Spin wave theory of dilute one-dimensional magnets†

A R McGurn‡ and M F Thorpe§
‡ Department of Physics, Western Michigan University, Kalamazoo, Michigan 49008, USA
§ Department of Physics, Michigan State University, East Lansing, Michigan 48824, USA

Received 21 July 1982, in final form 4 October 1982

Abstract. The low-temperature specific heat and inelastic neutron scattering from dilute one-dimensional Heisenberg magnets are computed using spin wave theory. The specific heat and inelastic neutron scattering are calculated exactly for segments of finite length and the properties for the random systems are computed by summing over segments. Analytical results in the limit of very low temperature for the specific heat are obtained for both ferromagnetic and antiferromagnetic systems. The results for the inelastic neutron scattering law are very similar to those obtained previously by computer simulation.

1. Introduction

The low-temperature thermodynamics and the inelastic neutron scattering law are computed using spin wave theory for dilute one-dimensional Heisenberg ferromagnets and antiferromagnets. These properties are calculated exactly for segments of finite length, and the corresponding properties of the dilute system are obtained by summing over segments weighted by their probability of occurrence.

From these results an analytic expression is obtained for the specific heat at very low temperature. This result shows an interesting exponential temperature dependence for both the dilute ferromagnet and the dilute antiferromagnet.

The results for the inelastic scattering law show good agreement with those obtained previously using the equation-of-motion technique (Endoh et al 1981). For small dilutions results have been obtained by extending the results for a single defect (Endoh et al 1981) and this theory gives good agreement with the results from the equation-of-motion technique. A low-concentration theory has also been considered by Lovesey (1981). Certain spectral features in the results are shown to be from particular segments or from even or odd segments.

We derive the eigenvalues and eigenvectors for ferromagnetic and antiferromagnetic segments in § 2. In § 3 we use these results to obtain the specific heat for the dilute ferromagnet and the dilute antiferromagnet. In § 4 we obtain the result for $S(q, \omega)$ for a single ferromagnetic segment using the eigenvectors in a direct calculation of the cross section. We show that an identical answer can be obtained more simply by cutting a single bond in a cyclcical chain and treating this bond as a defect in a Green function formalism.

† Work supported in part by NSF.
The result for $S(q, \omega)$ for the dilute ferromagnet is obtained by summing over segments. In § 5 a similar Green function calculation is done for the dilute antiferromagnetic chain.

2. Single segments

A single ferromagnetic segment with $n$ spins is described by the Hamiltonian

$$H = -J \sum_{i=1}^{n-1} S_i \cdot S_{i+1}$$

(1)

where the $S_i$ are spin operators obeying the usual commutation rules (see for example Kittel 1963). At low temperatures, it is reasonable to transform to Bose operators and keep only the quadratic terms (Endoh et al 1981) so that

$$H = JS \left( a_1^+ a_1 + a_n^+ a_n + 2 \sum_{i=2}^{n-1} a_i^+ a_i - \sum_{i=1}^{n-1} (a_i^+ a_{i+1}^+ + a_{i+1} a_i) \right)$$

(2)

If the ground state is $|0\rangle$, a general wavefunction $|\psi\rangle$ within the manifold of $n$ states involving a single spin deviation may be written

$$|\psi\rangle = \sum c_i a_i^+ |0\rangle$$

(3)

where the coefficients $c_i$ satisfy the linear equations obtained from the Schrödinger equation ($H|\psi\rangle = E|\psi\rangle$)

$$(\epsilon - 1) c_1 = -c_2$$

$$(\epsilon - 2) c_i = -c_{i-1} - c_{i+1}, \quad 2 \leq i \leq n - 1$$

$$(\epsilon - 1) c_n = -c_{n-1}$$

(4)

and the dimensionless energy $\epsilon = E/JS$. Solving these equations by standard techniques (see for example Thorpe and Miyazima 1981) we find that

$$\epsilon_K = 2(1 - \cos K)$$

(5)

where

$$K = \pi p/n \quad p = 0, 1, \ldots, n - 1$$

(6)

and the eigenvector amplitudes $c_i$ in the eigenstate $\epsilon_K$ are given by

$$c_i = A \cos \left[ K(i - \frac{1}{2}) \right]$$

(7)

and correspond to the standing waves that would be expected for an open segment. The normalisation constant is given by $\langle \psi | \psi \rangle = 1$ and leads to $A^2 = 2/n$ if $K \neq 0$ and $A^2 = 1/n$ if $K = 0$.

A similar calculation can be performed for an antiferromagnetic segment described by equation (1) but with $J \rightarrow -J$ (a convention that will be used throughout this paper). The eigenvalues are given by

$$\epsilon_K = 2|\sin K|$$

(8)
Spin wave theory of dilute one-dimensional magnets

with

\[ K = \pi p/n \quad p = 0, 1, \ldots, \frac{1}{2}n - 1 \quad (9) \]

for segments with an even number of spins where all the modes are doubly degenerate. For segments with an odd number of spins

\[ K = \pi(p + \frac{1}{2})/n \quad p = 0, 1, \ldots, \frac{1}{2}(n - 3) \quad (10) \]

where all the modes are also doubly degenerate. In addition there is a single excitation at \( K = 0 \) (which corresponds to a doubly degenerate ground state as required by Kramers' theorem (Kramers 1930)). In order to obtain the dispersion relation (equation (8)), it is necessary to do a Bogoliubov transformation after transforming to Bose operators (see, for example, Kittel 1963).

The dispersion relations (equations (5) and (8)) have the same form as for infinite segments. The finiteness of the segments selects certain discrete standing waves that satisfy the boundary conditions.

3. Specific heat

The specific heat \( C_n \) for a single spin segment (either ferromagnetic or antiferromagnetic) is given by

\[ C_n = k \sum_k [\frac{1}{2} \beta \varepsilon_k \cosh(\frac{1}{2} \beta \varepsilon_k)]^2 \quad (11) \]

where the spin excitations are treated as non-interacting bosons and \( \beta = (kT)^{-1} \).

In a dilute system with the spins randomly located at \( N \rightarrow \infty \) sites with probability \( x \), the probability of finding a spin segment of length \( n \) is given by

\[ P_n = N(1 - x)^2x^n \quad (12) \]

Examples of such spin segments are shown in figure 1. The specific heat \( C \) for the complete system is given by

\[ C = \sum_{n=1}^{N} P_n C_n \quad (13) \]

These summations can be performed numerically until convergence is obtained at some \( N \). Generally \( N \) was chosen to be about a factor ten greater than the mean length of a segment. Except for the very smallest values of \( 1 - x \), this causes no difficulties.

The results for the dilute ferromagnet and the dilute antiferromagnet are shown in figures 2 and 3 for low temperatures \( (kT \ll JS) \) where spin-wave theory should be valid. Sharply defined spin wave excitations have been seen in inelastic neutron scattering in the one-dimensional antiferromagnet TMMC (Hutchings et al 1972) and we would expect the spin wave approximation to be valid in the dilute chains of concern in this paper. Even though the spins do not order except at \( T = 0 \), they are highly correlated within segments at low temperatures.

At very low temperatures the specific heat (equation (13)) can be evaluated in closed form using the method of steepest descents (Thorpe and Miyazima 1982, Thorpe et al 1982). The major contribution to the specific heat comes from segments of intermediate length which is a trade-off between short segments, which are more probable, and long segments, which have a larger specific heat because of a smaller energy gap. For both
the dilute ferromagnet and the dilute antiferromagnet the result can be written
\[
\frac{C}{Nk} = B(T/T_0)^\alpha \exp[-(T/T_0)^\beta]
\] (14)
where for the dilute ferromagnet
\[
\begin{align*}
\alpha &= \frac{3}{4} \\
\beta &= \frac{3}{4} \\
B &= [2(1 - x)^2 \pi^{1/2}]/[27 \ln(1/x)] \\
T_0 &= \frac{2T}{J} \pi^2 [\ln(1/x)]^2
\end{align*}
\] (15)
and for the dilute antiferromagnet
\[
\begin{align*}
\alpha &= \frac{3}{4} \\
\beta &= \frac{3}{2} \\
B &= [(1 - x)^2 (2\pi)^{1/2}]/[8 \ln(1/x)] \\
T_0 &= 4JS\pi \ln(1/x).
\end{align*}
\] (16)
These results are valid for \( T < T_0 \) which is the region in the bottom left-hand corner in figures 2 and 3. These results have been discussed elsewhere (Thorpe et al 1982).

**Figure 2.** The specific heat per site \( C/Nk \) for a dilute ferromagnet as a function of temperature \( kT/2JS \) for \( x = 0.25, 0.5, 0.8, 0.9, 1.0 \) as shown. For \( x = 1 \), the usual \( T^5 \) behaviour is obtained.

**Figure 3.** The specific heat per site \( C/Nk \) as a function of \( kT/2JS \) for the dilute antiferromagnet for \( x = 0.5, 0.7, 0.8, 0.9, 1.0 \) as shown. For \( x = 1 \), the usual \( T \) behaviour is obtained.
Spin wave theory of dilute one-dimensional magnets

4. Evaluation of \( S(q, \omega) \) for a dilute ferromagnetic chain

The neutron scattering law for a single segment of \( n \) spins is given by the Fermi Golden Rule

\[
S_n(q, \omega) = \frac{2\pi}{S} \sum_{i,k} |\langle 0 | e^{i\mathbf{q}\cdot\mathbf{R}_i} | K \rangle|^2 \delta(\omega - \varepsilon_k)
\]

where the prefactor \( 2\pi/S \) is chosen for convenience and \( y \) is any direction perpendicular to the arbitrary assumed spin ordering direction. For a derivation of equation (17) with prefactors see Marshall and Lovesey (1971). The dimensionless frequency \( \omega \) is in units of \( JS \) with \( \hbar = 1 \). Transforming to Bose operators, the result for a single ferromagnetic segment becomes

\[
S_n(q, \omega) = n\pi \sum_K |\langle q | K \rangle|^2 \delta(\omega - \varepsilon_k)
\]

where \( |q\rangle \) are the plane-wave states

\[
|q\rangle = n^{-1/2} \sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i} a_i|0\rangle.
\]

For long segments only the \( q = K \) states contribute and we get the usual result that the scattering is a single \( \delta \)-function. However for finite segments, scattering takes places from all the states \( K \). Using the results of § 2, we find that

\[
|\langle q | K \rangle|^2 = (1/n^2)(1 + \cos K)(1 - \cos q)(1 - \cos nK \cos nq)/(\cos K - \cos q)^2
\]

for \( K \neq 0 \)

\[
= (1/n^2)(1 - \cos nq)/(1 - \cos q) \quad \text{for } K = 0.
\]

From these results the inelastic neutron scattering can be written

\[
S_n(q, \omega) = \frac{\pi}{n} \sum_{K \neq 0} \frac{(1 + \cos K)(1 - \cos q)(1 - \cos nK \cos nq)}{(\cos K - \cos q)^2} \delta(\omega - \varepsilon_k)
\]

\[
+ (\pi/n)(1 - \cos nq)/(1 - \cos q) \delta(\omega).
\]

The sum over \( K \) can be done using the relationship

\[
\frac{1}{n} \sum_{r=1}^{n} \frac{1}{\cos \theta - \cos(2\pi r/n)} = -[\sin \theta \tan(\pi n\theta)]^{-1}
\]

(22)

to obtain the very compact form

\[
S_n(q, \omega) = \frac{\varepsilon_q}{(\omega - \varepsilon_q)^2} \text{Im} \left[ \left( \frac{4 - \omega}{\omega} \right)^{1/2} \cos nq - \cos(2n \sin^{-1}(\frac{1}{2} \omega^{1/2})) \right] \left[ \sin(2n \sin^{-1}(\frac{1}{2} \omega^{1/2})) \right]
\]

(23)

with \( \delta \)-function responses at \( \varepsilon_k \) with appropriate weightings occur in \( S_n(q, \omega) \) due to the zeros of \( \sin(2n \sin^{-1}(\frac{1}{2} \omega^{1/2})) \).

The neutron scattering law for the dilute ferromagnet \( S(q, \omega) \) is obtained as sum over segments

\[
S(q, \omega) = \sum_{n=1}^{N} P_n S_n(q, \omega)
\]

(24)

using equations (12) and (23) and cutting off \( N \) in the same way as for the calculation of
the specific heat in the previous section. Results are shown in figure 4 for \( q = \pi / 2 \) and \( \pi \) and a spin concentration \( x = 0.8 \). Also shown in figure 4 are results obtained using the equation-of-motion technique (Thorpe and Alben 1976, Alben et al 1977, Endoh et al 1981) with parameters chosen to give the same width in \( \omega \). It can be seen that the results are very similar, with the equation-of-motion technique giving a little more background. The sharp features in the spectra are the standing waves on the various segments. As \( x \) increases to 1, \( S(\pi, \omega) \sim \delta(\omega - 4) \) and \( S(\pi / 2, \omega) \sim \delta(\omega - 2) \), the result for a single infinite segment.

![Figure 4. \( S(q, \omega) \) for a dilute ferromagnetic chain for \( x = 0.8 \). The results in (a) and (b) are from equation (24) in this paper and in (c) and (d), from using the equation-of-motion technique. The energy \( \omega \) is in units of \( JS \) and contains a small imaginary part 0.04.](image)

We note that the total integrated intensity for \( S(q, \omega) \) is independent of \( q \):

\[
\int_0^\infty S(q, \omega) \, d\omega = \pi N x
\]

and proportional to the total number of magnetic spins. This can easily be proved from equations (12), (18) and (24).

While this method of calculation using the eigenvectors that leads to equation (23) is direct and elegant we have found it more convenient to use another technique that is simpler for the antiferromagnet. It involves using a Green function technique and forming a segment of \( n \) spins by 'cutting' a cyclical ring of \( n \) spins.

The zero-temperature Green functions for a ring of \( n \) ferromagnetically coupled spins are given by

\[
P_m(t) = -i \theta(t) \langle [S^+_m(t), S_m(0)] \rangle / 2 S
\]
Spin wave theory of dilute one-dimensional magnets

where \( l, m = 1, 2, \ldots, n \) label the spin sites. (Here the spin labelled \( n \) is connected to the one labelled \( 1 \).) Within the spin wave treatment equation (26) becomes

\[
P_{lm}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \omega e^{-i\omega t} \frac{1}{n} \sum_{k} P_k(\omega) \exp[ik(l - m)]
\]

(27)

where \( P_k(\omega) = [\omega - 4 \sin^2(k/2)]^{-1} \) and

\[
k = 2p\pi/n \quad p = 0, 1, 2, \ldots, n - 1.
\]

(28)

We obtain the Green functions \( G_{lm} \) for a segment of \( n \) spins by breaking the bond between the spins labelled 1 and \( n \). The Green function matrix \( \mathbf{G} \) is related to the Green function matrix \( \mathbf{P} \) through the equation

\[
\mathbf{G} = \mathbf{P} + \mathbf{PVG}
\]

(29)

where \( \mathbf{V} \) has elements

\[
V_{lm} = \begin{cases} 
-1 & \text{if } l = m = 1 \text{ or } n \\
1 & \text{if } l = 1 \text{ and } m = n \text{ or } l = n \text{ and } m = 1 \\
0 & \text{otherwise}.
\end{cases}
\]

(30)

The potential \( \mathbf{V} \) removes the bond between the spins labelled 1 and \( n \), breaking the ring into an open segment. After some algebra, equation (29) yields the following form for the matrix elements of \( \mathbf{G} \):

\[
G_{ll'} = P_{ll'} - (P_{ll} - P_{nn})(P_{ll'} - P_{nn'})/[1 + 2(P_{ll} - P_{nn})].
\]

(31)

The inelastic neutron scattering law \( S_n(q, \omega) \) is given by the imaginary part of the space and time Fourier transform of \( \mathbf{G} \). We find

\[
S_n(q, \omega) = -\text{Im} \left\{ \frac{1}{n} \sum_{k} P_k(\omega) \left( \frac{\sin((k - q)n/2)}{\sin((k - q)/2)} \right)^2 \\
-\frac{4}{\omega n} \left[ \sum_{k} P_k(\omega) \cos\left(\frac{kn}{2}\right) \sin\left(\frac{k}{2}\right) \frac{\sin((q - k)n/2)}{\sin((q - k)/2)} \right]^2 \right\}
\]

(32)

where the \( k \)-sums are as in equation (28). The neutron scattering law \( S(q, \omega) \) is obtained using equation (24) to give the result for the dilute ferromagnetic chain. We have checked that this gives the same results as in figures 4(a) and (b). It is interesting to note that the \( \delta \)-functions in \( S_n(q, \omega) \) come from the poles of \( P_k(\omega) \) at \( \omega_k \) with \( k \)-values given by equation (28) and from the zeros of \( \sum_k P_k(\omega) \) which can be obtained with the help of equation (22) and shown to be at \( \omega_k \) which are those frequencies present in an open segment of length \( n \) that are not present in a cyclical segment of length \( n \). (Those can be obtained by comparing equations (6) and (28).) Careful algebraic manipulation shows that equation (32) is identical to equation (23).

In figure 5 we show results for \( S_n(q, \omega) \) for \( 2 \leq n \leq 10 \) obtained from equation (32) where a small imaginary part is added to the energy. We note that the peak at \( \omega = 2 \) is absent for all odd chains as can be seen from equations (5) and (6).

In figures 6(a) and (b) results are presented for \( S(q, \omega) \) against \( \omega \) for \( q = \pi/2 \) and \( \pi \) and spin concentration \( x = 0.5 \). In figures 6(c) and (d) we show the contributions to \( S(q, \omega) \) for \( q = \pi \) and \( x = 0.5 \) due to only odd segments and even segments respectively. We note that the peak at \( \omega = 2 \) is absent for odd-length segments as expected. This is
true for all $q$-values. By comparing figures 4(a) and 6(a), it can be seen that ‘$q$-selection’ has broken down much more at $x = 0.5$ that at $x = 0.8$. This can be understood in terms of summing over the segments in figure 5.

Figure 5. $S_q(q = \pi, \omega)$ for $2 \leq n \leq 10$ as indicated on the figures as a function of frequency $\omega$ for ferromagnetic segments. The response for each segment consists of a series of broadened $\delta$-functions. The vertical scale is arbitrary but the same for all nine subgraphs, so $S(q, \omega)$ for the dilute ferromagnet is obtained by adding these results weighted with $P_n$.

Figure 6. $S(q, \omega)$ for a dilute ferromagnetic chain for $x = 0.5$. The results are from equations (24) and (32). Parts (a) and (b) show the complete result for $q = \pi$ and $\pi/2$. In parts (c) and (d) the contributions of odd and even segments to (a) are shown separately. The energy $\omega$ is in units of $JS$ and contains a small imaginary part 0.04.
5. Evaluation of $S(q, \omega)$ for a dilute antiferromagnetic chain

The zero-temperature Green function for an antiferromagnetically coupled segment of $2n$ spins is given by

$$P_{\alpha \beta}(t) = -i \theta(t) \langle [S_i^\alpha(t), S_m^\beta(0)] \rangle/2S$$

(33)

where in spin wave theory $\alpha = +$ or $-$ indicates that the $l$ spin is on the up-spin or down-spin sublattice and $\beta = +$ or $-$ refers to the $m$ spin. From spin wave theory

$$P_{\alpha \beta}^\beta = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, e^{-i\omega t} \frac{1}{n} \sum_k P_k \omega_k \omega_{k-l} e^{i\omega(l-m)}$$

(34)

where

$$P_k^+ = (\omega + 2)/D$$
$$P_k^- = P_k^+ = -2 \cos k/D$$
$$D = \omega^2 - 4 \sin^2 k$$

(35)

and $k = p\pi/n (p = 0, 1, 2, \ldots, n-1)$. Here we label the spins such that the odd sites have spin up and the even sites have spin down.

The Green function matrix $G$ for a segment of $2n$ spins can be obtained from the $P$ matrix of equation (34) by breaking the bond between the spins labelled 1 and $2n$. Hence $G$ is related to $P$ by

$$G = P + PVG$$

(36)

where

$$V_{ln} = \begin{cases} -1, & \text{if } l = 1 \text{ or } 2n \text{ and } m = 1 \text{ or } 2n \\ 0, & \text{otherwise.} \end{cases}$$

(37)

From equation (36) we obtain

$$G_{lw} = P_{lw} - [(\omega + 2)/(\omega^2)] (P_{1n} + P_{lw})(P_{2n} + P_{lw})/P_{11}$$

(38)

The inelastic scattering law $S_{2n}(q, \omega)$ is given by the imaginary part of the space and time Fourier transforms of $G$ in equation (38). We find

$$S_{2n}(q, \omega) = -\text{Im} \left[ n \sum_k \frac{4[1 - \cos k \cos(q-k)]}{\omega^2 - 4 \sin^2 k} \left( \frac{\sin[(k-q)n]}{\sin(k-q)} \right)^2 - \frac{(\omega + 2) H_1 H_2}{P_{11}} \right]$$

(39)

where

$$H_1 = \frac{1}{n} \sum_k \exp[i(k-q)(n+1)] \frac{\sin[(k-q)n]}{\sin(k-q)} \left( \frac{1 - e^{i(k-q)}}{\omega^2 - 4 \sin^2 k} \right)$$
$$H_2 = \frac{1}{n} \sum_k \exp[-i(k-q)(n+1)] \frac{\sin[(k-q)n]}{\sin(k-q)} \left( \frac{1 - e^{-i(k-q)}}{\omega^2 - 4 \sin^2 k} \right)$$

(40)
We see from equation (38) that for our segments \( G_{ll'} = G_{l,l'} \), so \( S_{2n}(q, \omega) \) is the same for chains with left-end spins on the up lattice as for those with left-end spins on the down lattice. In our computation of \( S(q, \omega) \) of the random one-dimensional system with spin concentration \( x \), \( S_{2n}(q, \omega) \) has weight \( 2N(1-x)^2 x^{2n} \) where \( 2N \to \infty \) is the number of lattice sites.

The Green function matrix \( G \) for a chain of \( 2n-1 \) spins can be obtained from the \( P \) matrix of equation (34) by breaking the bonds between the spins labelled 1 and 2n and the spins labelled 2n-1 and 2n. Hence \( G \) is related to \( P \) by

\[
G = P + PVG
\]

where

\[
V_{lm} = \begin{cases} 
-1, & \text{if } l = m = 1 \text{ or } l = m = 2n - 1 \\
-1, & \text{if } l = 1, m = 2n \text{ or } l = 2n, m = 1 \\
-1, & \text{if } l = 2n, m = 2n - 1 \text{ or } l = 2n - 1, m = 2n \\
0, & \text{otherwise.} 
\end{cases}
\]

From equation (41) the matrix elements of \( G \) are found to be given by

\[
G_{ll'} = P_{ll'} - [(P_{ll'} + P_{l,2n-1}P_{2n-1,l})A \\
+ (P_{ll'}P_{2n,l} + P_{l,2n}P_{l',l} + P_{l,2n-1}P_{2n-1,l'})B \\
+ (P_{ll'}P_{2n-1,l} + P_{l,2n}P_{l',l})C + P_{l,2n}P_{l',l}D] / R
\]

where

\[
A = 1 + 2P_{1,2n} + P_{11} - P_{2n,2n} + 2(P_{1,2n})^2 - 2P_{11}P_{2n,2n} \\
B = (1 + 2P_{1,2n})(1 + P_{11} - P_{1,2n-1}) \\
C = -[2P_{1,2n} + P_{2n,2n} + P_{1,2n-1} - 2P_{1,2n-1}P_{2n,2n} + 2(P_{1,2n})^2] \\
D = -2(1 + P_{11} - P_{1,2n-1})(P_{11} + P_{1,2n-1}) \\
R = [(1 + P_{11} + P_{1,2n})^2 - (P_{1,2n-1} + P_{1,2n})^2(1 + 2P_{1,2n}) \\
+ 2(P_{1,2n-1} - 1 - P_{11})(P_{1,2n} + P_{2n,2n})(P_{1,2n-1} + P_{11})].
\]

The \( S_{2n-1}(q, \omega) \) can be obtained from the space and time Fourier transform of \( G \), i.e.,

\[
H(\omega) = \sum_{i,j=1}^{2n-1} \exp[iq(r_i - r_j)] G_{ij}(\omega).
\]

We find

\[
S_{2n-1}^{+}(q, \omega) = -\text{Im}[H(\omega)]
\]

for a segment with up spins either end and

\[
S_{2n-1}^{-}(q, \omega) = -\text{Im}[H(-\omega)]
\]
for a segment with down spins on either end. Here

\[
H(\omega) = \frac{1}{n} \sum_k \left[ P_k^+(\omega) \left( \frac{\sin((k-q)n)}{\sin(k-q)} \right)^2 + P_k^-(\omega) \left( \frac{\sin((k-q)(n-1))}{\sin(k-q)} \right)^2 \right. \\
+ 2P_k^-(\omega) \frac{\sin((k-q)n) \sin((k-q)(n-1))}{\sin(k-q)} \\
- (I_1(q, \omega)I_1(-q, \omega) + I_2(q, \omega)I_2(-q, \omega) - A/R) \\
+ (I_1(q, \omega)I_2(-q, \omega) + I_1(-q, \omega)I_2(q, \omega) + B/R) \\
+ 2(I_1(q, \omega)I_3(-q, \omega) + I_1(-q, \omega)I_3(q, \omega) - C/R) \\
- I_2(q, \omega)I_2(-q, \omega) - D/R \]
\]

(48)

where

\[
I_1(q, \omega) = \frac{1}{n} \sum_k \left( P_k^+(\omega) \frac{\sin((k-q)n)}{\sin(k-q)} + P_k^-(\omega) \frac{\sin((k-q)(n-1))}{\sin(k-q)} \right) \\
\times \exp[i(k(n-1) - qn)] \\
I_2(q, \omega) = \frac{1}{n} \sum_k \left( P_k^+(\omega) \frac{\sin((k-q)n)}{\sin(k-q)} + P_k^-(\omega) \frac{\sin((k-q)(n-1))}{\sin(k-q)} \right) \exp[i(k-q)n] \\
I_3(q, \omega) = \frac{1}{n} \sum_k \left( P_k^+(\omega) \frac{\sin((k-q)n)}{\sin(k-q)} + P_k^-(\omega) \frac{\sin((k-q)(n-1))}{\sin(k-q)} \right) \\
\times \exp[i((k-q)n + k)].
\]

For a chain of length \(2N \rightarrow \infty\) and spin concentration \(x\), the total neutron scattering can be written as

\[
S(q, \omega) = \sum_{n=2}^{\infty} C_{2n} S_{2n}(q, \omega) + \sum_{n=2}^{\infty} C_{2n-1} (S_{2n-1}^+(q, \omega) + S_{2n-1}^-(q, \omega)) \\
+ 2N(1-x)^2 x^{2n} S_2(q, \omega) \\
(50)
\]

where \(C_{2n} = 2N(1-x)^2 x^{2n}\) and \(C_{2n-1} = N(1-x)^2 x^{2n-1}\) and

\[
S_2(q, \omega) = -\text{Im}[2(1-\cos q)/\omega^2] \\
(51)
\]

is the scattering due to pairs of spins.

In figure 7 we show the results for the neutron scattering law for antiferromagnetic segments of length \(3 \leq n \leq 11\). For segments with an odd number of spins we average over the possibility that the two end spins are either up or down. From §2 we only expect a response at \(\omega = 1\) for segments of length \(3r\) where \(r\) is an integer (i.e. 3, 6, 9 etc). In fact for the segments shown there is only response at \(n = 3\) and \(n = 9\). The response is absent at \(n = 6\). These results are important with regard to the absence of Ising resonances as discussed by Endoh et al (1981). If we neglect the non-Ising terms in the Hamiltonian (equation (1)), then there are two kinds of excitations: the bulk modes at \(\omega = 2\), that correspond to making a spin deviation on a site with two neighbours and the modes at \(\omega = 1\), that came from spins at the ends of segments with only one neighbour. Those are the analogue of the Ising resonances that survive when the transverse terms in the
Hamiltonian (equation (1)) are switched on in 2D (Cowley et al 1977). This is not the case in 1D as explained by Endoh et al (1981) and confirmed experimentally. If it were so we would have expected a peak at $\omega = 1$ for all the subgraphs in figure 7 and all these peaks would have had equal weight. This is clearly not the case. We note that $q = \pi/2$ is

Figure 8. $S(q, \omega)$ for a dilute antiferromagnetic chain for $x = 0.75$ and $0.50$ as indicated. The results (a) and (b) are obtained by summing over segments, and (c) and (d) from the equation-of-motion technique. The energy $\omega$ in units of $JS$ and contains a small imaginary part 0.02.
the zone-boundary wavevector where Ising resonance effects are expected to be most prominent. Most of the response at $\omega = 1$ in subsequent graphs comes from segments with three spins where spin wave theory in the antiferromagnet is most unreliable. It is much better for longer segments where zero-point effects are less serious (McGurn and Thorpe 1979).

In figure 8 we show $S(q, \omega)$ for $q = \pi/2$ for spin concentrations of $x = 0.75$ and $x = 0.50$. In figures 8(a) and (b) the results are from equation (50) and those in figure 8(c) and (d) are obtained using the equation-of-motion method (Endoh et al 1981). A width was added by putting $\omega = \text{Re}(\omega) + i\ 0.02$ to permit a better comparison of the two methods. It can be seen that the results are very similar. A region near $\omega = 0$ cannot be directly compared as the equation-of-motion technique suppresses the response there due to a sine Fourier transform; the results from the method of this paper are the standard. Hence only the non-zero frequency modes stand comparison. In figures 9(a) and (b) we compare the contributions to the $q = \pi/2$ spectrum (see figure 8(b)) from even and odd segments respectively for $x = 0.5$. We see that the peak at $\omega = 1$ comes only from the odd segments and predominantly from three spin segments. In figures 9(c) and (d) we make a similar decomposition for $x = 0.75$ of the result in figure 8(a).

![Figure 9](image)

Figure 9. The contributions of even and odd segments to $S(q, \omega)$ in figure 8 for dilute antiferromagnetic chains with $x = 0.50$ and 0.75.

We have integrated the area under the curves $S(q, \omega)$ for the dilute antiferromagnet. Unlike the dilute ferromagnet, where the area is constant, there is considerable dependence on $q$ and $x$ as shown in figure 10 where we plot the total scattering per magnetic site. For $x = 1$ the result becomes proportional to $\tan(q/2)$ as expected for a linear chain (Thorpe 1976). For the pure chain the total scattered intensity diverges near the magnetic Bragg point $q = \pi$.

Note that in figures 4, 6, 8, 9 the vertical normalisation is arbitrary and such that the major spectral feature coincides in peak height.
6. Conclusions

We have used spin wave theory to calculate the specific heat and neutron scattering law $S(q, \omega)$ of dilute ferromagnetic and antiferromagnetic chains at low temperatures where we expect spin wave theory to be valid. These properties are obtained for single segments and then summed with the proper weighting. The series converge well and cause no numerical problems.

The specific heat changes from a power-law to an exponential behaviour at the very lowest temperatures, reflecting the discrete nature of the excitation spectrum.

The results for the neutron scattering law agree with those obtained previously from the equation-of-motion technique although in some cases the equation-of-motion technique gives a little more background. The present method has the advantage that contributions from particular segment types can be isolated. As the magnetic concentration $x$ decreases from 1, we find that 'q-selection' breaks down increasingly, as we expect from the destruction of the long-range periodicity. Not only does the $x = 1$ spin wave peak broaden but new peaks appear. Unfortunately all experiments to date have had $x$ sufficiently close to 1 for only the broadened peak to be seen (Endoh et al 1981).

It should be noted that the present method is restricted in its use to dilute systems, whereas the equation-of-motion technique can be used for any random magnetic system. We confirm the results of Endoh et al (1981) that Ising resonances do not occur in 1D by looking at the contributions of individual segments to the neutron scattering law.

References

Spin wave theory of dilute one-dimensional magnets

Kittel C 1963 *Quantum Theory of Solids* (New York: Wiley) ch 4
Kramers H A 1930 *Proc. Acad. Sci. Amsterdam* 33 959
Lovesey S W 1981 *Solid State Commun.* 38 953
Thorpe M F 1976 *Phys. Rev.* B 13 2186