Revisiting the Exact Dynamical Structure Factor of the Heisenberg Antiferromagnetic Model

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Résumé

We revisit our initial derivations of the exact 2-spinon \( S_2 \) and 4-spinon \( S_4 \) dynamical structure factors (DSF). First we show that the latter derivations had normalization factors that are twice and quadruple the correct ones respectively. This means that \( S_2 \) contributes not 72% as was previously thought but 36% to the total DSF. We also calculated the contribution of \( S_4 \) to be between 18% and 20% and not 27% as was calculated by Caux and Hagemans. In fact we show that the latter reference had also the normalization factor twice the correct value and had it done the numeric integrations correctly it would have obtained a contribution between 36% and 40% for \( S_4 \). Furthermore, we prove that its claim that our initial derivation of \( S_4 \) was also incorrect in its dependency on the spectral parameters is incorrect because fixing the momentum transfer \( k \) up to \( 2\pi \) as the latter reference did to justify its claim only amounts to multiplying the overall factor by 2 because as we will prove in this paper \( S_4 \) is periodic in \( k \) with period \( 2\pi \). Also in this paper we derive \( S_n \) for general \( n \) by following a different approach compared to our initial derivation of \( S_4 \). Although for \( S_4 \) both the new derivation and the initial one lead to equivalent formulas that are expressed differently, the new form presented in this paper is much more elegant and compact and also reveals new hidden and nontrivial symmetries which substantially simplify the numeric evaluation of \( S_4 \) and its sum rules. Moreover based on the results of this paper we propose a simple approximation to the total DSF of the Heisenberg model. Finally we comment on how our work might resolve the discrepancy between the exact theoretic results and experimental data as reported by Zaliznyak et al.

1 Introduction

It is well known that the family of 1D quantum spin chain models play a crucial role both from a physical point of view and a mathematical point of view as they lend themselves to exact solutions based on mathematical algebraic theories and they lend themselves to precise experiments in the lab [1-15]. This is due to the fact that these models exhibit symmetries that can be described rigorously by well known algebras and their spectrum of eigenspaces can be built from well structured representations of these algebras. Moreover in the thermodynamic limit, the symmetries of these models become infinite dimensional meaning that the latter models must satisfy an infinite number of constraints. Because of this only a finite number of representations survive, thus making these models exactly and completely solvable. By completely solvable we mean not only can we describe exactly their eigenspaces but also exactly calculate the physical quantities such as the \( S \) matrix, the form factors of their local operators, and the static

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and dynamic correlation functions. Although in the latter case the physical quantities are often expressed as sums of infinite series they nonetheless often converge and only a finite number of terms contribute to any given precision. This is to be contrasted with the finite chains case where the symmetries are described by finite algebras having an infinite number of representations thus rendering these models not completely and exactly solvable. The model by excellence that embodies this phenomenon is the anisotropic Heisenberg chain in the thermodynamic limit which was shown in \cite{12,13} to be symmetric under the infinite dimensional quantum affine algebra $U_q(sl(2))$. Since this algebra has only two representations therefore this model is exactly solvable. Indeed the static correlation functions and the form factors were exactly calculated in \cite{13}. Based on them the dynamical structure factors (DSF) due to 2 spinons and 4 spinons were exactly calculated in \cite{16} and \cite{17} respectively. Further studies in \cite{18} and \cite{19} using the sum rules showed that the 2-spinon DSF contributes 72% and the 4-spinon DSF contributes 27% to the total DSF, respectively. This would then mean that the contributions of both $S_2$ and $S_4$ would account for 99% of the total DSF. However experimental data obtained in \cite{20} and \cite{21} reveal that the observed contribution accounts roughly only for the third of the total theoretic DSF. Motivated by these experimental data and the inconsistency they raised with respect to the currently available exact theoretic results we decided to reexamine our initial derivations of the 2-spinon DSF in \cite{16} and 4-spinon DSF in \cite{17} and to relate them as a consistency check to the exact static correlation functions obtained in \cite{13} and \cite{22}. The main conclusion we reach and that we will explain in details in this paper is that the normalisation overall factor of $S_2$ was overevaluated by a factor 2 in \cite{16} and the normalisation overall factor of $S_4$ was also overevaluated by a factor of 4 in \cite{17} and by a factor of 2 in \cite{19}. This means $S_2$ contributes 36% instead of 72% and the 4-spinon DSF contributes $18 - 20\%$ instead of 27% to the total DSF, respectively. In fact we believe that if the numeric calculation was done correctly in \cite{19} they would have obtained a contribution of 36% – 40% and not 27%. This would have been a major inconsistency since at that time $S_2$ was believed to contribute already 72% which means that $S_2$ and $S_4$ together would contribute more than 100% which obviously is impossible. Therefore one of the results of the present paper is then the contributions of $S_2$ and $S_4$ add up to only $54 - 56\%$. We believe that the observed DSF as reported in \cite{20,21} which accounts for the third of the total DSF would be just the contribution of $S_2$ which we found to be 36% which is roughly the third of 100%.

Unlike our original derivations of $S_2$ and $S_4$ where we have calculated them first in the anisotropic case and then taken the isotropic limit at the last stage, this time around we decided to derive $S_n$ for the general case of $n$ spinons by starting out from the form factors directly in the isotropic limit. In the latter limit the form factors are expressed as integrals in the case of $n \geq 4$ but they have an incorrect overall factor in \cite{13} that we correct in this paper. We then analytically integrate the latter integrals explicitly. We get the same expression for $S_2$ as before but for $S_4$ we get a new formula that is equivalent to the old one but expressed in a different form. In particular our new derivation highlights the existence of hidden structures represented by the appearance of a new vector of function elements and a new matrix of function elements in terms of which $S_4$ is simply expressed. Both the latter function elements satisfy highly nontrivial symmetry relations with respect to the permutations of both their spectral parameters and their indices which identify the 4 spinons. As a byproduct of these symmetries which translate into a simple expression of $S_4$, the actual numerical computation for the purpose of sum rules and for the purpose of graphical plotting of $S_4$ are greatly simplified as we will see in the main text. As a new result presented in this paper we show that in the general case of $S_n$ the overall normalisation factor can be expressed simply in terms of the Glaisher-Kinkelin constant and only in the case of $S_2$ does this constant cancel out leading to a simple overall factor of $1/4$. This provides an analytic proof why the $S_2$ normalisation factor is exactly equal to $1/4$, a result which as far
as we know was only derived numerically in [18].

We make a comment on the expression for $S_4$ presented in [19] by noting that it is the same as the one originally computed by us in [17] up to an overall factor. To be more precise in [17] we had an incorrect extra multiplicative factor of 2 from adding contributions to the DSF from both sectors $i = 0, 1$ corresponding to the two possible representations of $U_q(sl(2))$, and an incorrect extra multiplicative factor of 4 from expressing the sums of exponentials of the energy terms and the sums of exponentials of the momenta terms in terms of the delta functions, and a missing multiplicative factor of 2 from the possibility of fixing the spinon momenta only up to $2\pi$. The reason why the last error amounts only to a missing 2 multiplicative factor is that in general $S_n$ is periodic with respect to the momentum transfer and spinon momenta with period $2\pi$. Therefore adding the contribution of the DSF when one of the spinon momenta is shifted by $2\pi$ (which in turn amounts to shifting the momentum transfer by $2\pi$) simply amounts to a multiplicative overall factor of 2. In [19] they justified the latter contribution by saying that the delta function fixes the momentum transfer only up to $2\pi$ but in fact it is not the momentum transfer that is fixed up to $2\pi$ and which should be exactly fixed but it is rather the momenta of the spinons which are fixed up to $2\pi$. Also in the latter reference it is not clear why they have not used the same argument with respect to the delta function of the energies to justify a fixing of the energy transfer only up to $2\pi$ in a similar manner as they did for the momenta. In fact part of our analysis is to prove that there is an asymmetry between the momenta of the spinons which are fixed only up to $2\pi$ and the energies of the spinons which are exactly fixed. Also in this reference the authors proposed an overall factor in an ad hoc manner without any justification of its derivation from first principles as we do in this paper but their overall factor also has the incorrect extra multiplicative factor of 2 from adding contributions to the DSF from both sectors of the eigenspace. Finally we also believe that their numerics are less precise when it comes to the computation of the sum rules in that they found $S_4$ to account for 27% when they should have found somewhere between 36% and 40%. So to sum up in the case of $S_4$ our initial paper [17] had an incorrect extra multiplicative factor of 4 in its normalization factor, whereas the paper in [19] has an incorrect multiplicative factor of 2 and less precise numeric evaluations of the sum rules. We also compare our initial expression for $S_4$ with the one used in [23] and conclude that their expression used a incorrect overall normalisation factor to start with and also their Monte Carlo integration was incorrect.

Since in this paper we show that $S_2$ and $S_4$ saturate the total DSF only up to 54% – 56% we need therefore to study the higher sectors as well. From the shapes of $S_2$ and $S_4$ as functions of energy transfer for fixed momentum transfer one can notice that they are very similar in that $S_4$ almost looks like a scaled down version of $S_2$ in the common first Brouillin zone $[0, 2\pi]$. Beyond $[0, 2\pi]$ $S_2$ is null and $S_4$ is extremely small. One is tempted then to conclude that this pattern would still hold true for the general $S_n$. Since $S_2$ is the only one which is very simple and expressed as a single term and captures the general shape of the general $S_n$ up to a scale factor we propose then an approximation to the total DSF as a scaled up version of $S_2$ such that it saturates the sum rules. This approximation is somewhere in the middle between the Muller ansatz and the exact one. It is better than the Muller ansatz because it has a much better shape that closely fits the experimental data and it is almost as simple as the Muller ansatz, and also it is much simpler that the exact total DSF which is very complex. The only drawback is that it misses all the spectral weight beyond the first Brouillin zone of $[0, 2\pi]$ although the latter is negligible for general $n$.

Finally we note that in this paper for the purpose of plotting $S_4$ and calculating its sum rules
we have used the Genz-Malik adaptive algorithm \[24\] for evaluating high dimensional integrals. As discussed in \[25\] the initial Genz-Malik adaptive integration method and its Berntsen-Espelid-Genz \[26\] enhanced version are highly superior to Monte Carlo or Quasi Monte Carlo methods because the latter can be inefficient if most of the randomly generated points lie outside the region where the integrand contributes the most to the integral. Even the better uniform properties of quasi-Monte Carlo sequences over Monte Carlo simulation can also be useless. In addition, both Monte Carlo and quasi-Monte Carlo methods are not able to take advantage of the regular behavior of the integrand. However, the Genz-Malik adaptive integration algorithm can be highly superior to Monte Carlo and quasi-Monte Carlo methods because it successively divides the integration region into subregions and detects the subregions where the integrand is most irregular (such as functions with peaks, singular points, discontinuities, oscillatory) and therefore places more points in those subregions. The Berntsen-Espelid-Genz enhanced version of the latter algorithm has a more sophisticated algorithm for the error estimation. The only disadvantage of the adaptive algorithms compared to Monte Carlo and Quasi Monte Carlo is that they do not scale well to very high dimensions because the number of evaluation points in each subregion increases exponentially, thus facing the dreaded curse of dimensionality again. In fact they are useful for small to moderate number of dimensions from 2 to 11, beyond which Monte Carlo and Quasi Monte Carlo are still the better option. Since in this paper we are faced with 2d integrations for $S_4$ and the sum rules of $S_2$, and 4d integration of the sum rules of $S_4$ we use the adaptive Berntsen-Espelid-Genz algorithm.

This paper is organized as follows in section 2. we compute analytically $S_n$ DSF for the general case of $n$ spinons and then we specialize it to 2-spinon et 4-spinon cases. Here we also prove that the physical DSF is obtained only from one sector of the eigenspace and not both sectors as was incorrectly done in our initial derivation. In section 3. we study the sum rules of $S_2$, $S_4$ and $S_n$ in general. In particular we show that $S_2$ contributes 36% and $S_4$ contributes between 18% and 20% depending on which sum rule is used. In section 4. we present our approximate total DSF of the Heisenberg model. Finally in section 5. we present our conclusions.

2 n-spinon DSF

The Hamiltonian of the anisotropic (XXZ) Heisenberg model is defined by

$$H_{XXZ} = -\frac{1}{2} \sum_{n=-\infty}^{\infty} (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z),$$

where $\Delta = (q + q^{-1})/2$ is the anisotropy parameter. Here $\sigma_n^x, y, z$ are the usual Pauli matrices acting at the $n_{th}$ position of the formal infinite tensor product

$$W = \cdots V \otimes V \otimes V \cdots,$$

where $V$ is the two-dimensional representation of $U_q(sl(2))$ quantum group. We consider the model in the anti-ferromagnetic regime $\Delta < -1$, i.e., $-1 < q < 0$. Refs. \[12\] \[13\] diagonalized $H_{XXZ}$ in terms of the set of eigenstates (spinons) denoted by $\mathcal{F} = \{ |\xi_1, \cdots, \xi_n > ; \xi_1, \cdots, \xi_n \geq 0, \ i = 0, 1 \}$. Here $i$ fixes the boundary conditions such that the allowable spin configurations are those for which the eigenvalues of $\sigma_n^z$ are $(-1)^{i+n}$ in the limit $n \rightarrow \pm \infty$. $\xi_j$ are the spectral parameters living on the unit circle, and $\epsilon_j = \pm 1$ are the spins of the spinons. The actions of
The dynamic structure function (DSF) corresponding to the operators

$$T|\xi_1, \cdots, \xi_n >_i = \prod_{i=1}^{n} \tau(\xi_i)^{-1} |\xi_1, \cdots, \xi_n >_{1-i}, \quad T|0 >_i = |0 >_{1-i},$$

$$H_{XXZ}|\xi_1, \cdots, \xi_n >_i = \sum_{i=1}^{n} e(\xi_i)|\xi_1, \cdots, \xi_n >_i,$$

where

$$\tau(\xi) = \xi^{-1} \theta_4(q\xi^2) = e^{-i\alpha}, \quad p(\alpha) = am(2K - \alpha) - \pi/2,$$

$$e(\alpha) = \frac{1-q^2}{2q} \frac{d}{d\alpha} \log \tau(\xi) = \frac{2K}{\pi} \sinh(\frac{\pi K'}{K}) \eta(2K - \alpha).$$

Here, $e(\alpha)$ and $p(\alpha)$ are the energy and the momentum of the spinon respectively, $am(\alpha)$ and $dn(\alpha)$ are the usual elliptic functions and delta functions respectively, with the complete elliptic integrals of the first kind $K$ and $K'$, and

$$q = -\exp(-\pi K'/K), \quad \xi = ie^{i\alpha},$$

$$\theta_x(y) = (x; y, x)_\infty(x^{-1}; y)_\infty,$$

$$\eta(x; y) = \prod_{n=0}^{\infty} (1 - xy^n).$$

Thus the anisotropic parameter $q$ in the anisotropic Heisenberg model XXZ plays also the dual role of being the nome of the latter elliptic functions and the deformation parameter of the quantum group $U_q(sl(2))$ under which XXZ is symmetric. The local operators $\sigma^{x,y,z}(t,n)$ at time $t$ and position $n$ are related to $\sigma^{x,y,z}(0,0)$ at time 0 and position 0 through :

$$\sigma^{x,y,z}(t,n) = \exp(itH_{XXZ})T^{n-1}\sigma^{x,y,z}(0,0)T^n \exp(-itH_{XXZ}).$$

The completeness relation over $\mathcal{F}$ reads [13] :

$$I = \frac{1}{n!} \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \sum_{m=1}^{\infty} \frac{1}{\eta(\xi_1, \cdots, \xi_n)} d\xi_1 \cdots d\xi_n |\xi_1, \cdots, \xi_n >_i \leq \xi_1, \cdots, \xi_n >_i, \xi_1 > \cdots > \xi_n >_i.$$

where $I$ is the identity operator acting on $\mathcal{F}$. In the case of the anisotropic ZZ model the dynamic structure function (DSF) corresponding to the operators $\sigma^z = (\sigma^x \pm i\sigma^y)/2$ and to the sector $i$ of $\mathcal{F}$ is defined by :

$$S^{i,-}(w,k) = \int_{-\infty}^{\infty} dt \sum_{m \in Z} e^{i(wt + km)} \xi < 0|\sigma^+(t,m)\sigma^-(0,0)|0 >_i,$$

where in the above Fourier transform $w$ and $k$ are the energy and momentum transfer respectively, and $Z$ is the set of integers. As we will see later it turns out that the DSF is in fact independent of $i$ and therefore the same for both sectors. One can always insert the identity operator between the operators $\sigma^+(t,n)$ and $\sigma^-(0,0)$ in (8) without affecting the value of $S^{i,-}(w,k)$, that is :

$$S^{i,-}(w,k) = \int_{-\infty}^{\infty} dt \sum_{m \in Z} e^{i(wt + km)} \xi < 0|\sigma^+(t,m)I\sigma^-(0,0)|0 >_i.$$
with the $n$-spinon DSF $S_{n}^{++}(w, k)$ being defined by:

$$S_{n}^{++}(w, k) = \frac{1}{\pi} \prod_{e_{n}=\pm 1} \int_{-\infty}^{\infty} dt \sum_{m \in Z} e^{i(w+km)t}$$

where we have used the orthogonality relations (13):

$$\int_{i} < 0|\sigma^{+}(t, m)|\xi_{n}, \cdots, \xi_{1} >_{e_{n}, \cdots, e_{1;i}; i < \xi_{n}, \cdots, \xi_{1} < \xi_{1}, \cdots, \xi_{n}|\sigma^{-}(0, 0)|0 >_{i},$$

where we have used the orthogonality relations (13):

$$\int_{i} < 0|\sigma^{+}(t, m)|\xi_{n}, \cdots, \xi_{1} >_{e_{n}, \cdots, e_{1}; i < \xi_{n}, \cdots, \xi_{1} < \xi_{1}, \cdots, \xi_{n}|\sigma^{-}(0, 0)|0 >_{i},$$

with the usual Kronecker symbol defined by $\delta_{ii} = 1$ and $\delta_{ij} = 0$ if $i \neq j$. $S_{n}^{++}$ can be expressed through (9) and (10) as:

$$S_{n}^{++}(w, k) = \frac{1}{\pi} \prod_{e_{n}=\pm 1} \int_{-\infty}^{\infty} dt \exp (it(w - \sum_{e_{n}=1}^{n} e(\xi_{i})))$$

where $i$ and $j$ are defined only modulo 2, we can split the sum over $Z$ in terms of even elements and odd elements and rewrite the latter formula as:

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To simplify the latter expression even further we use the fact that the form factors of the operators $\sigma^{+}$ and $\sigma^{-}$ satisfy the following relations (13):

$$i < 0|\sigma^{+}(0, 0)|\xi_{n}, \cdots, \xi_{1} >_{e_{n}, \cdots, e_{1;i}} = (i < 0|\sigma^{+}(0, 0)|\xi_{n}, \cdots, \xi_{1} >_{e_{n}, \cdots, e_{1;i}})^{*}$$

The last relation means that only $S_{n}^{++}$ with $n$ even are non-vanishing. Using the latter relations and for a reason that will make sense later when we consider the form factors in the isotropic limit we shift $k$ by $\pi$ to get:

$$S_{n}^{++}(w, k) = \frac{1}{\pi} \prod_{e_{n}=\pm 1} \int_{-\infty}^{\infty} dt \exp (it(w - \sum_{e_{n}=1}^{n} e(\xi_{i})))$$

Here by the symbol $\sum_{e_{n}=\pm 1}$ we mean the sum is constrained by the selection rule expressed by the second relation in (15). Now we will take the isotropic limit of the XXZ Heisenberg model
where the latter formula will simplify even further. The isotropic limit $q \to -1$ is performed by first making the following redefinitions:

$$
\xi = ie^{\frac{\pi}{2}}, \\
q = -e^{\epsilon}, \quad \epsilon \to 0^+,
$$

(17)

where $\beta$ is the spectral parameter corresponding to the isotropic Heisenberg model. Then, we find in this limit [13]:

$$
i < 0 | \sigma^+(0,0) | \xi_{\kappa}, ..., \xi_{\ell} > e_{\kappa}, ..., e_{\ell}i; \\
i < 0 | \sigma^+(0,0) | \beta_{\kappa}, ..., \beta_{1} > e_{\kappa}, ..., e_{1}; \\
\sim e^{-n/2} C_{1,i,n} \\
\times \prod_{n_{\ell} \geq 1} \left( \frac{A_{-(\beta_{\ell} - \beta_{\ell})}^{\pi i} \prod_{n=1}^{n_{\ell}} \prod_{b \in B} \left( \int \frac{d\alpha}{2\pi i} \right) \prod_{b' > b} \left( \int \frac{d\alpha'}{2\pi i} \right) \prod_{b = b+1}^{b+1} (\beta_{\ell} - \alpha_{b} + \frac{\pi i}{2}) \Gamma(-\frac{1}{2} - \frac{\alpha_{b} - \beta_{\ell}}{2\pi i}) \sinh(\alpha_{b}) \prod_{b' = b}^{b} \Gamma(-\frac{1}{2} - \frac{\alpha_{b} - \beta_{\ell}}{2\pi i}) \sinh(\alpha_{b}) \right) \right)
$$

(18)

where the set $B$ associated with a configuration $(\epsilon_{m}, ..., \epsilon_{1})$ is defined by

$$
B = \{ b : \epsilon_{b} = +1; \quad \sum_{\ell=1}^{n} \epsilon_{\ell} = -2 \}, \quad \dim (B) = n - 2 \equiv N.
$$

(19)

The contours $C_{b}$ are drawn in Figure 1. In the expression of $C_{1,i,n}$ and more precisely in $(i)^{-2i}$, the $i$ that is in the exponent refers to the sector index (i.e., $i = 0, 1$), whereas the $i$ that is not in the exponent refers to the unit complex imaginary number (i.e. $i^2 = -1$). Also in all terms $\pi i$, $i$ refers to the unit complex imaginary number. Note that there was an error in the formula of $C_{1,i,n}$, given in [13], and which has been corrected in the above expression by having $C_{1,i,n}$ proportional to the factor $\Gamma(3/4)^{-n/2}$ instead of $\Gamma(3/4)^{n/2}$ as was incorrectly done in [13]. Finally $\Gamma(z)$ is the usual gamma function and for a complex variable $z = x + iy$, with $x$ and $y$ being real, the complex functions $A_{\pm}(z)$ and their square modulus $|A_{\pm}(z)|^2$ are defined in terms of the following integrals:

$$
A_{\pm}(z) = \exp \left( -\int_{-\infty}^{\infty} dt \frac{\sin(1/2 \sinh^2(2t) \cosh(t))}{\sinh(2t) \cosh(t)} \exp(\mp t) \right),
$$

$$
|A_{\pm}(z)|^2 = \exp \left( -\int_{-\infty}^{\infty} dt \frac{\cosh(1/2 \sinh^2(2t) \cosh(t))}{\sinh(2t) \cosh(t)} \exp(\pm t) \right).
$$

(20)

From the latter relation one can show that the following constant terms which contribute to the overall normalization factor of $S_{n}^{\pm}$ can be expressed as:

$$
|A_{\pm}(i\pi/2)|^2 = \exp \left( -\int_{0}^{\infty} dx \frac{\cosh(x) - 1}{\sinh(2x) \cosh(x)} \exp(\mp x) \right) = \pi \Gamma(1/2 \pm 1/4)^{-2} (\sqrt{2} e A^{-6})^{1/2},
$$

$$
A = \exp \left( \frac{A_{0}}{12} - \psi'(-1) \right) = 1.282471291 \cdots,
$$

(21)
where $A$ is the Glaisher-Kinkelin constant and $\zeta(x)$ is the usual Riemann zeta function. Since as we will see later the final formula of $S_{n}^{k,+}$ will be expressed just in terms of $|A_{-}(\beta)|^2$ with the spectral parameter $\beta$ being real let us then define for the sake of simplifying the notation the real valued function $A(\beta)$ that we refer to henceforth as the "Jimbo Miwa function" (since they were the first authors to introduce it and this function seems to be an extremely important one in terms of which the Heisenberg model is exactly solved) as:

$$A(\beta) \equiv |A_{-}(\beta)|^2 = \exp \left( -\int_{0}^{\infty} dt \frac{\cosh(2t) \cos(\frac{2\beta}{\pi}) - 1}{t \sinh(2t) \cosh(t)} \exp(t) \right).$$  \hspace{1cm} (22)$$

From [18] the isotropic limit of $S_{n}^{k,+}$ as given by [10] is equal to:

$$
S_{n}^{k,+}(w, k - \pi) \to \epsilon^n C_{2,n} \sum_{\epsilon_1, \ldots, \epsilon_n} \int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_n \times \left( \sum_{m \in \mathbb{Z}} \exp(2im(k + \sum_{\ell=1}^{n} p(\beta_{\ell}))) \right) \times \left( \int_{-\infty}^{+\infty} dt \exp(it(w - \sum_{\ell=1}^{n} e(\beta_{\ell}))) \right) \times |i < 0|\sigma^+(0,0)|\beta_{n}, \ldots, \beta_{1} >_{\epsilon_n, \ldots, \epsilon_1}|^2 \times (1 + \exp(i(k + \sum_{\ell=1}^{n} p(\beta_{\ell})))) ,
$$

with

$$C_{2,n} = 2^{-n} \pi^{-2n} (n!)^{-1}. \hspace{1cm} (24)$$

Now a source of an error that plugged all existing papers dealing with the exact DSF in that they all got the normalization overall factor incorrect is due to the tricky step of expressing each of following sum : $\sum_{m \in \mathbb{Z}} \exp(2im(k + \sum_{\ell=1}^{n} p(\xi_{\ell})))$ and integral : $\int_{-\infty}^{+\infty} dt \exp(it(w - \sum_{\ell=1}^{n} e(\xi_{\ell})))$ in terms of the usual Dirac delta function $\delta(x)$. The difficulty lies in the fact that the Dirac delta function is not really a function but to be more precise a distribution that can be thought of just by what it does to other usual functions as opposed to any intrinsic and explicit functional form. Except for the 2-spinon DSF, all the current papers in the litterature used incorrect normalization factors when they expressed the latter sum and integral in terms of the delta function $\delta(x)$. We will see later the final formula of $\gamma$ and $\delta$ we have then from [25] :

$$
\lim_{M \to \infty} \sum_{M=-M}^{M} \exp imx = 2\pi \sum_{\ell=0}^{\ell-1} \delta(x - 2\pi \ell), \hspace{1cm} 0 \leq x \leq 2\pi \ell, \\
\lim_{M \to \infty} \sum_{M=-M}^{M} \exp imx = 2\pi \sum_{\ell=-\ell+1}^{\ell-1} \delta(x - 2\pi \ell), \hspace{1cm} -2\pi \ell \leq x \leq 0. \hspace{1cm} (25)$$

Let us note that the momenta $-\pi \leq p(\beta_{\ell}) \leq 0, \ell = 1, \ldots, n$ of the spinons are defined only modulo $2\pi$ inside the domain of definition of the total momentum of $n$ spinons $-k = \sum_{\ell=1}^{n} p(\beta_{\ell}) \in [-n\pi, 0]$. However the energies $0 \leq e(\beta_{\ell}) \leq \pi, \ell = 1, \ldots, n$ are not defined modulo $2\pi$ inside the domain of definition of the total energy of $n$ spinons $w = \sum_{\ell=1}^{n} e(\beta_{\ell}) \in [0, n\pi]$. Since we will be integrating over the two momenta $p(\beta_{1})$ and $p(\beta_{2})$ and thus the two corresponding energies $e(\beta_{1})$ and $e(\beta_{2})$ we have then from [25] :

$$
\int_{-\infty}^{\infty} dt \exp(it(w - \sum_{\ell=1}^{n} e(\beta_{\ell}))) = 2\pi \delta(w - \sum_{\ell=1}^{n} e(\beta_{\ell})), \hspace{1cm} 0 \leq e(\beta_{1}) + e(\beta_{2}) \leq 2\pi, \\
\sum_{m \in \mathbb{Z}} \exp(2im(k + \sum_{\ell=1}^{n} p(\beta_{\ell}))) = 2\pi \sum_{\ell=-n/2+1}^{0} \delta(2(k + \sum_{\ell=1}^{n} p(\beta_{\ell}) - 2\pi \ell')), \\
\pi \sum_{\ell=-n/2+1}^{\ell-1} \delta(k + \sum_{\ell=1}^{n} p(\beta_{\ell}) - 2\pi \ell'), \\
-\pi \leq p(\beta_{1}) + p(\beta_{2}) \leq 0. \hspace{1cm} (26)$$

Now in the last relation one can always shift the momenta of the spinons to cancel the term $2\pi \ell'$ in $\delta(k + \sum_{\ell=1}^{n} p(\beta_{\ell}) - 2\pi \ell')$ thus effectively leading to the following final form of formulæ
relating the sum \( \sum_{n \in \mathbb{Z}} \exp(2im(k + \sum_{\ell=1}^{n} p(\xi_{\ell}))) \) and integral \( \int_{-\infty}^{\infty} dt \exp(it(w - \sum_{\ell=1}^{n} e(\xi_{\ell}))) \) to the delta function \( \delta(x) \):

\[
\int_{-\infty}^{\infty} dt \exp(it(w - \sum_{n=1}^{n} e(\beta_{\ell}))) = 2\pi \delta(w - \sum_{\ell=1}^{n} e(\beta_{\ell})), \quad 0 \leq e(\beta_{1}) + e(\beta_{2}) \leq 2\pi
\]

It was possible to make the last shift in the spinon momenta because

\[
\beta_{\ell}(p_{\ell} + 2\pi) = \beta_{\ell}(p_{\ell}), \quad e(p_{\ell} + 2\pi) = e(p_{\ell}), \quad \ell = 1, \ldots, n
\]  

and therefore the integrand of the expression \(23\) is periodic in the spinon momenta and \(k\) with period \(2\pi\) since it depends just on the \(\beta_{\ell}\) and delta functions. Therefore \(S_{n}^{i+,\ell}(w, k - \pi)\) is also periodic in the spinon momenta and \(k\) with period \(2\pi\):

\[
S_{n}^{i+,\ell}(w, k - \pi + 2\pi) = S_{n}^{i+,\ell}(w, k - \pi).
\]  

It is worth mentioning that in the case of 4 spinons the authors of \[19\] assumed \(S_{n}^{i+,\ell}(w, k - \pi)\) and \(S_{n}^{i+,\ell}(w, k - \pi + 2\pi)\) to be different and therefore they evaluated them separately and because of this they concluded that our initial formula derived in \[17\] was incorrect in its dependency on the spectral parameters \(\beta_{\ell}\). In fact we have just proved that \(S_{n}^{i+,\ell}(w, k - \pi) = S_{n}^{i+,\ell}(w, k - \pi + 2\pi)\) and therefore our initial formula was incorrect just by factor of 2 in its overall factor and its dependency on the spectral parameters \(\beta_{\ell}\) was indeed correct contrary to the claim of \[19\]. Also note that in \[19\] the authors justified the inclusion of the contribution \(S_{n}^{i+,\ell}(w, k - \pi + 2\pi)\) by saying that the delta function fixes the momentum transfer \(k\) only up to \(2\pi\) but in fact it is not the momentum transfer that is fixed up to \(2\pi\) and which should be exactly fixed but it is rather the momenta of the spinons which are fixed up to \(2\pi\). Also in the latter reference it is not clear why the authors have not used the same argument with respect to the delta function of the energies to justify a fixing of the energy transfer only up to \(2\pi\) in a similar manner as they did for the momenta. We have just proved that there is an asymmetry between the momenta of the spinons which are fixed only up to \(2\pi\) and the energies of the spinons which are exactly fixed. So if we make usage of \(27\) back in \(23\) we obtain:

\[
S_{n}^{i+,\ell}(w, k - \pi) \rightarrow e^{n} C_{3,n} \sum_{n_{1}, \ldots, n_{n}} \int_{-\infty}^{+\infty} d\beta_{n} \times \delta(w - \sum_{\ell=1}^{n} e(\beta_{\ell})) \delta(k + \sum_{\ell=1}^{n} p(\beta_{\ell}))
\]

\[
\times |\beta_{1} \cdot \cdots \beta_{n}|^{2} \times (1 + \exp(i(k + \sum_{\ell=1}^{n} p(\beta_{\ell}))))
\]

with

\[
C_{3,n} = 2n\pi^{2} C_{2,n} = 2^{1-n} \pi^{2(1-n)}((n-1)!)^{-1}.
\]  

From the expression of the form factor as given by \(18\) it is clear that it has simple poles coming from the \(\Gamma(z)\) function. As shown in Figure 1. the contours \(C_{n}\) enclose the simple poles \(\beta_{\ell} + \frac{\pi}{2} - 2\pi_{\ell}, \pi i\) with \(1 \leq \ell_{b} \leq n\) and \(s_{\ell} \in N, i.e., any nonnegative integer. In Figure 1. these poles are represented by the cross x and not the disk. The contours \(C_{1}\) enclose also all the points denoted by the cross x with negative \(s_{\ell}\) but these are not poles of the integrand because the latter is analytic at these points and therefore their contribution to the integral is zero. For this
purpose let us recall that the \( \Gamma(z) \) function is analytic everywhere on the complex plane except at the negative integer simple poles \( z = -s \), with residues given by:

\[
Res_{z=-s}\Gamma(z) = \frac{(-1)^s}{s!}, \quad s \geq 0.
\]

(32)

Consequently, we can explicitly perform the complex integration of the form factor with respect to the integration variables \( a \) in (18). Indeed, using the following relations:

\[
\sinh(\beta + \frac{x}{2} - 2\pi i s) = i \cosh(\beta), \\
\Gamma(-i\beta - s) = \Gamma(s + 1) \sinh(\pi \beta),
\]

(33)

with \( s \) being any non-negative integer and \( \beta \) any real variable, we find:

\[
\begin{align*}
&\langle 0|\sigma^+(0,0)|\beta_1, \ldots, \beta_t \rangle \sim \epsilon^{-n/2} C_{4,t,n}^{b_{TN}, s_{1}, \ldots, s_t} f(\beta_1, \ldots, \beta_t) \\
&\times \sum_{t_1, \ldots, t_t = 1}^{\infty} \sum_{s_1, \ldots, s_t = 0}^{\infty} D_{b_{TN}, \ldots, b_t, t_1, \ldots, t_t}^{|\beta_1, \ldots, \beta_t|} H_{t_1, \ldots, t_t}^{s_1, \ldots, s_t}(\beta_1, \ldots, \beta_t), \\
&\sum_{l=0}^{\infty} \frac{s}{2\pi i (s+1)} \Gamma(s + 1) = \frac{1}{s!},
\end{align*}
\]

(34)

where again the infinitesimal error is defined by (17) and:

\[
H_{t_1, \ldots, t_t}^{s_1, \ldots, s_t}(\beta_1, \ldots, \beta_t) = \prod_{a=1}^{N} \cosh(\beta_a) \gamma(s_a) \prod_{a'=1}^{N} \cosh(\pi \rho_a \ell_{a'}),
\]

\[
D_{b_{TN}, \ldots, b_t, t_1, \ldots, t_t}^{|\beta_1, \ldots, \beta_t|}(\beta_1, \ldots, \beta_t) = \prod_{a=1}^{N} \prod_{a'=1}^{N} \prod_{a=1}^{N} \cosh(\pi \rho_a \ell_{a'}),
\]

\[
L_{t_1, \ldots, t_t}^{s_1, \ldots, s_t}(\beta_1, \ldots, \beta_t) = \prod_{a=1}^{N} \prod_{a'=1}^{N} \prod_{a=1}^{N} \cosh(\pi \rho_a \ell_{a'}),
\]

\[
S_{t_1, \ldots, t_t}^{s_1, \ldots, s_t}(\beta_1, \ldots, \beta_t) = \prod_{a=1}^{N} \prod_{a'=1}^{N} \prod_{a=1}^{N} \cosh(\pi \rho_a \ell_{a'}),
\]

\[
F(\beta_1, \ldots, \beta_t) = \prod_{a=1}^{N} \prod_{a'=1}^{N} \prod_{a=1}^{N} \cosh(\pi \rho_a \ell_{a'}),
\]

\[
C_{4,t,n}^{b_{TN}, s_{1}, \ldots, s_t} = \frac{1}{2\pi i (s+1)} \prod_{a=1}^{N} \cosh(\beta_a).
\]

(35)

Here \( N \) is defined by (19) and \( \Theta(x) \) is the usual Heaviside step function defined as \( \Theta(x) = 0 \) for \( x \leq 0 \) and \( \Theta(x) = 1 \) for \( x > 1 \). Furthermore, we have used relations (21) and introduced the notations:

\[
\rho_{ab} = \frac{\beta_a - \beta_b}{\pi}, \\
\gamma(z) = \Gamma(z + \frac{1}{2}) / \Gamma(z + 1).
\]

(36)

Given the latter we can easily check that for any non-negative integer \( s \) we have:

\[
\gamma(s) = \frac{(2s-1)!!}{(2s-1)!} \sqrt{\pi}, \quad s \geq 1,
\]

\[
\gamma(0) = -2\sqrt{\pi}.
\]

(37)
Also note the fact that the $A_-(\beta)$ function is an even function with respect to the permutation of the spectral parameters $\beta_1$ and $\beta_2$, i.e.,

$$A_-(2\pi \rho_{ab}) = A_-( -2\pi \rho_{ab}) = A_-(2\pi \rho_{ab}).$$

To optimize the numerical evaluations of the DSF it is worth expressing the functions $\Gamma(z-s+1)$ for any non-negative $s$ in terms of the function $\Gamma(z+1)$ without $s$ and the Pochhammer symbol $(z)_s$ defined as:

$$(z)_s = z(z-1)\cdots(z-s+1) = \frac{\Gamma(z+1)}{\Gamma(z-s+1)}, \quad s \geq 1,$$

$$(z)_0 = 1. \quad (39)$$

Substituting relation (34) back in (30) we find that the $n$-spinon DSF can be written in terms of $S^{s_2N,\ldots,s_1}_{\ell_2N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n)$ function as:

$$S^{i,+}_n(w,k-\pi) = C_{0,n} \int_{-\infty}^{+\infty} d\beta_1 \cdots \int_{-\infty}^{+\infty} d\beta_n$$

$$\times \delta(k + \sum_{l=1}^{n} p(\beta_l))$$

$$\times \delta(w - \sum_{l=1}^{n} e(\beta_l))$$

$$\times F(\beta_1,\ldots,\beta_n)$$

$$\times \sum_{\ell_2N,\ldots,\ell_1=1}^{n} \sum_{s_2N,\ldots,s_1=0}^{\infty} S^{s_2N,\ldots,s_1}_{\ell_2N,\ldots,\ell_1}(\beta_1,\ldots,\beta_n), \quad (40)$$

with

$$C_{0,n} = C_{3,n}C_{5,n} = n2^{(n^2-50n+60)/12} \pi^{2(2-n)} (n!)^{-1} e^{n(n-2)/4} A^{-3n(n-2)}. \quad (41)$$

Integrating the two delta functions over $\beta_1$ and $\beta_2$ we obtain:

$$S^{i,+}_n(w,k-\pi) = C_{0,n} \int_{-\infty}^{+\infty} d\beta_3 \cdots \int_{-\infty}^{+\infty} d\beta_n$$

$$\times \sum_{(\beta_1,\beta_2,\beta_3,\ldots,\beta_n) \in E} \sum_{r=1}^{n} \prod_{\ell=3}^{n} \frac{1}{\cosh(\beta_{\ell})}$$

$$\times \sum_{s_2N,\ldots,s_1=0}^{\infty} S^{s_2N,\ldots,s_1}_{\ell_2N,\ldots,\ell_1}(\beta_1,\beta_2,\beta_3,\ldots,\beta_n), \quad (42)$$

where

$$F(\beta_1,\beta_2,\beta_3,\ldots,\beta_n) = \cosh(\beta_1) \cosh(\beta_2) F(\beta_1,\beta_2,\beta_3,\ldots,\beta_n) = \prod_{\ell=3}^{n} \frac{A(2\pi p_{\rho_{ell}})}{\cosh(\beta_{\ell})},$$

$$W = e(\beta_1) + e(\beta_2) = w - \sum_{\ell=3}^{n} e(\beta_{\ell}) = w - \pi \sum_{\ell=3}^{n} \frac{1}{\cosh(\beta_{\ell})},$$

$$K = -p(\beta_1) - p(\beta_2) = k + \sum_{\ell=3}^{n} p(\beta_{\ell}) = k + \sum_{\ell=3}^{n} \arccot(\sinh(\beta_{\ell})),$$

$$W_u = 2\pi |\sin(K/2)|,$$

$$W_f = p|\sin(K)|,$$

$$\beta_1 = \arccosh \left( \cot \left( \frac{-K + \arccos \left( \frac{W}{\sqrt{\pi}} \right)}{2} \right) \right),$$

$$\beta_2 = \arcsinh \left( \cot \left( \frac{-K + \arccos \left( \frac{W}{\sqrt{\pi}} \right)}{2} \right) \right).$$

(43) and $E$ is the set of all $(\beta_1,\beta_2,\beta_3,\ldots,\beta_n)$ that satisfy the latter relations for fixed $k$ and $w$. This set is generated from the actions of the permutation elements $P_{12}$ and $P_{ij}$, $i \neq 1,2; j \neq 1,2; i \neq j$ on the naturally ordered set $(\beta_1,\beta_2,\beta_3,\ldots,\beta_n)$. This means $\dim(E) = 2 \times (n-2)!$. To show that all the elements of $E$ contribute the same value to the integral one can easily check that the
following identities hold true:

\[
\begin{align*}
X^{s_2, \ldots, s_1}(\beta_1, \ldots, \beta_n) &= X^{s_2, \ldots, s_1}(\beta_1, \ldots, \beta_n)^*, \\
X^{s_N, \ldots, s_1, s_2}(\beta_1, \ldots, \beta_n) &= X^{s_N, \ldots, s_1, s_2}(\beta_1, \ldots, \beta_n)^* \in R, \\
H^{s_N, \ldots, s_1, \ell_1, \ldots, \ell_N, \ldots, \ell_1, P_{a,b}}(\beta_1, \ldots, \beta_n, \beta_n) &= H^{s_N, \ldots, s_1, \ell_1, \ldots, \ell_N, \ldots, \ell_1, P_{a,b}}(\beta_1, \ldots, \beta_n, \beta_n), \\
F_{P_{a,b}}(\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n) &= F(\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n), \quad a, b = 1, \ldots, n, \quad a \neq b,
\end{align*}
\]

where for some function \(G(\beta_1, \ldots, \beta_n)\) with its arguments ordered in the natural ordering \((\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n)\) we have introduced the action of the permutation group on its arguments as:

\[
G_{P_{a,b}}(\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n) = G(\beta_{\tau(1)}, \beta_{\tau(2)}, \ldots, \beta_{\tau(n-1)}, \beta_{\tau(n)}), \quad (45)
\]

with the action of the transposition \(P_{a,b}\) operator on the naturally ordered set \((\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n)\) defined as usual by:

\[
P_{a,b}(\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n) = (\beta_{\tau(1)}, \beta_{\tau(2)}, \ldots, \beta_{\tau(n-1)}, \beta_{\tau(n)}). \quad (46)
\]

For example:

\[
G_{P_{1,3}}(\beta_1, \beta_2, \beta_3, \ldots, \beta_{n-1}, \beta_n) = G(\beta_3, \beta_2, \beta_1, \ldots, \beta_{n-1}, \beta_n). \quad (47)
\]

In the above identities we denote by \(X^{s_2, \ldots, s_1}(\beta_1, \ldots, \beta_n)\) either \(L^{s_2, \ldots, s_1}_{2N}(\beta_1, \ldots, \beta_n)\) or \(S^{s_2, \ldots, s_1}_{2N}(\beta_1, \ldots, \beta_n)\), that is, both of the latter functions satisfy exactly the same identities given by the first two relations in \([14]\). Let us note from the latter identities also that the function \(F(\beta_1, \beta_2, \ldots, \beta_{n-1}, \beta_n)\) is fully symmetric function under the permutation group acting on all its arguments. Furthermore let us note that the choice of the integration variables \(\beta_1, \beta_2\) in \([40]\) was arbitrary and we could have picked any other pair. The number of all possible pairs in \((\beta_1, \beta_2, \ldots, \beta_n)\) is \(n \times (n - 1)/2\). Because of the latter identities and redefinitions on the integration variables all the elements of the set \(E\) contribute equally for a total overall factor of \(2 \times (n - 2)! \times n(n - 1)/2 = n!\) which is just the multiplicity factor of the energy-momenta conservation laws \(k = -\sum_{\ell=1}^{n} p_\ell\) and \(w = \sum_{\ell=1}^{n} e_\ell\) since there are \(n!\) ways to permute the \(p_\ell\) such that all these configurations satisfy the latter laws. The \(n\)-spinon DSF \(S^{n+}\) simplifies then to:

\[
S^{n+}(w, k - \pi) = C_{7,n} \int_{-\infty}^{+\infty} d\beta_3 \cdot \ldots \cdot \int_{-\infty}^{+\infty} d\beta_n \\
\times \frac{F(\beta_1, \beta_2, \beta_3, \ldots, \beta_n)}{(\theta(W_\pi - W + \theta(W_\pi - W)) + F(W_\pi - W))} \\
\times \sum_{\ell_1=1}^{n} \sum_{\ell_{2N} = \ell_{N}, \ell_{2N} - 1, \ldots}^{n} \ldots (2 - \delta_{\ell_1+\ell_2} e_\ell) \frac{e_\ell}{A^{3n(n-2)}} A^{-3n(n-2)} \\
\times \sum_{s_{2N}, \ldots, s_1=0}^{n-1} (2 - \delta_{\ell_1 n} e_\ell) \text{Re}(S^{s_{2N}, \ldots, s_1}_{2N}(\beta_1, \beta_2, \beta_3, \ldots, \beta_n)), \quad (48)
\]

with

\[
C_{7,n} = n!C_{6,n} = n! \frac{n^2(n^2 - 50n + 60)/12 \pi^2(2-n)^{n(n-2)/4}}{A^{-3n(n-2)}}. \quad (49)
\]

Note that in general the overall factor \(C_{7,n}\) is simply expressed in terms of the Glaisher-Kinkelin constant \(A\). This is a new result as far as the author knows. Note also that \(C_{7,2} = 1/4\) which is also a new result that was previously unknown albeit this value was first used without any proof or justification in reference \([15]\) (to be more precise the latter reference used a value of 1/2 which is double the correct value due to the inclusion of both sectors \(i\) which was also incorrect as we will see shortly in the sequel). Since \(S^{n+}\) is independent of the sector index \(i\) we have decided to omit any reference to it in the sequel. This also means that both sectors contribute equally and we just need to focus on one of them. In fact we will prove next that only one sector leads to the full physical DSF. In the initial paper \([16]\) a mistake was made by adding
up the contributions from both sectors to get the physical DSF which in turn made the overall normalization factor overvalued by a factor of 2. Let us now prove why it was incorrect to do so in this initial paper \[16\]. For this purpose let us integrate both sides of the total $S^i(w, k)$ as given by relation \((5)\) with respect to both $w$ and $k$:

$$\frac{1}{(2\pi)^2} \int_0^\infty dw \int_{-\pi}^{\pi} dk S^{i,++}(w, k) = \frac{1}{(2\pi)^2} \int_0^\infty dw \int_{-\pi}^{\pi} dk \int_0^\infty dt \sum_{n\in Z} e^{i(wt+kn)}$$

$$\times \chi_i < 0|\sigma^+(t, n)\sigma^-(0, 0)|0 >_i$$

$$= \int_{-\infty}^\infty dt \sum_{n\in Z} \delta(t)\delta(n) < 0|\sigma^+(t, n)\sigma^-(0, 0)|0 >_i$$

$$= i < 0|\sigma^+(0, 0)\sigma^-(0, 0)|0 >_i = \frac{1}{2},$$

with

$$\sigma^+(0, 0)\sigma^-(0, 0) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} (0, 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} (0, 0).$$

This is an extremely important result known in the literature as the total integrated intensity sum rule. Also the value $1/2$ is the well known full physical value of the static one point function of the local operator $i < 0|\sigma^+(0, 0)\sigma^-(0, 0)|0 >_i$. The crucial point to note here is that it is obtained from just from one sector $i$ without summation over both sectors $i$ and is indeed independent of $i$ as was calculated in both references \[22\] and \[13\]. Since the full physical static one point function is a limiting particular case of the dynamic full physical DSF and is obtained from just one sector this means the latter must also be obtained from just one sector. Since it should not depend on which one of the two possible sectors $i = 0, 1$ the latter two must therefore contribute equally, or put otherwise, the DSF should be independent of $i$. Given that the full physical DSF is the sum of the $n$-spinon DSF $S^{i,++}_n$ the latter is also the full physical one and should also be independent of $i$ which is indeed the case as shown by \[18\]. This should be expected because recall that $i$ fixes the boundary conditions such that the allowable spin configurations are those for which the eigenvalues of $\sigma^z_\ell$ are $(-1)^{i+n}$ in the limit $n \to \pm \infty$. So the two eigenspaces corresponding to the two sectors are completely disjoint and it would take an infinite energy to jump from one state from one sector to another state in the other sector. Therefore there can be no interference between the two eigenspaces and the physical DSF is built on any one of them but not the two at the same time. This concludes the proof that we should not sum up the contributions of the 2 sectors $i = 0, 1$ to get the physical $n$-spinon DSF.

### 2.1 2-spinon DSF

This case is characterized by $n = 2$ and empty set $B$ for the only allowed configuration $(\epsilon_2, \epsilon_1) = (-, -)$ and therefore the general formulas \[18\] and \[35\] simplify considerably to:

$$i < 0|\sigma^+(0, 0)|\xi_2, \xi_1 >_{+-}$$

$$\rightarrow i < 0|\sigma^+(0, 0)|\beta_2, \beta_1 >_{+-}$$

$$\rightarrow -1 < 0|\sigma^+(0, 0)|\beta_2, \beta_1 >_{+-}$$

$$\sim \epsilon^{-1} C_{1,1,2} A_{-(\beta_2 - \beta_1)} \prod_{i=1}^\pi \sinh(\pi i / 4 - \beta_i / 2)$$

$$|i < 0|\sigma^+(0, 0)|\xi_2, \xi_1 >_{+-} |^2$$

$$\rightarrow |i < 0|\sigma^+(0, 0)|\beta_2, \beta_1 >_{+-} |^2$$

$$\sim \epsilon^{-2} C_{5,2} A(\beta_2 - \beta_1)$$

$$\begin{aligned}
C_{1,1,2} &= -\epsilon^{-1} \iota \Theta(3/4)^{-1} A_+(\pi i / 2)^{-1}, \\
C_{5,2} &= 2^{-\pi^2}, \\
p(\xi_2) &\rightarrow p(\beta_2), \cot(p(\beta_2)) = \sinh(\beta_2), -\pi \leq p(\beta_2) \leq 0, \\
e(\xi_2) &\sim e(\beta_2) = -\pi \sin(p(\beta_2)), 0 \leq e(\beta_2) \leq \pi, \quad 1 \leq \ell \leq 2, \\
\tilde{f} \frac{d\xi_2}{2\pi i} &\rightarrow \epsilon^{-2} 2^{-\pi^2} \int_{-\epsilon}^\epsilon d\beta_1 \int_{-\epsilon}^\epsilon d\beta_2.
\end{aligned}$$
Because of the latter simple relations the general formula of $n$-spinon $S_{n}^{\pm}$ simplifies substantially as well to:

$$S_{2}^{\pm}(w, k - \pi) = \frac{1}{4} \frac{A(\tilde{\beta}_{2} - \tilde{\beta}_{1})\Theta(W_{u} - w)\Theta(w - W_{l})}{\sqrt{W_{u}^{2} - w^{2}}},$$  \(53\)

where

$$W = w = e(\tilde{\beta}_{1}) + e(\tilde{\beta}_{2}), \quad 0 \leq w \leq 2\pi,$$

$$K = k = -p(\tilde{\beta}_{1}) - p(\tilde{\beta}_{2}), \quad 0 \leq k \leq 2\pi,$$

$$W_{u} = 2\pi \sin(k/2), \quad W_{l} = \pi \left| \sin(k) \right|,$$

$$\tilde{\beta}_{1}(w, k) = \text{arcsinh} \left( \cot \left( -\frac{k}{2} + \arccos \left( \frac{w}{W_{u}} \right) \right) \right),$$

$$\tilde{\beta}_{2}(w, k) = \text{arcsinh} \left( \cot \left( -\frac{k}{2} - \arccos \left( \frac{w}{W_{u}} \right) \right) \right).$$  \(54\)

Plotting the dispersion relation of $w$ as a function of $k$ in Figure 2 we can see that $w$ lies between two boundaries. The upper boundary is given by $W_{u}$ and the lower boundary is given by $W_{l}$ which is also known as des Cloizeaux-Pearson dispersion relation. For the sake of comparison with experimental data where the DSF is given for the local spins normalized as:

$$S_{x} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_{y} = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_{z} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$  \(55\)

we consider then the following nonvanishing components of the 2-spinon DSF:

$$S_{2}^{xx}(w, k - \pi) = S_{2}^{yy}(w, k - \pi) = S_{2}^{zz}(w, k - \pi) = \frac{1}{2} S_{z}^{\pm}(w, k - \pi).$$  \(56\)

The latter components are equal because of the isotropy of the Heisenberg model. In Figure 3 we plot $S_{2}^{zz}$ as a function of $w$ for fixed $k = \pi$. Note from relation $53$ despite the presence of the term $\sqrt{W_{u}^{2} - w^{2}}$ in the denominator of $S_{2}^{zz}$ the latter actually vanishes at this boundary. This is physically expected because this boundary is characterized by equal momenta of the 2 spinons (i.e., equal spectral parameters $\tilde{\beta}_{1}$ and $\tilde{\beta}_{2}$ as can be seen from $54$). Since the two spinons are fermions in nature and they have the same spin therefore they cannot have equal momenta due to the Pauli exclusion principle for fermions thus leading to vanishing DSF. To see that the upper boundary corresponds to equal spectral parameters $\tilde{\beta}_{1}$ and $\tilde{\beta}_{2}$ it is clear from relations $54$ $\tilde{\beta}_{1}(w, k) = \tilde{\beta}_{2}(w, k)$ if

$$\arccos \left( \frac{w}{W_{u}} \right) = 0,$$  \(57\)

that is:

$$w = W_{u}.$$  \(58\)

By analogy note from Figure 3 that at the other extreme lower boundary $W_{l}$ $S_{2}^{zz}$ diverges leading to a resonance. This is also physically expected because this boundary is characterized by one momentum being equal to $\pi$ and the other one being equal to $0$, that is, the two spinons which have equal spins are at their maximum difference through the momenta leading to an extreme opposite of the Pauli exclusion principle and which we call the inclusion principle for fermions when they are at their maximum difference, that is, fermions tend to favor being at states where they differ by a maximum amount. This is analogous to bosons which favor being at states which have have exactly equal quantum numbers. Between these two extremes $S_{2}^{zz}$ takes on non-zero finite values which correspond to the two spinons having equal spins but different momenta that differ by an amount between $0$ and $\pi$ exclusive. The transition between the latter three regimes is a smooth one.
2.2 4-spinon DSF

This case is characterized by $n = 4$ and $\dim(B) = 1$ meaning that there are four allowed configurations $(\epsilon_4, \epsilon_3, \epsilon_2, \epsilon_1)$ with all $\epsilon_\ell = \epsilon$, $\ell = 1, 2, 3, 4$ except one of them being equal to $+$. The general formulas in [15] take the following considerably simpler form:

\[
\begin{align*}
\begin{align*}
    i < 0|\sigma^+(0, 0)|\xi_4, \ldots, \xi_1 > & \sim e^{-2C_{4,4}} \\ 
    \sum_{b=1}^{4} |i < 0|\sigma^+(0, 0)|\beta_4, \ldots, \beta_1 > \sim & \sum_{b=1}^{4} |i < 0|\sigma^+(0, 0)|\beta_4, \ldots, \beta_1 > \sim e^{-2C_{4,4}} f(\beta_1, \ldots, \beta_4), \\
    & \times \sum_{\ell=1}^{4} \prod_{m=1}^{\infty} D_{b,m}^{\beta_1}(\beta_1, \ldots, \beta_4) H_{b,\ell}(\beta_1, \ldots, \beta_4).
\end{align*}
\end{align*}
\]

The infinitesimal $\epsilon$ is defined by (17) and the single contour $C_b$ is displayed in Figure 1. Moreover, the general relations (34) and (35) become for $n = 4$:

\[
\begin{align*}
    i < 0|\sigma^+(0, 0)|\beta_4, \ldots, \beta_1 > \sim e^{-2C_{4,4}} f(\beta_1, \ldots, \beta_4), \\
    \sum_{b=1}^{4} |i < 0|\sigma^+(0, 0)|\beta_4, \ldots, \beta_1 > \sim e^{-2C_{4,4}} f(\beta_1, \ldots, \beta_4), \\
    & \times \sum_{\ell=1}^{4} \prod_{m=1}^{\infty} D_{b,m}^{\beta_1}(\beta_1, \ldots, \beta_4) H_{b,\ell}(\beta_1, \ldots, \beta_4).
\end{align*}
\]

where:

\[
\begin{align*}
    H_{b,\ell}(\beta_1, \ldots, \beta_4) & = \cosh(\beta_\ell) \gamma(\pi) \prod_{m=1}^{\infty} \frac{\gamma(\pi \beta_m)}{\sinh(\pi \beta_m)}, \\
    D_{b,m}^{\beta_1}(\beta_1, \ldots, \beta_4) & = \prod_{m=1}^{4} \prod_{m \neq b}^{4} \frac{\pi \beta_m}{\sinh(\pi \beta_m)}, \\
    L_{b,\ell,\ell'}(\beta_1, \ldots, \beta_4) & = \sum_{\alpha_{\ell,\ell'}^{(b)}} D_{b,\ell,\ell'}^{(b)}(\beta_1, \ldots, \beta_4) D_{b,\ell,\ell'}^{(b)}(\beta_1, \ldots, \beta_4)\gamma(\pi \beta_{\ell,\ell'}^{(b)}), \\
    S_{b,\ell,\ell'}^{(b)}(\beta_1, \ldots, \beta_4) & = H_{b,\ell,\ell'}^{(b)}(\beta_1, \ldots, \beta_4) L_{b,\ell,\ell'}^{(b)}(\beta_1, \ldots, \beta_4)\gamma(\pi \beta_{\ell,\ell'}^{(b)}), \\
    f(\beta_1, \ldots, \beta_4) & = \prod_{\ell=1}^{4} \prod_{m=1}^{\infty} \frac{A_{\ell,\pi \beta_m}}{\cosh(\pi \beta_m)}, \\
    F(\beta_1, \ldots, \beta_4) & = \prod_{\ell=1}^{4} \prod_{m=1}^{\infty} \frac{A_{\ell,\pi \beta_m}}{\cosh(\pi \beta_m)}. \\
\end{align*}
\]

Finally setting $n = 4$ in the general expression [18] of $S_{n}^{++}$ we obtain:

\[
\begin{align*}
    S_{4}^{++}(w, k - \pi) & = C_{7,4} \int_{-\infty}^{+\infty} d\beta_\ell \int_{-\infty}^{+\infty} d\beta_4 \\
    & \times \frac{\prod_{\ell=1}^{4} \prod_{m=1}^{\infty} \frac{A_{\ell,\pi \beta_m}}{\cosh(\pi \beta_m)}}{\prod_{\ell=1}^{4} \prod_{m=1}^{\infty} \frac{A_{\ell,\pi \beta_m}}{\cosh(\pi \beta_m)}} \times \left( \sum_{\ell=1}^{4} \delta_{\ell,1} \delta_{\ell,1} \sum_{s_1, s_2, s_3, s_4=0}^{\infty} (2 - \delta_{\ell,1}) Re(S_{4}^{++}(s_1, s_2, s_3, s_4)(\beta_1, \beta_2, \beta_3, \beta_4)) \right),
\end{align*}
\]

\[
\begin{align*}
\end{align*}
\]

15
The latter two relations express all diagonal terms \( S \) of \( S \) the reason that allows us to substantially simplify the 4-spinon DSF to express it only in terms where 

\[
\begin{align*}
F(\beta_1, \beta_2, \beta_3, \beta_4) &= \cosh(\beta_1) \cosh(\beta_2) F(\beta_1, \beta_2, \beta_3, \beta_4) = \prod_{\ell=0}^{4} \frac{A(2\pi \rho_m)}{\cosh(\beta_1) \cosh(\beta_2)}, \\
W &= e(\beta_1) + e(\beta_2) = w - e(\beta_3) - e(\beta_4) = w - \pi \cosh(\beta_1) \cosh(\beta_2), \\
K &= -p(\beta_1) - p(\beta_2) = k + p(\beta_3) + p(\beta_4) = k + \arccot(\sinh(\beta_1)) + \arccot(\sinh(\beta_4)), \\
W_u &= 2\pi |\sin(K/2)|, \\
W_o &= \pi |\sin(K)|, \\
\beta_1 &= \arcsinh \left( \cot \left( \frac{\beta}{\pi} + \arccos \left( \frac{W}{W_{\beta}} \right) \right) \right), \\
\beta_2 &= \arcsinh \left( \cot \left( \frac{\beta}{\pi} - \arccos \left( \frac{W}{W_{\beta}} \right) \right) \right), \\
C_{4,4} &= 2^{-25/3} \pi^{-4} e^{2} A^{-24}.
\end{align*}
\]

Note that just in this particular case of \( n = 4 \) new symmetries embodied by new identities arise. Indeed, in addition to the relations (64) satisfied by the matrix functions \( X_{\ell,m}^{s,t}(\beta_1, \ldots, \beta_4) \), the vector functions \( H_{\ell}^{s,t}(\beta_1, \ldots, \beta_4) \), and the scalar function \( F(\beta_1, \ldots, \beta_4) \) which are given by:

\[
\begin{align*}
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4)^{*}, \\
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4)^{*} \in R, \\
H_{\ell}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= H_{m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4)^{*}, \\
F_{P_{\ell,m}}(\beta_1, \beta_2, \beta_3, \beta_4) &= F(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m, \quad \ell, m = 1, \ldots, 4, \quad s, t = 0, \ldots, \infty.
\end{align*}
\]

we also have the following extra identities satisfied by both matrix functions \( X_{\ell,m}^{s,t}(\beta_1, \ldots, \beta_4) = L_{\ell,m}^{s,t}(\beta_1, \ldots, \beta_4) \) and \( X_{\ell,m}^{s,t}(\beta_1, \ldots, \beta_4) = S_{\ell,m}^{s,t}(\beta_1, \ldots, \beta_4) \):

\[
\begin{align*}
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m, \quad \ell \neq m', \quad \ell' \neq m, \quad \ell' \neq m', \\
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m, \\
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m, \\
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m'. \\
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m, \\
X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= X_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell \neq m'.
\end{align*}
\]

Note that the first relation implies that the functions \( X_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) \) are real valued for any \( \ell = 1, \ldots, 4 \) and non-negative integer \( s \). The most important subset of relations that we will be using in the sequel to simplify even further the expression of 4-spinon \( S_4^{\beta} \) (62) is:

\[
\begin{align*}
S_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= S_{1,1}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell = 2, 3, 4, \\
S_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) &= S_{m,s}^{t,s}(\beta_1, \beta_2, \beta_3, \beta_4), \quad \ell = 1, 2, 3, 4.
\end{align*}
\]

The latter two relations express all diagonal terms \( S_{\ell,m}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4) \) in terms of the first diagonal term \( S_{1,1}^{s,t} \) and the first off diagonal term \( S_{1,2}^{s,t} \) respectively. This is the reason that allows us to substantially simplify the 4-spinon DSF to express it only in terms of \( S_{1,1}^{s,t} \) and \( S_{1,2}^{s,t} \) with \( t \geq s \) instead of all possible terms \( S_{\ell,m}^{s,t} \) and their complex conjugates.

Indeed using the latter relations (66), the invariance of the scalar function \( \frac{F(\beta, \beta_2, \beta_3, \beta_4)}{\sqrt{W_{\beta}^{2} - W^{2}}} \) under
the transpositions of \((\beta_1, \beta_2)\), and independently, that of \((\beta_3, \beta_4)\), and finally the redefinition of the integration variables from \((\beta_3, \beta_4)\) to \((\beta_1, \beta_3)\) respectively, we can substantially simplify the 4-spinon DSF \((62)\) to write it in the following form:

\[
S_{4}^{++}(w, k - \pi) = \sum_{t=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\beta_3 d\beta_4 \\
\times \left( \sum_{p \in Y_{11}} a_{s, t}^{11, p} \Re(S_{12}^{1, p}(\beta_1, \beta_2, \beta_3, \beta_4)) \\
+ \sum_{p \in Y_{12}} a_{s, t}^{12, p} \Re(S_{12}^{2, p}(\beta_1, \beta_2, \beta_3, \beta_4)) \right)
\]

\[
S_{4}^{--}(w, k - \pi) = \sum_{t=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\beta_3 d\beta_4 \\
\times \left( \sum_{p \in Y_{11}} a_{s, t}^{11, p} \Re(S_{12}^{1, p}(\beta_1, \beta_2, \beta_3, \beta_4)) \\
+ \sum_{p \in Y_{12}} a_{s, t}^{12, p} \Re(S_{12}^{2, p}(\beta_1, \beta_2, \beta_3, \beta_4)) \right)
\]

with the sets \(Y_{11}\) and \(Y_{12}\) being subsets of the permutation group acting on \((\beta_1, \beta_2, \beta_3, \beta_4)\) in its natural order, and defined by:

\[
Y_{11} = \{1, P_{12}, P_{12}P_{23}\}, \\
Y_{12} = \{1, P_{12}, P_{23}, P_{12}P_{23}, P_{13}P_{24}, P_{23}P_{12}, P_{12}P_{23}\},
\]

and the coefficients given by:

\[
a_{11, 1}^{s, t} = a_{12, 1}^{s, t} = 2 - \delta_{s, t}, \\
a_{11, 2}^{s, t} = a_{12, 2}^{s, t} = 2\delta_{s, t}, \\
a_{11, 3}^{s, t} = a_{12, 3}^{s, t} = 2, \\
a_{11, 4}^{s, t} = a_{12, 4}^{s, t} = 4, \\
2a_{12, 2}^{s, t} = a_{12, 3}^{s, t} = 4(1 - \delta_{s, t}).
\]

As we did in the 2-spinon case we consider the following non-vanishing components of the 4-spinon DSF:

\[
S_{4}^{xy}(w, k - \pi) = S_{4}^{yx}(w, k - \pi) = S_{4}^{yx}(w, k - \pi) = \frac{1}{2} S_{4}^{--}(w, k - \pi).
\]

We plot \(S_{4}^{xx}\) and \(S_{4}^{xy} + S_{4}^{yx}\) as functions of \(w\) for fixed \(k = \pi\) in Figures 4 and 5 respectively. As can be seen from Figure 4 \(S_{4}^{xx}\) is non-vanishing in the whole range \([0, 4\pi]\). In particular although very small it is not vanishing in the range \([2\pi, 4\pi]\). The latter fact can be used to detect the presence of 4 spinons experimentally since we know that in the latter range \(S_{4}^{xx}\) is vanishing so any non zero value of \(S_{4}^{xy}\) can be interpreted as a sign of the presence of 4 spinons and higher in the spectrum.
3 Sum Rules

Here we will compute the percentage of contribution of $S_n^+$ to the total $S^+$ analytically and numerically in the cases $n = 2, 4$ and only analytically in the general case of $n > 4$. For this purpose we consider the first sum rule satisfied by the total $S^+$, which is represented by the following total integrated intensity formula:

$$\int_0^\infty dw \int_0^{2\pi} dk S^+(w, k - \pi) = 2\pi^2. \quad (72)$$

Then we consider the following second sum rule satisfied by the total $S^+$ and which is also known as the first frequency moment at fixed momentum:

$$\int_0^\infty dw w S^+(w, k - \pi) = \frac{16\pi^2}{3} (1 - \cos(k)), \quad (73)$$

with $c_0 = \log(2) - 1/4$. To make analogous arguments and derivations as we will do in the sequel in the case of the first sum rule we rather use the following total integrated form of the second sum rule:

$$\int_0^\infty dw \int_0^{2\pi} dk w S^+(w, k - \pi) = \frac{16\pi^2}{3} \int_0^{2\pi} dk (1 - \cos(k)) = \frac{32\cos^2}{3}. \quad (74)$$

In the sequel we will refer to (72) and (74) as the first sum rule and second sum rule respectively.

As we will see below both sum rules involve integrals of $S_n^+$ that are totally symmetric with respect to the permutations of the spectral parameters $\beta_i, \ell = 1, \cdots, n$.

3.1 2-spinon

Now we present one of the main results of this paper and that is the contribution of $S_n^+$ to the total $S^+$ is about 36%. For this purpose, let us calculate the contribution of just the 2-spinon DSF to the integral given by the first sum rule (72) with $S^+$ being substituted by $S_2^+$. For this purpose it is convenient to make a change of variables from $(w, k)$ to $(\beta_1, \beta_2) \equiv (\beta_1, \beta_2)$ given by (54). We expect the integrand to be symmetrical with respect to the permutations of $\beta_1$ and $\beta_2$. Indeed we have:

$$\int_0^\infty dw \int_0^{2\pi} dk S_2^+(w, k - \pi) = \int_0^{2\pi} dw \int_0^{2\pi} dk S_2^+(w, k - \pi) = \frac{1}{4} \int_{-\infty}^{+\infty} d\beta_1 \int_{-\infty}^{+\infty} d\beta_2 \frac{A(\beta_2 - \beta_1)}{\cosh(\beta_1) \cosh(\beta_2)} = \frac{1}{4} \int_{-\infty}^{+\infty} d\beta_1 \int_{-\infty}^{+\infty} d\beta_2 \frac{A(\beta_2 - \beta_1)}{\cosh(\beta_1) \cosh(\beta_2)} = 7.17. \quad (75)$$

Figure 7 is a plot of the latter integrand as a function of $\beta_1$ and $\beta_2$. Figure 8 is also a plot of the latter integrand as a function of $\beta_1$ for fixed $\beta_2 = 0$. In both figures we see the manifestation of the existence of 2 spinons through 2 peaks in the graphs. We remark that in the integral over $\beta_1$ and $\beta_2$ the term $\Theta(W_n - w) \Theta(w - W_i)$ is always equal to 1 due to relations (54) so it is omitted. But this term allowed us to reduce the integral over $w$ from 0 to infinity to 0 to $2\pi$ since the maximum value of $W_n$ is $2\pi$ for 2 spinons. This remark holds true for the general case of $S_n$ with obvious changes so it will be understood there as well and we will not be repeating this argument again. If we compare this to the first sum rule (72) we conclude that $S_2^+$ accounts for 36.32% of the total $S^+$. This is a half of the currently known result in the litterature of 72% as first reported in reference [18]. Again using (74), an analogous calculation considering the second sum rule (74) leads to:

$$\int_0^\infty dw \int_0^{2\pi} dk w S_2^+(w, k - \pi) = \frac{1}{4} \int_{-\infty}^{+\infty} d\beta_1 \int_{-\infty}^{+\infty} d\beta_2 \frac{A(\beta_2 - \beta_1)}{\cosh(\beta_1) \cosh(\beta_2)} = 16.60. \quad (76)$$
If we compare this result to (74) we come to the conclusion that $S_2^{+-}$ accounts for 35.58% of the total $S^{+-}$, which confirms the conclusion reached through the first sum rule. As mentioned in the introduction experimental data obtained in [20] and [21] reveals that the observed contribution accounts roughly only for the third of the total theoretic DSF when the latter was incorrectly believed to be 99%. Since we have just shown that $S_2$ accounts for 36% which is roughly the third of 100% we believe that a reconciliation between experimental data and theoretical data can be made if the experimental data relates just to the 2-spinon sector.

3.2 4-spinon

In order to evaluate the contribution of $S_4^{+-} (w, k - \pi)$ relative to the total contribution given by the first sum rule (72) it is much convenient to consider the latter in the form

$$\int_0^\infty dw \int_0^{4\pi} dk S^{+-} (w, k - \pi) = 2 \int_0^\infty dw \int_0^{2\pi} dk S^{+-} (w, k - \pi) = 4\pi^2, \quad (77)$$

since as we will see below is much easier to calculate the contribution of $S_4^{+-}$ by considering both $w$ and $k$ in $[0, 4\pi]$. So we substitute $S^{+-}$ by $S_4^{+-}$ as given by (68) in the latter relation, and as we did in the 2-spinon case we make a change of variables from $(w, k)$ to $(\beta_1, \beta_2) \equiv (\beta_1, \beta_2)$ given by (63). We end up with the following expression:

$$\int_0^\infty dw \int_0^{4\pi} dk S_4^{+-} (w, k - \pi) = \int_0^{4\pi} dw \int_0^{4\pi} dk S_4^{+-} (w, k - \pi) = C_{7,4} \sum_{l \geq 0}^{\infty} \int_{-\infty}^{\infty} d\beta_1 \cdots \int_{-\infty}^{\infty} d\beta_4 F(\beta_1, \beta_2, \beta_3, \beta_4) \times \left( \sum_{p \in Y_{11}} \alpha_{11, p} \Re\left(S_{1,1}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4)\right) + \sum_{p \in Y_{12}} \alpha_{12, p} \Re\left(S_{1,2}^{s,t}(\beta_1, \beta_2, \beta_3, \beta_4)\right) \right), \quad (78)$$

where $Y_{11}$ and $Y_{12}$ are the sets of permutations acting on the four spectral parameters $\beta_\ell$ and are defined by (69). The coefficients $\alpha_{11, p}$ and $\alpha_{12, p}$ are given by (70). Using the defining relation (61) of $F(\beta_1, \ldots, \beta_4)$, one can easily check that it is invariant under the permutation group $G$ of the four spectral parameters $\beta_\ell$, that is:

$$F_P(\beta_1, \ldots, \beta_4) = F(\beta_1, \ldots, \beta_4). \quad (79)$$

where $P$ is any permutation acting on the latter parameters. For this reason and because of redefinitions of the latter spectral parameters, the above integrand is fully symmetric under the permutation group $G$ and hence simplifies substantially to:

$$\int_0^\infty dw \int_0^{4\pi} dk S_4^{+-} (w, k - \pi) = \int_0^{4\pi} dw \int_0^{4\pi} dk S_4^{+-} (w, k - \pi) = C_4 \int_{-\infty}^{\infty} d\beta_1 \cdots \int_{-\infty}^{\infty} d\beta_4 \times F(\beta_1, \beta_2, \beta_3, \beta_4) \times \sum_{l=1}^{2} \sum_{s \geq 0}^{\infty}(3 - 2\delta_{s,l})(2 - \delta_{s,l}) \times \Re\left(S_{1,1}^{s,t}(\beta_1, \ldots, \beta_4)\right), \quad (80)$$

with

$$C_4 = 4 \times C_{7,4} = 2^{-19/3} \pi^{-4} e^2 A^{-24}. \quad (81)$$

Figure 9 is a plot of one term of the latter integrand with $\ell = 1$ and $s = t = 0$ as a function of $\beta_1$ and $\beta_2$ for fixed $\beta_3 = 0$ and $\beta_4 = 1$. It shows the manisfestation of 4 spinons in the spectrum through 4 peaks in the graph. With the help of the Genz-Malik algorithm the numeric integration of the latter integral gives:

$$\int_0^\infty dw \int_0^{4\pi} dk S_4^{+-} (w, k - \pi) = 6.98 \pm 0.04. \quad (82)$$
With the first sum rule in its form given by (77), this means that $S_4^{++}$ contributes $17.68 \pm 0.10\%$ or almost $18\%$ to the total $S^{++}$. To make analogous derivations as we did in the case of the first sum rule we use the following form of the second sum rule:

$$
\int_0^\infty dw \int_0^{4\pi} dw S^{+-}(w, k - \pi) = \frac{2}{\pi} \int_0^\infty dw \int_0^{2\pi} dw S^{+-}(w, k - \pi)
$$

$$
= \frac{32\alpha_\pi}{3} \int_0^{2\pi} dk(1 - \cos(k)) = \frac{54\alpha_\pi^2}{3}
$$

(83)

Now since $w$ as given by (65) is symmetric with respect to the permutation group $G$ acting on the four spectral parameters $\beta_i$, and using exactly the same arguments as we did from (78) through (81) we find:

$$
\int_0^\infty dw \int_0^{4\pi} dw S_4^{+-}(w, k - \pi) = \int_0^{4\pi} dw \int_0^{4\pi} dw S_4^{+-}(w, k - \pi)
$$

$$
= C_4 \int_0^{4\pi} dw \int_0^{4\pi} dw S_4^{+-}(w, k - \pi)
$$

$$
\times \pi(\cosh(\beta_1) + \cdots + \cosh(\beta_4))
$$

$$
\times F(\beta_1, \beta_2, \beta_3, \beta_4)
$$

$$
\times \frac{2}{\pi} \sum_{\ell_1=1}^{2N} \sum_{t_1 \geq 2N} \left[ (3 - 2\delta_1, \ell_1)(2 - \delta_{s,t}) \right]
$$

$$
\times Re \left( S_4^{+-}(\beta_1, \ldots, \beta_4) \right)
$$

(84)

Again with the help of the Genz-Malik algorithm for the numeric integration of the latter integral we find:

$$
\int_0^\infty dw \int_0^{4\pi} dw S_4^{+-}(w, k - \pi) = 18.64 \pm 0.06,
$$

(85)

which given the second sum rule (83) means that $S_4^{+-}$ contributes $19.97\%$ or almost $20\%$ to the total $S^{+-}$. As a summary then the above two sum rules show that $S_4^{+-}$ contributes between $18\%$ and $20\%$ to the total $S^{+-}$.

3.3 n-spinon

The general case of $n$-spinons parallels closely the case of 4-spinon. In particular the first sum rule (77) generalizes as:

$$
\int_0^\infty dw \int_0^{2\pi} dw S^{i+}(w, k - \pi) = \frac{n}{2} \int_0^\infty dw \int_0^{2\pi} dw S^{i+}(w, k - \pi) = n\pi^2.
$$

(86)

If we substitute $S^{++}$ by $S_n^{++}$ as given by (48) in the latter relation, and make a change of variables from $(w, k)$ to $(\beta_1, \beta_2) \equiv (\beta_1, \beta_2)$ given by (43) as we did in the previous cases we find:

$$
\int_0^{2\pi} dw \int_0^{2\pi} dw S_n^{i+}(w, k - \pi) = C_{7,n} \int_0^{2\pi} dw \int_0^{2\pi} dw F(\beta_1, \cdots, \beta_n)
$$

$$
\times \left( \sum_{\ell_1N \geq 2N, \ell_2N \cdots, \ell_{N-1} = 1, t_1 = 0}^{2N, \cdots, s_{0} = 0} \delta_{\ell_2N, \ell_{N-1}} \right)
$$

$$
\times Re \left( S_n^{i+}(\beta_1, \cdots, \beta_n) \right)
$$

(87)

with $N$ given by (19) and $C_{7,n}$ given by (49). With powerful enough computing resources one should be able to compute the latter integral numerically through the Genz-Malik algorithm at least for the cases $n = 6, 8, 10, 12$. Unfortunately we do not possess such computing resources and therefore we left this computation for the future when they become available to us. This would of course allow us to find the contribution of the $n$-spinon $S_n^{i-}$ to the total $S_n$. The analogue of the second sum rule (83) in the case of $n$-spinon is:

$$
\int_0^{2\pi} dw \int_0^{2\pi} dw S^{i-}(w, k - \pi) = \frac{n}{2} \int_0^{2\pi} dw \int_0^{2\pi} dw S^{i-}(w, k - \pi)
$$

$$
\times \frac{54\alpha_\pi^2}{3} \int_0^{2\pi} \frac{3}{\pi} dk(1 - \cos(k)) = \frac{16\alpha_\pi^2}{3}
$$

(88)
Similar derivation that led to (87) gives:

\[ \int_{\infty}^{0} dw \int_{0}^{n \pi} dk w S_{n}^{i,+}(w, k - \pi) = \int_{0}^{n \pi} dw \int_{0}^{n \pi} dk w S_{n}^{i,-}(w, k - \pi) = \pi C_{T,n} \int_{-\infty}^{\infty} d\beta_{1} \cdots \int_{-\infty}^{\infty} d\beta_{n} F(\beta_{1}, \ldots, \beta_{n}) \]

\[ \times (\cosh(\beta_{1})^{-1} + \cdots + \cosh(\beta_{n})^{-1}) \]

\[ \times \left( \sum_{\ell_{2N} \geq \ell_{N}, \ell_{2N-1}, \ldots, \ell_{1}=1}^{\infty} \sum_{s_{2N}, \ldots, s_{1}=0}^{\infty} (2 - \delta_{\ell_{2N} \ell_{N}}) \right) \]

\[ \times \left( \sum_{\ell_{2N} \geq \ell_{N}, \ell_{2N-1}, \ldots, \ell_{1}=1}^{\infty} \sum_{s_{2N}, \ldots, s_{1}=0}^{\infty} (2 - \delta_{\ell_{2N} \ell_{N}}) \right) \]

\[ \times \left( \sum_{\ell_{2N} \geq \ell_{N}, \ell_{2N-1}, \ldots, \ell_{1}=1}^{\infty} \sum_{s_{2N}, \ldots, s_{1}=0}^{\infty} (2 - \delta_{\ell_{2N} \ell_{N}}) \right) \]

Again with powerful enough computing resources one should be able to evaluate the latter integrals a la Genz-Malik algorithm for at least \( n = 6, 8, 10, 12 \). Using the second sum rule (88) this would give us the contribution percentage of the \( n \)-spinon \( S_{n}^{+,-} \) to the total \( S_{n} \). This task is also left for the future computing resources permitting.

4 An approximation for the total DSF of the Heisenberg model

As mentioned in the introduction since in this paper we have shown that \( S_{2} \) and \( S_{4} \) saturate the total DSF only up to 54% – 56% we need therefore to study the higher sectors as well. From the shapes of \( S_{2} \) in Figure 3 and \( S_{4} \) in Figure 4 as functions of energy transfer for fixed momentum transfer one can notice that they are very similar in that \( S_{4} \) almost looks like a scaled down version of \( S_{2} \) in the common first Brouillin zone \([0, 2\pi]\). Beyond \([0, 2\pi]\) \( S_{2} \) is null and \( S_{4} \) is extremely small. One is tempted then to conclude that this pattern would still hold true for the general \( S_{n} \). Since \( S_{2} \) is the only one which is very simple and expressed as a single term and captures the general shape of the general \( S_{n} \) up to a scale factor we propose then an approximation to the total DSF as scaled up version of \( S_{2} \) such that it saturates the sum rules. This approximation is somewhere in the middle between the Muller ansatz and the exact one. It’s better than the Muller anstaz because it has a much better shape that closely fits the experimental data and it is almost as simple as the Muller anstaz, and also it is much simpler that the exact total DSF which is very complex. The only drawback is that it misses all the spectral weight beyond the first Brouillin zone of \([0, 2\pi]\) although the latter is negligible for general \( n \). To recap if we rescale the overall factor to saturate the sum rules we find then the approximate total DSF of the Heisenberg model to be

\[ S_{\text{Approx}}^{zz}(w, k - \pi) = S_{\text{Approx}}^{yy}(w, k - \pi) = S_{\text{Approx}}^{zz}(w, k - \pi) = \frac{25}{18} S_{2}^{+,-}(w, k - \pi). \]  

\( S_{\text{Approx}}^{zz} \) is plotted in Figure 6 as a function of \( w \) for fixed \( k = \pi \).

5 Conclusion

In this paper we have derived the \( n \)-spinon DSF \( S_{n} \) and we have proved why any sector among the two possible sectors of the eigenspace should be considered but not both at the same time. This allowed us to correct the overall factors in the existing formulas in the litterature. In particular we have shown that the overall factor of the \( n \)-spinon DSF can be expressed in terms of the Glaisher-Kinkelin constant. We have extensively studied the 2-spinon and 4-spinon cases and in particular we have shown that the 2-spinon DSF accounts for 36% of the total DSF and that the 4-spinon DSF account for between 18% and 20% for the total DSF depending on the sum rule. In the case of 4-spinon we have derived a set of highly nontrivial symmetry relations
involving permutations of the spectral parameters and indices of the DSF terms. It begs the question whether the latter symmetry relations can be generalized to the $n$-spinon case. We have derived analytically the integrals corresponding to the sum rules for the general case of $n$-spinon and all it remains is to evaluate them numerically at least for the cases $n = 6, 8, 10, 12$ using the Genz-Malik algorithm or any other one. We have proposed an approximation to the total DSF based on rescaling the overall factor of the 2-spinon DSF such that it saturates the sum rules. Finally we propose as an experiment to detect any non vanishing $S$ for fixed $k$ and $w$ greater than $W_u = 2\pi \sin (k/2)$ of the 2-spinon case which would signal the presence of 4 spinons and higher in the spectrum.

![Figure 1](image1.png)

Figure 1. : The $\frac{n-2}{2}$ contours $\bar{C}_n$ used in the $n$-spinon case

![Figure 2](image2.png)

Figure 2. : Dispersion relation in the 2-spinon case
Figure 3. $S_2$ as a function of $w$ for fixed $k = \pi$

Figure 4. $S_4$ as a function of $w$ for fixed $k = \pi$
Figure 5. \( S_2 + S_4 \) as a function of \( w \) for fixed \( k = \pi \)

Figure 6. \( S \) Total Approximate as a function of \( w \) for fixed \( k = \pi \)
Figure 7: Plot of the 2-spinon integrand of the total integrated intensity sum rule as a function of $\beta_1$ and $\beta_2$.

Figure 8: Plot of the 2-spinon integrand of the total integrated intensity sum rule as a function of $\beta_1$ for fixed $\beta_2 = 0$. 

25
Figure 9.: Plot of the 4-spinon integrand of the total integrated intensity sum rule as a function of $\beta_1$ and $\beta_2$ for fixed $\beta_3 = 0$ and $\beta_4 = 1$

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