k_2}{2}. \tag{3.16}$$

This equation is an important relation between the k's and ϕ. However it does not tell us the allowed values of k_1 and k_2. For this we need other equations, which come from the periodic boundary conditions.

Clearly $f_{\ell_1+N,\ell_2+N} = f_{\ell_1,\ell_2}$ and from (3.10) this implies

$$\begin{aligned}&e^{ik_1N}e^{ik_2N} = 1\\ \text{so}\quad &(k_1+k_2)N = \lambda 2\pi \quad \text{where } \lambda \text{ is an integer,}\end{aligned}$$

$$\text{and therefore}\quad k_1+k_2 = \lambda\frac{2\pi}{N}. \tag{3.17}$$

k_1+k_1 is the *total* wavevector, and the fact that this has to be an integer multiple of $2\pi/N$ merely reflects the translational symmetry.

More interestingly, however, we also have

$$f_{\ell_2,\ell_1+N} = f_{\ell_1,\ell_2}$$

since the (ℓ_1+N)'th site is the same as the ℓ_1'th site and our convention is that the second subscript is always greater than the first. Now (3.12) gives

$$e^{ik_1\ell_2}e^{ik_2(\ell_1+N)}e^{i\phi/2}+e^{ik_2\ell_2}e^{ik_1(\ell_1+N)}e^{-i\phi/2} = e^{ik_1\ell_1}e^{ik_2\ell_2}e^{i\phi/2}+e^{ik_2\ell_1}e^{ik_1\ell_2}e^{-i\phi/2}.$$

For this to be true for all ℓ_1, ℓ_2, the coefficients of $e^{ik_1\ell_1}e^{ik_2\ell_2}$ and also of $e^{ik_2\ell_1}e^{ik_1\ell_2}$ must be the same on both sides. The first of these gives

$$\begin{aligned}&e^{ik_1N}e^{-i\phi/2} = e^{i\phi/2}\\ \therefore\quad &e^{i(k_1N-\phi)} = 1\\ \therefore\quad &k_1N-\phi = \lambda_1 2\pi \quad \text{where } \lambda_1 \text{ is an integer.}\end{aligned}$$

$$\text{and so} \quad k_1 = \lambda_1 \frac{2\pi}{N} + \frac{\phi}{N}. \tag{3.18}$$

Similarly the second gives

$$k_2 = \lambda_2 \frac{2\pi}{N} - \frac{\phi}{N} \quad \text{where } \lambda_2 \text{ is an integer.} \tag{3.19}$$

Note that the sum of (3.18) and (3.19) is (3.17), so that only two of these are strictly needed.

Conclusion The eigenstates with two deviations from the fully aligned state have the form:

$$\psi = \sum_{\ell_1 \ell_2} f_{\ell_1,\ell_2} |\ell_1 \ell_2\rangle \qquad (\ell_2 > \ell_1) \tag{3.20}$$

$$f_{\ell_1,\ell_2} = C\left(e^{ik_1\ell_1} e^{ik_2\ell_2} e^{i\phi/2} + e^{ik_2\ell_1} e^{ik_1\ell_2} e^{-i\phi/2}\right) \tag{3.21}$$

where k_1, k_2 and ϕ satisfy the three equations

$$2\cot\phi/2 = \cot\frac{k_1}{2} - \cot\frac{k_2}{2} \tag{3.22}$$

$$k_1 = \lambda_1 \frac{2\pi}{N} + \frac{\phi}{N} \tag{3.23}$$

$$k_2 = \lambda_2 \frac{2\pi}{N} - \frac{\phi}{N}, \tag{3.24}$$

and the energy of this eigenstate is

$$\varepsilon \ = \ J(\cos k_1 + \cos k_2 - 2).$$

It is important to note here that k_1 and k_2 are *not* integer multiples of $\frac{2\pi}{N}$ and so the energy is *not* the same as for two single deviation states. In fact k_1 and k_2 may not even be real, since ϕ does not have to be real.

3.4.1 Form of the States

There are two types of two-deviation states as follows.

a. *Class C* These occur when $|\lambda_1 - \lambda_2| \geq 2$. It can be shown that in this case the ϕ are real, and therefore k_1, k_2 are also real.
   Since the k_1, k_2 are real the magnitude of each of the two terms in f_{ℓ_1,ℓ_2} is always 1, independent of the values of ℓ_1, ℓ_2. We say that the state consists of two 'free' deviations, or two 'free' spin waves or two 'free' magnons. Note they are 'free' but they still interact with each other and this causes the shift in k_1, k_2 from the values allowed for isolated spin waves. In other words they are not independent.

For a given value of total wavevector $k = k_1 + k_2$, the energy can be written as

$$\varepsilon = -J[2 - \cos k_1 - \cos(k - k_1)].$$

Choosing the ferromagnetic case with $J = -|J|$, this can be written as

$$\varepsilon = |J|\left[2 - 2\cos\frac{k}{2}\cos\left(k_1 - \frac{k}{2}\right)\right].$$

k_1 can take values in the range $0 \leq k_1 \leq 2\pi$ so the second cosine can effectively have any value between -1 and $+1$. This means that these states with two 'free' magnons have energies for a given k bounded by $|J|(2 - 2\cos\frac{k}{2})$ below and $|J|(2 + 2\cos\frac{k}{2})$ above. This is indicated in Fig. 3.2 by the curves marked P and Q. As $N \to \infty$ these states form a continuum.

b. *Class A/B* These occur for $\lambda_1 = \lambda_2$ and $|\lambda_1 - \lambda_2| = 1$, although there is no significant difference between these two cases. It can be shown that in these cases the ϕ and therefore k_1, k_2 are complex in such a way that $k_2 = k_1^*$.
Now the magnitude of the terms in f_{ℓ_1,ℓ_2} does depend on ℓ_1 and ℓ_2. In fact one of the terms in (3.12) diverges as $|\ell_2 - \ell_1| \to \infty$. This is unphysical and the coefficient of this term must be chosen to be zero. The other term then tends to 0 as $|\ell_2 - \ell_1| \to \infty$, which means that the two deviations are more likely to be found close to each other than further apart. For this reason such a state is called a bound state of the two deviations or of two spin waves. The two deviations form a complex which can then travel freely along the chain. Another term used to describe this state is a '2-string'.
Again it can be shown that energy of the bound state lies above that of two 'free' states with the same total k if $J > 0$, i.e. the antiferromagnetic case, but below them if $J < 0$, the ferromagnetic case.
The spectrum of the bound states can be obtained by writing

$$f_{\ell_1,\ell_2} = c_1 e^{i\frac{k}{2}(\ell_1+\ell_2)} e^{-g(\ell_2-\ell_1)}. \tag{3.25}$$

where k is the total wave-vector and g is a positive real constant. Comparing with the earlier form, Eq. (3.12), the second term has been omitted by choosing $c_2 = 0$ since if ℓ_1 and ℓ_2 are interchanged the term with g would diverge as $\ell_2 - \ell_1 \to \infty$, as mentioned earlier. The earlier form, Eq. (3.12), is valid for any value of N whereas this form, Eq. (3.25), is an approximation valid for large N as it requires $\ell_2 - \ell_1 << N$. Because of the exponential decay this is valid for the bound states.
Substituting (3.25) into Eqs. (3.8) and (3.9) gives

$$(E_A - E - 2J) + \frac{J}{2}\left(e^{-i\frac{k}{2}}e^{-g} + e^{i\frac{k}{2}}e^{g} + e^{-i\frac{k}{2}}e^{g} + e^{i\frac{k}{2}}e^{-g}\right) = 0 \tag{3.26}$$

and

$$(E_A - E - J) + \frac{J}{2}\left(e^{i\frac{k}{2}}e^{-g} + e^{-i\frac{k}{2}}e^{-g}\right) = 0 \tag{3.27}$$

which together yield

$$e^{-g} = \frac{1}{2}\left(e^{i\frac{k}{2}} + e^{-i\frac{k}{2}}\right) = \cos\frac{k}{2}. \tag{3.28}$$

Finally substituting back into (3.27) gives

$$E - E_A = -\frac{J}{2}(1 - \cos k)$$

This curve has the same form as the free magnon but with a coefficient which is half that of the free magnon. It is indicated by curve R in Fig. 3.2.

We see from (3.12) and (3.25) that for $c_2 = 0$, $e^{i\frac{k}{2}(l_1+l_2)}e^{-g(l_2-l_1)} \equiv e^{ik_1l_1}e^{ik_2l_2}$, so that $k_1 = k/2 - \mathrm{i}g$ and $k_2 = k/2 + \mathrm{i}g$. Hence this special solution is also the same as (3.23) and (3.24) provided

$$k_1 = \lambda_1\frac{2\pi}{N} + \frac{\phi}{N} = \frac{k}{2} - ig,$$

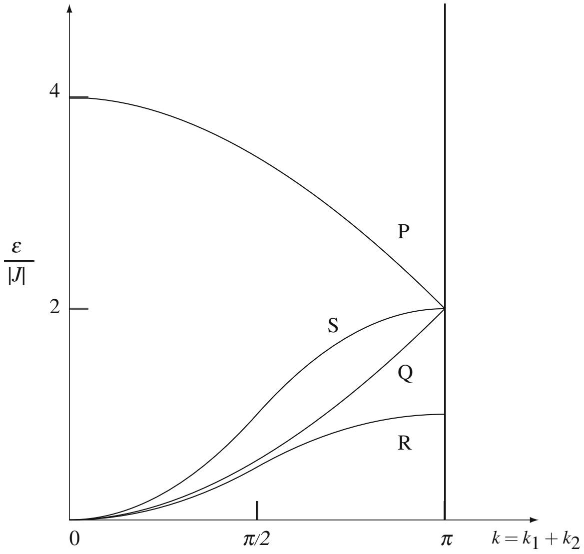

Fig. 3.2 Spectrum of two-deviation states in a 1D spin-$\frac{1}{2}$ chain with ferromagnetic isotropic nearest-neighbour Heisenberg exchange. P, Q are the top and bottom of the continuum of two 'free'-magnon states. R is the single branch of two-magnon bound states and S is the single spin-wave spectrum

$$\text{and} \quad k_2 = \lambda_2 \frac{2\pi}{N} - \frac{\phi}{N} = \frac{k}{2} + ig,$$

$$\text{which requires} \quad \phi = (\lambda_2 - \lambda_1)\pi - igN.$$

3.5 Three Deviation States

Now consider states with $S_T^z = \frac{N}{2} - 3$, i.e. three deviations from the aligned state. If we have three deviations then similar equations can be written down for the coefficients $f_{\ell_1\ell_2\ell_3}$ as were written for the two-deviation coefficients $f_{\ell_1\ell_2}$. Again there is one basic equation for the case where none of ℓ_1, ℓ_2, ℓ_3 are neighbours. This has a solution of the form

$$f_{\ell_1\ell_2\ell_3} = e^{ik_1\ell_1} e^{ik_2\ell_2} e^{ik_3\ell_3}$$

with $\varepsilon = -J(3 - \cos k_1 - \cos k_2 - \cos k_3)$. Clearly this is the same energy as three free magnons with wave vectors k_1, k_2, k_3, although, just as for the case of two deviations, these wave vectors will not be the same as for free magnons. For the same value of ε any permutation of k_1, k_2, k_3 will be a solution, so we expect in general

$$\begin{aligned} f_{\ell_1\ell_2\ell_3} = {} & A_1 e^{i(k_1\ell_1 + k_2\ell_2 + k_3\ell_3)} + A_2 e^{i(k_2\ell_1 + k_3\ell_2 + k_1\ell_3)} \\ & + A_3 e^{i(k_3\ell_1 + k_1\ell_2 + k_2\ell_3)} + B_1 e^{i(k_1\ell_1 + k_3\ell_2 + k_2\ell_3)} \\ & + B_2 e^{i(k_3\ell_1 + k_2\ell_2 + k_1\ell_3)} + B_3 e^{i(k_2\ell_1 + k_1\ell_2 + k_3\ell_3)} \end{aligned} \tag{3.29}$$

The ratio of the coefficients are determined by 'boundary condition' equations when two or three of ℓ_1, ℓ_2, ℓ_3 are neighbours. These equations are somewhat lengthy and are not given here. Again it is useful to introduce phase factors and write $A_p = Ce^{i\Phi_p/2}$ and $B_p = Ce^{-i\Phi_p/2}$ for $p = 1, 2, 3$.

3.5.1 Bethe Ansatz for $S_T^Z = \frac{N}{2} - 3$

Bethe [1] suggested (The German word 'ansatz' has no exact equivalent in English but roughly means 'starting point'), and subsequently proved, that the phase factors Φ_p should have the form of a sum of '2-body' phase factors of the sort we saw earlier. Specifically that

$$\left.\begin{aligned} \Phi_1 &= \phi_{12} + \phi_{13} + \phi_{23} \\ \Phi_2 &= \phi_{23} + \phi_{21} + \phi_{31} \\ \Phi_3 &= \phi_{31} + \phi_{32} + \phi_{12} \end{aligned}\right\} \begin{array}{l} \text{Note that the ordering of the} \\ \text{subscripts here is the same as the ordering} \\ \text{of the } k\text{'s in the corresponding term.} \end{array}$$

where the ϕ_{ij} satisfy the same equations as before, namely

$$2\cot\frac{\phi_{ij}}{2} = \cot\frac{k_i}{2} - \cot\frac{k_j}{2}\,. \tag{3.30}$$

These equations ensure that $\phi_{ji} = -\phi_{ij}$ and hence the phases of B_p are the negative of those of A_p.

Periodic boundary conditions applied to $f_{\ell_1\ell_2\ell_3}$ require

$$\left.\begin{aligned} Nk_1 &= 2\pi\lambda_1 + \phi_{12} + \phi_{13} \\ Nk_2 &= 2\pi\lambda_2 + \phi_{21} + \phi_{23} \\ Nk_3 &= 2\pi\lambda_3 + \phi_{31} + \phi_{32} \end{aligned}\right\}$$

where $\lambda_1, \lambda_2, \lambda_3$ are integers.

Again we find that if $|\lambda_i - \lambda_j| \geq 2$ for all i, j then the solutions have three real values of k_i. These are states with three 'free' spin waves. If some $|\lambda_i - \lambda_j| = 0$ or 1 then we get bound states or mixtures of bound and 'free'. A state may consist either of 1 'free' and 1 bound pair of deviations in which case one k is real and the other two complex or of a single bound state of 3 deviations in which case all the k are complex. The form of the bound state of 3 deviations is a generalisation of Eq. (3.25) but will not be given here.

3.6 States with an Arbitrary Number of Deviations

In general we may have r deviations from the fully aligned state, i.e. $S_T^Z = \frac{N}{2} - r$. Bethe showed that for r deviations the solution would be a generalised version of the three-deviation form Eq. (3.29). In particular there are now r values of k_i, denoted $k_1, k_2, \ldots, k_r$.

There will be $M = r!$ permutations of these which we label $P_1 \ldots P_M$. Let the ith k in the pth permutation be k_i^p, then

$$f_{\ell_1\ldots\ell_r} = \sum_{p=1}^{M} A_p\, e^{i(k_1^p\ell_1 + k_2^p\ell_2 \ldots k_r^p\ell_r)}$$

Note that the summation here is over the M permutations. The Bethe ansatz now requires

$$A_p = C\exp\left[\sum_{i=1}^{r}\sum_{j=i+1}^{r}\phi_{ij}^p\right]$$

where $\phi_{ij}^p = \pm\,\phi_{ij}$, the negative sign occurring if the order of k_i, k_j in the pth permutation is reversed. For example, referring back to the three-deviation case, $\Phi_2 = \phi_{23} - \phi_{12} - \phi_{13}$. In addition Eq. (3.30) still applies.

This form of $f_{\ell_1 \dots \ell_r}$ is clearly rather complicated, but in practice we do not need to use it (for some things!). Normally, the actual equations we work with are the following:

$$\text{the energy equation } \varepsilon = J \sum_{i=1}^{r} (\cos k_i - 1) \tag{3.31}$$

and the two equations relating k and ϕ

$$N k_i = 2\pi \lambda_i + \sum_{j \neq i} \phi_{ij} \tag{3.32}$$

$$2 \cot \frac{\phi_{ij}}{2} = \cot \frac{k_i}{2} - \cot \frac{k_j}{2}. \tag{3.33}$$

These are the equations that form the Bethe Ansatz and were first written down by Bethe in 1931 [1]. Bethe showed that they are correct for the $S = \frac{1}{2}$ Heisenberg model. They do not apply for $S > \frac{1}{2}$.

The fact that the Bethe Ansatz works for $S = \frac{1}{2}$ means that it is an example of what is called an *integrable* system. The $S > \frac{1}{2}$ systems are not integrable. Unfortunately there is no general way of predicting which systems are integrable. Each case has to be demonstrated directly.

Clearly integrable systems are special cases and in general most systems are not integrable. Nevertheless since many exact results are available for integrable systems they are extremely important and they have greatly increased our understanding of many-body systems.

Reference

1. Bethe, H.A.: Z. Phys. **71**, 205–226 (1931) 36, 38