Chapter 5
Antiferromagnetic Spin Waves

Abstract The ground state of the antiferromagnetic spin-1/2 linear chain is a made up of a linear combination of basis states with exactly half ($N/2$) the spins reversed. The elementary excitations from the ground state have $N/2 \pm 1$ spins reversed. To calculate the energies of these states, des Cloiseaux and Pearson used a modified version of the same method that Hulthén had used for the ground state energy. The modifications are quite significant and involve some rather different mathematical techniques. These are described in this chapter. The result is not a single branch of excitations as a function of the total wave vector, but rather a continuum of states. The lower boundary of this continuum has a simple sine-wave form, which is similar to that obtained using conventional antiferromagnetic spin-wave theory (covered in a later chapter). We finish this chapter with a discussion of the somewhat unexpected behaviour of the excitation spectrum when an external magnetic field is present.

5.1 The Basic Formalism

Bethe [1] gave the wave functions for the 1D $S = \frac{1}{2}$ Heisenberg chain in 1931 and the ground state energy was evaluated by Hulthén in 1938 [2]. In 1962 Des Cloiseaux and Pearson [3] obtained the exited states or elementary excitations, the antiferromagnetic spin waves. In this chapter we follow their treatment closely with some extra details. Note that the treatment given here determines the energies of the elementary excitations exactly. In Chap. 8 an approximate theory of the same excitations is given which is applicable much more generally than the $S = \frac{1}{2}$ Heisenberg chain.

The lowest-lying excited states (the elementary excitations) have $S_T = 1$ and $S_T^z = 0, \pm 1$. Once again, within the $S_T^z = 1$ subspace the lowest lying states are class C: states which are all or partly bound, with complex values of k_i, lie higher in energy.

For a state with $S_T^z = 1$ we require $\dfrac{N}{2} - 1$ deviations from the fully aligned state, and hence $\dfrac{N}{2} - 1$ values of k_i, with corresponding values of λ_i. For class C we require that the λ_i are separated by at 2 or more and are chosen from the integers

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$1, 2, 3, \ldots, N-2, N-1$. λ_i must not be chosen to be zero since this gives the $S_T^z = 1$ component of a multiplet with $S_T > 1$.

There are clearly many ways to do this. One way is to choose

$$\lambda = 1, 3, 5, \ldots, \Lambda, \Lambda+4, \Lambda+6, \ldots, N-3, N-1 \tag{5.1}$$

where Λ is an odd integer. Here we have a single gap of size 4. Alternatively we may have two gaps of size 3

$$\lambda = 1, 3, 5, \ldots, \Lambda_1, \Lambda_1+3, \Lambda_1+5, \ldots, \Lambda_2, \Lambda_2+3, \Lambda_2+5, \ldots, N-3, N-1 \tag{5.2}$$

where Λ_1 is an odd integer and $\Lambda_2 \geq \Lambda_1 + 3$ is an even integer. One could also have 'gaps' at the beginning

$$\lambda = 3, 5, 7, \ldots, N-5, N-3, N-1 \tag{5.3}$$

or

$$\lambda = 2, 4, 6, \ldots, \Lambda_2, \Lambda_2+3, \Lambda_2+5, \ldots, N-3, N-1 \tag{5.4}$$

or similar 'gaps' at the end.

$$\lambda = 1, 3, 5, 7, \ldots, N-5, N-3 \tag{5.5}$$

or

$$\lambda = 1, 3, 5, \ldots, \Lambda_1, \Lambda_1+3, \Lambda_1+5, \ldots, N-4, N-2 \tag{5.6}$$

These latter four can be regarded as special cases of Eq. (5.1) and Eq. (5.2), but in fact they are important as we shall see.

All these possibilities lead to a large number of states, forming a continuum in the limit $N \to \infty$. The lowest states for a given k were determined by Des Cloiseaux and Pearson [3] by studying numerically finite size chains with $N \leq 16$. They found that for $-\pi < k < 0$ or equivalently $\pi < k < 2\pi$ the choice that gives the lowest energy is given by Eq. (5.4), while for $0 < k < \pi$ the correct choice is Eq. (5.6). We shall follow des Cloiseaux and Pearson and present the calculation for $-\pi < k < 0$.

Two other preliminaries are necessary. Firstly it is convenient to work in the $S_T^z = 0$ subspace. As noted before an $S_T = 1$ state with $S_T^z = 0$ has an extra $\lambda = 0$ added since there need to be $\frac{N}{2}$ deviations, and this corresponds to an extra $k_i = 0$. Hence, writing $\Lambda_2 = 2n$, the set of λ is

$$\lambda = 0, 2, 4, 6, \ldots, 2n, 2n+3, \ldots, N-3, N-1 \tag{5.7}$$

Secondly the total wave-vector

$$k = \sum_{i=1}^{N/2} k_i = \sum_{i=1}^{N/2} \left(\frac{2\pi}{N}\lambda_i + \sum_{j=1}^{N/2}{}' \phi_{ij} \right) = \frac{2\pi}{N} \sum_{i=1}^{N/2} \lambda_i$$

since for every ϕ_{ij} in this sum there is an equal and opposite ϕ_{ji}. The prime on the second summation indicates $j \neq i$.

Using $1 + 3 + 5 + \cdots + (N-3) + (N-1) = \frac{N^2}{4}$ and noting that the set of λ in Eq. (5.7) differs from this by the first n terms being reduced by 1 we have

$$k = \frac{2\pi}{N} \left(\frac{N^2}{4} - n \right) = \frac{2\pi}{N}(-n) \mod 2\pi,$$

which is strictly only true if N is a multiple of 4 but this is not a significant restriction in the limit $N \to \infty$. Thus

$$n = N|k|/2\pi. \tag{5.8}$$

As in the previous chapter, we now pass to the continuum limit by writing $x_i = \frac{2i-1}{N}$, which becomes a *continuous* variable in the limit $N \to \infty$, running from 0 to 1. Note that $x_i \neq \frac{\lambda_i}{N}$ now as the λ are not evenly spaced. In fact the λ satisfy

$$\lambda_i = \frac{2i-2}{N} = \frac{x_i}{N} - \frac{1}{N} \quad \text{for } i \leq n, \tag{5.9}$$

$$\lambda_i = \frac{2i-1}{N} = \frac{x_i}{N} \quad \text{for } i > n. \tag{5.10}$$

In the large N limit we define

$$x_i \equiv \frac{2i-1}{N} \xrightarrow[N\to\infty]{} x; \qquad \frac{\lambda_i}{N} \xrightarrow[N\to\infty]{} \lambda(x); \qquad k_i \xrightarrow[N\to\infty]{} k(x); \qquad 0 \leq x \leq 1$$

The $i \leq n$ in Eq. (5.9) becomes $x < \dfrac{|k|}{\pi}$ and $i > n$ in Eq. (5.10) becomes $x > \dfrac{|k|}{\pi}$ and these two equations can be written together as

$$\lambda(x) = x - \left(\frac{1}{N}\right) \Theta \left(\frac{|k|}{\pi} - x \right) \tag{5.11}$$

where Θ is the step function.

The calculation given here differs from that in the previous chapter only in the choice of the λ_i. The other equations from the Bethe method are unchanged, namely

$$2 \cot \frac{1}{2} \phi(x, y) = \cot \frac{k(x)}{2} - \cot \frac{k(y)}{2}, \tag{5.12}$$

$$k(x) = 2\pi\lambda(x) + \frac{1}{2} \int_0^1 \phi(x, y)\, dy, \tag{5.13}$$

and

$$\varepsilon \;=\; -\frac{JN}{2}\int_0^1 [1-\cos k(x)]\,dx, \tag{5.14}$$

and again we take $-\pi \le \phi \le \pi$.

Substituting for $\lambda(x)$ from Eq. (5.11) gives

$$k(x) \;=\; 2\pi\left[x-\left(\frac{1}{N}\right)\Theta\left(\frac{|k|}{\pi}-x\right)\right]+\frac{1}{2}\int_0^1 \phi(x,y)\,dy, \tag{5.15}$$

and splitting the integral into two parts for the same reason as before

$$\begin{aligned}k(x) = 2\pi&\left[x-\left(\frac{1}{N}\right)\Theta\left(\frac{|k|}{\pi}-x\right)\right]\\ &+\frac{1}{2}\int_0^x \phi(x,y)\,dy+\frac{1}{2}\int_x^1 \phi(x,y)\,dy.\end{aligned} \tag{5.16}$$

Now differentiate with respect to x and note that $\frac{d}{dx}\theta\left(\frac{|k|}{\pi}-x\right)=-\delta\left(\frac{|k|}{\pi}-x\right)$.

$$\begin{aligned}\frac{dk}{dx} &= 2\pi\left[1+\frac{1}{N}\,\delta\left(\frac{|k|}{\pi}-x\right)\right]+\frac{1}{2}\phi_1(x,x)+\frac{1}{2}\int_0^x \frac{\partial\phi}{\partial x}dy\\ &\quad -\frac{1}{2}\phi_2(x,x)+\frac{1}{2}\int_x^1 \frac{\partial\phi}{\partial x}dy\end{aligned}$$

where

$$\phi_1(x,x) \;=\; \lim_{y\to x-}\phi(x,y) \;=\; -\pi,$$

and

$$\phi_2(x,x) \;=\; \lim_{y\to x+}\phi(x,y) \;=\; +\pi \quad \text{as before.}$$

Thus, putting $x_0=\dfrac{|k|}{\pi}$,

$$\begin{aligned}\frac{dk}{dx} &= 2\pi\left[1+\frac{1}{N}\,\delta(x_0-x)\right]+\frac{1}{2}(-\pi)-\frac{1}{2}(\pi)+\frac{1}{2}\int_0^x \frac{\partial\phi}{\partial x}\,dy+\frac{1}{2}\int_x^1 \frac{\partial\phi}{\partial x}\,dy\\ &= \pi+\frac{2\pi}{N}\,\delta(x_0-x)+\frac{1}{2}\int_0^1 \frac{\partial\phi}{\partial x}\,dy\,.\end{aligned}$$

Using the substitutions

$$\cot\frac{k(x)}{2} = \xi(x)$$
$$\cot\frac{k(y)}{2} = \eta(y),$$

so that $2\cot\frac{1}{2}\phi(x,y) = \xi(x) - \eta(y)$, and defining

$$f(\xi) = -\frac{dx}{d\xi}; \quad f(\eta) = -\frac{dy}{d\eta}$$

then

$$\frac{\partial\phi}{\partial x} = \frac{\partial\phi}{\partial\xi}\frac{d\xi}{dx} = -\frac{1}{f(\xi)}\frac{\partial\phi}{\partial\xi}.$$

But

$$\phi = \cot^{-1}\left[\frac{1}{2}(\xi-\eta)\right],$$

therefore

$$\frac{\partial\phi}{\partial\xi} = \frac{-1}{1+\frac{1}{4}(\xi-\eta)^2}\,\frac{1}{2}.$$

Also

$$dy = \frac{dy}{d\eta}\,d\eta = -f(\eta)\,d\eta,$$

$$\therefore \quad \frac{dk}{dx} = \pi + \frac{2\pi}{N}\delta(x_0 - x) + \frac{1}{2}\int\left(-\frac{1}{f(\xi)}\right)\frac{(-1)(-f(\eta)\,d\eta)}{1+\frac{1}{4}(\xi-\eta)^2}$$
$$= \pi + \frac{2\pi}{N}\delta(x_0 - x) - \frac{1}{2f(\xi)}\int\frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2}.$$

This is now an integral over η instead of y. As y goes from 0 to 1, $k(y)$ goes from 0 to 2π (not strictly proved here but can be shown from (5.15)) so $\cot\frac{k(y)}{2}$ goes from $+\infty$ to $-\infty$.

Putting $\xi_0 = \cot\frac{k(x_0)}{2}$ and using the standard relation for change of variable

$$\delta(x_0 - x) = \delta(\xi_0 - \xi)\frac{d\xi}{dx} = \delta(\xi_0 - \xi)\frac{-1}{f(\xi)}$$

and noting that $\delta(\xi_0 - \xi)\frac{-1}{f(\xi)} = \delta(\xi - \xi_0)\frac{1}{f(\xi)}$ since $f(\xi) = -f(-\xi)$, gives

$$\frac{dk}{dx} = \pi + \frac{2\pi}{Nf(\xi)}\delta(\xi - \xi_0) - \frac{1}{2f(\xi)}\int_{-\infty}^{\infty}\frac{f(\eta)\,d\eta}{1+\frac{1}{4}(\xi-\eta)^2}\,.$$

Finally $\displaystyle \frac{dk}{dx} = \frac{dk}{d\xi}\frac{d\xi}{dx} = -\frac{1}{f(\xi)}\frac{dk}{d\xi}$

and since $\xi = \cot\dfrac{k(x)}{2}$, $k(x) = 2\cot^{-1}\xi$ and $\dfrac{dk}{d\xi} = \dfrac{-2}{1+\xi^2}$.
Therefore

$$\frac{2}{1+\xi^2}\frac{1}{f(\xi)} = \pi + \frac{2\pi}{Nf(\xi)}\delta(\xi - \xi_0) - \frac{1}{2f(\xi)}\int_{-\infty}^{\infty}\frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2} \tag{5.17}$$

$$\text{i.e.}\quad f(\xi) = \frac{2}{\pi(1+\xi^2)} + \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{f(\eta)d\eta}{1+\frac{1}{4}(\xi-\eta)^2} - \frac{2}{N}\delta(\xi - \xi_0)\,. \tag{5.18}$$

Notice that the only difference between this equation and the corresponding $f(\xi)$ in the ground state calculation of the previous chapter is the extra delta function at the end. This comes from the choice of λ in Eqs. (5.9) and (5.10).

The method of solution of this equation is the same as in the previous chapter, using the Fourier Transform. We define

$$F(q) = \int_{-\infty}^{\infty} f(\theta)e^{iq\theta}d\theta$$

with inverse

$$f(\theta) = \frac{1}{2\pi}\int_{-\infty}^{\infty}F(q)e^{-iq\theta}dq.$$

Substituting in Eq. (5.18) gives

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}F(q)e^{-iq\xi}dq = \frac{2}{\pi(1+\xi^2)} - \frac{2}{N}\delta(\xi-\xi_0)$$
$$+\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\eta}{1+\frac{1}{4}(\xi-\eta)^2}\frac{1}{2\pi}\int_{-\infty}^{\infty}F(q)e^{-iq\eta}dq\,.$$

Now

$$\int_{-\infty}^{\infty}\frac{e^{-iq\eta}d\eta}{1+\frac{1}{4}(\xi-\eta)^2} = e^{-iq\xi}\int_{-\infty}^{\infty}\frac{e^{iq(\xi-\eta)}d\eta}{1+\frac{1}{4}(\xi-\eta)^2}\,.$$

so substituting $z = \dfrac{1}{2}(\xi - \eta)$, with $d\eta = -2dz$, gives

$$= -2e^{-iq\xi}\int_{-\infty}^{\infty}\frac{e^{2iqz}dz}{1+z^2}$$

$$= -2e^{-iq\xi}\pi e^{-2q}.$$

Therefore

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}F(q)e^{-iq\xi}dq = \frac{2}{\pi(1+\xi^2)} - \frac{2}{N}\delta(\xi-\xi_0) - \frac{1}{2\pi}\int_{-\infty}^{\infty}F(q)e^{iq\xi}e^{-2q}dq\,.$$

Multiply both sides by $e^{iq'\xi}$ and integrate $\int_{-\infty}^{\infty}d\xi$

$$F(q') = \frac{2}{\pi}\int_{-\infty}^{\infty}\frac{e^{iq'\xi}d\xi}{(1+\xi^2)} - e^{-2q'F(q')} - \frac{2}{N}e^{iq'\xi_0}$$

$$(1+e^{-2q'})F(q') = \frac{2}{\pi}\pi e^{-q'} - \frac{2}{N}e^{iq'\xi_0}$$

therefore

$$F(q') \quad = \quad \frac{1}{\cosh q'} - \frac{2e^{iq'\xi_0}}{N(1+e^{-2q'})}$$

As before the energy relative to the aligned state is

$$\varepsilon = -\frac{JN}{2}\int_{-\infty}^{\infty}\frac{2f(\xi)d\xi}{1+\xi^2} \tag{5.19}$$

$$= -JN\frac{1}{2\pi}\int_{-\infty}^{\infty}F(q)\pi e^{-|q|}dq$$

$$= -\frac{JN}{2}\int_{-\infty}^{\infty}\frac{2}{(e^q+e^{-q})}e^{-|q|}dq + J\int_{-\infty}^{\infty}\frac{e^{-|q|}e^{iq\xi_0}}{1+e^{-2q}}dq$$

$$= -JN2\int_{0}^{\infty}\frac{e^{-q}}{e^q+e^{-q}}dq + \frac{J}{2}\int_{-\infty}^{\infty}e^{iq\xi_0}\operatorname{sech} q\,dq$$

$$= -JN\ \ln 2 + \frac{J\pi}{2}\operatorname{sech}(\pi\xi_0/2) \tag{5.20}$$

Clearly the first term is the ground state energy and the second is the additional energy of the elementary excitations above the ground state.

Finally we need to relate ξ_0 to the wave-vector k. If we ignore terms of order $\frac{1}{N}$ in Eq. (5.15) we obtain the corresponding equation from the previous chapter. The relation between x and $k(x)$ in this calculation differs only to order $\frac{1}{N}$ from that in the previous so we can use the result obtained there:

$$-\frac{dx}{d\xi} = f(\xi) = \frac{1}{2}\,\text{sech}\left(\frac{\pi\xi}{2}\right)$$

When $x = 0$, $k(x) = 0$ so $\xi = \cot\frac{k(x)}{2} = +\infty$.
Hence

$$\int_0^{x_0} dx = -\int_\infty^{\xi_0} \frac{1}{2}\,\text{sech}\left(\frac{\pi\xi}{2}\right) d\xi = \frac{1}{\pi}\left[\cot^{-1}\sinh\left(\frac{\pi\xi}{2}\right)\right]_\infty^{\xi_0}$$
$$\therefore \quad x_0 = \frac{1}{\pi}\cot^{-1}\left[\sinh\left(\frac{\pi\xi_0}{2}\right)\right].$$

To order $\dfrac{1}{N}$, $\quad \pi x_0 = k$ so

$$\cot(k) = \sinh\left(\frac{\pi\xi_0}{2}\right)$$

and

$$\text{sech}\left(\frac{\pi\xi_0}{2}\right) = \frac{1}{\sqrt{1+\sinh^2(\frac{\pi\xi_0}{2})}} = \frac{1}{\sqrt{1+\cot^2(k)}}$$
$$= \frac{1}{\sqrt{\text{cosec}^2(k)}} = \sin k$$

Substituting into Eq. (5.20) gives

$$\varepsilon = -JN\ \ln 2 + \frac{J\pi}{2}\sin k \tag{5.21}$$

This is the energy relative to the aligned state so the excitation energy, the energy above the ground state is

$$E_k = \frac{J\pi}{2}\sin k \tag{5.22}$$

This is the exact result obtained by Des Cloiseaux and Pearson [3] for the energy of the antiferromagnetic spin-waves or magnons in the spin-$\frac{1}{2}$ chain with isotropic Heisenberg exchange.

It should be noted that the particular choice of λ given by Eqs. (5.9) and (5.10) is not the only possible one for class C states with $N/2-1$ deviations from the aligned state, i.e. with $S_T^z = 1$. Des Cloiseaux and Pearson showed numerically that it gives the lowest state for any particular k. The other choices lead to a continuum of states, bounded above by $E_k^{\max} = J\pi\sin\frac{k}{2}$ [4]. The energies of the class C states are shown in Fig. 5.1. One should also remember that there are numerous states which

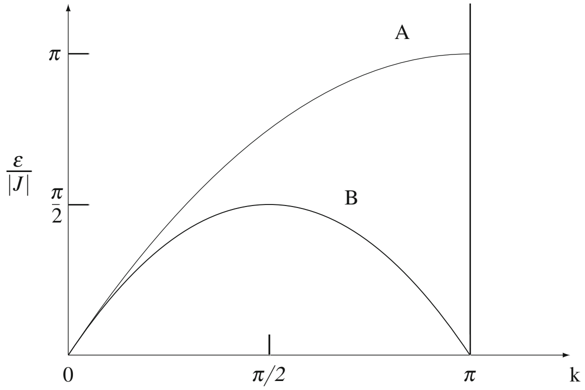

Fig. 5.1 Elementary excitation energies in a 1D spin-$\frac{1}{2}$ chain with antiferromagnetic isotropic nearest-neighbour Heisenberg exchange. There is a continuum of states from the lower boundary B to the upper boundary A. The states on the lower boundary B are the antiferromagnetic spin waves

are not pure class C but have one or more bound multiplets and which lie in general at higher energy than the class C states.

Nevertheless the des Cloiseaux and Pearson result is extremely important and in fact the response to a probe, for example by neutron scattering, is strongest at this lower boundary [5, 6].

5.2 Magnetic Field Behaviour

Finally in this chapter we discuss the elementary excitations in the presence of a magnetic field H applied in the z-direction. In this case the Hamiltonian for the chain becomes

$$\mathcal{H} = J \sum_{i=1}^{N} \mathbf{S}_i . \mathbf{S}_{i+1} - g\beta H \sum_{i=1}^{N} S_i^z \tag{5.23}$$

where g is the Landé g-factor mentioned in Chap. 1 and β is the Bohr magneton, the magnetic dipole moment associated with one unit of angular momentum.

For antiferromagnetic coupling, $J > 0$, the classical ground state consists of two sublattices, exactly as in the zero field case, but now the orientation of the spins on one sublattice is at an angle θ to the z-axis and on the other sublattice at an angle $-\theta$. In fact the ground state is the same as for an interacting pair of spins for which

$$\begin{aligned}\mathcal{H} &= J\mathbf{S}_1 \cdot \mathbf{S}_2 - \frac{1}{2} g\, \beta\, H (S_1^z + S_2^z) \\ &= J S^2 \cos 2\theta - g\, \beta\, H S \cos\theta \end{aligned} \tag{5.24}$$

and minimising with respect to θ gives

$$JS^2 2\sin 2\theta - g\beta HS\sin\theta = 0$$

from which $\quad \cos\theta = \dfrac{H}{K} \quad$ where $K = \dfrac{4JS}{g\beta}$

and so $\quad S^z = S\cos\theta = \dfrac{H}{2K}.$

Clearly the largest value of S^z is $\frac{1}{2}$ and this is reached when $H = K$. That this is the classical ground state for the whole system follows from the fact that this choice gives the minimum energy for every pair separately.

It should be pointed out that the magnetic fields needed in practice to produce values of θ significantly less than 90°, the zero-field value, are much too high to be realised experimentally, so for the present this remains a theoretical exercise. However, it is of interest because it is a striking example of the difference between classical and quantum behaviour.

The existence of two sublattices implies that the underlying periodicity of the system is $2a$, rather than a, the lattice spacing, which we shall take to be unity. The Brillouin zone (BZ) should then have a periodicity in k-space of $\frac{2\pi}{2a} = \pi$. This is precisely the periodicity observed in the elementary excitations described in the previous section, in the absence of a magnetic field.

The quantum treatment of the elementary excitations was first carried out by Ishimura and Shiba [7], see also [8], using the same Bethe Ansatz method as is used for the elementary excitations in zero field, but with a modified choice of the λ. The result is that the periodicity in k-space of the BZ is quite different from the classical periodicity. In fact the periodicity changes smoothly from π at $H = 0$ where the magnetisation per site $\langle S^z\rangle = 0$, to 0 at $H = K$ where $\langle S^z\rangle = \frac{1}{2}$. The spectrum is shown for various values of the magnetisation in Fig. 5.2. Note that the periodicity for the fully aligned state is actually 2π rather than zero and the behaviour when

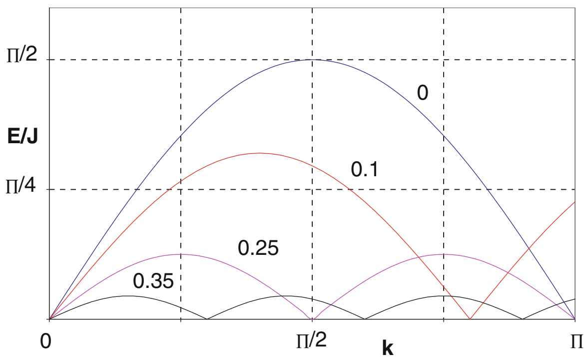

Fig. 5.2 The spectrum of elementary excitations for an antiferromagnetic spin 1/2 chain in a magnetic field. The curves are labelled by the magnetisation per site $\langle S^z\rangle$, which is zero in zero field and $\frac{1}{2}$ for fields $H \geq K$ where all the spins are aligned parallel to the field

the number of reversed atoms is small, of order $1/N$, i.e. when $\langle S^z \rangle \to \frac{1}{2}$, has to be handled differently.

This clearly indicates that the underlying magnetic structure does not have a periodicity of $2a$ in real space like the classical structure. A simple model [9] which fits the data quite well is one in which there are no sublattices as such but rather the spins all align parallel or antiparallel to the z-axis. Then as the magnetic field increases the antiparallel spins become fewer in number but regularly spaced, resulting in a steadily increasing periodicity in real space. This periodicity varies with the magnetisation in a way that precisely matches the observed variation of the periodicity of the BZ in k-space.

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