Specific heat and high-temperature series of lattice models: Interpolation scheme and examples on quantum spin systems in one and two dimensions

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We have developed a method for evaluating the specific heat of lattice spin systems. It is based on the knowledge of high-temperature series expansions, the total entropy of the system, and the low-temperature expected behavior of the specific heat as well as the ground-state energy. By the choice of an appropriate variable (entropy as a function of energy), a stable interpolation scheme between low and high temperature is performed. Contrary to previous methods, the constraint that the total entropy is $\log(2S+1)$ for a spin S on each site is automatically satisfied. We present some applications to quantum spin models on one- and two-dimensional lattices. Remarkably, in most cases, a good accuracy is obtained down to zero temperature.

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I. INTRODUCTION

The accurate knowledge of the thermodynamic quantities of quantum magnets is an important issue from the experimental point of view. It allows one to determine precisely exchange energies J from experimental data or to identify possible deviations from a given model. In this paper we propose a simple method to compute the heat capacity from a high-temperature (HT) expansion. Numerous techniques have been developed to study thermodynamical singularities from power series expansions.[1] However, in this work, the point of view is slightly different. We mainly focus on the computation of the heat capacity for systems *without a phase transition* at $T>0$ (here in one and two dimensions) and try to evaluate the specific heat $c_v(T)$ accurately in the largest possible temperature range. We devised a two-point Padé-like interpolation of a particular function, namely the entropy as a function of energy, which satisfies the energy and entropy sum rules obeyed by $c_v(T)$. These two constraints are nonlocal in temperature and improve significantly the convergence of standard Padé approximations.

Before describing the method itself, let us briefly review some commonly used methods to investigate the thermodynamic properties of spin systems.

High-temperature series expansion is the usual approach to evaluate the strength of microscopic interactions from experiments. Thermodynamic quantities such as magnetic susceptibility χ or specific heat c_v are expanded in powers of $\beta=1/T$. Presently computers do not allow to compute more than about 20 terms for quantum systems.[2] When analyzed through (differential) Padé approximants, HT series give reliable results for T greater than the typical magnetic exchange energy of the model. When the low-temperature form of a given quantity is known, Padé approximants can be improved to reproduce the correct asymptotic behavior. However, with this approach it is difficult to investigate temperatures much below J. In some cases, a detailed understanding of the low-energy regime allows one to construct *biased* approximants and to compute thermodynamics in a larger temperature range (see for instance Ref. 3 for the magnetic susceptibility of square- and triangular-lattice ferromagnets). Another series approach to thermodynamics is the finite-cluster expansion. This expansion in powers of the coupling constant may, in some cases, allows one to go to lower temperature. It has been applied in one[4] and two[5,6] dimensions.

Finite-size calculation. The previous approaches are exact at high temperature but do not satisfy the sum rule that the total entropy is $\ln(2S+1)$. An alternative is to compute the heat capacity of a finite system from the exact spectrum of a small cluster of spins, and then compute the partition function by summing over all eigenstates (example: spin-1 chain[7,8]). A direct finite-temperature lanczös algorithm can also be performed,[9] as well as transfer matrix techniques. These techniques automatically give the correct entropy, but they are limited to small systems ($N\leqslant 36$) and finite-size errors may be difficult to control, especially in two dimensions.

Quantitative extrapolations to $N=\infty$ of finite-size $c_{v,N}(T)$ data have been done in spin chains but are not really efficient at low temperatures. It has been applied to spin chains[8,10–12] and the triangular antiferromagnet.[13] Power-law behaviors at low temperature cannot be observed due to the important discretization of the low-energy spectrum in a small system.

Quantum Monte-Carlo simulations can reach a rather large number of spins for not frustrated systems (as the square lattice[14]). These calculations reproduce the correct HT behavior (up to small statistical errors) but cannot reach the very low-temperature regime. This technique is one of the most efficient in studying thermodynamics properties but it requires important numerical effort and is limited to small systems when the model contains frustration.

Sum rules. We propose a *simple* method to compute the heat capacity which involves a different kind of HT series analysis. In contrast to previous methods, we provide a procedure for $c_v(T)$ which satisfies a first sum rule:

$$\int_0^\infty \frac{c_v(T)}{T} dT = \ln(2S+1). \tag{1}$$

Moreover, we incorporate the knowledge of the ground-state energy e_0 and the energy e_m at infinite temperature. These energies are either known exactly or can be computed numerically. We use this information in a second sum rule:

$$\int_0^\infty c_v(T) dT = e(T=\infty) - e(T=0). \tag{2}$$

Finally, the low-temperature leading contribution of $c_v(T)$ is taken into account.

We claim that the implementation of these integral constraints increases in a significant way the range of validity of the HT series.[15] We will show that this method is indeed successful even at low or zero temperature for the models we have investigated. By ''successful,'' we mean that the specific heat is obtained *down to zero temperature* with a relative accuracy typically between 1 and 0.1 % with only ten terms in the high-temperature series. This accuracy should be considered as surprisingly high for low-temperature quantities obtained with a high-temperature series expansion.

II. INTERPOLATION PROCEDURE

A. Elementary thermodynamics: From $c_v(T)$ to $s(e)$

In the canonical ensemble, the energy per site e and the *entropy per site* s are increasing functions of temperature $T = 1/\beta$. Since e is a monotonic function of T, we can express s as a function of e rather than of temperature. The specific heat as a function of temperature is easily expressed with $s(e)$ in the following way. The entropy $s(T)$ obeys:

$$\frac{ds}{dT} = \frac{c_v}{T}, \tag{3}$$

where c_v is the specific heat per site. It follows that :

$$s'(e) = \frac{ds}{de} = \frac{c_v}{T}\frac{dT}{de}, \tag{4}$$

where the prime denotes differentiation with respect to e. Since $dT/de = 1/c_v$, we have (the Boltzmann constant k_B is set to unity in the whole paper):

$$s'(e) = \frac{1}{T} = \beta. \tag{5}$$

We use this relation to eliminate the variable temperature in c_v :

$$c_v = \frac{de}{dT} = \left[\frac{dT}{de}\right]^{-1} = \left[\frac{d}{de}\left(\frac{1}{s'}\right)\right]^{-1}. \tag{6}$$

We eventually find

$$c_v = -\frac{s'^2}{s''} \tag{7}$$

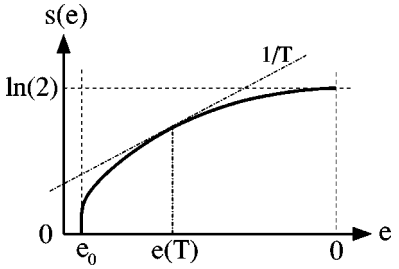

FIG. 1. Typical shape of the entropy s as a function of energy e for a spin-$\frac{1}{2}$ system.

Equations (5) and (7) are the basic relations that we shall use here. These relations can also be obtained by considering the density of states of a large but finite system.[16] For simplicity, we discuss the case of a quantum spin $\frac{1}{2}$ model on a lattice.[17] The simplest cases are the Heisenberg models:

$$H = 2J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \tag{8}$$

where the sum runs over the first nearest neighbors. $s(e)$ is defined inside an interval going from the ground-state energy e_0 up to the high-temperature energy e_m. e_m is the free-spin average of the energy, which is obtained straightforwardly since, at infinite temperature one has $\langle \vec{S}_i \cdot \vec{S}_j \rangle = 0$. For the Hamiltonian (8), one simply gets $e_m = 0$. If the ground state $|0\rangle$ is ferromagnetic [$J<0$ in Eq. (8)], one has $\langle 0|\vec{S}_i \cdot \vec{S}_j|0\rangle = \frac{1}{4}$ and $e_0 = Jz/4$ for a Bravais lattice of coordination number z. However, for antiferromagnetic models, e_0 is not known exactly but Monte-Carlo simulations, exact diagonalizations, or analytical calculation (spin-wave, mean-field Schwinger bosons, etc.) can be used. In summary the function $s(e)$, defined in the interval $[e_0,0]$ ($e_0<0$), is an increasing function of e, starting at 0 in e_0 with an infinite slope, and finishing at ln(2) in $e=0$ (see Fig. 1).

To find an approximation of $s(e)$, we combine three types of exact informations on $s(e)$:

(a)The entropy per spin is ln(2) at infinite temperature

$$s(e_m = 0) = \ln(2) \tag{9}$$

and vanishes at zero temperature:[18]

$$s(e_0) = 0 \tag{10}$$

(b) The behavior of $c_v(T \to \infty)$ is known from HT series. From the expansion of $c_v(T)$ in powers of $1/T$ up to order $1/T^n$, we get the expansion of $s(e)$ in the vicinity of $e \to e_m = 0$ in powers of e to order e^n:

$$s(e)_{e\to 0} = \ln(2) + \sum_{i=2}^{n} a_i e^i. \tag{11}$$

This expansion can be computed by solving Eqs. (5) and (7) order by order for $s(e)$ (details in Appendix A).

(c) When the low-energy physics of the model is understood, the low-temperature limit of the specific heat can often be predicted. In the case where the system exhibits some ferro- or antiferromagnetic long-range order at zero tempera-

ture, the low-lying excitations are spin waves. These gapless modes give a low-temperature heat capacity which is a power law. When the space dimension is D, a ferromagnet has $c_v(T) \sim T^{D/2}$ and an antiferromagnet has $c_v(T) \sim T^D$. In both a cases, we can write:

$$c_v(T)_{T\to 0} \sim T^{p/q}, \tag{12}$$

where p and q are integers. This low-temperature behavior translates into a behavior of $s(e)$ about the ground-state energy per site e_0.

$$s(e)_{e\to e_0} \sim (e-e_0)^{p/(p+q)}. \tag{13}$$

On the other hand, if elementary excitations are gapped the system has a thermally activated specific heat

$$c_v(T)_{T\to 0} \sim \exp(-\Delta/T) \tag{14}$$

and Eq. (13) is replaced by a logarithmic behavior about the ground-state energy (see Appendix C).

B. Interpolation by Padé approximants

We now define the interpolation procedure between low and high energy for $s(e)$. We look for an approximation of $s(e)$ which satisfies Eqs. (9), (10), (11), and (13). A two-point Padé interpolation is not directly possible since $s(e)$ is singular in $e=e_0$. We have to transform s to obtain regular behavior in the *whole* interval $[e_0,0]$. This is possible when p and q are two integers (but other low-temperature form will be used for thermally activated c_v in gapped systems, see Sec. IV). We define a function $G(e)$ as

$$G(e) = s(e)^{p+q}. \tag{15}$$

This function now behaves as $(e-e_0)^p$ when $e\to e_0$ and as $\ln(2)^{p+q} + \mathcal{O}(e^2)$ when $e\to 0$. It is now possible to look for approximations G^{app} of G which are of Padé form (details in Appendix B). This interpolation scheme fails if any of the functions $G(e)$, $s(e)$, $s'(e)$, or $-s''(e)$ becomes negative in the interval $[e_0,0]$. This provides a natural criterion to select the degrees $[u,d]$ for which Padé approximants give physical solutions. The curve for the specific heat $c_v(T)$ is eventually obtained in a parametric form $\{T(e),c_v(e)\}_{e\in[e_0,0]}$ thanks to Eqs. (5), (7), and (15).

III. LOW-TEMPERATURE POWER-LAW BEHAVIOR OF $C_v(T\to 0)$

We start by illustrating the method for systems where the specific heat is proportional to T^α at low temperature. Some cases where the specific heat is thermally activated will be described in the next section. Data files with the numerical results presented here (as well as colored versions of the figures) are available upon request.

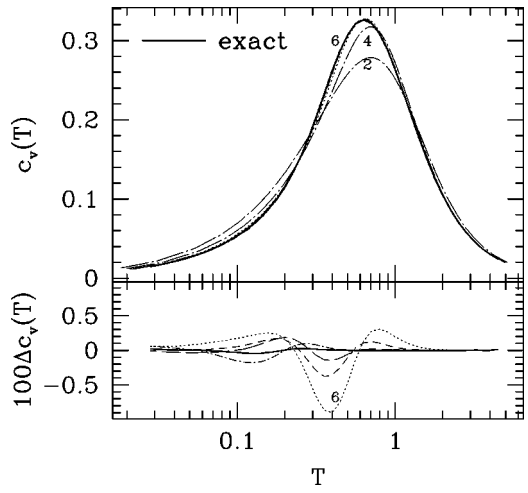

FIG. 2. One-dimensional $S=\frac{1}{2}$ XY model. *Top*: Exact specific heat (full line), approximations at orders $n=2$ and $n=4$ (dash-dot lines), $n=6$ (dotted line). *Bottom*: Differences with the exact result (notice the magnified scale). $n=6$ (Dotted line), $n=8$ (dash line), $n=10$ (long dash), $n=22$ (dash-dot), and $n=30$ (full line). Shown are diagonal Padé approximants: $[n/2,n/2]$.

A. One-dimensional $S=\frac{1}{2}$ XY model

As a first application, we consider the spin-$\frac{1}{2}$ XY chain:

$$H = 2\sum_i (S_i^x \cdot S_{i+1}^x + S_i^y \cdot S_{i+1}^y). \tag{16}$$

This spin problem can be solved exactly (the Jordan-Wigner transformation maps the XY model to free spinless fermions) and provides a check for a gapless spectrum. The energy per site at $T=0$ (respectively, at $T\to\infty$) is $e_0 = -2/\pi$ (respectively, $e_m=0$). The heat capacity is given by:[19]

$$c_v(\beta) = \frac{2\beta^2}{\pi}\int_0^{\pi/2} \frac{\cos^2(k)}{\cosh^2[\beta\cos(k)]}\,dk. \tag{17}$$

From this formula, the high- and low-temperature expansions can be computed. We find: $c_v(\beta\to 0) = \frac{1}{2}\beta^2 - \frac{3}{8}\beta^4 + \cdots$ and $c_v(T\to 0) = (\pi/6)\,T + \mathcal{O}(T^3)$. The linear law at low temperature gives $p=q=1$ in Eq. (15). Figure 2 shows the comparison between the exact $c_v(T)$ and the ones obtained from the Padé approximants. At each order n, a few approximants $[u,n-u]$ lead to the same variations. In Fig. 2, only diagonal Padé approximants $[n/2,n/2]$ are shown. A convergence of the specific heat is obtained with a relative accuracy of the order of one percent *down to zero temperature* with only six terms in the HT expansion. We want to emphasize that the slope $(dc_v/dT)(T=0)$ is not imposed in our procedure. Therefore, the method provides quantitative information on this low-energy parameter which characterizes the low-energy excitations. The value of the prefactor is exactly known for this XY model and we find that it oscillates around the exact value (i.e., $\pi/6$). It is a few percent below the exact value at the order $n=6$.

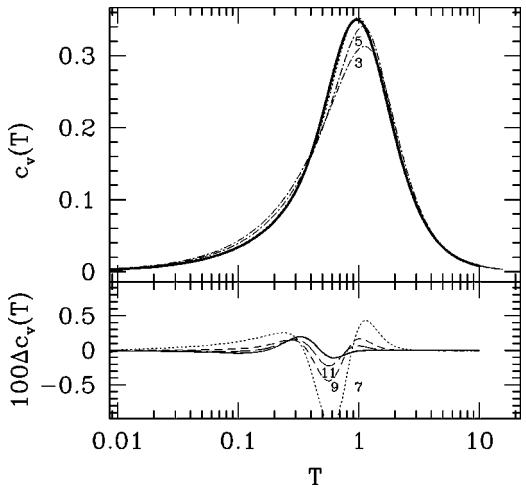

FIG. 3. Specific heat of the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain. *Top*: Result from Klümper *et al.* (Ref. 26) (full line), approximations at orders $n=3$ and $n=5$ (dash-dotted lines), and $n=7$ (dots). *Bottom*: Difference between Ref. 26 and present approach. $n=7$ (dot line), $n=9$ (dash line), $n=11$ (long dash), odd n from $n=13$ to $n=23$, and $n=24$ (full lines).

B. One-dimensional antiferromagnetic Heisenberg spin-$\frac{1}{2}$ model

$$H=2\sum_i \vec{S}_i\cdot\vec{S}_{i+1} \tag{18}$$

This model is solvable with the Bethe ansatz.[20] The ground-state energy is exactly known[21] to be $e_0=-2\ln(2)+\frac{1}{2}$. The low-temperature limit of the heat-capacity is[22] $c_v(T)=T/3+\mathcal{O}(T^2)$. The HT expansion computed by Baker *et al.*[23] was recently extended to order β^{24} by Bühler *et al.*[24] The heat capacity curve has been computed for anisotropic versions of the spin-$\frac{1}{2}$ chain,[25] but we are not aware of any exact computation of c_v for the isotropic Heisenberg model based on the *exact* Bethe ansatz equations (due to the existence of an infinite number of coupled equations at the isotropic point). However, an approximate solution was proposed recently by Klümper.[26] The accuracy of specific heat obtained by his method is claimed to be extremely high ($\sim 10^{-7}$).

Our results for this model are displayed Fig. 3. A good convergence is obtained down to zero temperature. If we truncate the HT expansion at order seven, an absolute precision of one percent can already be obtained. At the highest order, the specific heat is in excellent agreement with the result of Ref. 26. The height of the peak, for instance, agrees with an accuracy of 10^{-4}. The low temperature limit is also in good agreement with the exact result: we find $c_v(T)\simeq 0.329\ T$ at order 24 [instead of $c_v(T)=\frac{1}{3}T$]. The difference with result of Ref. 26 at intermediate temperatures (see bottom of Fig. 3) is due to the fact the low-temperature coefficient is off by 1% from the exact value $\frac{1}{3}$. This result is obtained without any extrapolation when $n\to\infty$. Taking into account finite-order corrections could improve further the accuracy. The position of the peak as well as the low temperature limit are summarized in Table I.

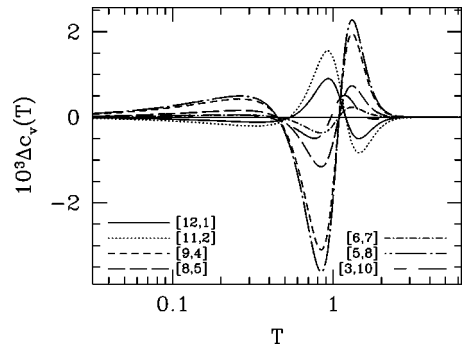

FIG. 4. Ferromagnetic spin-1/2 Heisenberg model on the triangular lattice. Comparison of the specific heats obtained from different Padé approximants at order $n=13$. The Padé approximant of reference has degrees [7,6]. Approximants [6,7], [8,5], [12,1], and [3,10] differ from the reference by less than 10^{-3}.

C. Triangular lattice Heisenberg models

First, we look at the convergence of this method on the ferromagnetic case where the ground-state energy is known exactly. Figure 4 shows the comparison of the various Padé interpolants $[u,d]$, with $n=u+d=13$ (highest available order[27]). Two of them have a singularity ([10,3] and [4,9]). If we exclude the polynomial form ($d=0$) and the cases $d>10$, all interpolations lead to the same variations of $c_v(T)$ in the whole range of temperature. Figure 4 also illustrates the very small dispersion of the different Padé approximants obtained with this method. It is also remarkable that the coefficient of the dominant term at low temperature depends weakly on the interpolation function used. As before, only the power of T is imposed, but the prefactor is not. We get $c_v(T)\sim 0.142(2)T$ at low temperature. Notice that this quantity is not given correctly by a linear spin-wave approximation (noninteracting magnons). We are not aware of any previous result for this quantity. A high-density monolayer of solid ^{3}He solid is, to our knowledge, the only experimental realization of a triangular-lattice spin-$\frac{1}{2}$ ferromagnet. The heat capacity has been measured by Ishida *et al.*[28] and their results are in very good agreement with our calculations.

In Figs. 5(a) and 5(b), we see now how the result converges when more terms are added in the HT expansion. For each HT expansion order n (as indicated in the figure), all possible fractions $[u,d]$ ($u+d=n$) are tried. Except for the lowest order, at each order several approximants fall on the ''same'' curve. A reasonable convergence is obtained even for $n=5$.

Figure 5(b) shows the approximated $c_v(T)$ with increasing HT order n for the antiferromagnet Hamiltonian. This model is frustrated, but it is now well established[29,30] that the ground-state is a three-sublattice Néel state. The low-temperature specific heat is thus proportional to T^2. The ground-state energy was estimated from exact diagonalization data.[29] Again here, we see a convergence for $n>5$. This should be compared with direct Padé approximants to the specific heat, which was done in Ref. 27 [dotted curve in Fig. 5(b)]. The comparison with our results shows indeed that the direct approach does not even allow to get correctly the maximum of $c_v(T)$. Our method converges with a relative

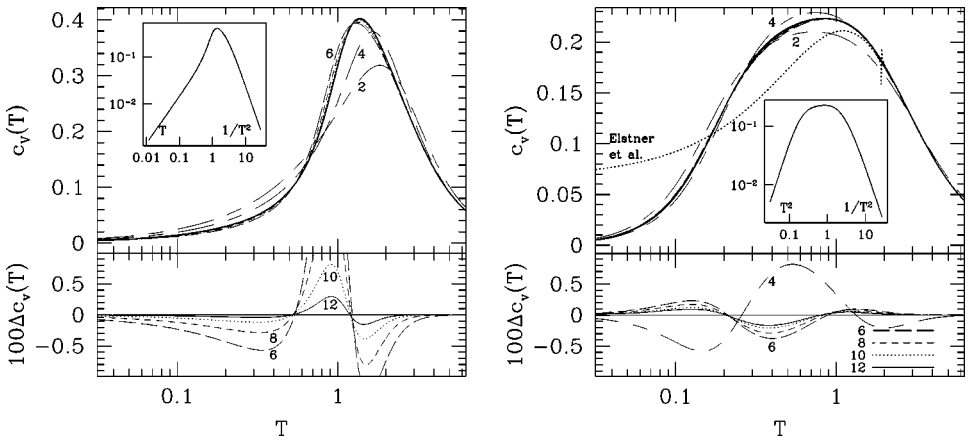

FIG. 5. Spin-1/2 Heisenberg model on the triangular lattice. (a) - *Top*: Variations of $c_v(T)$ with respect to the number of terms in the HT expansion in the ferromagnetic case. The even n from 2 to 8 and $n=13$ are shown. Inset: data for $n=13$ in a log-log plot. *Bottom*: Difference with the highest order ($n=13$). Even n from 6 to 12 are shown. Order 12 and 13 differ by less than 3.10^{-3}. (b): Same as (a) for the antiferromagnetic case. Order 12 and 13 differ by less than 2.10^{-3}. The dotted line (with the spike) is from Elstner *el al.*[27]

accuracy of about 1% down to zero temperature and we get $c_v(T)\sim 5.3(2)T^2$. It would be interesting to compare this result with spin-wave calculations taking magnon-magon interactions into account.

D. Square lattice Heisenberg model

We evaluated the specific heat for the $S=\frac{1}{2}$ Heisenberg model on the square lattice. Figure 6 shows the convergence of the specific heat with respect to the number of terms in the HT expansion. The convergence with the HT expansion order is faster in the antiferromagnetic case than in the ferromagnetic one. At low temperature we obtain $c_v(T)=0.25(0.01)T$ [respectively, $c_v(T)=0.25(0.01)T^2$] for the ferromagnetic (respectively antiferromagnetic) case. The result in the antiferromagnetic case can be compared with the modified spin-wave theory of Takahashi[31] which is $c_v(T)=0.214T^2$ in our units.

IV. SYSTEMS WITH THERMALLY ACTIVATED HEAT CAPACITY

A. One-dimensional Ising model

$$H=2\sum_i S_i^z\cdot S_{i+1}^z \tag{19}$$

This model is the simplest one with a gapped spectrum. It allows to check the convergence of our method to the exact result in the case of a low-temperature activated heat capacity. The energy per site at $T=0$ is $e_0=-1$ and $e_m=0$ at $T=\infty$. The specific heat per spin is given by $c_v(\beta=1/T)=[\beta/\cosh(\beta)]^2$. The HT expansion starts as $c_v(\beta=1/T)\sim\beta^2-\beta^4+\ldots$, while the spectrum has a gap $\Delta=2$. The heat capacity is thermally activated at low temperature:

$$c_v(\beta\to\infty)\sim\beta^2\exp(-\Delta\beta). \tag{20}$$

For such behavior, the entropy behaves as

$$s(e)\sim-(e-e_0)\log(e-e_0)/\Delta, \tag{21}$$

when $e\to e_0$. We need a transformation which converts this logarithmic singularity into a regular behavior. We choose the transformation

$$G(e)=(e-e_0)\frac{d}{de}\left[\frac{s(e)}{e-e_0}\right] \tag{22}$$

and we approximate G by a Padé approximant (see appendix C for details). The convergence is shown in Fig. 7. The gap also converges rapidly to the exact value 2. The best Padé approximants are those of the form $[d,d]$ with $d\sim n/2$.

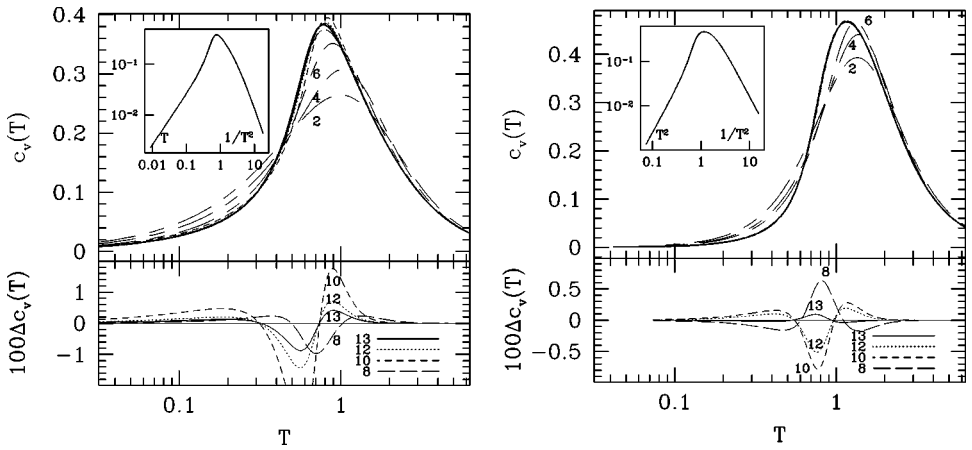

FIG. 6. spin-$\frac{1}{2}$ Heisenberg model on the square lattice. Same as Fig. 5 for the (a) square lattice ferromagnet and (b) square lattice antiferromagnet. Even n from 2 to 14 and $n=13$ are shown. Orders $n=13$ and 14 differ by less than 4.10^{-3} in the ferromagnetic case and by less than 10^{-3} in the antiferromagnetic case.

TABLE I. Parameters of the different models. Column two indicates whether the couplings are ferromagnetic (F) or antiferromagnetic (AF). e_0 is the ground-state energy per spin, e_m is the mean energy at infinite temperature (here $e_m=0$). n is the highest known order of the HT expansion of the specific heat. The three last columns are parameters extracted from our analysis: low-temperature limit and position of the peak. These result are obtained from the highest order available. The error bars reflects the dispersion of the different Padé approximants at the highest order. Figures with a star (*) are those for which the exact value is known (see text).

Heisenberg model		e_0-e_m	n	$c_v(T\to 0)$	$T^{\max}$	$c_v^{\max}$
$S=\frac{1}{2}$ chain	AF	$-2\ln 2+1/2$[a]	24[b]	0.329^*T	0.9618(2)	0.3497
$S=1$ chain	AF	-1.401[c]	20[d]	$\exp(-0.40^*/T)$	0.861(1)	0.543(1)
Triangular lat.	F	$-3/2$	13[e]	$0.142(2)T$	1.375(5)	0.403(3)
Triangular lat.	AF	-1.11[f]	13[e]	$5.3(2)T^2$	0.84(1)	0.2231(5)
Square lat.	F	-1	14[g]	$0.25(0.01)T$	0.785(4)	0.383(3)
Square lat.	AF	-1.34[h,i]	14[g]	$0.25(0.01)T^2$	1.163(2)	0.467(2)

[a]Reference 21.
[b]Reference 24.
[c]Reference 33.
[d]Reference 34.
[e]Reference 27.
[f]Reference 29.
[g]Reference 37.
[h]Reference 38.
[i]Reference 39.

B. One-dimensional $S=1$ Heisenberg model

$$H=\sum_i \vec{S}_i\cdot\vec{S}_{i+1} \tag{23}$$

It is known that this system exhibits a spin gap (Haldane phase) and the heat capacity is thermally activated. More precisely, a nonlinear sigma model approach[32] gives:

$$c_v(T)=\frac{\Delta}{\sqrt{2\pi}}\left(\frac{\Delta}{T}\right)^{3/2}\exp(-\Delta/T). \tag{24}$$

More generally, if elementary excitations are weakly interacting massive bosons, one expects $c_v(T)\sim\exp(-\Delta/T)T^{D/2-2}$ in space dimension D.

The value of the ground-state energy and spin gap is known very accurately (from the density-matrix renormalization-group calculations done by White and Huse[33]) to be $e_0=-1.401484038971(4)$ and $\Delta=0.41050(2)$. We use the HT series data obtained up to order 20 by Elstner, Jolicœur, and Golinelli.[34] We apply the same transformation as with the one-dimensional Ising model. The result is shown in Fig. 8. Notice that Eq. (21) implies $c_v(T)\sim\exp(-\Delta/T)/T^2$ instead of $\sim\exp(-\Delta/T)/T^{3/2}$ as it should be from Eq. (24). The consequence of this little inconsistency is that, at fixed order in the HT series, we overestimate the value of the gap Δ. Note that the correct low-T behavior would only give a logarithmic correction to $s(e)$ [Eq. (21)]. This can be rectified, in principle, by a more sophisticated transformation of $s(e)$. Nevertheless, we obtain

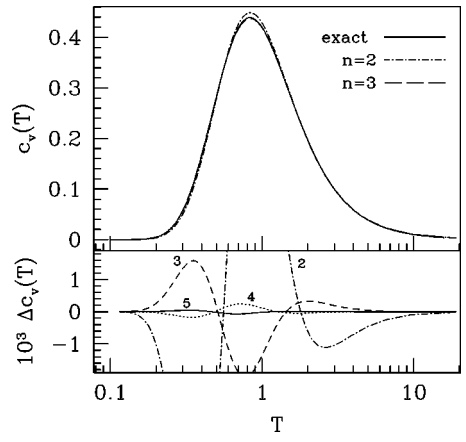

FIG. 7. One-dimensional Ising model. *Top*: comparison between the exact specific heat (full line) and those obtained from second (dot-dashed line) and third (dashed line) orders. *Bottom*: difference between exact result and the approximations at orders $n=2$, 3, 4, and 5.

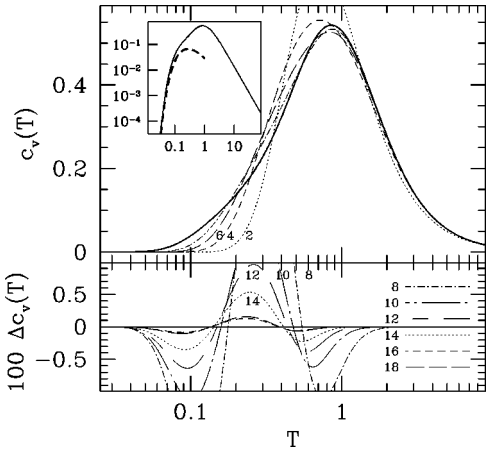

FIG. 8. Specific heat of the antiferromagnetic Heisenberg spin-1 chain. *Top*: HT orders are $n=2$, 4, 6, 8, and 20 (full line). *Inset*: Log-log plot of $n=20$ and theoretical prediction of Eq. (24) (dashed). *Bottom*: Difference between $n=20$ and even n from 8 to 18. $n=16,18$ differ from $n=20$ by less than 2×10^{-3}.

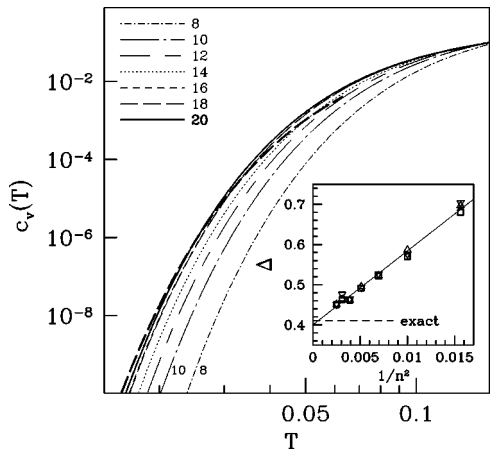

FIG. 9. Convergence of $c_v(T)$ at low temperature for the antiferromagnetic Heisenberg spin-1 chain. Even orders from 8 to 20 are shown. Full bold line is $n=20$, the dashed bold line is from Ref. 32 (Eq. 24). Notice that $n=16$ and 18 are almost identical at the scale of the figure. *Inset*: Spin gap for orders $n=8,10,12,14,16,18,20$. The horizontal dashed line is the exact value (0.41) and the full line is a least-square fit to the data. It extrapolates to $\Delta=.40$. Upward triangles are for approximants with degrees $[n/2+1,n/2-1]$, square for $[n/2,n/2]$ and downward triangles for degrees $[n/2-1,n/2+1]$.

a gap which varies roughly as $1/n^2$ (n is the order of the HT expansion) and the extrapolation shown Fig. 9 gives 0.40. So, very surprisingly, this HT approach is able to provide some quantitative and nontrivial information about the low-energy physics.

V. CONCLUSIONS

We have presented a new and simple method to analyze HT series expansion for the specific heat of spin systems. It requires only : the ground-state energy and the qualitative behavior of $c_v(T)$ at low temperature. These two pieces of information allow us to constrain the specific heat with two sum rules which improve drastically the convergence of the HT expansion. This technique is particularly appropriate to analyze specific heat measurements in a large temperature range. Since in many cases it is able to predict the position and the height of the maximum of $c_v(T)$, this method can simplify and improve the determination of exchange parameter(s) and of the number of spins in the sample. Remarkably, the method converges down to zero temperature with only ten terms of the HT series in most of the cases we have investigated. This method can even provide some quantitative information on the low-energy physics [see, e.g., the value of the spin gap of the Haldane chain, or the zero-temperature entropy of the Kagome antiferromagnet (Ref. 35)].

It would be interesting to apply this technique to more sophisticated models such as the $t-J$ or Hubbard models. It also seems worthwhile to investigate other interpolation methods than the simple Padé approximants presented here. The application of this HT analysis to systems with finite-temperature phase transitions is another promising direction we are currently investigating.

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APPENDIX A: SERIES FOR $s(e\to 0)$

We describe how the series for $s(e\to 0)$ is obtained from the series for $c_v(T\to\infty)$. Assume the expansion of the specific heat is known up to order n:

$$c_v(T)_{T\to\infty}=\sum_{i=2}^{n}\frac{a_i}{T^i}+\mathcal{O}\left(\frac{1}{T^{n+1}}\right). \tag{A1}$$

Equations (5) and (7) imply

$$s''(e)c_v[T=1/s'(e)]=-[s'(e)]^2$$

$$s''(e)\left[\sum_{i=2}^{n}a_i s'(e)^i\right]=-[s'(e)]^2. \tag{A2}$$

Expanding Eq. (A2) in powers of e gives the series for $s(e\to 0)$. For instance, if we have

$$c_v(T)_{T\to\infty}=\frac{a_2}{T^2}+\frac{a_3}{T^3}+\frac{a_4}{T^4}+\mathcal{O}\left(\frac{1}{T^5}\right) \tag{A3}$$

we obtain

$$s(e)_{e\to 0}=\ln(2)-\frac{1}{2a_2}e^2-\frac{a_3}{6a_2^3}e^3$$

$$+\frac{2a_4a_2-3a_3^2}{24a_2^5}e^4+\mathcal{O}(e^5). \tag{A4}$$

In fact, solving Eq. (A2) can be done very simply with a software like MAPLE:

$$n:=4;\quad \text{Order}:=n+1:$$

$$\text{cv}:=\mathbf{add}(a[i]/T^{**}i,\quad i=2..n);$$

$$\text{eq}:=-\mathbf{D}(s)(e)^{**}2/\mathbf{D}(\mathbf{D}(s))(e)=\mathbf{subs}(T=1/\mathbf{D}(s)(e),cv);$$

$$\mathbf{dsolve}(\{\text{eq},s(0)=\ln(2),\quad \mathbf{D}(s)(0)=0\},$$

$$s(e),'\mathbf{type}=\mathbf{series}');$$

APPENDIX B: PADÉ APPROXIMANT FOR $G(e)$

When the system has a specific heat with a power law $T^{p/q}$ at low temperature the function $G(e)=s(e)^{p+q}$ is regular at the ground-state energy $e=e_0$ as well as at high temperature $e=0$. We can therefore approximate G by

$$G^{\rm app}(e)=\ln(2)^{p+q}\left(1-\frac{e}{e_0}\right)^p {\rm Pade}_{[u,d]}(e), \qquad \text{(B1)}$$

where ${\rm Pade}_{[u,d]}(e)=N(e)/D(e)$, N (respectively, D) is a polynomial of degree u (respectively, d) and $N(0)=D(0)=1$. By construction, Eq. (B1) guarantees that $G^{\rm app}$ has the correct behavior at low temperature $G^{\rm app}\sim(e-e_0)^p$. One has to evaluate the Padé approximant so that the HT expansion of $G(e)$ [and thus of $s(e)$ and $c_v(T)$] is exact up to order $n=u+d$. As usual, this is done by expanding both sides of Eq. (B1) in powers of e and solving a linear system to determine the unknown coefficients of the two polynomials N and D. As an example, we give here the general expression for the three possible approximants at order $n=2$:

$${\rm Pade}_{[2,0]}(e)=1+p\frac{e}{e_0}+\frac{1}{2}[p(p+1)-x]\left(\frac{e}{e_0}\right)^2 \qquad \text{(B2)}$$

$${\rm Pade}_{[1,1]}(e)=\frac{1+\frac{1}{2}\left[p-1+\frac{x}{p}\right]\frac{e}{e_0}}{1+\frac{1}{2}\left[-p-1+\frac{x}{p}\right]\frac{e}{e_0}} \qquad \text{(B3)}$$

$${\rm Pade}_{[0,2]}(e)^{-1}=1-p\frac{e}{e_0}+\frac{1}{2}[p(p-1)+x]\left(\frac{e}{e_0}\right)^2, \qquad \text{(B4)}$$

where

$$x=\frac{e_0^2}{a_2}\frac{p+q}{\ln(2)}. \qquad \text{(B5)}$$

APPENDIX C: $G(e)$ FOR GAPPED SYSTEMS

With gapped systems, the specific heat has the form: $c_v(T)=\exp(\Delta/T)T^{\alpha-2}$. We obtain the low-energy limit:

$$s(e)\simeq-\frac{e-e_0}{\Delta}\left\{\ln[(e-e_0)\Delta]+\alpha\ln\left[\frac{-\ln(e-e_0)}{\Delta}\right]\right\}. \qquad \text{(C1)}$$

For $\alpha=0$, we recover Eq. (21) and the transformation of Eq. (22) holds. When $\alpha\neq0$, in order to remove the logarithmic singularities, one has to differentiate several times. But such transformations provide singular behavior for $s(e)$, mainly because of the change of sign in the arguments of the log between $e=e_0$ and $e=e_m=0$. More work has to be done in these cases.

Unlike the case of a power-low behavior at low temperature, cases with a gap require an integration in order to go back from $G(e)$ defined Eq. (22) to the entropy and the specific heat. Since we look for approximations of $G(e)$ in a Padé form, this integration can be performed analytically. The value of the gap Δ can be obtained directly from G, without integration, since $G(e=e_0)=1/\Delta$.

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