The Three-Magnon Contribution to the Spin Correlation Function in Integer-Spin Antiferromagnetic Chains

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The exact form factor for the O(3) non-linear $\sigma$ model is used to predict the three-magnon contribution to the spin correlation function, $S(q, \omega)$, near wavevector $q = \pi$ in an integer spin, one-dimensional antiferromagnet. The 3-magnon contribution is extremely broad and extremely weak; the integrated intensity is $< 2\%$ of the single-magnon contribution.

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The Hamiltonian for the one dimensional Heisenberg antiferromagnet of spin $s$ is

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}. \quad (1)$$

Based upon the large-$s$ limit we write the spin operators as

$$\vec{S}_j \approx s(-1)^j \phi(j) + \vec{l}(j), \quad (2)$$

where $s\phi$ and $l$ represent the staggered and uniform magnetization of the spin chain. We set the lattice spacing to 1.

The low energy behaviour of this Hamiltonian can be described by the O(3) non-linear $\sigma$ model \cite{1}. Recently, the exact form factors for this field theory were calculated \cite{2,3}. The resulting prediction for $S(q, \omega)$ at $q \approx 0$ was discussed in \cite{5}. Here we comment on the prediction at $q \approx \pi$. In the continuum approximation, the (zero temperature) spin correlation function at $q = \pi + k \approx \pi$ is

$$S_{ab}(\pi + k, \omega) = s^2 \int dx \int dt \exp(i \omega t - k x) < \Omega | \phi^a(x, t) \phi^b(0, 0) | \Omega > \equiv \delta_{ab} S(\pi + k, \omega), \quad (3)$$

where $| \Omega >$ is the groundstate.

We insert a complete set of asymptotic states. It is known that the spectrum consists of a triplet of massive magnons. Thus, the asymptotic states will be characterized by a spin index and a momentum for each particle in the state.

$$| n > = | a_1, p_1; a_2, p_2; \ldots ; a_n, p_n >$$

It is convenient to label the particles’ momenta by the rapidities, $\theta_i$:

$$E_i = \Delta \cosh \theta_i, \quad p_i = (\Delta / v) \sinh \theta_i \quad (4)$$

where $v$ is the spin-wave velocity corresponding to the velocity of light in the quantum field theory and $\Delta$ is the gap corresponding to the rest mass energy in the quantum field theory. ($v \approx 2.49 J$ and $\Delta \approx .4107 J$ for the $s=1$ chain.) Thus we may write:

$$S_{ab}(\pi + k, \omega) = s^2 \int dx \int dt \exp(i \omega t - k x) \sum_n \frac{1}{n!} \prod^n_{i=1} \int \frac{d\theta_i}{4\pi} < \Omega | \phi^a(x, t) | n > \langle n | \phi^b(0, 0) | \Omega > . \quad (5)$$

We use

$$< \Omega | \phi(x, t) | n > = < \Omega | \phi(0) | n > \exp[-i(E_n t - P_n x)], \quad (6)$$

where $P_n$ and $E_n$ refer to the total momentum and energy of the state $| n >$, to obtain

$$S(\pi + k, \omega) = s^2 \frac{(2\pi)^3}{3} \sum a \sum n \frac{1}{n!} \prod^n_{i=1} \int \frac{d\theta_i}{4\pi} \delta(k - P_n) \delta(\omega - E_n) | < \Omega | \phi^a(0, 0) | n > |^2 . \quad (7)$$
The field is renormalized
\[ \Phi^a(x) = \frac{1}{\sqrt{Z}} \phi^a(x) \] (8)
in order that we satisfy the relation \( \langle \Omega | \Phi^a(0) | b, p \rangle = \delta^{ab} \). Symmetry arguments guarantee that only asymptotic states with an odd number of magnons will offer non-zero matrix elements.

For the one particle contribution,
\[ S_1(\pi + k, \omega) = s^2 v Z \pi \frac{\delta(\omega - \sqrt{v^2 k^2 + \Delta^2})}{\sqrt{v^2 k^2 + \Delta^2}}. \] (9)

The integrated intensity is,
\[ S_1(q) \equiv \int dw S_1(q, w) = s^2 v Z \pi \frac{1}{\sqrt{v^2 k^2 + \Delta^2}}. \] (10)

Numerical simulations on the \( s = 1 \) antiferromagnet \[6\] indicate that \( Z \approx 1.26 \).

The three particle contribution can be written:
\[ S_3(\pi + k, \omega) = s^2 v Z \frac{\pi}{\sqrt{\omega^2 - v^2 k^2}} \int_0^\infty \frac{d(\theta_1 - \theta_2) d(\theta_2 - \theta_3)}{(4\pi)^2} \delta(\sqrt{\omega^2 - v^2 k^2} - M(\theta_1, \theta_2, \theta_3)) \]
\[ \frac{1}{3} \sum_{a,a_1,a_2,a_3} \langle \Omega | \Phi^a(0,0) | a_1,p_1; a_2,p_2; a_3,p_3 \rangle^2, \] (11)
where:
\[ M \equiv \sqrt{\left( \sum_{i=1}^{3} E_i \right)^2 - v^2 \left( \sum_{i=1}^{3} p_i \right)^2} \] and \( \theta_{ij} \equiv \theta_i - \theta_j. \) (12)

Remarkably, the 3-particle form factor has been calculated exactly using the integrability of the non-linear \( \sigma \) model \[3,4\]:
\[ \frac{1}{3} \sum_{a,a_1,a_2,a_3} \langle \Omega | \Phi^a(0,0) | a_1,p_1; a_2,p_2; a_3,p_3 \rangle^2 = \pi^6 |\psi(\theta_1, \theta_2, \theta_3)|^2 [2(\theta_{21}^2 + \theta_{12}^2 + \theta_{31}^2) + 12\pi^2], \]
\[ \psi(\theta_1, \theta_2, \theta_3) \equiv \prod_{i>j} \psi(\theta_{ij}), \]
\[ \psi(\theta) \equiv \frac{\theta - i\pi}{2(2\pi i - \theta)} \tanh \frac{\theta}{2}. \] (13)

The resulting integral in Eq. (11) can be easily performed numerically. The result for \( S(\pi, \omega) \) is shown in Fig. 1.

![Graph](image-url)  
**FIG. 1.** 1-magnon and 3-magnon contribution to spin-correlation function, \( S(\pi, \omega) \). The factor of \( s^2 v Z \pi / \Delta \) in Eq. (3) has been divided out so that the peak at \( \omega = \Delta \) has unit integral.
The three-magnon contribution vanishes below $3\Delta$. In the limit $\omega \to 3\Delta$, it behaves as:

$$S_3(\pi, \omega) \rightarrow s^2 v Z \times .01045(\omega - 3\Delta)^3/\Delta^5. \quad (14)$$

It has a rounded, asymmetric peak at $\omega \approx 6.33\Delta$ then decays at high energy as $s^2 v Z \times 19.9/\{\omega^2[\ln(\omega/\Delta)]^2\}$. The integrated intensity of the three particle contribution at $q = \pi$ is

$$S_3(\pi) \approx .0193S_1(\pi). \quad (15)$$

This 3-particle contribution to $S(q, \omega)$ is very weak and very broad. It is instructive to calculate the average frequency of the 3-particle term:

$$\bar{\omega}_3 \equiv \frac{\int d\omega S_3(\pi, \omega)}{\int d\omega S_3(\pi, \omega)} \quad (16)$$

Using the result of [4] for the integral in the numerator of Eq. (16) we find:

$$\bar{\omega}_3 \approx 75.2\Delta. \quad (17)$$

It can be seen that the maximum possible energy of a 3 magnon state with total crystal momentum $\pi$ is only about $17\Delta$. $S(\pi, \bar{\omega}_3)$ in the field theory gets significant contributions from bosons with momenta considerably larger than $\pi$, the maximum possible in the lattice model. In fact the relativistic approximation to the dispersion relation seems to break down significantly for $\rho > 2\pi$. We note that, for $\omega < 9\Delta$, only magnons with $\rho < 2\pi$ contribute to $S_3(\pi, \omega)$. Thus we might hope that $S_3(q, \omega)$ calculated from the field theory is fairly accurate for $\pi - q < 2\pi$ and $\omega < 9\Delta$. The non-relativistic corrections to the magnon dispersion relation make $S_3(\pi, \omega)$ vanish for $\omega \geq 17\Delta$. If we only integrate over $S_3(\pi, \omega)$ up to $\omega = 17\Delta$ this reduces $S_3(\pi)$ to about $0.02S_1(\pi)$. However, the non-relativistic corrections may also tend to increase $S_3(\pi, \omega)$ for $9\Delta < \omega < 17\Delta$ since they flatten the dispersion relation hence increasing the density of states. Clearly the value of $\bar{\omega}_3$ in the s=1 chain must be less than the maximum possible frequency of about $17\Delta$. If we make a rough estimate that $\bar{\omega}_3 \approx 10\Delta$ and $S_3(\pi) \approx 0.02S_1(\pi)$ then we can estimate the overall average frequency (also ignoring 5 and more magnon contributions) as:

$$\bar{\omega} \approx \frac{\int d\omega[S_3(\pi, \omega) + S_3(\pi, \omega)]\omega}{\int d\omega[S_3(\pi, \omega) + S_3(\pi, \omega)]} \approx \Delta + \frac{S_3(\pi)}{S_3(\pi, \omega)}\bar{\omega}_3 \approx \Delta[1 + 0.2 \times 10] = 1.2\Delta. \quad (19)$$

This estimate can be compared to the numerically determined value. We may use an exact sum rule for the Heisenberg antiferromagnet:

$$\int d\omega S(q, \omega) = -(1/2) < [H, S^z(q), S^z(-q)] > = (2/3)|e_0|(1 - \cos q), \quad (20)$$

where $e_0$ is the groundstate energy per site. Using the numerically determined value of $S(q)$ and $e_0$ gives $\bar{\omega}(q)$. This is plotted in Fig. (18) of Ref. 3 where it is referred to as $\omega_{\text{SMA}}$. From this figure we see that at $q = \pi$, $\bar{\omega} \approx 1.2\Delta$ in agreement with our crude estimate of Eq. (19). This lends some confidence to our prediction that the 3-magnon contribution to $S(q, \omega)$ near $q \approx \pi$ is extremely broad and extremely weak, with $\bar{\omega}_3$ of order the maximum possible 3-magnon energy, $\approx 10\Delta$ and the relative integrated intensity of order 2%. As such, it will be extremely difficult to observe experimentally. We note that the 2-particle contribution to $S(q, \omega)$ near $q = 0$ is also extremely difficult to observe since it appears to only occur for $q < 2\pi$ and since $S(q, \omega) \propto q^2$ as $q \to 0$. Thus experimental applications of the beautiful exact results [8,2–4] on the non-linear $\sigma$ model remain elusive.

If we assume that the 3-particle form factor in Eq. (13) goes to a non-zero constant at the top of the 3-particle continuum, $\omega \approx 17\Delta$, then it follows from phase space considerations that $S_3(\pi, \omega)$ drops discontinuously to 0 at that
energy. This is quite different than the continuous vanishing of $S_3$ at the bottom of the 3-particle continuum which is entirely due to the vanishing of the form factor there. Possibly this discontinuous drop at the top of the continuum might be easier to observe experimentally than other features. However clearly the tiny size of the drop would make even this extremely difficult.

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