On the 3-particle scattering continuum in quasi one dimensional integer spin Heisenberg magnets

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We analyse the three-particle scattering continuum in quasi one dimensional integer spin Heisenberg antiferromagnets within a low-energy effective field theory framework. We exactly determine the zero temperature dynamical structure factor in the O(3) nonlinear sigma model and in Tsvelik’s Majorana fermion theory. We study the effects of interchain coupling in a Random Phase Approximation. We discuss the application of our results to recent neutron-scattering experiments on the spin-1 Haldane-gap material CsNiCl$_3$.

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I. INTRODUCTION

In recent inelastic neutron scattering experiments $^{1}$ on the quasi one dimensional spin-1 Heisenberg magnet CsNiCl$_3$ $^{2}$, the existence of incoherent multiparticle scattering continua in the one dimensional phase was investigated. If was found, that close to the antiferromagnetic wave vector (along the chain direction), there is significant spectral weight above the coherent magnon peak.

Motivated by these experimental results we determine the dynamical structure factor for weakly coupled integer spin Heisenberg chains in a low-energy effective field theory framework. In particular, we calculate the ratio of spectral weights of multiparticle scattering continua to the coherent magnon peak.

An appropriate model Hamiltonian for CsNiCl$_3$ is

\[ H = J \sum_{<ij>} S_i \cdot S_j + J' \sum_{<ij'>} S_i \cdot S_j + D \sum_n (S_n^z)^2 , \]

where the first and second sums are over nearest neighbour spins along and between the chains respectively. The exchange constants are estimated to be $J \approx 2.8\text{meV}$, $J' \approx 0.045\text{meV}$ and the single-ion anisotropy is estimated to be $D \approx -0.004\text{meV}$. Above the ordering temperature of about 4.84K, CsNiCl$_3$ is considered to be a good realisation of a one dimensional Haldane-gap system, although there is a sizeable dispersion perpendicular to the chain direction due to the interchain coupling. As $D$ is very small, we neglect it from now on.

As a first approximation we can neglect the effects due to $J'$, so that we arrive at the purely one dimensional Heisenberg Hamiltonian

\[ H_{1D} = J \sum_n S_n \cdot S_{n+1} . \]

The dynamical susceptibility for (2) has been calculated numerically for a chain of 20 sites by Takahashi $^{3}$. He found, that about three percent of the total intensity above the antiferromagnetic wave vector are due to incoherent multiparticle scattering continua. A recent dynamical density matrix renormalisation group calculation on large systems of up to 320 sites quotes a result of about 2.5 percent $^{4}$ for this quantity. The purpose of the present work is to determine the incoherent contribution to the structure factor by analytical means in the thermodynamic limit. At present, the best way to do this is by using a low-energy effective field theory description of (2) and taking the interchain coupling in (1) into account perturbatively. The dynamical magnetic susceptibility for a spin chain is given by

\[ \chi_{\alpha\beta}(\omega, q) = -\frac{i}{\mathcal{Q}_0} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt e^{i\omega t - iqx} \times \langle [S^\alpha(t, x), S^\beta(0, 0)] \rangle . \]

Note that we use units in which $\hbar = 1$. The dynamical structure factor is obtained as (see e.g. $^5$)

\[ S_{\alpha\beta}(\omega, q) = -\frac{1}{\pi} \text{Im} \chi_{\alpha\beta}(\omega, q) . \]

Due to the spin-rotational symmetry of (2), we can restrict our attention to the case $\alpha = \beta = \pi$. We denote the corresponding susceptibility and structure factor by $\chi(\omega, q)$ and $S(\omega, q)$, respectively. Below we will calculate the structure factor in two different low-energy effective field theories. We concentrate on the region $q \approx \pi$, which is of experimental relevance. It is known that in this region there exists a coherent one magnon excitation with a gap $\Delta$ and incoherent three, five, seven etc magnon scattering continua. We constrain our analysis to the case of three magnons, which gives the dominant contribution. We also investigate the effects of the coupling between chains, but do not take into account the single-ion anisotropy. We note that the analysis of section $^{11}$ can be easily extended to the case $D \neq 0$.

The outline of this paper is as follows. In section $^{11}$ we determine the dynamical structure factor of the one dimensional model (2) for general integer spin $S$ in the framework of the O(3) nonlinear sigma-model (NL$\sigma$M) description. In section $^{12}$ we study the effects of the coupling between chains in (1), using the NL$\sigma$M results as an input. In section $^{111}$ we determine the structure factor within a second low-energy effective field theory description, which holds for $S = 1$ in the presence of a (strong)
biquadratic exchange interaction \( J \) between spins in addition to (3). Although the structure of the excitation spectrum as a function of wave number along the chain direction is essentially the same as in the NLσM, the structure factor turns out to be rather different. In section V we discuss temperature effects and in section VII we summarise and discuss our results.

II. O(3) NONLINEAR SIGMA MODEL

At energies much smaller than the exchange \( J \), the lattice model (2) (for integer spin \( S \)) can be approximated by a field theory, the O(3) NLσM (see e.g. [8]). The Lagrangian density of the NLσM is given by

\[
\mathcal{L} = \frac{1}{2g} \left[ \left( \frac{\partial m^a}{\partial t} \right)^2 - v \left( \frac{\partial m^a}{\partial x} \right)^2 \right], \quad \vec{m} \cdot \vec{m} = 1 , \quad (5)
\]

where \( \vec{m} \) is a three-component vector and \( v \) is the magnon velocity. The relation between lattice and field theory variables is given by (4).

\[
\hat{S}(x) \approx S(-1)^{x/a_0} \vec{m}(x) + \frac{1}{vg} \vec{m}(x) \times \frac{\partial \vec{m}(x)}{\partial t} , \quad (6)
\]

where \( a_0 \) is the lattice spacing. In order for the NLσM to give an accurate description of the low-energy physics of the spin chain, the spin \( S \) is supposed to be large. However, previous investigations [9] indicate that even for \( S = 1 \) is described rather well by the NLσM. In order for the NLσM to be applicable, the magnon mass gap \( M \) is given by

\[
M = \frac{1}{2} \sqrt{\left( \frac{\partial m^a}{\partial t} \right)^2 - v \left( \frac{\partial m^a}{\partial x} \right)^2} , \quad \vec{m} \cdot \vec{m} = 1 , \quad (5)
\]

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Here we are interested in wave-number transfers close to the antiferromagnetic point \( q \approx \frac{2\pi}{a_0} \). Using (3), we see that the dynamical susceptibility is given by

\[
\chi(\omega, q) = -\frac{i S^2}{a_0} \int_{-\infty}^{\infty} dx \int_{0}^{\infty} dke^{i\omega t - i q x} \times \langle [m_3(t, x), m_3(0, 0)] \rangle . \quad (7)
\]

The two-point function \( \langle m_3(t, x) m_3(0, 0) \rangle \) has been calculated using the formfactor approach [11] in [12,13]. Let us briefly review some relevant formulas. The exact spectrum of the O(3) NLσM consists of three massive magnons \( A_a, a = 1, 2, 3 \), that form the vector representation of O(3). We denote the magnon mass gap by \( M \). Due to factorisability of the exact scattering matrix [6], multi magnon scattering states form a basis of the Hilbert space. Let us introduce some notations. We parametrise energy and momentum of one magnon states in terms of a rapidity variable \( \theta \)

\[
E_k = M v^2 \cosh \theta , \quad P_k = M v \sinh \theta . \quad (8)
\]

A scattering state of \( N \) magnons with rapidities \( \{ \theta_j \} \) and O(3) indices \( \{ \varepsilon_j \} (\varepsilon_j = 1, 2, 3) \) is denoted by

\[
| \theta_1, \theta_2, \ldots , \theta_N \rangle_{\varepsilon_1, \varepsilon_2, \ldots , \varepsilon_N} . \quad (9)
\]

Its energy and momentum are

\[
E_N = M v^2 \sum_{j=1}^{N} \cosh \theta_j , \quad P_N = M v \sum_{j=1}^{N} \sinh \theta_j . \quad (10)
\]

The resolution of the identity is given by

\[
1 = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} d\theta_j \frac{d\theta}{4\pi} | F^{(n)}(\theta_1, \ldots , \theta_n) | ^2 \times | \theta_1, \ldots , \theta_n \rangle_{\varepsilon_1, \ldots , \varepsilon_n} \langle \theta_1, \ldots , \theta_n | . \quad (11)
\]

The two-point function of some operator \( O \) can now be expressed in the spectral representation as

\[
\langle O^1(t, x) O(0, 0) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} d\theta_j \frac{d\theta}{4\pi} | F^{(n)}(\theta_1, \ldots , \theta_n) | ^2 \times \exp \left( -it \sum_{k=1}^{n} \frac{v^2 M \cosh \theta_k + ix v M \sinh \theta_k }{2} \right) . \quad (12)
\]

Here

\[
| F^{(n)}_{O} (\theta_1, \ldots , \theta_n) | ^2 = \sum_{\varepsilon_{j}} | \langle 0 | O^1(0, 0) | \theta_1, \ldots , \theta_n \rangle_{\varepsilon_1, \ldots , \varepsilon_n} | ^2 . \quad (13)
\]

The matrix elements for several operators \( O \) in (13) have been determined in [12,13]. In order to calculate the structure factor, we are interested in matrix elements of (any of the components of) the fundamental field of the NLσM, e.g. \( O = m_3 \). The summed absolute values of the first few matrix elements for this case are

\[
| F^{(2k)} (\theta) | ^2 = 0 , \quad k = 1, 2, \ldots ,
\]

\[
| F^{(1)} (\theta) | ^2 = Z ,
\]

\[
| F^{(3)} (\theta_1, \theta_2, \theta_3) | ^2 = Z r^6 \left[ 12 \pi^2 + 2 \sum_{j<k} (\theta_j - \theta_k)^2 \right] \prod_{k<l} \left( \frac{\theta_k - \theta_l}{2} \right)^4 \left( \frac{\theta_k - \theta_l}{2} \right)^4 \left( \frac{\theta_k - \theta_l}{2} \right)^4 . \quad (14)
\]

Here the overall factor \( Z \) is due to the field renormalisation in the NLσM. In order to determine the dynamical susceptibility, we now use (13) and (12) in (8) and then carry out the \( x \) and \( t \) integrations. In this way we arrive at
\[ \chi(\omega, q) = \frac{Z'}{\omega^2 - v^2q^2 - \Delta^2 + i\varepsilon} + \frac{\pi^2 Z'}{3} \int_{-\infty}^{\infty} \frac{dz}{4\pi} \int_{-\infty}^{\infty} \frac{dy}{4\pi} \left[ 12\pi^2 + 4(3z^2 + y^2) \right] f(z + y)f(z) \]
\[ \times \left( \frac{f(y - z)f(y + z)f(2z)}{\omega^2 - v^2q^2 - \Delta^2 - 4\Delta^2 \cosh z(\cosh z + \cosh y) + i\varepsilon} \right) + \text{contributions from 5, 7, 9... particles,} \]

where \( Z' = S^2 Zv/a_0, \Delta = Mv^2 \) and
\[
 f(z) = \left[ \tanh(z/2) \right]^4 \frac{z^2 + \pi^2}{z^2[z^2 + 4\pi^2]} .
\]

The structure factor close to the antiferromagnetic wave number is obtained from this using (3).

\[
 S(\omega, q) = \frac{Z'}{2\sqrt{v^2q^2 + \Delta^2}} \delta(\omega - \sqrt{v^2q^2 + \Delta^2}) + \frac{\pi^2 Z'}{3} \int_{z_0}^{\infty} dz \left[ 3\pi^2 + 3z^2 + Y \right] f(2z)f(z + Y)f(z - Y) \]
\[ \times \frac{1}{\sqrt{\left[ (\omega^2 - v^2q^2 - \Delta^2 - 4\Delta^2 \cosh \Delta z)^2 - 16\Delta^4 \cosh^2 \Delta z \right]}} + \text{contributions from 5, 7, 9... particles.} \]

(17)

Here \( z_0 = \text{arccosh} \frac{1}{2} \) and \( Y = \text{arccosh} \frac{\sqrt{v^2q^2 + \Delta^2}}{4\cosh \Delta z} \). An important difference between (17) and (13) is the way, in which states with 3, 5, 7... magnons contribute. It can be easily seen from the upper limit of integration, that three magnon states contribute to the structure factor only if \( s^2 = \omega^2 - v^2q^2 > 9\Delta^2 \), i.e. above the three magnon threshold. Similarly, \( 2n + 1 \) magnon states only contribute if \( s > (2n + 1)\Delta \). In other words, (17) is exact as long as \( s < 5\Delta \). The situation is quite different for \( \Re \chi(\omega, q) \): here multi magnon states contribute for all values of \( s \). However, their contribution is negligible at small \( s \) (see e.g. (13)). The first contribution in (17) is due to the coherent one magnon states with dispersion \( \omega = \sqrt{v^2q^2 + \Delta^2} \), which is known to be a good approximation to the lattice-dispersion as long as \( q \) is sufficiently small (recall that in our notations \( q \) denotes the deviation from \( \pi/a_0 \)). The total spectral weight cannot be calculated within the NL\( \sigma \)M framework, so that one has to resort to a direct numerical analysis of the quantum spin chain. For the spin-1 case this yields (14) \( Z' \approx 1.28\frac{S^2}{a_0} \), \( v = 2.51a_0 \).

The remaining integral in the three magnon contribution to (13) can be evaluated numerically. The result is shown in Fig. 3.

![Fig. 1. NL\( \sigma \)M result for the three magnon contribution to the dynamical structure factor close to the antiferromagnetic point. Here \( M \) is the magnon mass-gap, \( v \) the spin velocity and \( s = \sqrt{v^2q^2 + \Delta^2} \).](image)

The behaviour of the structure factor just above the three magnon threshold can easily be determined by Taylor-expanding the integrand in (17). The result is
\[
 S(\omega, q) \approx \frac{Z'}{\Delta^2} \frac{\pi^7}{16\sqrt{3}} [s - 3\Delta]^3, \quad 0 < s - 3\Delta \ll 1 .
\]

The ratio of total spectral weights of the one magnon (1) and three magnon (3) contributions can be calculated as well. Numerically we find that that ratio of spectral weights at wave number \( \pi/a_0 \) is roughly equal to
\[
 \frac{I_3(\pi)}{I_1(\pi)} \approx 0.02 .
\]

We note that a sizeable fraction of the three magnon spectral weight is located at very high energies, where the field theory does not relate to the lattice spin model. If we restrict \( \omega \) to be smaller than twenty times the magnon gap, the ratio (14) diminishes to about 0.013.

The NL\( \sigma \)M result is somewhat at odds with the numerical results (14) on the spin 1 chain. The most likely reason is that the NL\( \sigma \)M does not work as well for \( S = 1 \) as previously thought. Irrespective of the one percent difference between NL\( \sigma \)M and numerical results it seems clear that the three magnon continuum of a single spin-1 chain is extremely weak! In quasi one dimensional materials like CsNiCl\(_3\) such a faint contribution would hardly be measurable experimentally as it would go under in the inevitable errors due to e.g. background subtraction.

Another relevant quantity as far as the experiments of (2) are concerned, is the ratio of three and one magnon spectral weights for \( q \neq 0 \). We find that e.g.
\[
 \frac{I_3([1 \pm 0.2\pi])}{I_1([1 \pm 0.2\pi])} \approx 0.04 .
\]

The increase in (20) as compared to (13) is mainly due to the decrease in spectral weight of the single magnon peak
\[ \frac{I_1([1 \pm 0.2][\pi])}{I_1(\pi)} \approx 0.45 . \] (21)

Let us now determine the real part of the dynamical susceptibility, which we will need in section III. Neglecting contributions of more than three magnons we arrive at the results shown in Fig. 2.

The coherent one magnon contribution to the structure factor is found to be

\[ S(\omega, q, \vec{k}) \bigg|_{\text{1 magnon}} = \frac{Z'}{2 \sqrt{\omega^2 q^2 + \Delta^2 + Z' J(\vec{k})}} \times \delta \left( \omega - \sqrt{\omega^2 q^2 + \Delta^2 + Z' J(\vec{k})} \right) . \] (25)

We see that the total spectral weight due to one magnon processes depends on the transverse wave-number transfer \( \vec{k} \).

From now on we consider the particular case of wave-number transfer \( \vec{k} = (\eta, \eta, 0) \) along the \((1,1,0)\) direction in CsNiCl₃, which is of direct experimental relevance \[1\,2\]. The \( \eta \) dependence of \( J(\vec{k}) \) is of the form

\[ J(\vec{k}) = 2J' \left( \cos 4\eta \pi + 2 \cos 2\eta \pi \right) . \] (26)

We note that at the special point \( \vec{k}_0 = (0.19, 0.19, 0) \) we have \( J(\vec{k}) = 0 \), so that (in our approximation) we are dealing with an ensemble of uncoupled chains. By fitting \((24)\) with \((26)\) to the experimentally observed magnon dispersion along the \((1,1,0)\) direction \[3\], we obtain

\[ \Delta \approx 1.32 \text{meV} , \quad Z' J' \approx 0.475 \text{meV}^2 . \] (27)

The resulting value of \( J' \approx 0.05 \text{meV} \) is by construction close to \[3\]. The variation of the total spectral weight \( I_1(\pi, \eta) \) of the one magnon peak with \( \eta \) \[23\] (with fixed wave number \( \pi/a_0 \) along the chain) is shown in Fig. 3.

\[ I_1(\pi, \eta) \bigg|_{\eta = 0.19} \] (23)

Note that \((23)\) involves both the real and imaginary parts of the one dimensional dynamical susceptibility. The

\[ m \] magnon dispersion close to the antiferromagnetic point along the chains is easily extracted from the poles of \((23)\)

\[ \omega^2 = v^2 q^2 + \Delta^2 + Z' J(\vec{k}) . \] (24)
The three magnon contribution to the structure factor is of the form

\[ S(\omega, q, \vec{k})|_{3 \text{ magnons}} = \frac{S(\omega, q)|_{3 \text{ magnons}}}{1 - J(\vec{k})\chi(\omega, q)} \].

(28)

Here we used the fact that the real part of the one-dimensional dynamical susceptibility did not exhibit any singularities. A result of this is that the three magnon continuum for fixed \( \eta \) starts at three times the magnon gap only at the special point \( \eta = 0.19 \).

From the analysis in section II we know that the dominant contribution to \( \chi(\omega, q) \) for \( \omega > 3\Delta \) is due to the real part of the one magnon contribution, which gives us an easy way to estimate the effects of the interchain coupling on the three magnon continuum

\[ S(\omega, \pi/\alpha_0, \vec{k})|_{3 \text{ magnons}} \approx S(\omega, \pi/\alpha_0)|_{3 \text{ magnons}} \times \left(1 - 0.547 \frac{\cos 4\pi \eta + 2 \cos 2\pi \eta}{(\omega/M)^2 - 1}\right)^{-2}. \]

(29)

In order to estimate the ratio of spectral weights of the three and one magnon states as a function of \( \eta \) we define

\[ I'_3(\pi, \eta) = \int_0^{20 M} d\omega S(\omega, \pi/\alpha_0, \vec{k})|_{3 \text{ magnons}}. \]

(30)

Here the cutoff at twenty times the magnon gap has been chosen arbitrarily. Note that the introduction of a cutoff is necessary to ensure the applicability of the field-theory description. The ratio of the three magnon spectral weight \( I'_3(\pi, \eta) \) to the one magnon spectral weight \( I_1(\pi, \eta) \) for wave-number transfer \( \eta \) along the \((1,1,0)\) direction to the total one magnon spectral weight \( I_1(\pi, \eta) \) is shown in Fig.4.

FIG. 4. Ratio of the total spectral weights of the three magnon continuum \( I'_3(\pi, \eta) \) to the one magnon spectral weight \( I_1(\pi, \eta) \) for wave-number transfer \( \eta \) along the \((1,1,0)\) direction.

We see that in all cases only a very small fraction of the total spectral weight sits in the incoherent three magnon scattering continuum. This fraction is at most two percent, which is much smaller than what has been observed experimentally in CsNiCl\(_3\). We conclude that the coupling between chains cannot account for the observed intensity in the incoherent scattering continuum at \( \pi/a_0 \) as long as we use a NLS\( \sigma \)M description for a single chain.

IV. TSVELIK’S MAJORANA FERMION THEORY

Apart from the NLS\( \sigma \)M there is a second low-energy effective field theory for Haldane-gap systems, due to A. M. Tsvelik [16]. It applies to spin-1 models of the type

\[ H = J \sum_{n=1}^{L} \vec{S}_n \cdot \vec{S}_{n+1} - b \left( \vec{S}_n \cdot \vec{S}_{n+1} \right)^2 + D(S_n^z)^2. \]

(31)

where \( b \approx 1 \). We note that one of the effects of \( b \neq 0 \) is to reduce the magnitude of the Haldane gap, which rules out a very large value of \( b \) in CsNiCl\(_3\). Using the Bethe Ansatz solution of (31) at the Armenian point \( b = 1 \), \( D = 0 \) [17], it is possible to derive (14) the following low-energy effective field theory of three interacting Majorana fermions valid for small \( 1 - b \) and \( D \)

\[ \mathcal{L} = i\gamma_a \gamma_\mu \partial_\mu \chi_a - m_a \chi_a \chi_a + g_a J_{\mu}^a J_{\mu}^a. \]

(32)

Here \( a = 1, 2, 3 \), \( \chi_a \) are two-component Majorana (real) fermions, \( \chi_a = \chi^T_a \gamma_0 \), \( J_{\mu}^a = \varepsilon^{abc} \gamma_\mu \gamma_a \chi_c \) are the components of SU(2) currents and our conventions for gamma matrices are

\[ \gamma_0 = \sigma_x, \quad \gamma_1 = i\sigma_y. \]

(33)

In the absence of a single-ion anisotropy \( (D = 0) \), the model is SU(2) symmetric and all Majorana masses and couplings \( g_a \) equal. We will constrain our discussion to this case only. Following [18] we will furthermore neglect the current-current interaction i.e. set \( g_a = 0 \). This is certainly justified as long as the mass gaps are not too small and we are only interested in single-particle properties as can be seen from a standard one-loop renormalisation group calculation. However, it is presently not clear whether this remains a good approximation for the calculation of the three magnon scattering continuum. In fact, it was recently argued [15] that the current-current interaction may become rather important for the calculation of finite-temperature properties of spin-1/2 ladder models, which have a very similar field-theory description [19]. After setting \( g_a = 0 \), (32) reduces to a theory of three noninteracting Ising models and exact information on correlation functions is available. The staggered components of the lattice spin operators are expressed in terms of order (\( \sigma \)) and disorder (\( \mu \)) operators of the three Ising models as

\[ (-1)^{x/a_0} S^x(t, x) = \sqrt{2} \sigma^1(t, x) \mu^2(t, x) \mu^3(t, x). \]

(34)
where the coefficient $A$ is presently not known. The dynamical susceptibility close to the antiferromagnetic wave number $\pi$ is thus given by

$$
\chi(\omega, q) = \frac{-iA}{\omega_0} \int_{-\infty}^{\infty} dx \int_{0}^{\infty} dt e^{-i\omega t+iq x} \times \langle \left[ (\sigma^1 \mu^2 \mu^3)(t, x), (\sigma^1 \mu^2 \mu^3)(0, 0) \right] \rangle \, .
$$

(35)

In order to determine (35) we therefore need to calculate $(G_\mu(t, x))^2 G_\sigma(t, x)$, where

$$
G_\sigma(t, x) = \langle \sigma(t, x) \sigma(0, 0) \rangle \, ,
$$

$$
G_\mu(t, x) = \langle \mu(t, x) \mu(0, 0) \rangle \, ,
$$

(36)

are correlation functions of order and disorder operators in the two-dimensional Ising model. These are known exactly [21]. For our purposes it is most convenient to work in the Minkowski-space spectral representation, which reads [21]

$$
\langle \mathcal{O}^1(t, x) \mathcal{O}(0, 0) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} \prod_{j=1}^{n} \frac{d\theta_j}{2\pi} \left| \mathcal{F}^{(n)}(\theta_1, \ldots, \theta_n) \right|^2 \times \exp \left( -i t \sum_{k=1}^{n} v^2 M \cosh \theta_k + i x \sum_{k=1}^{n} v M \sinh \theta_k \right) \, ,
$$

(37)

where

$$
\mathcal{F}^{(2n+1)}(\theta_1, \ldots, \theta_{2n+1}) = i^{2n+1} \prod_{i<j=1}^{2n+1} \tanh \frac{\theta_i - \theta_j}{2} \, ,
$$

$$
\mathcal{F}^{(2n)}(\theta_1, \ldots, \theta_{2n}) = i^n \prod_{i<j=1}^{2n} \tanh \frac{\theta_i - \theta_j}{2} \, .
$$

(38)

After performing the Fourier integrals we arrive at the following representation for the dynamical structure factor

$$
S(\omega, q) = \frac{v A}{\sqrt{v^2 q^2 + \Delta^2}} \delta(\omega - \sqrt{v^2 q^2 + \Delta^2})
$$

$$
+ \frac{4v A}{\pi^2 \Delta^2} \int_{0}^{z_0} dz \frac{\tanh^2 z + \frac{1}{6} \left[ \tanh z \tanh \frac{Y_{\pi/2} + z}{2} \tanh \frac{Y_{\pi/2} - z}{2} \right]^2}{\sqrt{(x^2 - 1 - 4 \cosh^2 z)^2 - 16 \cosh^2 z}}
$$

$$
+ \text{contributions from 5, 7, 9... particles} \, ,
$$

(39)

where $x^2 = (\omega^2 - v^2 q^2)/\Delta^2$ and $z_0$ and $Y$ are defined above. The one and three particle contributions in (39) give the exact result as long as $s \leq 5 \Delta$. For frequencies just above the three-particle threshold the integral in (39) can be easily evaluated by Taylor-expanding the integrand

$$
S(\omega, q) = \frac{A v^2 - v^2 q^2 - 9 \Delta^2}{24 \sqrt{3} \Delta^4} \, .
$$

(40)

Eqn. (40) agrees with a result obtained for correlation functions of the spin-1/2 ladder [19,22].

Performing the remaining integral in (39) numerically, we obtain the three magnon contribution to (39) as shown in Fig. 3.

FIG. 5. Result for the three magnon contribution to the dynamical structure factor close to the antiferromagnetic point in Tsvelik’s Majorana fermion theory. Here $M$ is the magnon mass-gap, $v$ the spin velocity and $s = \sqrt{v^2 q^2 + \Delta^2}$.

The ratio of spectral weights of three-particle and one-particle contributions to the structure factor (39) for frequencies restricted to $\omega < 20 M$ is roughly equal to

$$
\frac{I_3(\pi)}{I_1(\pi)} \approx 0.17 \, .
$$

(41)

Thus the three-particle scattering continuum is much stronger than in the NLσM! The coupling between chains can be taken into account in complete analogy with the NLσM case. Furthermore it is in principle possible to analytically study the effects of the single-ion anisotropy in the Majorana fermion theory.

V. TEMPERATURE

An additional complication in CsNiCl$_3$ is that the ordering temperature 4.84K is of the same order of magnitude as the Haldane gap $\Delta \approx 15.4$K. Clearly temperature effects will therefore not be negligible in the temperature range in which Neutron scattering experiments are conducted (5K-10K). One way of taking them into account would be to use recent results for finite-temperature correlation functions of the Ising model [23] in order to extend the analysis of section [18]. This is nontrivial, so that we constrain ourselves to a rather preliminary discussion based on recent results of [18]. There it was shown, that the finite temperature lineshape of the one magnon peak at very low temperatures $T \ll \Delta$ is given by

$$
S(\omega, q) = A' T \exp(-\Delta/T)
$$

where
\times \frac{1}{(\omega - \sqrt{\Delta^2 + v^2 q^2})^2 + (1.2T \exp(-\Delta/T))^2}.
\end{equation}

In other words, at temperatures much smaller than the Haldane gap the lineshape is Lorentzian. Although (42) does not really apply to CsNiCl$_3$ because $T = \mathcal{O}(\Delta)$, it can be taken as an indication that in the experimentally relevant temperature range, a sizeable fraction of what used to be the one magnon spectral weight at $T = 0$ may get transferred to energies significantly above the single magnon gap $\Delta$.

\section{VI. SUMMARY AND CONCLUSIONS}

Using a low-energy effective field theory description (that needs to be supplemented by numerical results in order to fix overall normalisations) we have studied the dynamical structure factor for weakly coupled integer spin Heisenberg chains. The three particle incoherent scattering continuum calculated in the $O(3)$ NL$\sigma$M is found to be too small to be observed in neutron scattering experiments.

On the other hand, Tsvelik's Majorana fermion theory yields a very strong three particle scattering continuum, which would be easily observable in experiments. The main difference between the NL$\sigma$M and the Majorana fermion theory is that in the latter the spin Hamiltonian contains strong biquadratic interactions of the form

\begin{equation}
\sum_n (\vec{S}_n \cdot \vec{S}_{n+1})^2.
\end{equation}

The presence of such interactions in e.g. CsNiCl$_3$ cannot a priori be ruled out. As a matter of fact we believe that spin-1 materials generically have at least small interaction terms of the form (43).

In the neutron scattering experiments a significant incoherent scattering continuum has been observed for several different temperatures. These findings are incompatible with the NL$\sigma$M results. However, the results of section IV indicate that biquadratic exchange interactions lead to a transfer of spectral weight from the coherent magnon peak to the incoherent scattering continuum. One possible scenario for reconciling (field) theory with the experimental findings is thus to postulate the existence of a sizeable biquadratic exchange interaction in CsNiCl$_3$. To the best of our knowledge no detailed (beyond 2D) theoretical study of the effects of biquadratic exchange interactions on the dynamical structure factor has been carried out. We believe that it would be interesting to do so.

As far as the present analysis is concerned, it has several shortcomings that ought to be improved upon in future work. Firstly, our analysis is restricted to zero temperature. As we argued above, temperature effects are important in the experimentally realised range of parameters. However, we believe it is unlikely that the finding of the large magnon spectral weight due to temperature effects only. Secondly, the analysis in the framework of the Majorana fermion theory did not take into account the current-current interaction. The results of section V therefore should be regarded with some caution. It would be very interesting to carry out a systematic analysis of the effects of the current-current interaction.

Finally, we would like to mention that the analysis of section V applies with minor modifications to the case of the spin-$1/2$ ladder as well. This is because the effective field theory description is very similar.

While this paper was being written, a preprint (cond-mat/9907431) by M.D.P. Horton and I. Affleck appeared, in which the three magnon contribution to the dynamical structure factor in the NL$\sigma$M was calculated. Their results have a strong overlap with our section I.

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