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2003 J. Phys.: Condens. Matter 15 8527

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The thermodynamics of the anisotropic spin- S XXZ chain in the high-temperature region

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Received 15 September 2003

Published 25 November 2003

Online at stacks.iop.org/JPhysCM/15/8527

Abstract

We report analytical calculations of the Helmholtz free energy of non-integrable anisotropic quantum XXZ chains in the high-temperature regime for several values of the spin S . Single-ion anisotropy and interaction with an external magnetic field are taken into account. The seven lowest-order terms in the high-temperature expansion of Helmholtz free energy are obtained. Our results contribute to the existing literature on high-temperature expansions and numerical studies of those models by discussing the effects of anisotropy upon their high-temperature thermodynamic properties, such as the average energy per site, the specific heat and magnetic susceptibility.

1. Introduction

One-dimensional quantum spin chains have been extensively studied by condensed matter physicists for many decades from both theoretical and experimental points of view. In particular, a number of exact results about the thermodynamic quantities have been obtained for $S = 1/2$ [1] through the thermodynamic Bethe ansatz technique, and for the classical Heisenberg chain ($S \rightarrow \infty$), originally solved by Fisher [2]. Unfortunately, systems with an intermediate value of S cannot be solved by the Bethe ansatz technique and still offer resistance to analytical methods.

After Haldane's conjecture [3] in 1983, there has been renewed interest in this field, since half-odd-integer spin chains would behave as gapless excitations with power-law decay in the spin correlations, whereas integer spin chains would show an excitation gap and exponentially decaying correlations. The existence has been verified of higher-spin quasi one-dimensional magnetic systems such as CsVCl₃ and CsVBr₃ ($S = 3/2$) [4–6] (investigated by inelastic neutron scattering), (2, 2'-bipyridine) trichloromanganese (III), or

simply denoted by $(\text{C}_{10}\text{H}_8\text{N}_2)\text{MnCl}_3$ ($S = 2$) [7], and $(\text{CD}_3)_4\text{NMnCl}_3$, usually denoted by TMMC ($S = 5/2$) [8, 9]. All these antiferromagnetic structures exhibit nearly ideal one-dimensional behaviour over a considerable range of temperature. Encouraged by these features, the magnetic and thermodynamic properties of higher-spin chains were first investigated numerically for the antiferromagnetic spin $S = 3/2$ chain using the quantum Monte Carlo (QMC) method (by Itoh *et al* [5, 6]), the density matrix renormalization group (DMRG) method (by Moukouri and Caron [10]) and the thermodynamic density matrix renormalization group (TDMRG) method (Xiang [11]). Yamamoto investigated the thermodynamic properties of the antiferromagnetic XXZ $S = 2$ chain using the QMC [12] method; more recently, he applied the modified spin wave theory to this model [13]. For higher-spin models ($S \leq 5/2$) there are also some reports about exact numerical diagonalization for small rings with $N = 5$ that were developed [14] before Haldane's conjecture. In 1989 Kim *et al* [15] used the numerical QMC to study the thermodynamic properties of spin models up to $S = 5/2$. Recently the semiclassical approach [16] was applied to study the thermodynamic properties of the antiferromagnetic and ferromagnetic XXZ chains, at their isotropic points. Very recently, Fukushima *et al* [17] obtained the specific heat and magnetic susceptibility of a ferromagnetic mixed-spin model with two kinds of spins, s and S , arranged alternately and coupled by a Heisenberg-type nearest-neighbour exchange for arbitrary values of s and S . They obtained numerical results through the exact diagonalization method and the analytical high-temperature expansions for both thermodynamic functions at the isotropic point (ferromagnetic exchange) for arbitrary values of s and S . Their high-temperature expansion of the specific heat, in the absence of an external magnetic field, goes up to $(\beta J)^{11}$ and their expansion of the magnetic susceptibility, calculated at vanishing magnetic field, goes up to $(\beta J)^6$ with a single-ion anisotropy term in one of the spins. With $s = S$ the thermodynamic quantities calculated by Fukushima *et al* reduce to those of isotropic XXZ spin- S model.

The Hamiltonian of the anisotropic spin- S XXZ chain is

$$\mathbf{H} = \sum_{i=1}^N J(\mathbf{S}_i, \mathbf{S}_{i+1})_{\Delta} - hS_i^z + D(S_i^z)^2, \quad (1)$$

where we use the notation $(\mathbf{S}_i, \mathbf{S}_{i+1})_{\Delta} \equiv S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z$. Here, S_i^x , S_i^y and S_i^z stand for the spin- S matrices in the i th site of the chain; N is the number of sites in the periodic chain; Δ is the anisotropy constant in the z -direction; h is the external magnetic field in the z -axis and D is the single-ion anisotropy parameter. For $S \geq 1$ there may be non-trivial higher-order anisotropic single-ion terms, e.g. in the case of thin ferromagnetic films [18, 19]. For this material, in addition to the single-ion anisotropy term $D(S_i^z)^2$, we take into account the single-ion quartic term $K(S_i^z)^4$. The method of Rojas *et al* for calculating the β -expansion of the Helmholtz free energy can be extended in order to incorporate this quartic (and higher-order) single-site term. In the present paper we restrict our discussion to the simplest case of the Hamiltonian (1), which models many quasi-1D materials [20].

Numerical and analytical results can be found in the literature about the high-temperature thermodynamic properties of quantum spin models at the isotropic points. The aim of the present communication is to study the effects of anisotropy in the spin- S XXZ model upon such properties. Both the single-ion anisotropy term and an external magnetic field are taken into account.

The paper is organized as follows: in section 2 we give a brief description of the β -expansion method, which allowed us to obtain thermodynamic properties such as average energy, specific heat and magnetic susceptibility, among others, in the high-temperature region. In the first subsection of section 3, we compare our results with the classical limit ($S \rightarrow \infty$) of the Heisenberg chain [2] for the isotropic case. We also verify if our results are in agreement

with the results of [17] for the ferromagnetic chains. In the second subsection of section 3 we explore our results to include the effect of the anisotropy parameter Δ and the presence of D and h in the Hamiltonian (1). Finally, in section 4 we give our conclusions.

2. A survey of the method

It has been recently shown in [21] that an auxiliary function φ can be defined from which one is allowed to systematically obtain the high-temperature expansion of the Helmholtz free energy for the thermodynamic limit of any one-dimensional chain model subject to periodic boundary conditions, spatial translation invariance and nearest-neighbour interactions. The coefficients of such expansion can be obtained for arbitrary order in β^n , where $\beta = 1/kT$, T is the absolute temperature and k is the Boltzmann constant. A detailed analysis of the convergence issues was carried out by Moura-Melo *et al* [22] for exactly solvable Ising chains.

The auxiliary function approach has also been successfully applied to the study of the thermodynamic properties in the high-temperature regime of the non-integrable spin-1 XXZ chain [23].

In the thermodynamic limit, the Helmholtz free energy per site of a quantum spin- S XXZ chain can be written as the β -expansion [21]

$$\mathcal{W}(\beta) = -\frac{1}{\beta}[\ln(2S + 1) + \ln(1 + \xi(\beta))], \tag{2}$$

where

$$\xi(\beta) = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \frac{\partial^n}{\partial \lambda^n} (\varphi(\lambda)^{n+1})|_{\lambda=1} \tag{3}$$

and the auxiliary function $\varphi(\lambda)$ is given by

$$\varphi(\lambda) = \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} \frac{(-\beta)^n}{\lambda^m} H_{1,m}^{(n)}. \tag{4}$$

The functions $H_{1,m}^{(n)}$ correspond to the ‘connected’ strings with n operators $\mathbf{H}_{i,i+1}$ ($\mathbf{H} = \sum_{i=1}^N \mathbf{H}_{i,i+1}$) so that m of them are distinct, that is,

$$H_{1,m}^{(n)} = \sum_{\{n_i\}}'' \left\langle \prod_{i=1}^m \frac{\mathbf{H}_{i,i+1}^{n_i}}{n_i!} \right\rangle_g. \tag{5}$$

The notation $\sum_{\{n_i\}}''$ stands for the restriction $\sum_{i=1}^m n_i = n$ and $n_i \neq 0$ for $i = 1, 2, \dots, m$. The index m satisfies the condition $1 \leq m \leq n$. The g -traces can be related to the normalized traces

$$\langle \mathbf{H}_{i_1,i_1+1}^{n_1} \mathbf{H}_{i_2,i_2+1}^{n_2} \cdots \mathbf{H}_{i_m,i_m+1}^{n_m} \rangle_g \equiv \frac{n_1! \cdots n_m!}{n!} \sum_{\mathcal{P}} \langle \mathcal{P}(\mathbf{H}_{i_1,i_1+1}^{n_1}, \mathbf{H}_{i_2,i_2+1}^{n_2}, \dots, \mathbf{H}_{i_m,i_m+1}^{n_m}) \rangle, \tag{6}$$

where $\sum_{i=1}^m n_i = n$ with $n_i \neq 0$ and the indices $i_k, k = 1 \cdots m$ are all distinct. By definition, $\langle \mathcal{P}(\mathbf{H}_{i_1,i_1+1}, \mathbf{H}_{i_2,i_2+1}, \dots, \mathbf{H}_{i_m,i_m+1}) \rangle$ represents the normalized traces of all distinct permutations of the n operators inside the parentheses. We refer the reader to [21] for details of this approach. In appendix D of [21] the function $H_{1,m}^{(n)}$ can be found written in terms of the normalized traces for $n, m = 1, \dots, 4$.

3. The high-temperature behaviour of the quantum spin- S XXZ chain

The thermodynamic properties of the quantum spin- S XXZ chain, in the high-temperature region can be described in terms of a β -expansion series. We apply the method of [21] to obtain the β -expansion of the Helmholtz free energy of Hamiltonian (1) for arbitrary values of J , Δ , h and D . We present in the appendix our results for the Helmholtz free energy per site $\mathcal{W}_s(\beta)$, up to order $(\beta J)^6$, for several values of spin S (namely, $S = 3/2, 5/2, 3, 7/2$ and 4). We presented elsewhere [24] the Helmholtz free energy of the spin-2 XXZ chain. In [24] we compared our results for $S = 2$ with the numerical QMC results of the antiferromagnetic chain obtained by Yamamoto [12]. For the sake of completeness, we include here the $S = 2$ case and explore the effects due to the presence of anisotropy in the spin-2 XXZ chain, not considered in [12]. From each expression of the free energy $\mathcal{W}_s(\beta)$ contained either in the appendix or in [24], it can be readily seen that the simultaneous change of sign $\Delta \rightarrow -\Delta$ and $D \rightarrow -D$ will only affect the even-power coefficients β^{2m} , for $m = 1, 2, \dots$, which in turn will get an overall sign. Those changes in sign yield different thermodynamic behaviours associated with the model in the high-temperature regime, corresponding to its distinct phases.

Due to the fact that the β -expansion of the Helmholtz free energy of the spin- S XXZ chain is analytical in the parameters J , Δ , D and in the external magnetic field h , thermodynamic functions can be obtained from it by suitable derivatives of $\mathcal{W}_s(\beta)$ such as the average energy, the specific heat, the magnetic susceptibility, the average of the squared z -component of magnetization, and the first-neighbours z -component of the spin correlation function.

The range of validity in β of our high-temperature expansions certainly depends on the choice of values for the set of parameters in the Hamiltonian (1). We take $J > 0$ and let Δ refer to either the ferromagnetic ($\Delta < 0$) or the antiferromagnetic ($\Delta > 0$) phases.

Finally we rescaled all the constants in the Hamiltonian (1), so that our expansion of the Helmholtz free energy is expressed in powers of the product $J\beta$.

3.1. Thermodynamics at the isotropic points ($\Delta = \pm 1$)

The classical limit of the spin models corresponds to having $S \rightarrow \infty$ in the Hamiltonian (1). In 1964 Fisher [2] solved this limit exactly for the isotropic cases ($\Delta = \pm 1$), with $D = 0$ and $h = 0$. In order to accommodate the limit $S \rightarrow \infty$ to the thermodynamics of the Hamiltonian (1), it is conveniently rewritten it in terms of the unit vectors $s_i \equiv S_i / \sqrt{S(S+1)}$. We replace each S_i by its corresponding unit vector s_i in the Hamiltonian (1); the constant J is replaced by $J \rightarrow JS(S+1)$. In the classical limit ($S \rightarrow \infty$) the expression of the specific heat for $\Delta = \pm 1$ is [2]

$$C(S \rightarrow \infty, T) = 1 - \frac{(J/k\tilde{T})^2}{\sinh^2(J/k\tilde{T})}. \quad (7)$$

We have $\tilde{T} \equiv T/S(S+1)$.

From our β -expansions (contained in the appendix) we obtain the expressions for the specific heat per site for $S = 3/2, \dots, 4$, in the high-temperature region ($C(S, T) = -\beta^2 \partial^2(\beta \mathcal{W}_s(\beta)) / \partial \beta^2$).

Figure 1 shows the specific heat per site as a function of kT , with $\Delta = 1$, $h = 0$ and $D = 0$. The four curves correspond to distinct values of S . The range of kT shown in figures 1(a) and (b) is that in which the expansions are reliable; those plots show that the specific heat per site for distinct values of S has distinct orders of magnitude. Figure 1(c) shows the specific heat per site for $S = 3/2$ and $5/2$ in a larger interval of kT , where both expansions are valid. A suitable normalization allows us to plot together and compare the

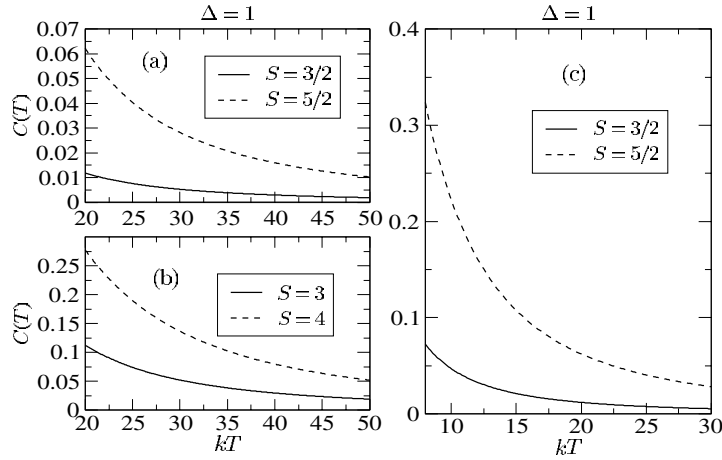


Figure 1. Specific heat per site as a function of kT , for $D = 0$, $h = 0$ and $\Delta = 1$, for distinct values of S . The range of kT in figures (a) and (b) is the range in which all four expansions are valid. In figure (c) the curves of figure (b) are extended up to $kT = 8$, showing their behaviour at higher temperatures.

curves of the specific heat per site for $S = 3/2, 2, \dots, \infty$. In figure 2 we have the specific heat times $(k\tilde{T})^2$ as a function of $1/k\tilde{T}$ for the isotropic points ($\Delta = \pm 1$) of the spin- S Heisenberg chain. They are compared with the classical limit result (7). The isotropic ferromagnetic point ($\Delta = -1$) and isotropic antiferromagnetic point ($\Delta = 1$) for $D = 0$ and $h = 0$ are plotted separately. For $\Delta = -1$, we verify that as we increase the value of S in $C(S, T)(k\tilde{T})^2$ it approaches the classical limit ($S \rightarrow \infty$) (solid curve) from below. For $\Delta = 1$ that same thermodynamic function monotonically approaches the classical limit curve from above. The curves of $C(S, T)$ for the antiferromagnetic chains get closer to the $C(\infty, T)$ as S increases faster than the curves of the ferromagnetic chains do. We can also conclude that the higher the value of S , the closer the behaviour of ferromagnetic and antiferromagnetic phases in the high-temperature region. In the $S \rightarrow \infty$ limit, according to equation (7), the phase becomes irrelevant to this thermodynamic function. Our β -expansion results for $\Delta = -1$ are valid up to $1/k\tilde{T} \sim 1$, whereas for $\Delta = 1$ its validity goes up to $1/k\tilde{T} \sim 1.5$. In order to determine the range of β in which the expansion of a given thermodynamic function is valid, we have let the relative weight of its highest-order term be 5% at most.

Fisher [2] also obtained the expression for the magnetic susceptibility at the isotropic points, namely,

$$\chi(S \rightarrow \infty, T) = \frac{1}{3k\tilde{T}} \frac{1 + u(S, T)}{1 - u(S, T)} \tag{8}$$

where $u(S, T)$ is given by

$$u(S, T) = \coth\left(\frac{J}{\tilde{T}}\right) - \frac{\tilde{T}}{J}, \tag{9}$$

with $\tilde{T} = T/S(S + 1)$.

The relation between the magnetic susceptibility $\chi(S, T)$ and the Helmholtz free energy is $\chi(S, T) = -\partial^2 \mathcal{W}_S(\beta) / \partial h^2$. In figure 3 we display the static magnetic susceptibility ($\chi(S, T)|_{h=0}$) times $k\tilde{T}$ versus $1/k\tilde{T}$ at the isotropic ferromagnetic point for a set of spins from $S = 3/2$ up to 4 and the classical limit $S \rightarrow \infty$ (solid curve). For the ferromagnetic case

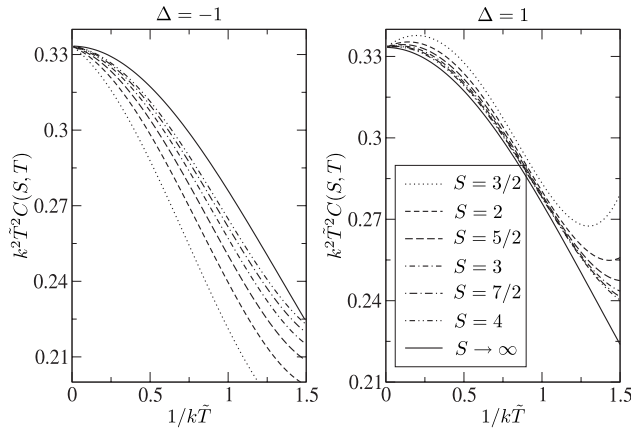


Figure 2. Specific heat per unit of $1/k^2 \tilde{T}^2$ (where $\tilde{T} \equiv T/S(S+1)$) as a function of $1/k\tilde{T}$, for the following values of spin $S = 3/2, 2, 5/2, 3, 7/2, 4$, and for the limit case $S \rightarrow \infty$, for the isotropic cases ($\Delta = \mp 1$). We take $D = 0$, and $h = 0$.

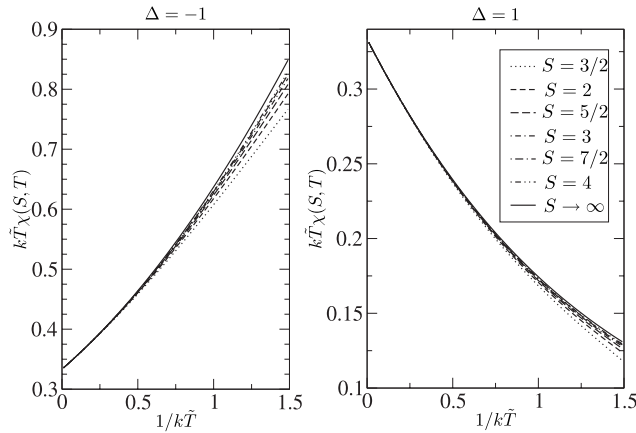


Figure 3. The static magnetic susceptibility times $k\tilde{T}$ as a function of $1/k\tilde{T}$, for a set of spin values $S = \{3/2, 2, 5/2, 3, 7/2, 4, \infty\}$, for the isotropic case ($\Delta = \pm 1$).

($\Delta = -1$) the curves of the static magnetic susceptibility times $k\tilde{T}$ for all the spin- S models under consideration are equal up to $1/k\tilde{T} \sim 0.5$, whereas for $1/k\tilde{T} \gtrsim 0.5$ the curves begin to split. For the antiferromagnetic case ($\Delta = 1$) we have an identical behaviour in the region $1/k\tilde{T} \sim 0.75$. The curves of each spin- S are not visually distinguishable in those plots, but if one takes the difference between two curves with different values of spins it is not null; e.g. the difference between the magnetic susceptibility of the model with spin $S = 3/2$ and $S \rightarrow \infty$, at $1/k\tilde{T} = 0.45$, is 0.8%, whereas the difference between the same thermodynamic function for $S = 3/2$ and 4 is 0.6%. For lower normalized temperature, $1/k\tilde{T} = 0.75$, the difference between the magnetic susceptibility of $S = 3/2$ and $S \rightarrow \infty$ increases to 2%; the same difference for the $S = 3/2$ and 4 cases goes to 1.5%.

The correlation function of the z -component of the spin between nearest neighbours for isotropic spin models in the classical limit is given by [2]

$$\langle S_i^z S_{i+l}^z \rangle (S \rightarrow \infty, T) = \frac{1}{3} u(S, T)^{|l|}, \quad (10)$$

where the function $u(S, T)$ is given by equation (9) and $l = 0, 1, 2, \dots$

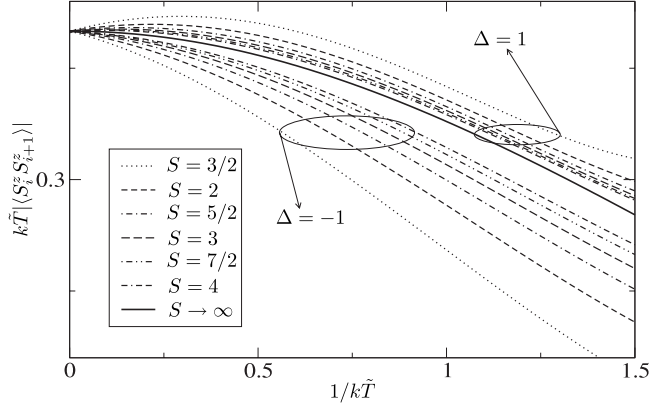


Figure 4. The absolute value of the correlation function $\langle S_i^z S_{i+1}^z \rangle$ times $k\tilde{T}$ is plotted as a function of $1/k\tilde{T}$ for $\Delta = -1$ and 1 .

The correlation function $\langle S_i^z S_{i+1}^z \rangle$ can be derived from the Helmholtz free energies $\mathcal{W}_s(\beta)$, whose expansions are given in the appendix, that is $\langle S_i^z S_{i+1}^z \rangle = \partial \mathcal{W}_s(\beta) / \partial \Delta$. In figure 4 we plot the scaled absolute value of the correlation function between nearest neighbours $k\tilde{T} |\langle S_i^z S_{i+1}^z \rangle|$ as a function of $1/k\tilde{T}$. For $\Delta = -1$ a bigger splitting (slow convergence in the values of S) is shown between the curves of consecutive spins compared with the approximations of the curves for different values of S at $\Delta = 1$. The classical limit of the spin model (solid curve) is much closer to the curves of the antiferromagnetic chains. For the ferromagnetic chains our β -expansions are valid up to $1/k\tilde{T} \sim 1$ and for the antiferromagnetic chains our β -expansions are valid up to $1/k\tilde{T} \sim 1.5$.

We also compared our results derived from the Helmholtz free energies, whose expressions are given in the appendix, with the results of Fukushima *et al* [17]. Our results are fully in agreement with the analytical results of [17] for the $S = s$ high-temperature expansion of the specific heat and the magnetic susceptibility.

3.2. Thermodynamics off the isotropic points ($\Delta \neq \pm 1$)

From now on we consider thermodynamic quantities taking into account the presence of the anisotropic constant Δ in the Hamiltonian (1) and including in it the single-ion anisotropy term and an external magnetic field.

The plots of the average energy $E(S, T)$ ($E(S, T) = \partial \mathcal{W}_s(\beta) / \partial \beta$) times $k\tilde{T}$ versus $1/k\tilde{T}$ from $S = 3/2$ up to 4 are displayed in figure 5 for the anisotropic parameters $\Delta = \pm 2$ and $\pm 1/2$. For the ferromagnetic chains ($\Delta = -1/2$ and -2) the curves of $k\tilde{T} E(S, T)$ are well separated and move apart as the temperature is lowered. For the antiferromagnetic cases ($\Delta = 1/2$ and 2), the curves are closer to one another and as the temperature decreases the curves tend to narrow the difference between them. Our β -expansions for the ferromagnetic case are valid up to $1/k\tilde{T} \sim 0.5$ whereas for the antiferromagnetic chains they are valid up to $1/k\tilde{T} \sim 1$.

In order to exemplify the effect of the anisotropic parameter Δ upon thermodynamic functions of spin- S XXZ models, the specific heat at a fixed temperature in units of $S(S+1)$ is displayed in figure 6. The quantity $k^2 \tilde{T}^2 C(S, T)$ is plotted as a function of the anisotropic parameter Δ for the set of spins from $S = 3/2$ up to 4. The rescaled temperature at $k\tilde{T} = 4/3$ and $5/3$ is taken; in all plots, $h = 0$. The distance between any two curves in the region $\Delta < -1$ goes to zero as the spin increases for both values of D . For the case $\Delta > 1$ the curves

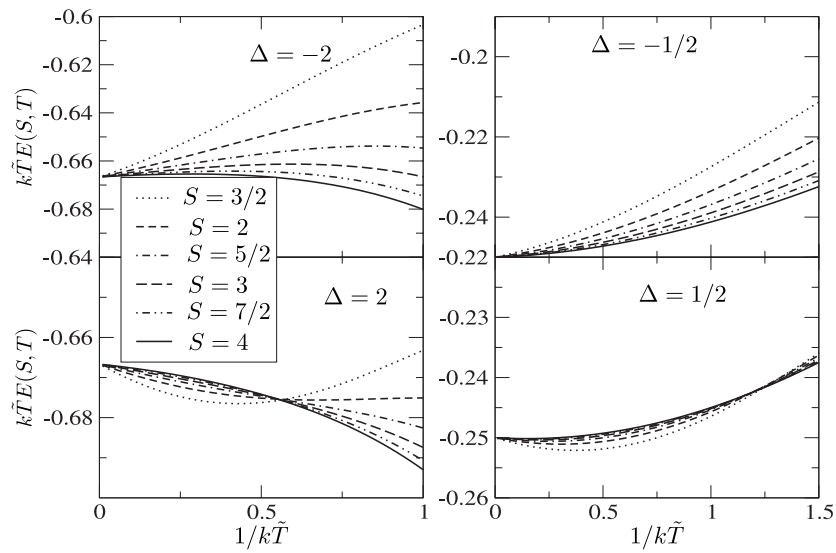


Figure 5. The average energy times $k\tilde{T}$ as a function of $1/k\tilde{T}$ for the spin- S model for $S = 3/2$ up to 4 with the anisotropic parameter taking the values $\Delta = \pm 1/2, \pm 2$.

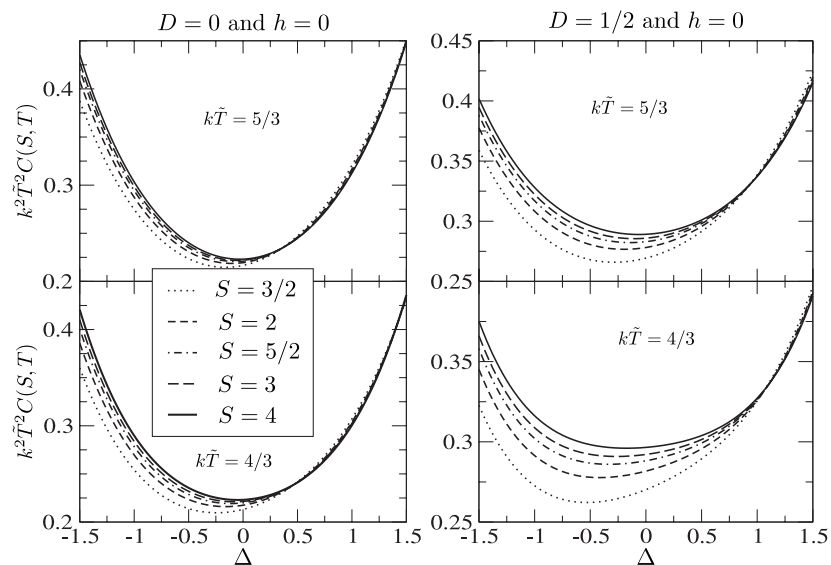


Figure 6. The specific heat $C(S, T)$ times $k^2\tilde{T}^2$ is plotted as a function of anisotropic parameter Δ , for two fixed temperatures in units of $S(S+1)$, $k\tilde{T} = 5/3$ and $4/3$ with $D = 0$ and $1/2$. In all plots $h = 0$.

are almost superimposed on one another. In the interval $|\Delta| < 1$ there exists a minimum, located at $\Delta \sim 0$ for $D = 0$ (the spin- S XX chain [25, 26]). In the ferromagnetic region the spreading of curves is more significant than in the antiferromagnetic region, mainly in the presence of a non-null D and lower temperatures.

In figure 7 we present the magnetic susceptibility times $k\tilde{T}$ as a function of the anisotropic parameter Δ at fixed rescaled temperatures in the presence and absence of the single-ion

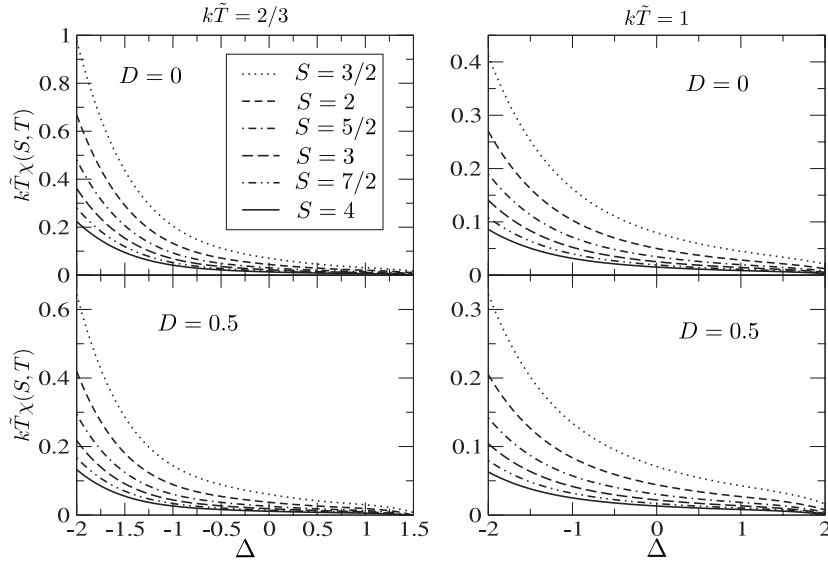


Figure 7. The magnetic susceptibility times $k\tilde{T}$ as a function of anisotropic parameter Δ for two fixed temperatures $k\tilde{T} = 2/3$ and 1, with $D = 0$ and 0.5. In all plots $h = 0$.

anisotropy term. It shows curves for spin values S ranging from $3/2$ to 4; in all plots we have $h = 0$. For $\Delta < 1$ the curves are a monotonically decreasing function of Δ , but decreasing more slowly in the antiferromagnetic region. There is no minimum of the amount $k\tilde{T}\chi(S, T)$ as a function of the anisotropic parameter Δ . In the presence of the single-ion anisotropy term with $D = 0.5$, the main qualitative characteristics of the curves still remain. From the range of validity of our results, it is not clear whether this function will increase for higher values of Δ .

In figure 8 we display the on-site correlation function $\langle (S_i^z)^2 \rangle$ per unit of $S(S + 1)$ as a function of the anisotropy parameter Δ at a fixed temperature in units of $S(S + 1)$, that is $k\tilde{T} = 2/3$. In the plot corresponding to $D = 0$ and $h = 0$ we are able to verify that, at the isotropic points $\Delta = \pm 1$, the quantity $\langle (S_i^z)^2 \rangle$ has the constant value $S(S + 1)/3$ for any value of S in the whole interval of temperature, since at this point (with $D = 0$ and $h = 0$) $\langle (S_i^x)^2 \rangle = \langle (S_i^y)^2 \rangle = \langle (S_i^z)^2 \rangle = \frac{1}{3}\langle (\mathbf{S}_i)^2 \rangle = \frac{1}{3}S(S + 1)$. The purpose of this figure is to show how this function becomes dependent on the temperature and how the curves begin to deviate from one another as the parameter Δ leaves the isotropic point. If we include the effect due to the presence of an external magnetic field, but keeping $D = 0$, the function $\langle (S_i^z)^2 \rangle$ continues to be constant at $\Delta = 1$ but this constant becomes h -dependent. When we include the contribution of the single-ion anisotropy term with $D = -1$ and $h = 0$, there is no more intersection of curves and the on-site correlation per units of $S(S + 1)$ exhibits systematically increasing functions as the spin increases. For the single-ion anisotropy parameters $D = 1$ and $h = 0$, the plots exhibit different behaviour in comparison to the case $D = -1$: now the curves decrease as the value of the spin increases and all the curves for different values of S in the regions $|\Delta| > 1$ tend to superpose.

Finally in figure 9 we plot the ratio of the absolute value of the correlation function between first neighbours and the on-site correlation function of the z -component of the spin, based on equation (10), which gives the correlation function between first neighbours for $S \rightarrow \infty$ as a power-law decay. Hence, the family of curves to be plotted could be of the same kind as

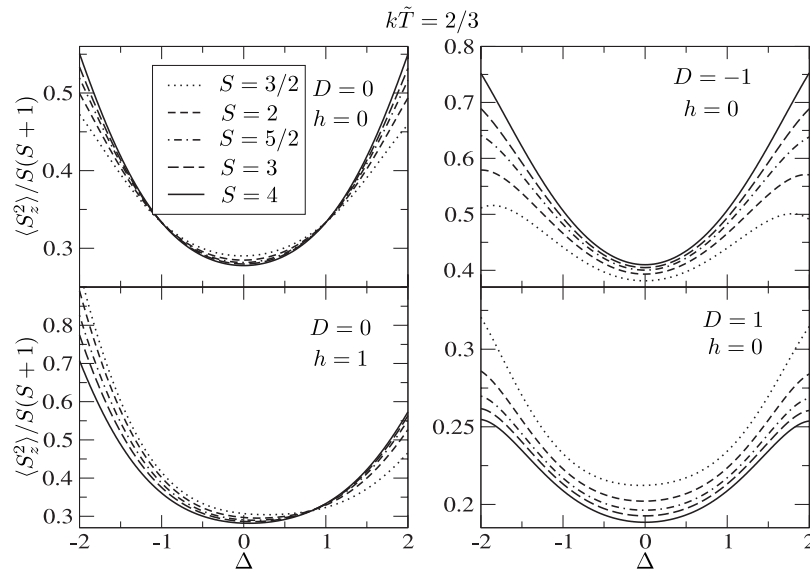


Figure 8. The on-site correlation function per unit of $S(S+1)$ as a function of the anisotropic parameter for a fixed temperature $k\tilde{T} = 2/3$ for $(D, h) = \{(0, 0), (-1, 0), (0, 1), (1, 0)\}$.

the $u(S, T)$ functions for higher values of S . In all plots we considered the two anisotropic points $\Delta = \pm 1/2$. In each graph the case $\Delta = 1/2$ corresponds to the set of curves that decrease as the value of S increases and the case $\Delta = -1/2$ corresponds to the curves that increase as the value of S increases. The set of curves (for S ranging from $3/2$ to 4) at each anisotropic point are well separated in each plot of figure 9. As the spin value S increases, the curves for $\Delta = \pm 1/2$ get closer together (as it should be, because in the limit $S \rightarrow \infty$ they are described by the same function). For $\Delta = -1/2$ the presence of an external magnetic field makes the curves of distinct values of S get closer together, in the high-temperature region. This approximation between curves is stronger when $D > 0$. For $\Delta = 1/2$ the curves get closer for distinct values of S , in the presence of D and an external magnetic field.

4. Conclusions

In summary, we discuss the thermodynamics of the anisotropic spin- S XXZ chain with a single-ion anisotropy term in the presence of an external magnetic field in the high-temperature region. We obtain the analytical β -expansion of the Helmholtz free energies for $S = 3/2, 5/2, 3, 7/2$ and 4 , up to order β^6 . From those free energies we obtain some thermodynamic functions, e.g. the specific heat, magnetic susceptibility and the correlation function of the z -component of the spin between first neighbours, among others. Recently, Fukushima *et al* [17] obtained the high temperature expansion of the specific heat and the magnetic susceptibility of a mixed ferromagnetic chain ($\Delta = -1$) with two alternating kinds of spin, S_i and s_i , in a unit cell along the chain for arbitrary values of s and S . When the spins S_i and s_i are the same, their calculation gives the β -expansion of the specific heat (in the absence of the single-ion anisotropy term and the external magnetic field) up to $(\beta J)^{11}$ and the magnetic susceptibility (at $h = 0$) up to order $(\beta J)^6$ of the isotropic ferromagnetic spin- S XXZ model. From our results we recover for the spin- S models, for the values of S considered in this paper, their results up to order $(\beta J)^4$ for the specific heat and the magnetic susceptibility and extend them

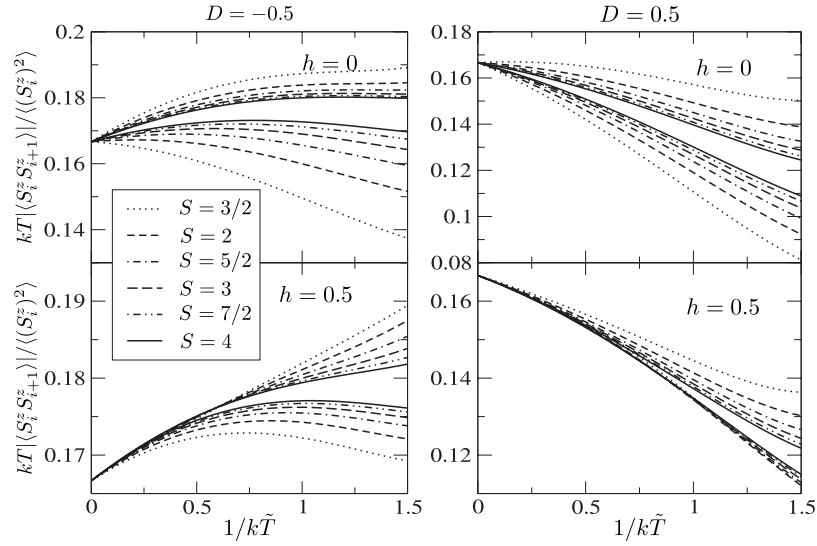


Figure 9. The absolute value of the correlation function between first neighbours times kT divided by $\langle (S_i^z)^2 \rangle$ is plotted versus $1/k\tilde{T}$ for anisotropic ($\Delta = \pm 1/2$) ferromagnetic and antiferromagnetic points for $D = -0.5, 0.5$ with $h = 0$ and 0.5 .

to the anisotropic models including the contribution of the single-ion anisotropy term and an external magnetic field.

We also compare our results, at the isotropic points ($\Delta = \pm 1$), with the classical spin model ($S \rightarrow \infty$). We show that as the value of S increases, the curves of the thermodynamic functions approach those of the $S \rightarrow \infty$ spin model.

Off the isotropic points ($\Delta \neq \pm 1$) we show how the thermodynamic functions depend on the anisotropic constant Δ , the single-ion anisotropy parameter D and the external magnetic field h . The comparisons are performed at a suitably rescaled temperature \tilde{T} that is kept fixed. In doing so, we show how the thermodynamic functions behave in the high-temperature region in the distinct phases of the anisotropic spin- S model.

As a final comment, we should say that in the nice calculations done by Fukushima *et al* in [17] it is essential that the model be invariant under rotation in order to simplify the calculation of the coefficients of their β -expansions. Those simplifications allow the β -expansion of the magnetic susceptibility to be calculated up to $(J\beta)^6$ and that of the specific heat to be calculated up to $(J\beta)^{11}$. We stress that our results are valid off the isotropic point, as well. This offers the interesting possibility of increasing the number of parameters in the model to fit the experimental data. The price one pays for not taking advantage of the invariance of the model under rotation is that the β -expansion of the Helmholtz free could only be obtained up to order $(J\beta)^6$. Nowadays, our calculations are limited by the RAM available on our personal computers. We hope in the near future to extend the order in β of our high-temperature expansion of the Helmholtz free energy of the anisotropic XXZ model.

Acknowledgments

OR thanks FAPEMIG for financial support. SMdeS thanks FAPEMIG for partial financial support. MTT thanks CNPq and FAPERJ for partial financial support.

Appendix. β -expansion of the free energy for the higher spin- S XXZ chain

In this appendix we present [27] the high-temperature expansions of the Helmholtz free energies per site $\mathcal{W}_s(\beta)$, up to order $n = 7$, for spin S , where $S = 3/2, 5/2, 3, 7/2$ and 4 for arbitrary sets of values for the parameters of the Hamiltonian (1).

For spin $S = 3/2$:

$$\begin{aligned}
 \mathcal{W}_{3/2}(\beta) = & -\ln(4)\beta^{-1} + \frac{5}{4}D + \left(-\frac{25}{32}\Delta^2 - \frac{5}{8}h^2 - \frac{25}{16} - \frac{1}{2}D^2\right)\beta \\
 & + \left(-\frac{25}{64}\Delta + \frac{5}{4}\Delta^2 D + \frac{1}{2}h^2 D - \frac{5}{4}D + \frac{25}{16}\Delta h^2\right)\beta^2 + \left(\frac{17}{192}h^4 + \frac{65}{64}h^2 + \frac{371}{1536} + \frac{3}{8}D^2\right. \\
 & + \frac{1}{12}D^4 - \frac{1}{2}\Delta^2 D^2 - \frac{1103}{3072}\Delta^4 - \frac{165}{64}\Delta^2 h^2 - \frac{5}{2}\Delta h^2 D + \frac{737}{384}\Delta^2\left.\right)\beta^3 + \left(\frac{83}{16}\Delta^2 h^2 D\right. \\
 & - \frac{85}{96}\Delta h^4 - \frac{3}{8}h^2 D + \frac{755}{3072}\Delta^3 + \frac{1489}{384}\Delta^3 h^2 + \frac{325}{192}D - \frac{15}{8}\Delta^2 D - \frac{5}{12}\Delta^2 D^3 \\
 & + \frac{35}{192}\Delta^4 D - \frac{5}{24}h^4 D + \frac{755}{1536}\Delta + \frac{1}{32}\Delta D^2 + \Delta h^2 D^2 - \frac{533}{128}\Delta h^2 - \frac{1}{6}h^2 D^3 \\
 & + \frac{2}{3}D^3\left.\right)\beta^4 + \left(-\frac{4895}{1024}\Delta^4 h^2 + \frac{2221}{30720}\Delta^4 - \frac{373003}{122880}\Delta^2 + \frac{3355}{36864}\Delta^6 + \frac{1}{8}h^4 D^2\right. \\
 & + \frac{67}{24}\Delta h^4 D - \frac{1}{45}D^6 + \frac{1021}{960}D^2 - \frac{19}{120}D^4 + \frac{389}{960}\Delta D - \frac{333}{160}\Delta^2 D^2 - \frac{389}{960}\Delta^3 D \\
 & + \frac{5}{6}\Delta h^2 D^3 + \frac{1}{3}\Delta^2 D^4 - \frac{33}{32}h^2 D^2 + \frac{101}{96}\Delta^4 D^2 + \frac{2111}{512}\Delta^2 h^4 + \frac{1}{240}\Delta D^3 + \frac{3995}{512}\Delta^2 h^2 \\
 & + \frac{9}{2}\Delta h^2 D - \frac{25}{8}\Delta^2 h^2 D^2 + \frac{11719}{46080} - \frac{13}{576}h^6 - \frac{205}{24}\Delta^3 h^2 D - \frac{209}{384}h^4 - \frac{685}{512}h^2\left.\right)\beta^5 \\
 & + \left(-\frac{109319}{245760}\Delta + \frac{1069}{2304}\Delta h^6 - \frac{2019683}{172032}\Delta^3 h^2 + \frac{1}{15}h^2 D^5 + \frac{5}{72}h^4 D^3 + \frac{61}{720}h^6 D\right. \\
 & + \frac{329435}{1032192}h^2 D^3 - \frac{35}{12}\Delta h^4 D^2 - \frac{2}{3}\Delta h^2 D^4 + \frac{34679}{368640}\Delta^5 - \frac{143653}{430080}D^5 \\
 & - \frac{33148757}{20643840}D^3 - \frac{59}{48}\Delta^2 h^2 D^3 - \frac{726245}{516096}h^2 D + \frac{29}{32}h^4 D + \frac{3666913}{516096}\Delta h^2 \\
 & - \frac{15665}{1152}\Delta^3 h^4 + \frac{3910241}{1032192}\Delta h^2 D^2 - \frac{1475}{96}\Delta^2 h^4 D + \frac{8573}{768}\Delta^4 h^2 D - \frac{466673}{368640}\Delta^3 \\
 & + \frac{5701951}{1474560}\Delta^4 D + \frac{9481141}{3440640}\Delta^2 D^3 + \frac{1}{6}\Delta^2 D^5 - \frac{153179}{92160}\Delta^2 D - \frac{361}{5120}\Delta D^2 \\
 & + \frac{17827}{107520}\Delta^3 D^2 - \frac{11215537}{1032192}\Delta^2 h^2 D - \frac{4397}{4608}\Delta^6 D + \frac{31}{6}\Delta^3 h^2 D^2 + \frac{3}{160}\Delta D^4 \\
 & - \frac{755}{576}\Delta^4 D^3 + \frac{212741}{36864}\Delta h^4 + \frac{31445}{6144}\Delta^5 h^2 - \frac{12814579}{10321920}D\left.\right)\beta^6 + \mathcal{O}(\beta^7). \quad (\text{A.1})
 \end{aligned}$$

For spin $S = 5/2$:

$$\begin{aligned}
 \mathcal{W}_{5/2}(\beta) = & -\ln(6)\beta^{-1} + \frac{35}{12}D + \left(-\frac{1225}{144} - \frac{28}{9}D^2 - \frac{35}{24}h^2 - \frac{1225}{288}\Delta^2\right)\beta \\
 & + \left(\frac{1225}{144}\Delta h^2 + \frac{28}{9}h^2 D + \frac{490}{27}\Delta^2 D + \frac{80}{81}D^3 - \frac{1225}{576}\Delta - \frac{490}{27}D\right)\beta^2 + \left(-\frac{365687}{27648}\Delta^4\right. \\
 & + \frac{259}{576}h^4 + \frac{19355}{1728}h^2 - \frac{980}{27}\Delta h^2 D + \frac{32977}{41472} - 28\Delta^2 D^2 + \frac{196}{81}D^4 + \frac{565019}{10368}\Delta^2 \\
 & - \frac{58555}{1728}\Delta^2 h^2 - \frac{40}{27}h^2 D^2 + \frac{217}{27}D^2\left.\right)\beta^3 + \left(\frac{62125}{648}D + \frac{28315}{648}\Delta^4 D - \frac{833}{324}\Delta D^2\right. \\
 & - \frac{217}{27}h^2 D + \frac{48265}{4608}\Delta - \frac{392}{81}h^2 D^3 - \frac{11305}{81}\Delta^2 D - \frac{9065}{864}\Delta h^4 - \frac{25}{9}h^4 D - \frac{560}{243}D^5 \\
 & + \frac{10087}{54}\Delta^2 h^2 D + \frac{1298843}{10368}\Delta^3 h^2 + \frac{10402}{243}D^3 - \frac{2380}{243}\Delta^2 D^3 + \frac{48265}{9216}\Delta^3 \\
 & + 56\Delta h^2 D^2 - \frac{390971}{3456}\Delta h^2\left.\right)\beta^4 + \left(\frac{727822177}{11197440} + \frac{24962}{81}\Delta h^2 D - \frac{32375}{81}\Delta^2 h^2 D^2\right. \\
 & + \frac{7063}{81}\Delta h^4 D + \frac{4760}{243}\Delta h^2 D^3 - \frac{192535}{243}\Delta^3 h^2 D - \frac{30872}{10935}D^6 - \frac{2422385}{41472}h^2 \\
 & - \frac{136283}{10368}h^4 - \frac{1333}{5184}h^6 + \frac{4808671}{41472}\Delta^2 h^4 + \frac{22043035}{41472}\Delta^2 h^2 - \frac{96336625}{248832}\Delta^4 h^2 \\
 & + \frac{8617}{2430}\Delta D^3 + \frac{45521}{3240}\Delta D - \frac{45521}{3240}\Delta^3 D + \frac{65204}{729}\Delta^2 D^4 - \frac{2219}{36}h^2 D^2 \\
 & + \frac{94547}{972}\Delta^4 D^2 - \frac{1116943}{4860}\Delta^2 D^2 - \frac{123304}{3645}D^4 + \frac{91288}{405}D^2 + \frac{476}{81}h^4 D^2 \\
 & - \frac{11724397249}{29859840}\Delta^2 - \frac{13029335}{8957952}\Delta^6 + \frac{168976781}{2488320}\Delta^4 + \frac{1400}{243}h^2 D^4\left.\right)\beta^5 \\
 & + \left(-\frac{1951787957}{59719680}\Delta - \frac{18507771191}{358318080}D + \frac{62916601}{23328}\Delta^4 h^2 D - \frac{41405}{36}\Delta^2 h^4 D\right. \\
 & + \frac{100333}{729}\Delta^2 h^2 D^3 - \frac{130408}{729}\Delta h^2 D^4 - \frac{23170}{81}\Delta h^4 D^2 + \frac{14393371121}{35831808}\Delta h^2 D^2 \\
 & - \frac{24178636835}{11943936}\Delta^2 h^2 D + \frac{1243618822261}{1074954240}\Delta^2 D^3 - \frac{57557180303}{89579520}\Delta^2 D
 \end{aligned}$$

$$\begin{aligned}
& + \frac{16680463}{466560} \Delta D^2 - \frac{37156}{729} \Delta^2 D^5 - \frac{3045}{4} \Delta^4 D^3 + \frac{40876867297}{39813120} \Delta^4 D \\
& - \frac{28559335}{31104} \Delta^3 h^4 - \frac{12289559251}{5971968} \Delta^3 h^2 + \frac{1603451735}{1492992} \Delta^5 h^2 + \frac{28189}{2304} \Delta h^6 \\
& + \frac{332998967}{995328} \Delta h^4 + \frac{5122720283}{5971968} \Delta h^2 + \frac{7395323}{466560} \Delta^3 D^2 - \frac{46457117}{139968} \Delta^6 D \\
& + \frac{4594}{405} \Delta D^4 + \frac{1371334}{729} \Delta^3 h^2 D^2 + \frac{679}{270} h^6 D - \frac{70}{243} h^4 D^3 + \frac{30872}{3645} h^2 D^5 \\
& + \frac{5621}{108} h^4 D + \frac{2313699323}{35831808} h^2 D^3 - \frac{4252177889}{17915904} h^2 D + \frac{437261279}{29859840} \Delta^5 \\
& - \frac{3700833073}{29859840} \Delta^3 - \frac{587896837}{5598720} D^5 - \frac{848128834859}{2149908480} D^3 + \frac{10976}{2187} D^7) \beta^6 + \mathcal{O}(\beta^7).
\end{aligned} \tag{A.2}$$

For spin $S = 3$:

$$\begin{aligned}
\mathcal{W}_3(\beta) = & -\ln(7)\beta^{-1} + 4D + (-2h^2 - 16 - 8\Delta^2 - 6D^2)\beta \\
& + (16\Delta h^2 + 6h^2 D + 48\Delta^2 D + \frac{22}{7} D^3 - 48D - 4\Delta)\beta^2 + (-96\Delta h^2 D \\
& - 88\Delta^2 h^2 + \frac{572}{3} \Delta^2 + \frac{113}{14} D^4 - \frac{768}{7} \Delta^2 D^2 + 28h^2 + \frac{180}{7} D^2 - \frac{146}{3} \Delta^4 \\
& + \frac{5}{6} h^4 - 2 - \frac{33}{7} h^2 D^2)\beta^3 + (-\frac{101}{14} h^4 D - 16\Delta^2 D^3 - 12\Delta D^2 + \frac{3062}{7} D + \frac{1420}{7} D^3 \\
& - 392\Delta h^2 - \frac{4794}{7} \Delta^2 D + \frac{1352}{3} \Delta^3 h^2 + 34\Delta + \frac{1732}{7} \Delta^4 D - \frac{113}{7} h^2 D^3 - \frac{185}{14} D^5 \\
& - \frac{180}{7} h^2 D + \frac{1536}{7} \Delta h^2 D^2 + 17\Delta^3 - \frac{80}{3} \Delta h^4 + \frac{4800}{7} \Delta^2 h^2 D)\beta^4 + (\frac{993199}{2205} \\
& + \frac{10344}{7} \Delta h^2 D - \frac{15096}{7} \Delta^2 h^2 D^2 + \frac{2176}{7} \Delta h^4 D + 32\Delta h^2 D^3 - \frac{28432}{7} \Delta^3 h^2 D \\
& - \frac{43489}{2940} D^6 - \frac{1769}{7} h^2 - \frac{935}{21} h^4 - \frac{817}{1260} h^6 + \frac{8516}{21} \Delta^2 h^4 + \frac{53720}{21} \Delta^2 h^2 - \frac{40678}{21} \Delta^4 h^2 \\
& + \frac{824}{35} \Delta D^3 + \frac{256}{5} \Delta D - \frac{256}{5} \Delta^3 D + \frac{29756}{49} \Delta^2 D^4 - \frac{2046}{7} h^2 D^2 + \frac{23060}{49} \Delta^4 D^2 \\
& - \frac{67152}{49} \Delta^2 D^2 - \frac{56839}{245} D^4 + \frac{378233}{245} D^2 + \frac{625}{28} h^4 D^2 - \frac{1819661}{735} \Delta^2 - \frac{81169}{2205} \Delta^6 \\
& + \frac{128393}{245} \Delta^4 + \frac{925}{28} h^2 D^4)\beta^5 + (-\frac{19049}{105} \Delta + \frac{76843}{315} D + \frac{948652}{49} \Delta^4 h^2 D \\
& - \frac{39572}{7} \Delta^2 h^4 D + \frac{82280}{49} \Delta^2 h^2 D^3 - \frac{59512}{49} \Delta h^2 D^4 - \frac{10288}{7} \Delta h^4 D^2 \\
& + \frac{1067260}{441} \Delta h^2 D^2 - \frac{30172328}{2205} \Delta^2 h^2 D + \frac{23269096}{2205} \Delta^2 D^3 - \frac{1847816}{315} \Delta^2 D \\
& + \frac{70113}{245} \Delta D^2 - \frac{181852}{245} \Delta^2 D^5 - \frac{1043656}{147} \Delta^4 D^3 + \frac{2661271}{315} \Delta^4 D - \frac{279016}{63} \Delta^3 h^4 \\
& - \frac{6093980}{441} \Delta^3 h^2 + \frac{5524898}{735} \Delta^5 h^2 + \frac{13304}{315} \Delta h^6 + \frac{492146}{315} \Delta h^4 + \frac{1299891}{245} \Delta h^2 \\
& + \frac{2314}{49} \Delta^3 D^2 - \frac{296446}{105} \Delta^6 D + \frac{18806}{245} \Delta D^4 + \frac{703408}{49} \Delta^3 h^2 D^2 + \frac{3727}{420} h^6 D \\
& - \frac{701}{84} h^4 D^3 + \frac{43489}{980} h^2 D^5 + \frac{1689}{7} h^4 D + \frac{976118}{2205} h^2 D^3 - \frac{700033}{441} h^2 D \\
& + \frac{56797}{630} \Delta^5 - \frac{227888}{315} \Delta^3 - \frac{221457}{245} D^5 - \frac{7036243}{2205} D^3 + \frac{152651}{2940} D^7) \beta^6 + \mathcal{O}(\beta^7).
\end{aligned} \tag{A.3}$$

For spin $S = 7/2$:

$$\begin{aligned}
\mathcal{W}_{7/2}(\beta) = & -\ln(8)\beta^{-1} + \frac{21}{4} D + (-\frac{21}{8} h^2 - \frac{21}{2} D^2 - \frac{441}{32} \Delta^2 - \frac{441}{16})\beta \\
& + (\frac{441}{4} \Delta^2 D - \frac{441}{64} \Delta - \frac{441}{4} D + 8D^3 + \frac{441}{16} \Delta h^2 + \frac{21}{2} h^2 D)\beta^2 + (-\frac{693}{2} \Delta^2 D^2 \\
& - \frac{151557}{1024} \Delta^4 + \frac{91}{4} D^4 + \frac{71883}{128} \Delta^2 + \frac{91}{64} h^4 - \frac{12789}{64} \Delta^2 h^2 + \frac{567}{8} D^2 + \frac{3969}{64} h^2 \\
& - \frac{7791}{512} - \frac{441}{2} \Delta h^2 D - 12h^2 D^2)\beta^3 + (-\frac{146853}{128} \Delta h^2 + 777D^3 - \frac{1323}{32} \Delta D^2 \\
& - \frac{567}{8} h^2 D - \frac{21483}{8} \Delta^2 D - \frac{1911}{32} \Delta h^4 - \frac{91}{2} h^2 D^3 - 56D^5 + \frac{48657}{1024} \Delta^3 \\
& + 693\Delta h^2 D^2 + \frac{105}{4} \Delta^2 D^3 + \frac{104307}{64} D + \frac{67557}{64} \Delta^4 D + \frac{48657}{512} \Delta + \frac{33327}{16} \Delta^2 h^2 D \\
& + \frac{173019}{128} \Delta^3 h^2 - \frac{131}{8} h^4 D)\beta^4 + (\frac{12015007}{5120} + \frac{11403}{2} \Delta h^2 D - \frac{71757}{8} \Delta^2 h^2 D^2 \\
& + \frac{7413}{8} \Delta h^4 D - \frac{105}{2} \Delta h^2 D^3 - \frac{131019}{8} \Delta^3 h^2 D - \frac{907}{15} D^6 - \frac{465885}{512} h^2 - \frac{16443}{128} h^4
\end{aligned}$$

$$\begin{aligned}
& -\frac{1387}{960}h^6 + \frac{611583}{512}\Delta^2h^4 + \frac{5070555}{512}\Delta^2h^2 - \frac{7878255}{1024}\Delta^4h^2 + \frac{8799}{80}\Delta D^3 \\
& + \frac{49539}{320}\Delta D - \frac{49539}{320}\Delta^3D + 3093\Delta^2D^4 - \frac{35973}{32}h^2D^2 + \frac{55875}{32}\Delta^4D^2 \\
& - \frac{1036377}{160}\Delta^2D^2 - \frac{48201}{40}D^4 + \frac{2561127}{320}D^2 + \frac{553}{8}h^4D^2 - \frac{500089497}{40960}\Delta^2 \\
& - \frac{5777809}{20480}\Delta^6 + \frac{29807823}{10240}\Delta^4 + 140h^2D^4) \beta^5 + \left(-\frac{67700717}{81920}\Delta + \frac{750204371}{163840}D\right. \\
& + \frac{26575275}{256}\Delta^4h^2D - \frac{710157}{32}\Delta^2h^4D + \frac{182823}{16}\Delta^2h^2D^3 - 6186\Delta h^2D^4 \\
& - \frac{23709}{4}\Delta h^4D^2 + \frac{190057743}{16384}\Delta h^2D^2 - \frac{5774469723}{81920}\Delta^2h^2D \\
& + \frac{11554850001}{163840}\Delta^2D^3 - \frac{201457011}{5120}\Delta^2D + \frac{8202651}{5120}\Delta D^2 - \frac{61593}{10}\Delta^2D^5 \\
& - \frac{3050299}{64}\Delta^4D^3 + \frac{1724320395}{32768}\Delta^4D - \frac{2199449}{128}\Delta^3h^4 - \frac{581312967}{8192}\Delta^3h^2 \\
& + \frac{406295427}{10240}\Delta^5h^2 + \frac{157913}{1280}\Delta h^6 + \frac{121566417}{20480}\Delta h^4 + \frac{1056989643}{40960}\Delta h^2 \\
& + \frac{18891}{5120}\Delta^3D^2 - \frac{45675581}{2560}\Delta^6D + \frac{12207}{32}\Delta D^4 + \frac{159675}{2}\Delta^3h^2D^2 + \frac{6307}{240}h^6D \\
& - \frac{1225}{24}h^4D^3 + \frac{907}{5}h^2D^5 + \frac{29169}{32}h^4D + \frac{189134217}{81920}h^2D^3 - \frac{333228711}{40960}h^2D \\
& + \frac{17639391}{40960}\Delta^5 - \frac{138258281}{40960}\Delta^3 - \frac{23836641}{4096}D^5 - \frac{6445757611}{327680}D^3 \\
& + \frac{5488}{15}D^7) \beta^6 + \mathcal{O}(\beta^7). \tag{A.4}
\end{aligned}$$

For spin $S = 4$:

$$\begin{aligned}
\mathcal{W}_4(\beta) = & -\ln(9)\beta^{-1} + \frac{20}{3}D + \left(-\frac{400}{9} - \frac{154}{9}D^2 - \frac{10}{3}h^2 - \frac{200}{9}\Delta^2\right)\beta \\
& + \left(\frac{400}{9}\Delta h^2 - \frac{6160}{27}D + \frac{6160}{27}\Delta^2D + \frac{1430}{81}D^3 - \frac{100}{9}\Delta + \frac{154}{9}h^2D\right)\beta^2 + \left(\frac{41}{18}h^4\right. \\
& - \frac{2816}{3}\Delta^2D^2 - \frac{11080}{27}\Delta^2h^2 + \frac{117652}{81}\Delta^2 - \frac{4546}{81} + \frac{9185}{162}D^4 - \frac{715}{27}h^2D^2 \\
& - \frac{12320}{27}\Delta h^2D + \frac{4708}{27}D^2 - \frac{10562}{27}\Delta^4 + \frac{3380}{27}h^2) \beta^3 + \left(\frac{421850}{81}D - \frac{4708}{27}h^2D\right. \\
& + \frac{355}{3}\Delta^3 - \frac{3280}{27}\Delta h^4 - \frac{94315}{486}D^5 + \frac{286744}{81}\Delta^3h^2 - \frac{721270}{81}\Delta^2D + \frac{73040}{243}\Delta^2D^3 \\
& - \frac{9185}{81}h^2D^3 - \frac{9548}{81}\Delta D^2 + \frac{148544}{27}\Delta^2h^2D - \frac{605}{18}h^4D + \frac{299420}{81}\Delta^4D + \frac{710}{3}\Delta \\
& + \frac{615868}{243}D^3 + \frac{5632}{3}\Delta h^2D^2 - \frac{79768}{27}\Delta h^2) \beta^4 + \left(\frac{108647677}{10935} + \frac{1513688}{81}\Delta h^2D\right. \\
& - \frac{2505800}{81}\Delta^2h^2D^2 + \frac{195712}{81}\Delta h^4D - \frac{146080}{243}\Delta h^2D^3 - \frac{13449040}{243}\Delta^3h^2D \\
& - \frac{9066239}{43740}D^6 - \frac{230095}{81}h^2 - \frac{26539}{81}h^4 - \frac{949}{324}h^6 + \frac{250292}{81}\Delta^2h^4 + \frac{2636600}{81}\Delta^2h^2 \\
& - \frac{6254890}{243}\Delta^4h^2 + \frac{495704}{1215}\Delta D^3 + \frac{165088}{405}\Delta D - \frac{165088}{405}\Delta^3D + \frac{9351260}{729}\Delta^2D^4 \\
& - \frac{33154}{9}h^2D^2 + \frac{1283612}{243}\Delta^4D^2 - \frac{31150768}{1215}\Delta^2D^2 - \frac{18589711}{3645}D^4 \\
& + \frac{13692217}{405}D^2 + \frac{59873}{324}h^4D^2 - \frac{181963703}{3645}\Delta^2 - \frac{3193415}{2187}\Delta^6 + \frac{15620203}{1215}\Delta^4 \\
& + \frac{471575}{972}h^2D^4) \beta^5 + \left(-\frac{11700557}{3645}\Delta + \frac{2652703169}{76545}D + \frac{327628268}{729}\Delta^4h^2D\right. \\
& - \frac{662860}{9}\Delta^2h^4D + \frac{41324392}{729}\Delta^2h^2D^3 - \frac{18702520}{729}\Delta h^2D^4 - \frac{1621840}{81}\Delta h^4D^2 \\
& + \frac{712785596}{15309}\Delta h^2D^2 - \frac{1514289848}{5103}\Delta^2h^2D + \frac{85849022936}{229635}\Delta^2D^3 \\
& - \frac{16027679512}{76545}\Delta^2D + \frac{25787267}{3645}\Delta D^2 - \frac{26919724}{729}\Delta^2D^5 - \frac{2269240}{9}\Delta^4D^3 \\
& + \frac{751937119}{2835}\Delta^4D - \frac{13749320}{243}\Delta^3h^4 - \frac{217421660}{729}\Delta^3h^2 + \frac{123919630}{729}\Delta^5h^2 \\
& + \frac{952}{3}\Delta h^6 + \frac{32772686}{1701}\Delta h^4 + \frac{76137109}{729}\Delta h^2 - \frac{550066}{729}\Delta^3D^2 - \frac{197837882}{2187}\Delta^6D \\
& + \frac{622006}{405}\Delta D^4 + \frac{258030256}{729}\Delta^3h^2D^2 + \frac{36839}{540}h^6D - \frac{205885}{972}h^4D^3 \\
& + \frac{9066239}{14580}h^2D^5 + \frac{79541}{27}h^4D + \frac{150347702}{15309}h^2D^3 - \frac{74699131}{2187}h^2D \\
& + \frac{12445691}{7290}\Delta^5 - \frac{48292496}{3645}\Delta^3 - \frac{328827899}{10935}D^5 - \frac{22620679997}{229635}D^3 \\
& + \frac{17390369}{8748}D^7) \beta^6 + \mathcal{O}(\beta^7). \tag{A.5}
\end{aligned}$$

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