

**Analytical results for the high-temperature expansion of the one-dimensional  $s=1$  XXZ model**Onofre Rojas,<sup>1</sup> E. V. Corrêa Silva,<sup>2</sup> Winder A. Moura-Melo,<sup>3</sup> S. M. de Souza,<sup>4</sup> and M. T. Thomaz<sup>2,\*</sup><sup>1</sup>*Departamento de Física, Universidade Federal de São Carlos, CEP 13565-905, São Carlos, São Paulo, Brazil*<sup>2</sup>*Instituto de Física, Universidade Federal Fluminense, Avenida General Milton Tavares de Souza, CEP 24210-340, Niterói, Rio de Janeiro, Brazil*<sup>3</sup>*Faculdades Federais Integradas de Diamantina, Rua da Glória No. 187, CEP 39100-000, Diamantina, Minas Gerais, Brazil*<sup>4</sup>*Departamento de Ciências Exatas, Universidade Federal de Lavras, Caixa Postal 37, CEP 37200-000, Lavras, Minas Gerais, Brazil*

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Recently Rojas *et al.* [J. Math. Phys. **43**, 1390 (2002)] obtained a closed analytical expression for the coefficients of arbitrary order in the cumulant expansion of a one-dimensional periodic chain model with nearest-neighbor interaction and spatial translation invariance; that approach can be applied equally well to both nonintegrable and exact integrable models. Here, we obtain the exact analytic expressions for the six lowest-order terms of the high-temperature expansion of the Helmholtz free energy per site of the nonintegrable one-dimensional spin-1 XXZ Heisenberg model. Our analytical results for the specific heat and the static magnetic susceptibility are compared, up to order  $\beta^6$  for the ferromagnetic and antiferromagnetic phases, with the respective numerical results of a periodic chain with ten sites ( $N=10$ ) and numerical results in the literature [Blöte, Physica B **79**, 427 (1975)]. A very good agreement is obtained for both phases in the high-temperature regime.

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Integrable one-dimensional models can be solved exactly through the algebraic Bethe ansatz method,<sup>3</sup> e.g. the one-dimensional Hubbard model<sup>4-6</sup> and the spin-1/2 XXZ model.<sup>7,8</sup> The thermodynamic quantities of these models are obtained from nonlinear integral equations (NLIE) valid for whole range of  $\beta=1/kT$ ,  $k$  being Boltzmann's constant and  $T$  being the absolute temperature). On the other hand, high-temperature expansions of thermodynamic functions are *bona fide* for a finite region of values of  $\beta$  only. However, those expansions are analytical, thus being easily handled to yield the thermodynamic properties of a chain model. In particular, the cumulant series<sup>9</sup> has the advantage of being equally applicable to both nonintegrable and exact integrable models. Such a method has been widely applied to the study of the high-temperature thermodynamic behavior of quantum models in  $D$ -dimensional space ( $D=1,2,3$ ). Recently Rojas *et al.*<sup>1</sup> showed, for any one-dimensional chain model with periodic boundary condition, invariance under spatial translation and interaction between nearest neighbors, that in the thermodynamic limit the coefficient of the high-temperature expansion of arbitrary order  $\beta^n$  can be derived from an auxiliary function  $\varphi$ . In Ref. 1 we applied this approach to the spin- $\frac{1}{2}$  XXZ model and obtained the high-temperature expansion of the Helmholtz free energy per site up to order  $\beta^3$ . In the high-temperature regime, our analytical results agreed with the numerical solutions of the NLIE for its free energy per site<sup>8</sup> and we corrected some of the coefficients of their  $\beta$  expansion derived from these NLIE.

Contrary to previous examples, the spin-1 XXZ model is nonintegrable and, therefore, cannot be solved by the algebraic Bethe ansatz method. In the 1970s, Blöte<sup>2</sup> and Neef<sup>10</sup> studied the temperature dependence of the specific heat of this model. More recently, Yamamoto and Miyashita<sup>11-13</sup> applied the Monte Carlo method to study numerically the specific heat, static magnetic susceptibility, and the magnetiza-

tion of rings and chains of different sizes as functions of temperature, and extrapolated results to the thermodynamic limit. Their numerical results agree with those contained in Ref. 2. Bao *et al.*<sup>14</sup> applied the Green-function approach to get an approximation to the thermodynamics of this model in whole range of temperature. They obtained a set of self-consistent equations, solved numerically to yield thermodynamic quantities for the spin-1 XXZ model.

Our aim in this work is to derive an analytical  $\beta$  expansion of the Helmholtz free energy per site of the anisotropic spin-1 XXZ model with single-ion anisotropy up to order  $\beta^5$ , where each coefficient in the  $\beta$  expansion is exact.

The Hamiltonian of the spin-1 XXZ model with anisotropy<sup>15</sup> is

$$\mathbf{H} = \sum_{i=1}^N J(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \Delta S_i^z S_{i+1}^z - h S_i^z + D(S_i^z)^2, \quad (1a)$$

where  $N$  is the number of sites in the periodic chain,  $\Delta$  is the anisotropy constant,  $h$  is the external magnetic field in the  $z$  axis, and  $D$  is the single-ion anisotropy parameter. The spin-1 operators  $S_i^+$ ,  $S_i^-$ , and  $S_i^z$ , written in the basis of  $S^z$  eigenvectors, are

$$S_i^+ = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \quad S_i^- = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix},$$

$$S_i^z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (1b)$$

The operators  $S_i^+$  and  $S_i^-$  are defined as  $S_i^\pm = 1/\sqrt{2}(S_i^x \pm iS_i^y)$ . We do not fix the sign of any constant in Eq. (1a).

From Ref. 1 it is found that the thermodynamic limit of the Helmholtz free energy per site of the present model can be written as

$$\mathcal{W}(\beta) = -\frac{1}{\beta} [\ln(3) + \ln\{1 + \xi(\beta)\}], \quad (2a)$$

where

$$\xi(\beta) = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \frac{\partial^n}{\partial \lambda^n} [\varphi(\lambda)^{n+1}]|_{\lambda=1} \quad (2b)$$

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

$$\varphi(\lambda) = \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} \frac{(-\beta)^n}{\lambda^m} H_{1,m}^{(n)}. \quad (2c)$$

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,

$$H_{1,m}^{(n)} = \sum_{\{n_i\}} \left\langle \prod_{i=1}^m \frac{\mathbf{H}_{i,i+1}^{n_i}}{n_i!} \right\rangle_g. \quad (2d)$$

The notation  $\Sigma_{\{n_i\}}^n$  stands for the restriction  $\Sigma_{i=1}^m n_i = n$  and  $n_i \neq 0$  for  $i=1, 2, \dots, m$ . The index  $m$  satisfies the condition  $1 \leq m \leq n$ . Finally, we relate the  $g$  traces to the normalized traces

$$\begin{aligned} & \langle \mathbf{H}_{i_1, i_1+1}^{n_1} \mathbf{H}_{i_2, i_2+1}^{n_2} \cdots \mathbf{H}_{i_m, i_m+1}^{n_m} \rangle_g \\ & \equiv \frac{n_1 \cdots n_m!}{n!} \sum_{\mathcal{P}} \langle \mathcal{P}(\mathbf{H}_{i_1, i_1+1}^{n_1}, \mathbf{H}_{i_2, i_2+1}^{n_2}, \dots, \mathbf{H}_{i_m, i_m+1}^{n_m}) \rangle, \end{aligned} \quad (2e)$$

where  $\Sigma_{i=1}^m n_i = n$  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 Ref. 1 for details on this approach; in Appendix D of that reference, the reader may find the function  $H_{1,m}^{(n)}$  written in terms of the normalized traces for  $n, m=1, \dots, 4$ .

The sums (2b) and (2c) allow us to write down a  $\beta$  expansion of the thermodynamic function  $\mathcal{W}(\beta)$ . In the Appendix we present the expressions of the functions  $H_{1,m}^{(n)}$  for  $n$  and  $m$  from 1 up to 6; using those in Eqs. (2b) and (2c), we obtain the  $\beta$  expansion of  $\mathcal{W}(\beta)$ , up to the fifth order in  $\beta$ ,

$$\begin{aligned} \mathcal{W}(\beta) = & -\frac{\ln(3)}{\beta} + \frac{2}{3}D + \left( -\frac{1}{9}D^2 - \frac{4}{9}J^2 - \frac{1}{3}h^2 - \frac{2}{9}\Delta^2 \right) \beta + \left( -\frac{1}{81}D^3 + \frac{4}{9}\Delta h^2 + \frac{4}{27}\Delta^2 D - \frac{4}{27}J^2 D + \frac{1}{9}h^2 D - \frac{1}{9}J^2 \Delta \right) \beta^2 \\ & + \left( \frac{1}{36}h^4 - \frac{1}{54}\Delta^4 + \frac{1}{324}D^4 + \frac{13}{81}J^2 \Delta^2 + \frac{1}{54}h^2 D^2 + \frac{7}{162}J^4 - \frac{8}{27}\Delta h^2 D + \frac{5}{27}J^2 h^2 - \frac{10}{27}\Delta^2 h^2 + \frac{1}{27}J^2 D^2 \right) \beta^3 \\ & + \left( \frac{7}{243}J^2 D^3 + \frac{1}{18}J^4 \Delta + \frac{1}{972}D^5 - \frac{1}{27}DJ^2 h^2 + \frac{1}{81}J^2 \Delta D^2 - \frac{1}{81}D \Delta^4 - \frac{11}{162}DJ^2 \Delta^2 - \frac{4}{243}\Delta^2 D^3 \right. \\ & \left. + \frac{22}{81}h^2 \Delta^3 - \frac{10}{27}J^2 \Delta h^2 - \frac{1}{36}Dh^4 + \frac{8}{27}\Delta^2 h^2 D - \frac{1}{162}D^3 h^2 + \frac{1}{36}J^2 \Delta^3 + \frac{13}{162}DJ^4 - \frac{4}{27}h^4 \Delta \right) \beta^4 \\ & + \left( -\frac{1}{18}D^2 h^2 J^2 + \frac{16}{81}Dh^4 \Delta - \frac{2}{81}D^2 h^2 \Delta^2 + \frac{5}{243}D^2 \Delta^4 - \frac{77}{486}h^2 \Delta^4 + \frac{13}{1620}D^2 J^4 - \frac{31}{324}J^4 h^2 - \frac{5}{1944}D^4 h^2 \right. \\ & \left. - \frac{7}{14580}D^4 J^2 - \frac{53}{4860}J^2 \Delta^4 + \frac{29}{81}h^4 \Delta^2 - \frac{1241}{14580}\Delta^2 J^4 - \frac{19}{324}J^2 h^4 + \frac{1}{648}D^2 h^4 - \frac{1}{729}D^4 \Delta^2 \right. \\ & \left. + \frac{8}{243}h^2 D^3 \Delta - \frac{52}{243}h^2 D \Delta^3 + \frac{26}{81}J^2 h^2 \Delta^2 - \frac{76}{1215}J^2 D^2 \Delta^2 + \frac{2}{1215}\Delta D^3 J^2 - \frac{2}{81}DJ^2 \Delta^3 \right. \\ & \left. + \frac{2}{81}D \Delta J^4 - \frac{7}{87480}D^6 - \frac{13}{3240}h^6 + \frac{173}{43740}\Delta^6 - \frac{131}{43740}J^6 + \frac{14}{81}h^2 D \Delta J^2 \right) \beta^5 + O(\beta^6). \end{aligned} \quad (3)$$

We point out that this analytic expansion is valid for any arbitrary set of values of parameters  $J$ ,  $\Delta$ ,  $D$ , and  $h$ , in the  $\beta$  interval where this expansion is sound. This equation applies equally well to any phase of the one-dimensional spin-1

XXZ model.<sup>16–18</sup> These calculations have been implemented in the computational language MAPLE.<sup>19</sup>

In addition, from Eq. (3), we see that the thermodynamic properties of this model are insensitive to the sign of the

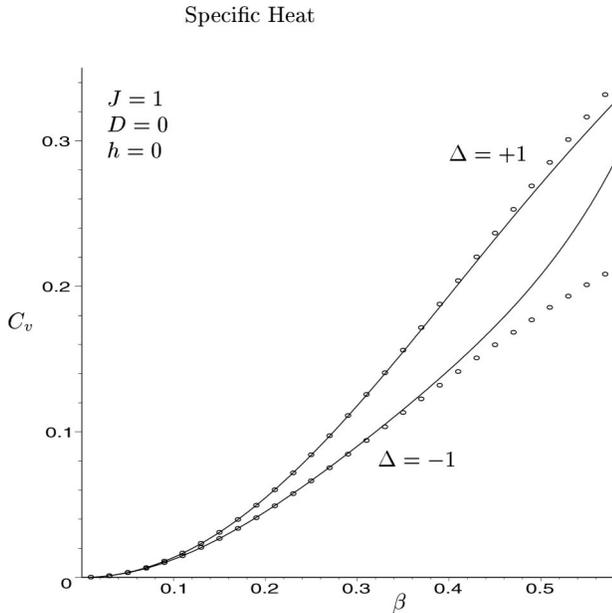


FIG. 1. Specific heat for the isotropic Heisenberg models with parameter values  $J=1$ ,  $D=0$ ,  $h=0$ , and  $\Delta=\pm 1$ . Solid lines stand for the specific heat calculated from the analytical expression of the Helmholtz free energy per site [cf. Eq. (3)]. Dotted lines correspond to numerical calculations in a ring with  $N=10$  sites.

constants  $J$  and  $h$ . The invariance upon changing the sign of  $J$  comes from the fact that the thermodynamic properties of any model result from the evaluation of traces. The functions  $H_{1,m}^{(n)}$  [Eq. (2d)] consist of traces of powers of the Hamiltonian (1a); given its particular structure, only even powers of  $J$  will contribute. The dependence on even powers of  $h$  in Eq. (3) comes from the isotropy of space. From now on we take  $J \geq 0$ ; moreover, we can redefine all the parameters in Hamiltonian (1a) dividing them by  $J$  and factorizing it out; expansion (3) then becomes an expansion in powers of  $(J\beta)^n$ , as it typically appears in the literature.

From Eq. (3) we see that if we simultaneously change the signs:  $\Delta \rightarrow -\Delta$  and  $D \rightarrow -D$ , only the coefficients of even powers  $\beta^{2m}$ , ( $m=1,2,\dots$ ) get an overall sign. These changes in the sign lead us to a different phase of the model.

Due to the fact that Eq. (3) is analytical in the parameters  $J, \Delta, D$  of the  $XXZ$  model and the external magnetic field  $h$ , we may derive from it the thermodynamic functions through the definition of suitable derivatives of  $\mathcal{W}(\beta)$ . For example, directly from Eq. (3) we may obtain the following thermodynamic quantities per site: the average energy, the specific heat, the average of the square of the  $z$  component of magnetization, the correlation of the  $z$  component of spin between first neighbors, among others. The collection of these quantities helps us to comprehend the behavior of the model in all its different phases (characterized by different sets of values for the parameters of the model) in the high-temperature region.

Our aim here is to verify the correctness of the  $\beta$  expansion (3) and to do so, we apply several distinct tests. The first verification is the case  $J=0$ , when we recover the  $s=1$  Ising model. In a previous work<sup>20</sup> we calculated, using the present

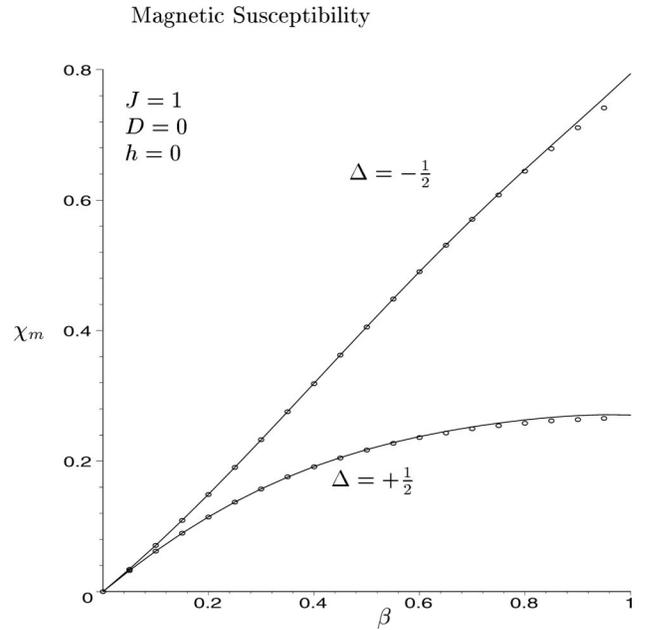


FIG. 2. Magnetic susceptibility for anisotropic Heisenberg models with parameter values  $J=1$ ,  $D=0$ ,  $h=0$ , and  $\Delta=\pm \frac{1}{2}$ . Solid lines represent the magnetic susceptibility calculated from the analytical expression of the Helmholtz free energy per site [cf. Eq. (3)]. Dotted lines correspond to numerical calculations in a ring with  $N=10$  sites.

approach, the first 80 terms of the  $\beta$  expansion of the Helmholtz free energy of the  $s=1$  Ising model in the absence of the external magnetic field ( $h=0$ ). Substituting  $J=0$  and  $h=0$  in Eq. (3), we recover the results of Ref. 20 up to order  $\beta^5$ .

Yamamoto and Miyashita<sup>11</sup> applied a Monte Carlo method to study the temperature dependence of some thermodynamic quantities (specific heat, internal energy, and static magnetic susceptibility) for the isotropic  $s=1$  Heisenberg model with no external magnetic field ( $h=0$ ), for rings containing 8–96 sites. From their graphs we see that for  $\beta J \leq 0.3$  all rings give the same numerical results irrespective of the number of sites in the ring. To compare those results with ours, including the contribution from the spin-flipping term proportional to  $J$  in Eq. (1a), we calculated numerically the temperature dependence of the specific heat and the static susceptibility of a ring with ten sites for  $D=0$  and  $h=0$ . Once the expansions can be written in powers of  $\beta J$ , we took  $J=1$  in Figs. 1 and 2. In Fig. 1 we have the  $\beta$  dependence of the specific heat

$$C_v(\beta) = -\beta^2 \frac{\partial^2}{\partial \beta^2} [\beta \mathcal{W}(\beta)] \quad (4)$$

in the high-temperature region for  $\Delta=\pm 1$ ,  $D=0$ , and  $h=0$ . The dotted lines correspond to the specific heat for a ring with ten sites and the solid lines represent our analytical expression derived from Eq. (3) for the Helmholtz free energy  $\mathcal{W}(\beta)$ . From Fig. 1 we see that in both cases,  $\Delta=\pm 1$ , the analytical and numerical curves coincide in the high-temperature region. For the ferromagnetic phase ( $\Delta=-1$ ) the

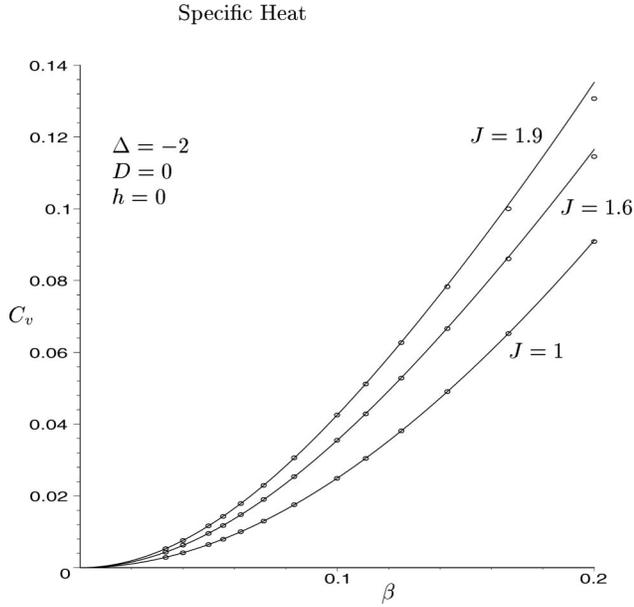


FIG. 3. Comparison of our analytical result of the specific heat and Blöte's numerical results (Ref. 2) in the ferromagnetic phase. We take the parameter values  $\Delta = -2$ ,  $D = 0$ ,  $h = 0$  and  $J = 1, 1.6$ , and  $1.9$ . Solid lines represent our analytical expression of the specific heat and the dotted lines correspond to data from Ref. 2.

relative error between the analytical and the numerical results is not greater than 1% for  $\beta \in [0, 0.31]$ . In Fig. 2 we compare the static magnetic susceptibility

$$\chi(\beta) = - \left. \frac{\partial^2 \mathcal{W}(\beta)}{\partial h^2} \right|_{h=0} \quad (5)$$

of a uniaxial Heisenberg model ( $\Delta = \pm 1/2$ ) for a ring with ten sites (dotted lines) and the analytical expression of  $\chi(\beta)$  (solid lines) derived from the free energy per site (3). For the ferromagnetic phase ( $\Delta = -1/2$ ) the difference between the analytical and numerical results is not greater than 1% for  $\beta \in [0, 0.87]$ , while in the antiferromagnetic phase ( $\Delta = 1/2$ ) the same holds true for  $\beta \in [0, 0.66]$ .

A beautiful numerical work by Blöte<sup>2</sup> tabulates numerical values for the specific heat at varied temperatures (including the high-temperature region) for the  $s = 1/2$  and  $s = 1$  Heisenberg models. In all his calculations Blöte has set  $h = 0$ . Comparison of the Hamiltonian (1) in Ref. 2 and ours, given by Eq. (1a), yields the following correspondence of parameters:  $J_{\parallel} = -\Delta/2$  and  $J_{\perp} = -J/2$ . In Fig. 3 we compare our analytical expression for the specific heat derived from Eq. (3) for anisotropic Heisenberg models in the absence of single-ion anisotropy ( $D = 0$ ) in the ferromagnetic case, while Fig. 4 focuses on the antiferromagnetic phase. In both figures, our curves fit pretty well the Blöte's numerical results in the high-temperature region.

From Figs. 5 and 6 we compare our results with those in Ref. 2 for the isotropic Heisenberg models with distinct values for the single-ion anisotropy parameter  $D$ . We take both positive and negative values of  $D$ . The ferromagnetic case is depicted in Figs. 5(a) and 5(b); the antiferromagnetic case, in Figs. 6(a) and 6(b). In all cases, our curves fit very well

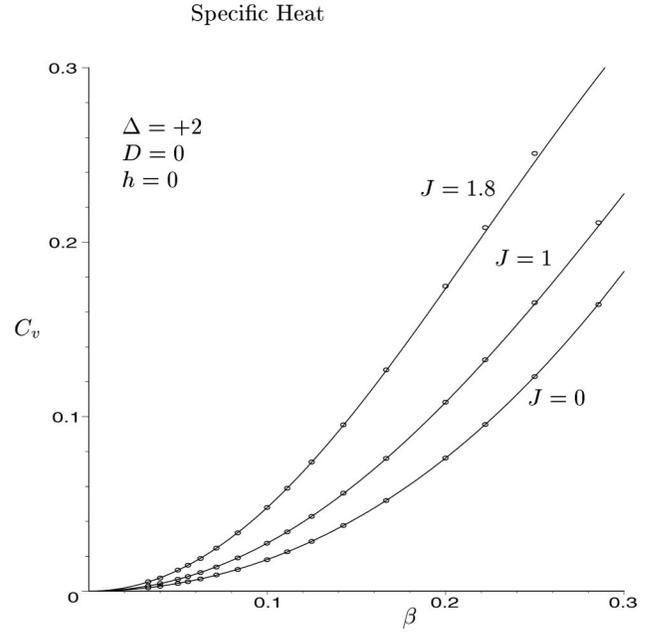


FIG. 4. Comparison of our analytic expression for the specific heat and Blöte's numerical results (Ref. 2) for the parameter values  $\Delta = 2$ ,  $D = 0$ ,  $h = 0$  and  $J = 0, 1, 0$ , and  $1.8$ . Solid lines show the specific heat of our analytical result and the dotted lines correspond to data from Ref. 2.

Blöte's numerical results in the high-temperature region. From Fig. 5 and 6 we see that the interval of  $\beta$  where our solution (3) is bona fide gets smaller as the absolute value of  $D$  increases.

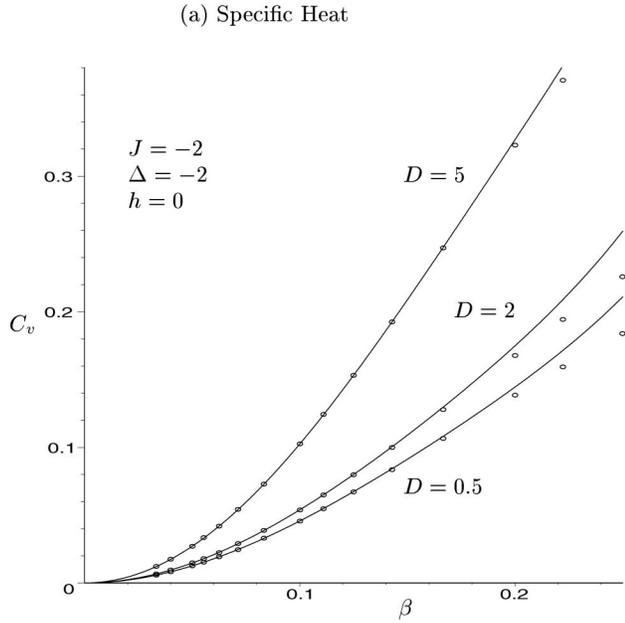
Our analytical results for the specific heat, obtainable from Eq. (3), fully agree in its isotropic limit with that of Sec. 5.2 of Ref. 2 in the high-temperature limit. We also recover the high-temperature static magnetic susceptibility for the isotropic Heisenberg model [Eq. (4.5a) of Ref. 12]. However, we do not agree with the high-temperature limit of the correlation function for the  $z$  component of spin between nearest neighbors  $\langle S_0^z S_1^z \rangle$  of Ref. 14. The correct limit is  $\langle S_0^z S_1^z \rangle \approx -\frac{4}{9} \Delta \beta$ .

Finally, in Ref. 21 Fisher gets the classical limit of the Helmholtz free energy of the  $s = 1$  isotropic Heisenberg model  $\mathcal{W}_{class}$ . The relation between the parameters in our Hamiltonian (1a) and that of Ref. 21 is  $J_{Fisher} = -2J$ . Subtracting the lowest term in  $\beta$  of our expression of  $\mathcal{W}(\beta)$  [up to the term  $-\ln(3)/\beta$ ] from the classical free energy  $\mathcal{W}_{class}$  we get

$$\mathcal{W}_{class} - \mathcal{W}(\beta) = \frac{1}{2} J^2 \beta, \quad (6)$$

which means that the classical model is not recovered from the quantum isotropic Heisenberg model even in the limit  $\beta \rightarrow 0$ .

In summary, in this work we applied the method of Ref. 1 to a nonintegrable spin-1  $XXZ$  model with single-ion anisotropy. We obtained the analytical  $\beta$  expansion of the Helmholtz free energy per site of the model up to order  $\beta^5$ . Each coefficient in expansion (3) is exact and valid for any values of the parameters in the Hamiltonian (1a). Several thermo-



(b) Specific Heat

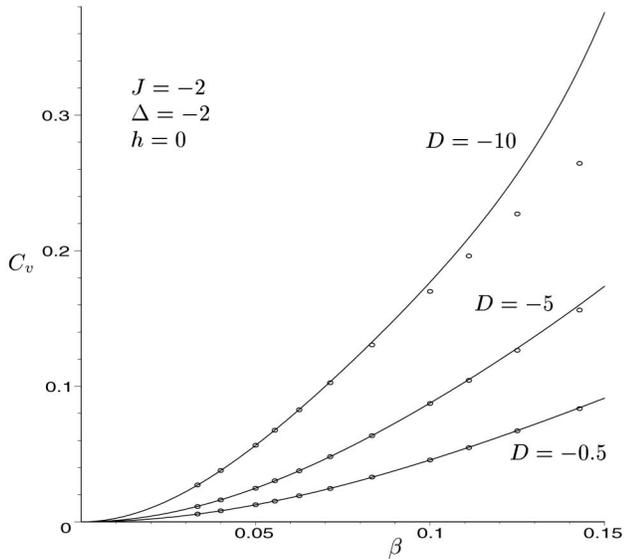
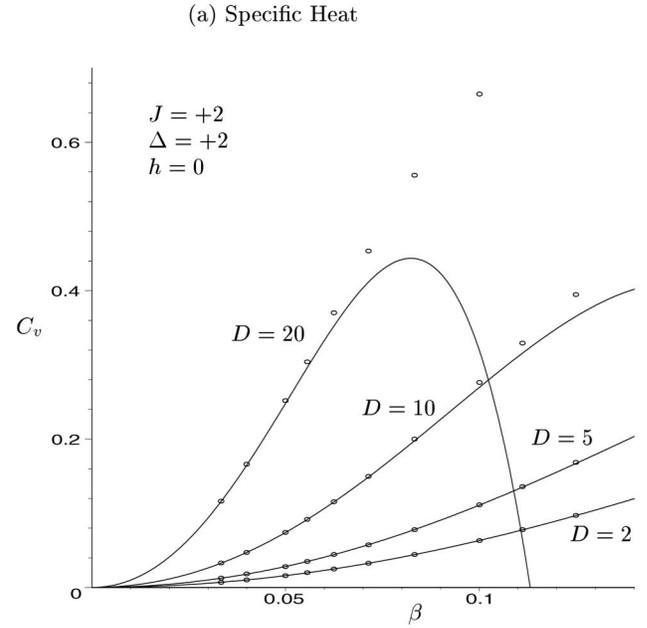


FIG. 5. Comparison of our analytic expression for the specific heat and Blöte's numerical results (Ref. 2) for the parameter values  $J = -2$ ,  $\Delta = -2$ , and  $h = 0$ . Solid lines represent our results and the dotted lines correspond to data from Ref. 2: (a)  $D = 0.5, 2$  and  $5$ ; (b)  $D = -0.5, -5$ , and  $-10$ .

dynamic quantities can be derived directly from suitable derivatives of  $\mathcal{W}(\beta)$  defined in terms of the parameters of the model and the external magnetic field.

To verify our analytical results we have compared them with numerical results, including those of Blöte's.<sup>2</sup> Our curves in the high-temperature region fit well those numerical results for both isotropic and anisotropic XXZ models in their ferromagnetic and antiferromagnetic phases, even if the single-ion anisotropy term is taken into account.

From expansion (3) we recover the analytical results



(b) Specific Heat

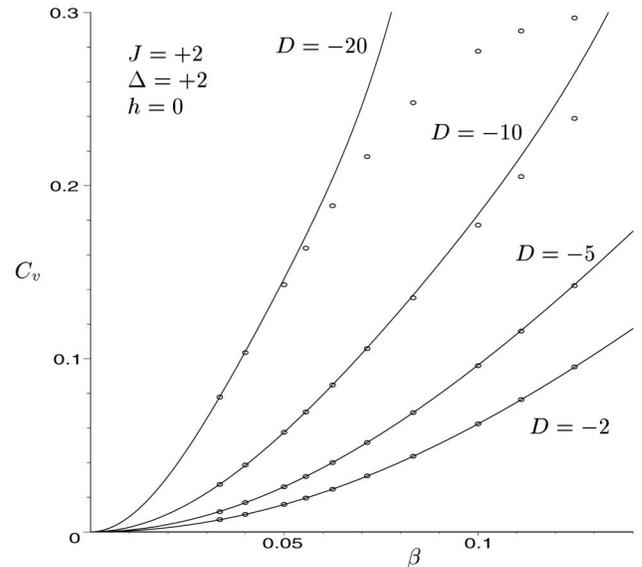


FIG. 6. Comparison of our analytic expression for the specific heat and Blöte's numerical results (Ref. 2) for the parameter values  $J = 2$ ,  $\Delta = 2$ , and  $h = 0$ . Solid lines show our analytical results and the dotted lines correspond to data from Ref. 2: (a)  $D = 2, 5, 10$ , and  $20$ ; (b)  $D = -2, -5, -10$ , and  $-20$ .

known in the literature<sup>2,12</sup> about the isotropic spin-1 Heisenberg model. We correct the high-temperature limit of  $\langle S_0^z S_1^z \rangle$  of Ref. 14. We also show that the thermodynamics of the classical spin-1 isotropic Heisenberg model differ in order  $\beta$  of the quantum spin-1 model.

Finally we should mention that the calculations involving Eqs. (2) have been implemented in the symbolic computational language MAPLE.<sup>19</sup> Currently, refinements are being made so that the expansion of the Helmholtz free energy (3)

for the  $s=1$  Heisenberg model can be extended to higher orders in  $\beta$ .

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**APPENDIX: ANALYTICAL EXPRESSIONS OF THE  $H_{1,m}^{(n)}$  FUNCTIONS UP TO  $n=6$**

We have calculated the  $H_{1,m}^{(n)}$  functions in terms of an arbitrary set of the parameters  $(J, \Delta, h, D)$  and obtained the following results. For  $n=1$

$$H_{1,1}^{(1)} = \frac{2}{3}D. \quad (A1)$$

For  $n=2$

$$H_{1,1}^{(2)} = \frac{4}{9}J^2 + \frac{2}{9}\Delta^2 + \frac{1}{3}h^2 + \frac{1}{3}D^2. \quad (A2)$$

$$H_{1,2}^{(2)} = \frac{4}{9}D^2. \quad (A3)$$

For  $n=3$

$$H_{1,1}^{(3)} = \left(\frac{2}{9}D - \frac{1}{9}\Delta\right)J^2 + \frac{1}{9}D^3 + \frac{2}{9}\Delta^2D + \frac{1}{3}h^2D, \quad (A4)$$

$$H_{1,2}^{(3)} = \frac{14}{27}J^2D + \frac{10}{27}\Delta^2D + \frac{4}{9}h^2D + \frac{4}{9}D^3 + \frac{4}{9}\Delta h^2, \quad (A5)$$

$$H_{1,3}^{(3)} = \frac{8}{27}D^3. \quad (A6)$$

For  $n=4$

$$\begin{aligned} H_{1,1}^{(4)} = & \frac{1}{27}\Delta^2J^2 + \frac{1}{18}J^4 + \frac{1}{54}\Delta^4 - \frac{2}{27}DJ^2\Delta \\ & + \frac{2}{27}J^2D^2 + \frac{2}{27}J^2h^2 + \frac{1}{9}\Delta^2D^2 + \frac{1}{9}\Delta^2h^2 \\ & + \frac{1}{36}h^4 + \frac{1}{6}h^2D^2 + \frac{1}{36}D^4, \end{aligned} \quad (A7)$$

$$\begin{aligned} H_{1,2}^{(4)} = & \frac{8}{9}\Delta h^2D + \frac{13}{27}J^2D^2 + \frac{2}{3}h^2D^2 - \frac{4}{27}DJ^2\Delta + \frac{5}{27}J^2h^2 \\ & + \frac{5}{9}\Delta^2D^2 + \frac{5}{27}\Delta^2h^2 + \frac{1}{9}h^4 + \frac{7}{27}D^4 + \frac{8}{81}\Delta^2J^2 \\ & + \frac{16}{81}J^4 + \frac{2}{27}\Delta^4, \end{aligned} \quad (A8)$$

$$\begin{aligned} H_{1,3}^{(4)} = & \frac{16}{27}D\Delta h^2 + \frac{8}{27}\Delta^2h^2 + \frac{32}{81}D^2\Delta^2 + \frac{4}{9}D^2h^2 \\ & + \frac{40}{81}D^2J^2 + \frac{4}{9}D^4 \end{aligned} \quad (A9)$$

$$H_{1,4}^{(4)} = \frac{16}{81}D^4. \quad (A10)$$

For  $n=5$

$$\begin{aligned} H_{1,1}^{(5)} = & -\frac{1}{36}J^2\Delta D^2 - \frac{1}{36}J^2\Delta h^2 + \frac{1}{36}DJ^4 + \frac{1}{54}D\Delta^4 \\ & + \frac{1}{36}DJ^2\Delta^2 + \frac{1}{27}\Delta^2D^3 + \frac{1}{18}DJ^2h^2 + \frac{1}{9}\Delta^2h^2D \\ & + \frac{1}{54}J^2D^3 + \frac{1}{180}D^5 + \frac{1}{36}Dh^4 + \frac{1}{18}D^3h^2 \\ & - \frac{1}{54}J^4\Delta - \frac{1}{108}J^2\Delta^3, \end{aligned} \quad (A11)$$

$$\begin{aligned} H_{1,2}^{(5)} = & \frac{1}{9}D^5 + \frac{7}{27}Dh^4 - \frac{55}{324}J^2\Delta D^2 + \frac{14}{27}D^3h^2 + \frac{29}{324}J^2\Delta h^2 \\ & + \frac{35}{81}\Delta^2D^3 + \frac{53}{162}DJ^2h^2 + \frac{5}{9}\Delta^2h^2D + \frac{43}{162}J^2D^3 \\ & + \frac{2}{9}h^2\Delta^3 + \frac{4}{27}\Delta h^4 + \frac{8}{9}\Delta h^2D^2 - \frac{2}{27}J^4\Delta + \frac{85}{324}DJ^4 \\ & + \frac{29}{162}D\Delta^4 + \frac{65}{324}DJ^2\Delta^2 - \frac{1}{27}J^2\Delta^3, \end{aligned} \quad (A12)$$

$$\begin{aligned} H_{1,3}^{(5)} = & \frac{10}{27}D^5 + \frac{2}{9}Dh^4 - \frac{4}{27}J^2\Delta D^2 + \frac{8}{9}D^3h^2 + \frac{20}{81}J^2\Delta h^2 \\ & + \frac{64}{81}\Delta^2D^3 + \frac{32}{81}DJ^2h^2 + \frac{104}{81}\Delta^2h^2D + \frac{56}{81}J^2D^3 \\ & + \frac{20}{81}h^2\Delta^3 + \frac{8}{27}\Delta h^4 + \frac{40}{27}\Delta h^2D^2 + \frac{80}{243}DJ^4 \\ & + \frac{14}{81}D\Delta^4 + \frac{70}{243}DJ^2\Delta^2, \end{aligned} \quad (A13)$$

$$\begin{aligned} H_{1,4}^{(5)} = & \frac{32}{81}D^5 + \frac{32}{81}D^3h^2 + \frac{88}{243}\Delta^2D^3 + \frac{32}{81}\Delta^2h^2D \\ & + \frac{104}{243}J^2D^3 + \frac{16}{81}h^2\Delta^3 + \frac{16}{27}\Delta h^2D^2, \end{aligned} \quad (A14)$$

$$H_{1,5}^{(5)} = \frac{32}{243} D^5. \quad (\text{A15})$$

For  $n=6$

$$\begin{aligned} H_{1,1}^{(6)} = & \frac{1}{45} D^2 h^2 J^2 + \frac{1}{270} J^2 h^4 - \frac{1}{135} \Delta D^3 J^2 - \frac{1}{45} h^2 D \Delta J^2 \\ & + \frac{1}{72} D^2 h^4 + \frac{1}{108} D^4 \Delta^2 + \frac{1}{90} J^2 D^2 \Delta^2 + \frac{1}{90} J^2 h^2 \Delta^2 \\ & + \frac{1}{108} D^2 \Delta^4 + \frac{1}{108} h^2 \Delta^4 + \frac{1}{120} D^2 J^4 + \frac{7}{1080} J^4 h^2 \\ & + \frac{1}{1080} D^6 + \frac{1}{1080} h^6 + \frac{1}{72} D^4 h^2 - \frac{1}{90} D \Delta J^4 \\ & - \frac{1}{135} D J^2 \Delta^3 + \frac{1}{270} D^4 J^2 + \frac{1}{18} D^2 h^2 \Delta^2 + \frac{1}{108} h^4 \Delta^2 \\ & + \frac{1}{1620} \Delta^6 + \frac{1}{324} J^6 + \frac{1}{540} J^2 \Delta^4 + \frac{1}{180} \Delta^2 J^4, \quad (\text{A16}) \end{aligned}$$

$$\begin{aligned} H_{1,2}^{(6)} = & \frac{8}{27} D h^4 \Delta + \frac{4}{9} h^2 D \Delta^3 + \frac{16}{27} h^2 D^3 \Delta + \frac{31}{270} h^2 D \Delta J^2 \\ & - \frac{44}{405} D \Delta J^4 - \frac{31}{405} D J^2 \Delta^3 + \frac{35}{54} D^2 h^2 \Delta^2 \\ & + \frac{13}{810} J^2 h^2 \Delta^2 + \frac{74}{405} J^2 D^2 \Delta^2 - \frac{29}{270} \Delta D^3 J^2 \\ & + \frac{217}{810} D^2 h^2 J^2 + \frac{23}{540} J^2 h^4 + \frac{5}{18} D^2 h^4 + \frac{25}{108} D^4 \Delta^2 \\ & + \frac{7}{36} D^2 \Delta^4 + \frac{29}{324} h^2 \Delta^4 + \frac{559}{3240} D^2 J^4 + \frac{217}{3240} J^4 h^2 \\ & + \frac{5}{18} D^4 h^2 + \frac{59}{540} D^4 J^2 + \frac{35}{324} h^4 \Delta^2 + \frac{8}{405} J^2 \Delta^4 \\ & + \frac{11}{270} \Delta^2 J^4 + \frac{31}{810} D^6 + \frac{1}{54} h^6 + \frac{1}{81} \Delta^6 + \frac{2}{45} J^6, \quad (\text{A17}) \end{aligned}$$

$$\begin{aligned} H_{1,3}^{(6)} = & \frac{88}{81} D h^4 \Delta + \frac{88}{81} h^2 D \Delta^3 + \frac{152}{81} h^2 D^3 \Delta + \frac{151}{243} h^2 D \Delta J^2 \\ & - \frac{359}{2430} D \Delta J^4 - \frac{241}{2430} D J^2 \Delta^3 + \frac{68}{27} D^2 h^2 \Delta^2 \\ & + \frac{202}{1215} J^2 h^2 \Delta^2 + \frac{743}{1215} J^2 D^2 \Delta^2 - \frac{59}{243} \Delta D^3 J^2 \\ & + \frac{194}{243} D^2 h^2 J^2 + \frac{2}{27} J^2 h^4 + \frac{16}{27} D^2 h^4 + \frac{200}{243} D^4 \Delta^2 \\ & + \frac{113}{243} D^2 \Delta^4 + \frac{23}{81} h^2 \Delta^4 + \frac{1271}{2430} D^2 J^4 + \frac{269}{2430} J^4 h^2 \\ & + \frac{25}{27} D^4 h^2 + \frac{44}{81} D^4 J^2 + \frac{28}{81} h^4 \Delta^2 + \frac{47}{1215} J^2 \Delta^4 \\ & + \frac{68}{1215} \Delta^2 J^4 + \frac{2}{9} D^6 + \frac{1}{27} h^6 + \frac{2}{81} \Delta^6 + \frac{107}{1215} J^6, \quad (\text{A18}) \end{aligned}$$

$$\begin{aligned} H_{1,4}^{(6)} = & \frac{104}{243} D^6 + \frac{8}{27} D^2 h^4 + \frac{80}{81} D^4 h^2 + \frac{16}{9} h^2 D^3 \Delta + \frac{16}{27} D h^4 \Delta \\ & + \frac{32}{81} h^4 \Delta^2 + \frac{196}{243} D^4 J^2 + \frac{44}{81} D^2 h^2 J^2 + \frac{220}{243} D^4 \Delta^2 \\ & + \frac{52}{27} D^2 h^2 \Delta^2 + \frac{320}{243} h^2 D \Delta^3 - \frac{32}{243} \Delta D^3 J^2 \\ & + \frac{128}{243} h^2 D \Delta J^2 + \frac{40}{243} h^2 \Delta^4 + \frac{292}{729} D^2 J^4 + \frac{20}{81} D^2 \Delta^4 \\ & + \frac{4}{27} J^2 h^2 \Delta^2 + \frac{320}{729} J^2 D^2 \Delta^2, \quad (\text{A19}) \end{aligned}$$

$$\begin{aligned} H_{1,5}^{(6)} = & \frac{80}{243} D^6 + \frac{80}{243} D^4 h^2 + \frac{128}{243} h^2 D^3 \Delta + \frac{256}{729} D^4 J^2 \\ & + \frac{224}{729} D^4 \Delta^2 + \frac{32}{81} D^2 h^2 \Delta^2 + \frac{64}{243} h^2 D \Delta^3 + \frac{32}{243} h^2 \Delta^4, \quad (\text{A20}) \end{aligned}$$

$$H_{1,6}^{(6)} = \frac{64}{729} D^6. \quad (\text{A21})$$

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