High-temperature expansion of the tetrahedral spin-1/2 and spin-2 XXZ models

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We apply the cummulant method to obtain the high-temperature expansion of the Helmholtz free energy of the tetrahedral spin-1/2 and spin-2 XXZ models. The tetrahedral model is written as a composite spin-1 XXZ model, and some of its thermodynamic functions are compared to those of the ordinary spin-1 XXZ model. The composite spin-1 model is then mapped onto a fermion model, and it is shown that the contribution of the string Hamiltonian to thermodynamic functions at high temperatures cannot be neglected. The high-temperature expansion of the Helmholtz free energy of the anisotropic spin-2 XXZ chain is obtained up to order β^6. Our results fit well the numerical quantum Monte Carlo data calculated by Yamamoto [Phys. Rev. B **53**, 3364 (1996)] for the isotropic antiferromagnetic Heisenberg chain. We complement his high-temperature expansions for thermodynamic functions with terms of higher order in β.

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I. INTRODUCTION

Quasi-one-dimensional models such as ladder models, tetrahedral spin models, dimer chains, and mixed spin models have been attracting the attention of theoreticians and experimentalists, because they represent a transition from one-dimensional to bidimensional models and show interesting topological features.

A surprising aspect about ladder models is that the spin-1/2 antiferromagnetic Heisenberg chain is a gapless model, whereas the even-legged antiferromagnetic Heisenberg ladder model has a gap in its energy spectrum.[1] Besides those important topological differences between chain and m-legged antiferromagnetic Heisenberg ladder models, there are materials whose experimental data can be fitted by those models. For example, the vanadyl pyrophosphate $(VO)_2P_2O_7$ (Ref. 2) and $SrCu_2O_3$ (Ref. 3) are well fitted by the two-legged antiferromagnetic Heisenberg ladder. Another important point about these quasi-one-dimensional models is the exciting possibility that a doped ladder can be associated with high-temperature superconductivity.[4,5]

A complete frustration occurs in the two-legged ladder model when diagonal couplings[6] are present. Recently, spin-1/2 tetrahedral clusters have attracted substantial interest due to the unconventional magnetic phases they present.[7–9] Tetrahedral spin-1/2 clusters have been applied to the study of properties of tellurate materials $Cu_2Te_2O_5X_5$ ($X=$Cl or Br). On the basis of experimental results it was argued that these materials can be appropriately described by the noninteracting tetrahedral spin-1/2 model.[8] This model can be mapped onto composite spin models, which have a sum of two or more spins at each site. Sólyom and Timonen[10,11] applied the Jordan-Wigner transformation to have the composite spin-1/2 model mapped onto the one-dimensional extended Hubbard model plus a string Hamiltonian with interactions along all the chain sites. For different sets of parameter values, they compared the $T=0$ phase diagrams of the anisotropic composite spin $S=1$ Heisenberg chain and the one-dimensional extended Hubbard model.

Zero- and low-temperature properties of the aforementioned quasi-one-dimensional models are well known; the same cannot be said, however, of their thermodynamic properties. In the nice work by Troyer, Tsunetsugu, and Würtz,[12] the thermodynamics of the two-legged Heisenberg model is calculated numerically in the whole range of temperature. There are few analytical results such as high-temperature expansions, even for models that have been studied extensively.

In Ref. 13 Niggemann, Uimin, and Zittartz considered an alternated spin chain where at each second site there is a kind of dumbbell configuration. At each vertex of the dumbbell there is a spin-1/2 (see Fig. 1). They obtained a set of coupled equations that give the thermodynamics of what

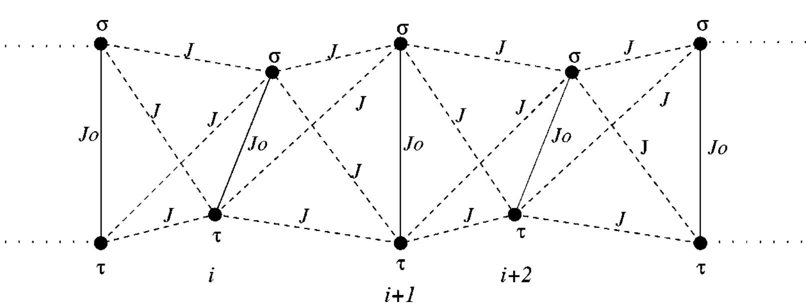

FIG. 1. The dumbbell structure of the tetrahedral spin-1/2 model. Along the ρ line we have the spin-1/2 σ_i at each site and along the r line another spin-1/2 τ_i.

they called model A.[14] In the thermodynamics of model A they explicitly verify the consequence of the equivalent chain model fragmentation due to the presence of $S=0$ states. The model B, also defined in Ref. 13, is a tetrahedral spin-1/2 model and also exhibits a rich phase diagram at $T=0$, but its thermodynamic properties are unknown. For a special choice of constants, model B becomes a noninteracting tetrahedral spin-1/2 model with the tetrahedral spin model being of a direct sum of two spins-1/2 at each site, with all interactions being of the isotropic Heisenberg type.

The spin-2 antiferromagnetic Heisenberg chains (AFH) have been less studied than the corresponding spin-1 model. Probably, this rests on the $S=2$ model having a larger number of degrees of freedom than lower-value spin models. Nevertheless, the ground-state energy of the $S=2$ AFH chain as well as its lowest excited states and low-temperature properties have been calculated.[15–17] On the other hand, there also are relatively few calculations on the thermodynamical functions of the spin-2 Heisenberg model.[18–20] Moreover, quasi-one-dimensional $S=2$ AFH materials have been synthesized,[21,22] hence the study of properties of the spin-2 XXZ model at zero and finite temperatures have risen in importance.

In 1995 Yamamoto[19] did a nice quantum Monte Carlo calculation (QMC) to obtain the thermodynamic properties of the $S=2$ AFH chain. He calculated the temperature dependence of the mean energy, specific heat, and static magnetic susceptibility per spin for either periodic or open chains with N sites for $N=32$, 64, and 96. Using the least-squares method, he extrapolated his results to the thermodynamic limit ($N\to\infty$). In the high-temperature region he derived a β expansion for each calculated physical quantity that fitted the numerical data in this limit.

To the best of our knowledge a study of thermodynamic properties of the anisotropic spin-2 XXZ chain with single ion-anisotropy term in the presence of an external magnetic field is still missing in the literature.

In Ref. 23 we presented a method to calculate the coefficients of the cummulant expansion of the Helmholtz free energy, in the thermodynamic limit, of any chain with periodic boundary condition, invariance under spatial translation, and interactions between nearest neighbors. The aim of the present work is to obtain the high-temperature expansion of the Helmholtz free energy of the tetrahedral spin-1/2 model and the spin-2 XXZ chain by applying the method presented in Ref. 23. The dimensions of parameter spaces of both models have been increased: in the tetrahedral model, we include anisotropic Heisenberg-type interactions along the diagonals (cf. Fig. 1); in the spin-2 XXZ we introduce anisotropy in the z direction. Both models are in the presence of an external magnetic field in the z direction. As mentioned previously, in Refs. 10 and 11 Sólyom and Timonen mapped the composite spin-1 model onto the one-dimensional extended Hubbard model plus a string Hamiltonian. We sought to clarify the importance of the contribution of the string Hamiltonian to the thermodynamics of the composite spin model in the high-temperature limit.

In Sec. II we obtain the Helmholtz free energy of the tetrahedral spin-1/2 model, up to order β^5. We compare some thermodynamics functions (such as the specific heat per site, the correlation of the z component of the spin between nearest neighbors, and the average of the squared z component of spin per site) of this model with those of the spin-1 XXZ model (spin-1 in the irreducible representation), obtained in Ref. 24. In Sec. III we compare the specific heat, mean energy, and static magnetic susceptibility of the one-dimensional extended Hubbard model[25] and a modified version of the tetrahedral spin-1/2 model. We do so to quantitatively verify the importance of the string Hamiltonian to the thermodynamics of the model in the high-temperature region. In Sec. IV we calculate the β expansion, up to order β^6, of the Helmholtz free energy of the $S=2$ XXZ model with anisotropy in the z direction and the single-ion anisotropy term in the presence of an external magnetic field in the z direction. The analytical results are compared to thermodynamic functions data calculated by the QMC method in Ref. 19. In Sec. V we present our conclusions. Finally, in the Appendix we give the β expansion of the Helmholtz free energy of the modified tetrahedral spin-1/2 model, up to order β^5, that is mapped onto to the fermionic chain model by Sólyom and Timonen.

II. THE THERMODYNAMICS OF THE TETRAHEDRAL SPIN-1/2 MODEL IN THE HIGH-TEMPERATURE LIMIT

The Hamiltonian of the tetrahedral spin-1/2 model (see Fig. 1) is

$$H_t=\sum_{i=1}^{N}\{J_0(\sigma_i,\tau_i)_1+J[(\sigma_i,\sigma_{i+1})_\Delta+(\sigma_i,\tau_{i+1})_\Delta+(\tau_i,\sigma_{i+1})_\Delta+(\tau_i,\tau_{i+1})_\Delta]-h(\sigma_i^z\otimes\mathbf{1}_\tau+\mathbf{1}_\sigma\otimes\tau_i^z)\}. \tag{1}$$

Along the ρ line of the dumbbell we have the spin-1/2 σ_i whereas along the r line we have the distinct spin-1/2 τ_i. We use the notation $(A_l,B_k)_\Delta\equiv A_l^x\otimes B_k^x+A_l^y\otimes B_k^y+\Delta A_l^z\otimes B_k^z$, with $A_l\equiv(A_l^x,A_l^y,A_l^z)$ and $B_k\equiv(B_k^x,B_k^y,B_k^z)$ to introduce the anisotropy in the z direction. We impose periodic boundary conditions to the Hamiltonian (1).

Hamiltonian (1) is a modified version of model B of Ref. 13 with $r_1=\rho_1$ and $r_2=\rho_2$. We introduce an anisotropy in the z direction in the crossing interactions as well as in the interaction between first neighbors (see Fig. 1). It is also a special case of the generalized spin ladder proposed by Kolezhuk and Mikeska[26] to interpolate some quasi-one-dimensional gapped models. Hamiltonian (1) is the special case, $J_2=J_3=J_4$, of the Hamiltonian in Ref. 8 that describes a frustrated spin ladder with diagonal couplings.

Defining the composite spin $\vec{S}_i$ at each site as

$$\vec{S}_i=\vec{\sigma}_i\otimes\mathbf{1}_\tau+\mathbf{1}_\sigma\otimes\vec{\tau}_i, \tag{2}$$

with $\mathbf{1}_\sigma$ being the identity in the σ space and $\mathbf{1}_\tau$ being the identity in the τ space, it is simple to realize that the tetrahedral spin-1/2 model (1) is mapped into the chain model:

$$H_t=\sum_{i=1}^{N}\left\{-\frac{3}{4}J_0\mathbf{1}_{4\times4}+\frac{J_0}{2}S_i^2+J[S_i^+S_{i+1}^-+S_i^-S_{i+1}^+ +\Delta S_i^zS_{i+1}^z]-hS_i^z\right\}, \tag{3a}$$

where $S_i^{\pm}\equiv(1/\sqrt{2})(S_i^x\pm iS_i^y)$ and $S_i^2\equiv\vec{S}_i\cdot\vec{S}_i$. The matrices in Hamiltonian (3a), written in the basis of the eigenstates of S_i^z and S_i^2, are

$$S_i^2=\begin{pmatrix}2&0&0&0\\0&2&0&0\\0&0&2&0\\0&0&0&0\end{pmatrix}_i,\quad S_i^z=\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix}_i, \tag{3b}$$

$$S_i^+=\begin{pmatrix}0&1&0&0\\0&0&1&0\\0&0&0&0\\0&0&0&0\end{pmatrix}_i,\quad S_i^-=\begin{pmatrix}0&0&0&0\\1&0&0&0\\0&1&0&0\\0&0&0&0\end{pmatrix}_i. \tag{3c}$$

The model described by Hamiltonian (3a) is also subject to a periodic boundary condition. In matrices (3b) and (3c) we recognize the sectors $S=0$ (singlet state) and $S=1$ (triplet state) that come from the composite spin (2).

The method developed in Ref. 23 can be directly applied to the Hamiltonian (3a) to obtain its thermodynamics in this region of temperature. The advantage of describing the tetrahedral spin-1/2 model in Fig. 1 by Hamiltonian (3a) is that of recognizing a one-dimensional composite spin model that has already been studied in the literature.[10,11,13]

By applying the results of Ref. 23 to the Hamiltonian (3a) we get the high-temperature expansion of the Helmholtz free energy of the tetrahedral spin-1/2 model (1), in the thermodynamic limit, up to order β^5:

$$\begin{aligned}\mathcal{W}_t(\beta)=&-\frac{\ln(4)}{\beta}+\frac{3J_0}{4}+\left(-\frac{J^2}{4}-\frac{3J_0^2}{32}-\frac{h^2}{4}-\frac{J^2\Delta^2}{8}\right)\beta+\left(-\frac{J^3\Delta}{16}+\frac{J_0h^2}{16}+\frac{J^2\Delta^2J_0}{16}-\frac{J_0^3}{64}+\frac{J\Delta h^2}{4}+\frac{J^2J_0}{8}\right)\beta^2\\&+\left(\frac{J^2J_0^2}{64}+\frac{J^2h^2}{16}-\frac{7J^4\Delta^4}{384}+\frac{J_0^4}{1024}-\frac{3J^2\Delta^2h^2}{16}+\frac{h^4}{96}+\frac{J^4\Delta^2}{32}-\frac{J_0J\Delta h^2}{8}+\frac{J_0^2h^2}{64}+\frac{J_0^2J^2\Delta^2}{128}+\frac{J_0J^3\Delta}{32}-\frac{J^4}{48}\right)\beta^3\\&+\left(-\frac{J_0h^4}{96}-\frac{J_0J^4}{64}-\frac{5J^4\Delta^2J_0}{96}-\frac{J^2\Delta^2J_0^3}{192}+\frac{J_0J^4\Delta^4}{192}-\frac{3J^3\Delta h^2}{32}+\frac{J^3\Delta J_0^2}{256}+\frac{J^5\Delta}{192}+\frac{13J^3\Delta^3h^2}{96}-\frac{J_0h^2J^2}{16}\right.\\&\left.-\frac{h^2J_0^3}{768}+\frac{J_0^5}{1024}+\frac{J^5\Delta^3}{384}-\frac{J_0^3J^2}{96}-\frac{J\Delta J_0^2h^2}{64}+\frac{7J_0J^2\Delta^2h^2}{64}-\frac{J\Delta h^4}{24}\right)\beta^4+\left(\frac{11J^4\Delta^4J_0^2}{3072}-\frac{5J^4\Delta^4h^2}{64}-\frac{11J^2\Delta^2J_0^4}{6144}\right.\\&+\frac{11J^2\Delta^2h^4}{128}+\frac{5J^4\Delta^2J_0^2}{384}+\frac{11J^4\Delta^2h^2}{128}-\frac{J^3\Delta J_0^3}{384}+\frac{J_0^2J^2h^2}{256}-\frac{7J^5\Delta^3J_0}{768}-\frac{7J_0J^5\Delta}{384}-\frac{J^2h^4}{96}-\frac{J^6\Delta^6}{2880}-\frac{h^2J^4}{192}\\&+\frac{J^6\Delta^2}{2560}+\frac{7J_0^2J^4}{512}-\frac{J_0^2h^4}{1536}-\frac{5h^2J_0^4}{3072}-\frac{11J^2J_0^4}{3072}+\frac{9J^6\Delta^4}{1280}+\frac{13J_0^6}{122\,880}+\frac{73J^6}{11\,520}-\frac{h^6}{1440}-\frac{J^3\Delta^3J_0h^2}{12}+\frac{J\Delta J_0^3h^2}{96}\\&\left.+\frac{5J\Delta J_0h^4}{96}+\frac{J^2\Delta^2J_0^2h^2}{128}+\frac{15J_0h^2J^3\Delta}{128}\right)\beta^5+O(\beta^6).\end{aligned} \tag{4}$$

In Ref. 24 we obtained the β expansion of the Helmholtz free energy of the XXZ Heisenberg model with spin-1, where the spin-1 is considered as a fundamental spin (i.e., the irreducible representation of spin-1), under periodic boundary conditions. For $J_0=0$, the Hamiltonian (3a) has the same form as the Hamiltonian (1a) of Ref. 24, in the absence of the single-ion anisotropy $(D=0)$.

Certainly it is interesting to compare the behavior of the thermodynamic quantities for the spin-1 model when it is a composite model and when it is a fundamental one.

The thermodynamics of both models is independent of the sign of the constant J. From now on we choose it to be positive. We factor the constant J in Hamiltonian (3a) and have the others constants redefined as J_0/J and H/J. The expression (4) for $\mathcal{W}_t(\beta)$ becomes an expansion with respect to the product (βJ), with $J>0$.

In what follows, we take $J=1$ and $D=0$ in expression (3) of Ref. 24 for the Helmholtz free energy of the spin-1 XXZ model and $J_0=0$ in Eq. (4).

From the Helmholtz free energy we calculate the specific

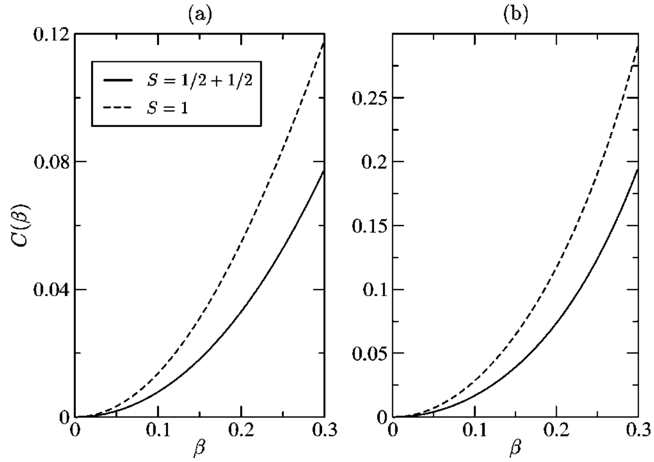

FIG. 2. Dashed lines represent the specific heat per site for the spin-1 XXZ model, whereas solid lines are for the tetrahedral spin-1/2 model with (a) $\Delta=1$ and $h=0$, and (b) $\Delta=-2$ and $h=0.5$.

heat per site, $C_L(\beta)$ $(C_L(\beta)=-\beta^2\partial^2[\beta\mathcal{W}(\beta)]/\partial\beta^2$, where $\mathcal{W}(\beta)$ is the Helmholtz free energy of the respective model). In the high-temperature region ($\beta\in[0{,}0.3]$), the specific heat per site of the spin-1 XXZ model is always higher than that of tetrahedral spin-1/2 model for the ferromagnetic ($\Delta<0$) and the antiferromagnetic ($\Delta>0$) phases. In Fig. 2(a) we compare the specific heat per site of both models in the absence of an external magnetic field, while in Fig. 2(b) we have an external magnetic field $h=0.5$. These figures exemplify the fact that in this region of temperature the specific heat per site of the spin-1 XXZ model is higher than that of the composite model. This happens due to the presence of composite spin $S=0$ along the chain. For both models the specific heat per site vanishes for $\beta\rightarrow0$, just like β^2, but with different positive coefficients.

In the high-temperature region, the correlation function between the z components of the nearest spins $\langle S_i^zS_{i+1}^z\rangle$ $[\langle S_i^zS_{i+1}^z\rangle=\partial\mathcal{W}(\beta)/\partial\Delta]$ of the spin-1 XXZ model is, in general, stronger than for the composite spin model. However, for $\Delta\in(-0.8{,}0)$ the curves of $\langle S_i^zS_{i+1}^z\rangle$ for both models cross each other. In Fig. 3(a) we have $\Delta=-0.06$ and $h=0$. For the interval of Δ mentioned above, the presence of an external magnetic field h takes the crossing point to a lower value of temperature, as we have in Fig. 3(b). The correlation function between nearest neighbors of both models vanishes as $\beta\rightarrow0$ but with different values of its derivative at $\beta=0$.

The mean energy per site $\varepsilon(\beta)$ $(\varepsilon(\beta)=\partial[\beta\mathcal{W}(\beta)]/\partial\beta)$ of the spin-1 XXZ model is lower than that of the tetrahedral spin-1/2 model in the high-temperature region. This is true for both models, even in the presence of the same nonvanishing external magnetic field h. Again, this fact is associated with the presence of immobile $S=0$ spins in the chain. Those composite spins $S=0$ are responsible for the breaking of the original chain into subchains of composite spin $S=1$, each one with nonzero mean energy per site. The union of those subchains is always smaller than the original chain,

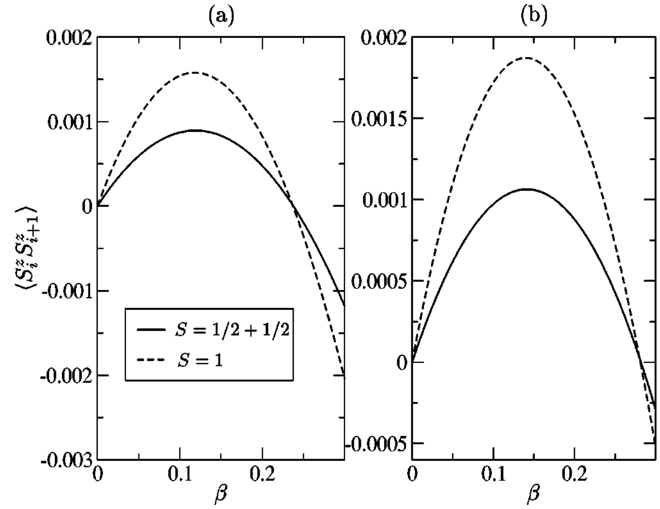

FIG. 3. The correlation function $\langle S_i^zS_{i+1}^z\rangle$ for both models with $\Delta=-0.06$. In (a) we have $h=0$ and in (b) we have an external magnetic field $h=0.2$. In the presence of the external magnetic field, the intersection of curves has gone higher in β, i.e., occurs at a lower temperature.

which implies that the mean energy per site of the composite model is always smaller than that of the spin-1 XXZ model. Figure 4 exemplifies this behavior for $\Delta=-2$ and $h=0.5$. In the vicinity of $\beta=0$, both models give a straight line but with different negative slopes.

In the region of high temperatures, the static magnetic susceptibility per site $\chi(\beta)$ $(\chi(\beta)=-\partial^2[\mathcal{W}(\beta)]/\partial h^2|_{h=0})$ of the spin-1 XXZ model is higher than that of the composite model. The static magnetic susceptibility is defined as the ratio of the magnetic moment per unit of length to the norm of the external magnetic field. The spins-0 in the chain work as nonmagnetic impurities, such that the magnetic susceptibility of the composite spin model is smaller than that of the fundamental spin-1 XXZ model. Varying the anisotropy con

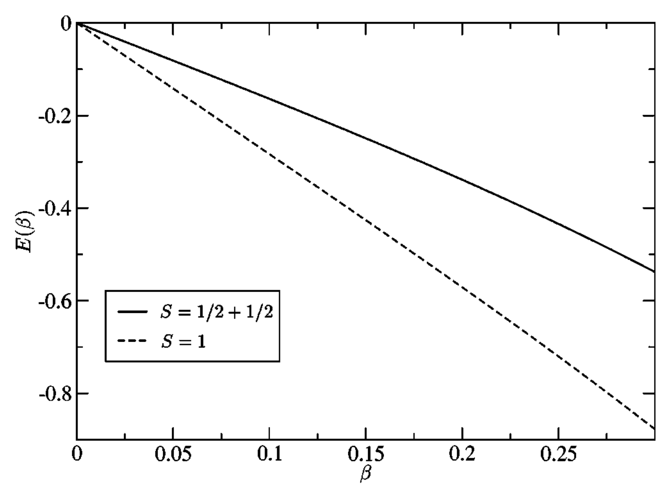

FIG. 4. The mean energy of the spin-1 XXZ is the dashed line and the solid line is the equivalent curve of the tetrahedral spin-1/2 model. For both curves we have $\Delta=2$ and $h=0.5$.

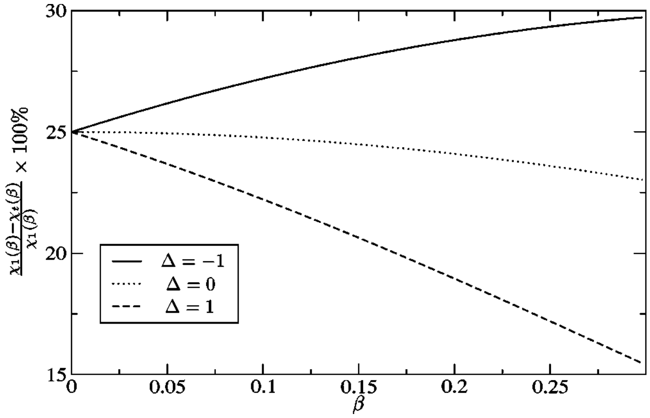

FIG. 5. We plot the percentage difference between the static magnetic susceptibility of the two models [Diff% = ([$\chi_1(\beta) - \chi_t(\beta)]/\chi_1(\beta)) \times 100\%$]. For the continuous line we have $\Delta = -1$; for the dotted line we have $\Delta = 0$; and for the dashed line we have $\Delta = 1$.

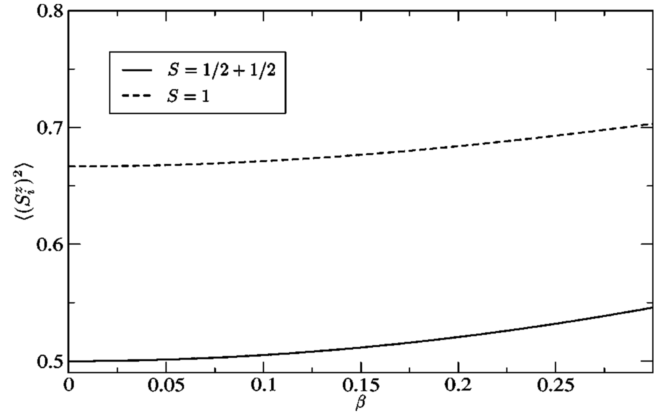

FIG. 6. We plot the mean value of the squared z component of spin per site $\langle (S_i^z)^2 \rangle$. We take $\Delta = 2$ and $h = 0.4$. The dashed line gives the curve for the spin-1 XXZ model; the solid line gives the curve for the composite spin-model.

stant Δ from negative (ferromagnetic state) to positive values (antiferromagnetic state), the difference between the static magnetic susceptibility per site of the spin-1 XXZ model, χ_1, and the analogous thermodynamic quantity of the tetrahedral spin-1/2 model, χ_t, diminishes. In Fig. 5 we plot the percentual relative difference. $[(\chi_1 - \chi_t)/\chi_1] \times 100\%$. For $\beta \to 0$ both models satisfy Curie's law, but with different coefficients.

Finally, we cannot obtain the mean value of the squared z component of spin at each site $\langle (S_i^z)^2 \rangle$ from a simple derivative of the Helmholtz free energy (4). To get $\langle (S_i^z)^2 \rangle$ for the composite model we apply the method of Ref. 22 to the modified Hamiltonian:

$$H_{t-mod} = \sum_{i=1}^{N} \left\{ J[S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + \Delta S_i^z S_{i+1}^z] - h S_i^z + \frac{G}{2} (S_i^z)^2 \right\}. \quad (5)$$

In the Appendix we give the expression of the β expansion, up to order β^5, of the Helmholtz free energy associated with this Hamiltonian, $\mathcal{W}_{t-mod}(\beta)$. The temperature dependence of the thermodynamic function $\langle (S_i^z)^2 \rangle$ of the composite spin model can be easily calculated as

$$\langle (S_i^z)^2 \rangle = 2 \frac{\partial \mathcal{W}_{t\text{-}mod}(\beta)}{\partial G} \Big|_{G=0}. \quad (6)$$

The thermodynamic function $\langle (S_i^z)^2 \rangle$ of the spin-1 XXZ model is larger than that of the tetrahedral spin-1/2 model in the high-temperature region for arbitrary ratio of the constants Δ/J and h/J. In Fig. 6 we compare the temperature dependence of the function $\langle (S_i^z)^2 \rangle$ of the two models for $\Delta = 2$ and $h = 0.4$. Differently from the other thermodynamic quantities presented, the limit $\beta \to 0$ of the $\langle (S_i^z)^2 \rangle$ is not the same for the two models, as we verify directly from Fig. 6. This is a direct consequence of the immobile $S = 0$ sites that work as "nonmagnetic impurities" in the chain.[10,11]

III. COMPARISON OF THE THERMODYNAMICS OF THE COMPOSITE SPIN-1 MODEL AND THE ONE-DIMENSIONAL EXTENDED HUBBARD MODEL

In Refs. 10 and 11, Sólyom and Timonen apply the Jordan-Wigner transformation to the spin variables to map their Hamiltonian (2.1),

$$H_{st} = -\sum_{i=1}^{N} [J_{xy}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z S_i^z S_{i+1}^z - D(S_i^z)^2], \quad (7)$$

into the Hamiltonian of the one-dimensional extended Hubbard model plus a string Hamiltonian with infinite correlation. This string Hamiltonian is proportional to the constant J_{xy}, only. In Refs. 10 and 11 the phase diagrams at $T = 0$ of Hamiltonian (7) and the one-dimensional extended Hubbard model are compared. They concluded that both models have a similar phase diagram in the strong-U limit ($J_{xy} = 0$) and consequently the effect due to the string Hamiltonian is negligible at $T = 0$ in this limit. However the models have different phase diagrams when $J_{xy} \neq 0$. Certainly both models do not have the same energy spectrum.

In Ref. 25 we calculated the high-temperature expansion of the grand potential of the one-dimensional generalized Hubbard model up to order β^2. In order to have a quantitative check of the effect due to the presence of the string Hamiltonian in the thermodynamics of the model described by the Hamiltonian (7) we consider the case: $J_{xy} = -J$, $J_z = -J\Delta$, and $D = G/2$. For these choices of constants, Hamiltonian (7) becomes identical to the modified Hamiltonian (5). We should note that the modified model corresponds to a tetrahedral spin-1/2 model where the term $J_0 S_i^2/2$ is replaced by $G(S_i^z)^2/2$. This new term is obtained in substituting the term $(\sigma_i, \tau_i)_1$ in Hamiltonian (1) by $(\sigma_i^z, \tau_i^z)_1$. In the Appen-

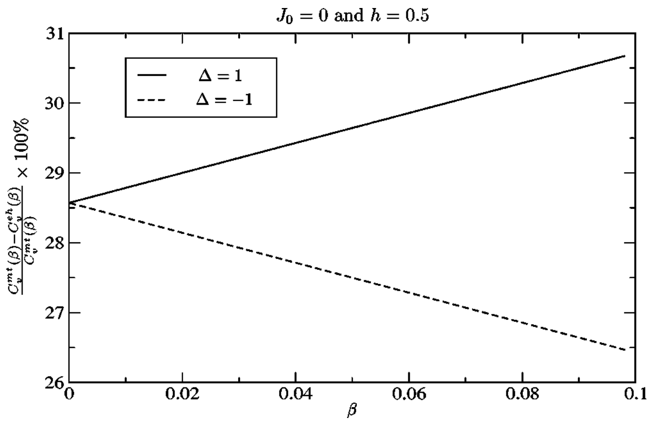

FIG. 7. The percentual relative difference of the specific heat per site given by the one-dimensional extended Hubbard model and the modified tetrahedral spin-1/2 model. For both plots we have set $G=0$ and $h=0.5$. The curves correspond to the cases $\Delta=-1$ (dashed line) and $\Delta=1$ (solid line).

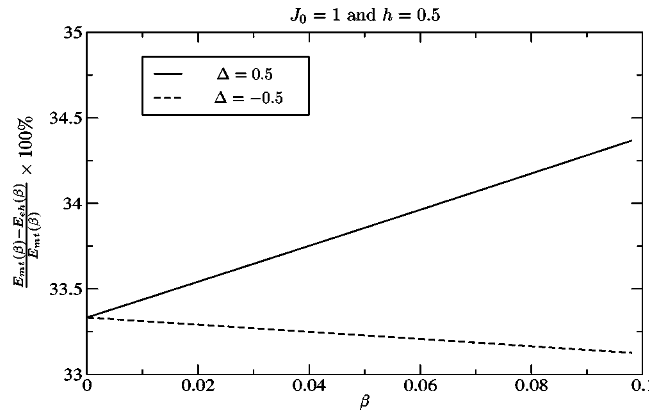

FIG. 8. The percentual relative difference of the mean energy per site given by the one-dimensional extended Hubbard model and the modified spin model. In the two curves we set $G=1$ and $h=0.5$. We plot the curves for $\Delta=-0.5$ (dashed line) and $\Delta=0.5$ (solid line).

dix we present the expression of the Helmholtz free energy of this modified model, up to order β^5, but since the results of the one-dimensional extended Hubbard model go up to order β^2, in the following β expansion for $\mathcal{W}_{t\text{-}mod}(\beta)$ we only keep terms up to order β^2:

$$\mathcal{W}_{t\text{-}mod}(\beta)=-2\frac{\ln(2)}{\beta}+\left(-\frac{J^2}{4}-\frac{J^2\Delta^2}{8}-\frac{G^2}{32}-\frac{h^2}{4}\right)\beta+\left(\frac{Gh^2}{16}+\frac{J^2\Delta^2G}{16}-\frac{J^3\Delta}{16}+\frac{J\Delta h^2}{4}\right)\beta^2+O(\beta^3). \tag{8}$$

To compare the results of the modified Hamiltonian (5) and the one-dimensional extended Hubbard model, in Eqs. (63) and (73) of Ref. 25, we made the following substitutions: $t=J/2$, $\lambda_B=0$, $E_0=-(G/2+2J\Delta+h)$, $U=G$, $V=Jh/2$, $\mu=0$, and $X=0$.

To verify the importance of the contribution of the string Hamiltonian to the thermodynamics functions in the high-temperature region, we calculate the relative difference (in percent) of the specific heat, mean energy, and static magnetic susceptibility per site obtained from the Hamiltonian (5) and the one-dimensional extended Hubbard model. In Fig. 7 we plot the relative difference in the specific heat per site of the one-dimensional extended Hubbard model $[C_L^{eh}(\beta)]$ and the modified tetrahedral spin-1/2 model $(C_L^{t-mod}(\beta))$, that is, $\Delta C_L(\beta)\equiv[(C_L^{eh}-C_L^{t-mod})/C_L^{t-mod}]\times 100\%$. In Fig. 7 we plot this relative difference, in the high-temperature region, for two values of Δ: $\Delta=\pm 1$. For both values of Δ we set $G=0$ and $h=0.5$. In the two curves the relative difference is larger than 20%. In particular, when we only have the "flip term" in the Hamiltonian (5) ($\Delta=h=G=0$), which is mapped into the hopping term of the one-dimensional Hubbard model plus a string Hamiltonian, the relative difference $\Delta C_L(\beta)$ is 50% for any value of β in the high-temperature region. In Fig. 8 we plot the difference of the mean energy per site of the one-dimensional extended Hubbard model (E_{eh}) and of the modified tetrahedral spin-1/2 model (E_{mt}), that is, $\Delta E(\beta)\equiv([E_{mt}(\beta)-E_{eh}(\beta)]/E_{mt}(\beta))\times 100\%$. In Fig. 8 we have set $\Delta=\pm 0.5$ and for both curves we have $G=1$ and $h=0.5$. We verify directly from the plots that the relative difference in the two plots is larger than 30%. As in the case of the specific heat per site when we set $\Delta=h=G=0$, the relative difference (in percent) $\Delta E(\beta)$ is equal to 50%, and it is independent of β in the high-temperature region.

Finally, up to order β^2, the static magnetic susceptibility is the same for both models. In units of J, we have

$$\chi_{eh}(\beta)=\chi_{t\text{-}mod}(\beta)=-\left(\frac{\Delta}{2}+\frac{G}{8}\right)\beta^2+\frac{\beta}{2}, \tag{9}$$

where $\chi_{eh}(\beta)$ is the static magnetic susceptibility of the one-dimensional extended Hubbard model and $\chi_{t\text{-}mod}(\beta)$ is the static magnetic susceptibility of the modified composite spin model.

IV. THE THERMODYNAMICS OF THE SPIN-2 XXZ CHAIN IN THE HIGH-TEMPERATURE REGION

The Hamiltonian of the anisotropic spin-2 XXZ model is identical to the modified Hamiltonian (5), but now the operators S_i^x, S_i^y, and S_i^z are the components of the fundamental $S=2$ spin matrices of the ith site. To simplify the notation we take $D=G/2$ in Hamiltonian (5).

Applying the method of Ref. 23 to the Hamiltonian (5) of the fundamental spin-2 XXZ model, we obtain its Helmholtz free energy, up to order β^6, for either positive or negative values of Δ and D:

$$
\begin{aligned}
\mathcal{W}_2(\beta)=&-\frac{\ln(5)}{\beta}+2D+\Bigg(-2J^2\Delta^2-h^2-\frac{7D^2}{5}-4J^2\Bigg)\beta+\Bigg(\frac{28J^2\Delta^2D}{5}-\frac{28J^2D}{5}+\frac{7h^2D}{5}-J^3\Delta+4J\Delta h^2+\frac{D^3}{5}\Bigg)\beta^2\\
&+\Bigg(\frac{101J^4}{150}+\frac{169D^4}{300}+\frac{919J^4\Delta^2}{75}+\frac{51J^2D^2}{25}+\frac{13h^4}{60}-\frac{128J^2\Delta^2D^2}{25}+\frac{19J^2h^2}{5}-\frac{409J^4\Delta^4}{150}-\frac{3h^2D^2}{10}-\frac{54J^2\Delta^2h^2}{5}\\
&-\frac{56J\Delta h^2D}{5}\Bigg)\beta^3+\Bigg(-\frac{169h^2D^3}{150}-\frac{212J^2\Delta^2D^3}{75}-\frac{51J^2h^2D}{25}-\frac{207J^4\Delta^2D}{10}+\frac{79J^5\Delta^3}{60}+\frac{256J\Delta h^2D^2}{25}-\frac{53h^4D}{60}\\
&+\frac{79J^5\Delta}{30}-\frac{646J^3\Delta h^2}{25}+\frac{2018J^3\Delta^3h^2}{75}+\frac{503J^2D^3}{75}+\frac{968J^2\Delta^2h^2D}{25}+\frac{95J^4D}{6}-\frac{52J\Delta h^4}{15}+\frac{73J^4\Delta^4D}{15}-\frac{23D^5}{100}\\
&-\frac{7J^3\Delta D^2}{25}\Bigg)\beta^4+\Bigg(\frac{1182J^3\Delta h^2D}{25}-50J^2\Delta^2h^2D^2+\frac{1424J\Delta h^4D}{75}+\frac{424J\Delta h^2D^3}{75}-\frac{1636J^3\Delta^3h^2D}{15}-\frac{66\,611J^6\Delta^2}{1500}\\
&-\frac{937J^2h^4}{300}-\frac{197J^2D^4}{60}-\frac{211J^4h^2}{20}+\frac{6563J^4D^2}{300}+\frac{227h^4D^2}{200}+\frac{23h^2D^4}{40}+\frac{451J^6\Delta^6}{900}+\frac{7643J^6\Delta^4}{1500}-\frac{31h^6}{360}\\
&-\frac{1106J^5\Delta^3D}{375}+\frac{1033J^4\Delta^4D^2}{75}+\frac{2034J^4\Delta^2h^2}{25}-\frac{3492J^4\Delta^2D^2}{125}+\frac{106J^3\Delta D^3}{375}+\frac{1106J^5\Delta D}{375}+\frac{653J^2\Delta^2h^4}{25}\\
&-\frac{2783J^4\Delta^4h^2}{50}-\frac{489J^2h^2D^2}{50}-\frac{3287D^6}{9000}+\frac{3161J^2\Delta^2D^4}{375}+\frac{27\,439J^6}{4500}\Bigg)\beta^5+\Bigg(-\frac{2924J\Delta h^4D^2}{75}-\frac{12\,763J^2\Delta^2h^4D}{75}\\
&-\frac{6322J\Delta h^2D^4}{375}-\frac{3\,193\,459J^4\Delta^2h^2D}{15\,750}+\frac{385\,729J^3\Delta h^2D^2}{7875}+\frac{92\,059J^4\Delta^4h^2D}{375}-\frac{134J^2\Delta^2h^2D^3}{75}+\frac{2284J^3\Delta^3h^2D^2}{15}\\
&-\frac{12\,187J^2D^5}{1500}+\frac{3287h^2D^5}{3000}+\frac{503h^4D^3}{1800}-\frac{1\,055\,363J^4D^3}{31\,500}+\frac{1003h^6D}{1800}-\frac{429\,461J^6D}{31\,500}+\frac{14\,699J^7\Delta^5}{9000}-\frac{35\,237J^7\Delta^3}{2250}\\
&-\frac{1141J^7\Delta}{250}+\frac{634J\Delta h^6}{225}-\frac{31\,606J^3\Delta^3h^4}{225}-\frac{55\,852J^4\Delta^4D^3}{1125}+\frac{11\,107J^5\Delta D^2}{5000}+\frac{2\,668\,067J^6\Delta^4D}{31\,500}+\frac{100\,073J^2h^2D^3}{15\,750}\\
&+\frac{897\,401J^5\Delta h^2}{9000}-\frac{109\,709J^4h^2D}{4500}+\frac{247J^3\Delta D^4}{250}-\frac{57\,067J^6\Delta^6D}{2250}-\frac{26\,173J^5\Delta^3h^2}{125}+\frac{847J^2h^4D}{100}-\frac{359\,167J^6\Delta^2D}{7875}\\
&+\frac{170\,119J^3\Delta h^4}{3150}-\frac{71J^2\Delta^2D^5}{375}+\frac{142\,021J^4\Delta^2D^3}{1750}+\frac{15\,341J^5\Delta^5h^2}{150}+\frac{19\,631J^5\Delta^3D^2}{7500}+\frac{731D^7}{3000}\Bigg)\beta^6+O(\beta^7). \qquad (10)
\end{aligned}
$$

In order to compare our result (10) with the high-temperature expansion in Ref. 19, we obtain from the free energy (10), the mean energy per spin $E_2^{AF}(\beta)$ and the static magnetic susceptibility per spin $\chi_2^{AF}(\beta)$ of the antiferromagnetic Heisenberg chain in the absence of an external magnetic field ($\Delta=1,\ D=0,$ and $h=0$):

$$
\begin{aligned}
E_2^{AF}(\beta)=&-12\beta-3\beta^2+\frac{204}{5}\beta^3+\frac{79}{4}\beta^4-\frac{4907}{25}\beta^5\\
&-\frac{15\,617}{120}\beta^6+O(\beta^7), \qquad (11a)
\end{aligned}
$$

$$
\begin{aligned}
\chi_2^{AF}(\beta)=&\,2\beta-8\beta^2+14\beta^3-\frac{32}{15}\beta^4-\frac{303}{10}\beta^5\\
&+\frac{13\,319}{900}\beta^6+O(\beta^7). \qquad (11b)
\end{aligned}
$$

Comparing Eq. (11a) with expression (3.2a) of Ref. 19 for the mean energy per spin, we see that in this last expression the even-power terms of (βJ) are missing. Consequently, the odd-power terms of (βJ) are missing from the expression of the specific heat, in Eq. (3.5a) of this same reference. Finally, we also notice a misprint in Eq. (3.10a) of Ref. 19 at order β^3, when comparing it to our Eq. (11b).

In Fig. 9 we compare our results (11) to the QMC data and the high-temperature expansion contained in Ref. 19. Equations (11) extend the interval of temperature where the β expansions of those thermodynamic functions are *bona fide*.

Our results in Fig. 9 are valid in the thermodynamic limit, showing that numerical data in Ref. 19 correspond to th limit $N\to\infty$, being valid for temperatures lower than those inferred from the β expansion in Yamamoto's original paper.[19] Our exact β expansion for the average energy per spin deviates from the numerical results of QMC method by 0.8% for $kT=4$, and by less than 1.3% for $kT=3.8$. The β expansion

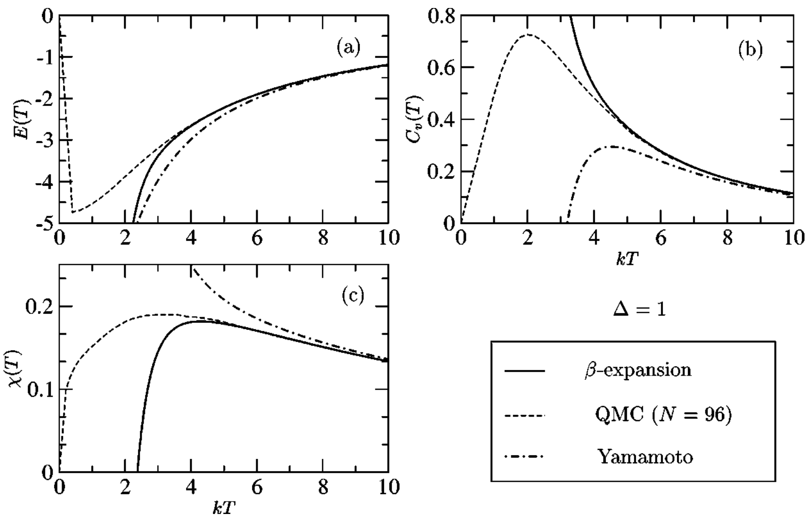

FIG. 9. We compare our results (3) (solid line) with the QMC data ($N=96$) (dashed line) and the high-temperature expansion in Ref. 1 (dotted-dashed line). The plots show (a) the mean energy per spin; (b) the specific heat per spin, and (c) the static magnetic susceptibility per spin. In all plots, $\Delta=1$, $D=0$, and $h=0$.

for the specific heat per spin noticeably deviates from numerical data for lower temperatures ($k\lesssim 4.5$) as wee see from Fig. 9(b).

The relative errors of the β expansion around $kT\sim 5$ with respect to QMC are the following: for $kT=5$ the error is 2.8% but for $kT=4.8$ this error becomes 2.2%. Certainly we expect a systematically increasing deviation when the temperature decreases and this eventual reduction happens due to the precision in the QMC calculation. A similar behavior is shown by the specific heat per spin in higher temperatures; that is, for $kT=5.6$ the relative error is 1% but for $kT=5.8$ the error becomes 1.3%, although it globally decreases as the temperature is increased. From Fig. 9(c), comparison of the magnetic susceptibility per spin, obtained by the β expansion (11b) and by QMC method, shows that the worsening of their relative error is smoother than that of the specific heat per site. For $kT=5$ we have an error of about 1%, whereas for $kT=4.6$ we have 1.5%.

V. CONCLUSIONS

The method presented in Ref. 23 has been applied up to now to obtain the high-temperature expansion of the Helmholtz free energy of one-dimensional models (the spin-1/2 integrable model[23] and the spin-1 nonintegrable model[24]) whose Hamiltonians are identified by one site label only. In this present communication we obtain the thermodynamics of the quasi-one-dimensional tetrahedral spin-1/2 model in the high-temperature region by applying the method of Ref. 23. We do so by mapping the tetrahedral spin-1/2 model into a composite spin model with $S=0$ and $S=1$ chains. The $T=0$ properties of this composite spin model have been studied previously.[10,11,13]

To verify the effect of the fragmentation of the chain due to the presence of $S=0$ spin,[13] in the high-temperature region we compare the thermodynamics of the tetrahedral spin-1/2 model to the thermodynamics of the spin-1 XXZ model.[24] In this region of temperature the specific heat and the static magnetic susceptibility per site of the spin-1 XXZ model are larger than those of the composite spin model. The mean energy per site of the spin-1 XXZ model is lower than that of the tetrahedral spin-1/2 model. In general, the correlation function between first neighbors is stronger in the spin-1 model than it is in the composite model, but there is an interval of values of Δ where this inequality is reversed. For $\beta\to 0$, all these thermodynamic functions have the same limit for both models. The function $\langle (S_i^z)^2\rangle$ expresses in a very clear way the effect of the immobile $S=0$ sites that work as ''nonmagnetic impurities'' in the chain. In the high-temperature region, this function for the spin-1 XXZ model has higher values than that of the tetrahedral spin-1/2 model. For $\beta\to 0$, the limit of this function is different for the two models.

In the literature the composite spin model has been mapped onto a fermionic model. This fermionic model is the one-dimensional extended Hubbard model plus a string Hamiltonian. The phase diagram of the composite spin model is compared to the phase diagram of the one-dimensional extended Hubbard model.[10,11] The purpose of this is showing that the effect of the string Hamiltonian could be neglected in the strong-U limit. To verify the importance of the contribution of the string Hamiltonian to the thermodynamics of the composite spin model, for any ratio among the constants of the model, in the high-temperature region, we compare its specific heat, static magnetic susceptibility, and mean energy per site with the ones obtained from the one-dimensional extended Hubbard model.[25] We obtain in the high-temperature limit that the β expansion, up to order β^2, that the static magnetic susceptibility per site is the same for both models. The relative difference of the specific heat per site of theses models is higher than 20% for the isotropic ferromagnetic and antiferromagnetic models ($\Delta=\pm 1$) in the presence of an external magnetic field. The relative difference of the mean energy per site is larger than 30% for $\Delta=\pm 0.5$, also in the presence of an external magnetic field. This relative difference decreases as much the anisotropic parameters Δ and G are much larger than J. When $\Delta=G=h=0$, the relative difference of these two physical quantities for both models is 50% and it is temperature independent in the high-temperature region.

We conclude that, at least in the high-temperature region, we cannot neglect the contribution of the string Hamiltonian to the thermodynamics of the composite spin model, mainly in the Heisenberg point ($\Delta = \pm 1$). Our results let us affirm that the energy spectra of the composite spin model and the one-dimensional extended Hubbard model are different.

Finally we extend the analytic β expansion for the thermodynamic functions of the isotropic antiferromagnetic spin-2 Heisenberg chain obtained by Yamamoto[19] to the anisotropic case and to a larger interval of temperature in the high-temperature region. The results presented are valid for the anisotropic spin-2 XXZ chain in the presence of an external magnetic field. Our results fit well the QMC data in Ref. 19 and the latter are used to obtain the interval of temperature where our expansion is reliable.

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APPENDIX: THE HELMHOLTZ FREE ENERGY OF THE MODIFIED TETRAHEDRAL SPIN-1/2 MODEL

The free energy of the modified tetrahedral spin-1/2 model described by Hamiltonian (5), up to order β^5, is

$$\begin{aligned}
\mathcal{W}_{t-mod}(\beta) = {} & -\frac{\ln(4)}{\beta} + \frac{D}{2} + \left(-\frac{J^2\Delta^2}{8} - \frac{h^2}{4} - \frac{J^2}{4} - \frac{D^2}{8} \right)\beta + \left(\frac{J^2\Delta^2 D}{8} + \frac{Dh^2}{8} - \frac{J^3\Delta}{16} + \frac{J\Delta h^2}{4} \right)\beta^2 \\
& + \left(\frac{J^2h^2}{16} - \frac{3J^2\Delta^2h^2}{16} + \frac{J^2D^2}{24} + \frac{J^3\Delta D}{48} + \frac{J^4\Delta^2}{32} - \frac{J^4}{48} - \frac{J^2\Delta^2D^2}{32} + \frac{D^4}{192} + \frac{h^4}{96} - \frac{J\Delta Dh^2}{4} - \frac{7J^4\Delta^4}{384} \right)\beta^3 \\
& + \left(\frac{7J^2\Delta^2h^2D}{32} + \frac{J^3\Delta D^2}{192} + \frac{J\Delta D^2h^2}{16} - \frac{h^2D^3}{96} - \frac{Dh^4}{48} - \frac{h^2J^2D}{16} \right. \\
& \left. + \frac{J^5\Delta^3}{384} - \frac{5J^4\Delta^2D}{96} - \frac{3J^3\Delta h^2}{32} + \frac{J^5\Delta}{192} + \frac{J^4\Delta^4D}{96} - \frac{J^2\Delta^2D^3}{96} - \frac{J\Delta h^4}{24} + \frac{13J^3\Delta^3h^2}{96} \right)\beta^4 \\
& + \left(-\frac{5J^4\Delta^4h^2}{64} + \frac{11J^2\Delta^2h^4}{128} + \frac{11J^4\Delta^2h^2}{128} - \frac{J^2h^4}{96} - \frac{J^6\Delta^6}{2880} - \frac{h^2J^4}{192} + \frac{J^6\Delta^2}{2560} + \frac{9J^6\Delta^4}{1280} + \frac{73J^6}{11\,520} - \frac{h^6}{1440} \right. \\
& - \frac{J^3\Delta^3Dh^2}{6} + \frac{D^3J\Delta h^2}{48} + \frac{5DJ\Delta h^4}{48} - \frac{5J^2\Delta^2h^2D^2}{64} + \frac{25J^3\Delta Dh^2}{192} + \frac{h^4D^2}{128} - \frac{J^2D^4}{160} - \frac{7D^2J^4}{1920} \\
& \left. - \frac{7J^5\Delta D}{960} - \frac{J^3\Delta D^3}{320} - \frac{7DJ^5\Delta^3}{640} + \frac{19J^4\Delta^2D^2}{1920} - \frac{J^2D^2h^2}{192} + \frac{7D^2J^4\Delta^4}{768} + \frac{J^2\Delta^2D^4}{192} - \frac{D^6}{2880} \right)\beta^5 + O(\beta^6).
\end{aligned} \tag{A1}$$

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