Specific heat of the $S=\frac{1}{2}$ Heisenberg model on the kagome lattice: high-temperature series analysis

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We compute specific heat of the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg model on the kagome lattice. We use a recently introduced technique to analyze high-temperature series expansion 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. In the case of kagome-lattice antiferromagnet, this method predicts a low-temperature peak at $T/J \lesssim 0.1$.

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I. INTRODUCTION

We consider the nearest-neighbor Heisenberg model on the kagome lattice:

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

Because of its unconventional properties, the spin-$\frac{1}{2}$ kagome antiferromagnet (KAF) has been subject to an intense activity these last years. All studies agree that this frustrated two-dimensional magnet has no long-ranged magnetic order at zero temperature. Precise high-temperature calculation methods like Padé approximants agree reasonably well down to zero temperature, which is not the case if one does a direct Padé analysis of the series. For the present kagome model we show that this method provides rich semi-quantitative informations on the specific heat curve, although a full convergence down to zero temperature cannot be achieved.

II. DIRECT HIGH-TEMPERATURE EXPANSION OF THE SPECIFIC HEAT

In this paper, we revisit the question of the specific heat with the help of a new method to analyze high-temperature series data. Compared to the usual Padé approximant approach, this method takes advantage of additional information on the system: the two sum rules on the energy and on the entropy are exactly satisfied.

We reproduce here the first attempt by Elstner and Young to compute the specific heat from its high-temperature expansion alone. We use Padé approximants to extrapolate the series. We impose the specific heat to vanish at low temperature as $T$, $T^2$ or $T^3$. At orders 9 to 17, only 6 such approximants do not develop poles or zeros in the interval $T \in [0, \infty]$ (Fig. 1). One should notice at this point that the remaining Padé approximants agree reasonably well down to zero temperature. This is usually not the case in 2D antiferromagnets where even the position of the peak ($T \approx 1$) can hardly be obtained by the use of direct Padé approximants to the series for the specific heat. From this point of view, the HT series expansion of the kagome model seems to have a faster convergence than models such as the triangular-lattice antiferromagnet.

By integration of these approximants, we evaluate the ground-state energy $e_0 = \int_0^\infty c_v(T) dT$ and the ground-state entropy $s_0 = \log(2) - \int_0^\infty c_v(T) dT$. These values are indicated in Fig. 1. The ground-state energy is about
series are plotted in Fig. 2. Using Eq. 2, the entropy can be obtained from the ground-state energy

\[ T = \exp(e_{0}) \]

\[ -0.845 \text{, only slightly higher (0.02)} \text{ than estimations obtained from exact diagonalizations. The entropy deficit is very large: 0.3 (40\% of log(2)). Elstner and Young argued that a low-temperature peak should be present in the specific heat in order to compensate the deficit of 40\% of log(2). However this low-temperature peak should “contain” almost no energy (2\%), which means that such peak would have to occur at very low temperatures. In order to estimate this temperature, one can add a $\delta$-function peak to the curves of Fig. 1 in order to recover the correct energy and entropy variations. This constrains both the location (temperature $T_1$) and the weight of the $\delta$-peak. By averaging over the different curves of Fig. 1 one finds $T_1 \simeq 0.05$ (resp. $T_1 \simeq 0.08$) for a ground-state energy $e_0 = -0.865$ (resp. $e_0 = -0.875$). These estimates are in agreement with the conclusions of the more elaborate treatment described below.

III. ENTROPY METHOD

In this section we briefly summarize the method we use to compute the specific heat. More details can be found in Ref. 17. The specific heat $c_v$ and the temperature $T$ can be obtained from the entropy $s$ as a function of the energy $e$ using basic thermodynamic relations:

\[ T(e) = 1/s'(e) \]

\[ c_v(e) = -s'(e)^2/s''(e) \]

From Eq. 2 one can convert\cite{3} a high-temperature series for $c_v(T \to \infty)$ into a series for $s(e \to 0)$ ($e = 0$ at $T = \infty$ for the Hamiltonian of Eq. 1). The truncated series are plotted in Fig. 2. Using Eq. 3, the entropy can be plotted as a function of temperature (right of Fig. 2). A good convergence is observed down to relatively low energies ($e \sim -0.75$) but the corresponding entropy remains very large (more than 60\% of ln(2)), although the ground-state energy is not much lower (the ground-state energy lies between the dashed vertical lines in Fig. 2). These result are consistent with a direct analysis of the series for $c_v(T)$ (Fig. 1). In addition, it appears that the “true” $s(e)$ must be bent downward below the curves of the truncated series (shown in Fig. 2) between $e_0$ and $\sim -0.75$ in order to reach $s = 0$ at $e = e_0$. Due to Eq. 3, this almost certainly implies a low-energy (and therefore low-temperature) peak in $c_v(T)$. This paper makes this idea more precise by computing the specific heat obtained by forcing the entropy to vanish at $e = e_0$.

The advantage of working on $s(e)$ rather than $c_v(T)$ is that a two-point Padé interpolation can be used to set the ground-state energy and the total entropy of the system. However, $s(e)$ is singular at $e = e_0$ (since $T = 1/s'(e) \to 0$ when $e \to e_0$). For this reason one cannot directly approximate $s(e)$ by a rational fraction (Padé approximant). If we assume that the specific-heat behaves as

\[ c_v \simeq (T/c_0)^\alpha \]

at low temperature ($c_0$ has the dimension of an energy) and $s(e_0) = 0$, $s(e)$ behaves as:

\[ s(e \to e_0) \simeq (\alpha + 1)^{\alpha+1} \left( e - e_0 \right)^{\alpha+1} \]

The quantity

\[ G(e) = s(e)^{1+1/\alpha} \]

\[ e - e_0 \]
is then non-singular at \( e = e_0 \) and can be approximated by a Padé form.\(^8\) The series for \( s(e \to 0) \) must therefore be transformed into a series for \( G(e \to 0) \) before Padé approximants can then be computed in the usual way. In what follows all the Padé approximants will be approximations to this function \( G(e) \). If no finite-temperature phase transition is expected, all approximants where \( G(e) \) has a pole or a zero, or where \( s'(e) \) or \( s''(e) \) vanishes somewhere in the interval \( |e_0, 0| \) must be discarded. The remaining ones are called “physical” for brevity.

A. Low-temperature behavior of \( c_v(T) \)

Unlike some simpler magnets where the nature of the ground-state and elementary excitations is known,\(^3\) the qualitative behavior of the specific heat when \( T \to 0 \) is unknown, although a \( \sim T^2 \) scenario has been proposed.\(^5,6\) However, one of the striking facts about the model is the unusually high density of states immediately above the ground-state.\(^3\) From this it is natural to expect gapless elementary excitations. If we assume quasi-particles with a dispersion relation \( \epsilon_k \sim k^\gamma \) we get a specific heat \( c_v \sim T^\alpha \) with \( \alpha = D/\gamma \) in space dimension \( D \). The (many body) density of states is \( \rho(E_0 + W) \sim \exp\left[ N(W/N)^{\alpha/(\alpha + 1)} \right] \) where \( N \) is the system size (consequence of Eq. 4 with \( e - e_0 = W/N \)). For an energy \( W \) of order one above the ground-state, a density of states \( \rho \sim 1.15^N \) was observed in exact spectra up to \( N = 36 \) sites.\(^3\) If this indeed holds up to the thermodynamic limit, it would imply \( \alpha = 0 \) (\( \gamma = \infty \)) and an extensive entropy at zero temperature. This is unlikely in the present model\(^3\) but this result points to a rather flat dispersion relation of the excitations, probably with \( \gamma > 1 \). In the following we will consider the two cases \( \gamma = 1 \) (\( \alpha = 2 \)) and \( \gamma = 2 \) (\( \alpha = 1 \)).\(^3\)

B. Ground-state energy and convergence of the different Padé approximants

In principle, the method above requires the knowledge of the ground-state energy \( e_0 \). If the value of \( e_0 \) is exact we expect the procedure to converge to the exact \( e_0 \) if the number of known terms in the HT series increases to infinity. This is in agreement with our experience on solvable models (such as the spin-\( \frac{1}{2} \) XY chain for instance)\(^9\) where the full series as well as \( e_0 \) are known exactly. Inversely, wrong values of \( e_0 \) cannot lead to any convergence as the limiting \( c_v \) would have to satisfy the HT series at all orders but would have a different energy sum rule. As a consequence, when \( e_0 \) differs from the true ground-state energy, the physical approximants gets fewer (and/or more scattered) when the order of expansion gets larger. Of course, the smaller the error on \( e_0 \) the longer series is needed to observe this departure from convergence. From this we assume that the existence of a larger number of physical approximant is an indication that \( e_0 \) (and \( \alpha \)) is closer to the exact value. However, because a limited number of terms of the series are known, this only provides a qualitative information and does not allow determine the energy completely.

From exact diagonalizations on systems with up to 36 sites, \( e_0 \) was evaluated by Waldtmann et al.\(^6\) to be \( e_0 = -0.865 \pm 0.015 \) (see also Refs.\(^7,8\)). Variational calculations as well as rigorous bounds on \( e_0 \) will be discussed in a separate paper.\(^9\)

The specific heat curve can be rather sensitive to the choice of \( e_0 \). Since \( e_0 \) is not exactly known, it is important to perform scans in order to see how the specific-heat curve depends on \( e_0 \). We observe that, for some choice of \( e_0 \) many Padé approximants at a given order give almost the same specific-heat curve whereas some other choice of \( e_0 \) leads to some significant scattering in the specific heat curves. This can conveniently be seen, for instance, by looking at the value of the different Padé approximants at \( e = e_0 \). Since \( G(e_0) \) and \( c_0 \) (defined by Eq. 4) are simply related by

\[
G(e_0) = \frac{\alpha + 1}{e_0 \alpha^{1 + 1/\alpha}}
\]

we plot \( c_0 \) (which has a direct physical meaning in term of \( c_v(T \to 0) \)) in Fig. 1 as a function of \( e_0 \) for all physical Padé approximants at order \( \beta^{16} \) and \( \beta^{17} \) (both for \( c_v(T) \sim T \) and \( \sim T^2 \) at low temperature). It turns out that \( c_0 \) is representative of the full specific-heat curve in the sense that if two Padé approximants give “close” values of \( c_0 \) (say a relative difference less than \( 10^{-3} \)), their corresponding specific-heat curves are similar (typical relative difference of \( 10^{-2} \) for all temperatures). This low-temperature coefficient \( c_0 \) is therefore a useful quantity to monitor how the \( c_v(T) \) result depends on the choice of the degree of the Padé approximant.\(^6\) In all cases the “optimal” energy region is around \( e_0 \approx -0.88 \pm 0.02 \).\(^6\) We also observe a gradual shift of the optimal region to higher energies as the order of the series is increased. We analyzed this effect and performed several extrapolations to the infinite-order limit (data not shown). It is not clear, however, that this indirect method to determine the ground-state energy is more accurate than the other available estimates.\(^6\)

C. Low temperature peak in \( c_v(T) \)

The curves corresponding to all physical approximants at order \( \beta^{17} \) for \( e_0 = -0.865, e_0 = -0.88 \) and \( e_0 = -0.89 \), and for \( c_v \sim T \) and \( c_v \sim T^2 \) are shown in Fig. 1. Although some uncertainties remain concerning the ground-state energy of the model as well as the low-temperature behavior of the specific heat, the results are relatively well converged down to \( T \approx 0.7 \) and the location of the high temperature peak is almost independent from the unknowns (\( e_0 \) and \( \alpha \)) and in agreement with previous studies.\(^6,7,9\) In addition, all the scenarios we
FIG. 3: (color online) Zero temperature limit of $c_0$ (see Eq. 4) for the different Padé approximants as a function of the ground-state energy. Top: a $c_v \sim (T/c_0)$ behavior is assumed at low temperature. Bottom: $c_v \sim (T/c_0)^2$. The degree $u$ of the numerator of each approximant is given. The degree of the denominator is $d = n - u$ where $n$ is the order of the series. Left: Order $n = 16$. Right: Order $n = 17$. The number of physical approximant ($N_{\text{Phys}}$) is plotted as a function of $e_0$ in each lower panel.

investigated give rise to a low-temperature peak (or a shoulder) in the specific heat at $T \simeq 0.02 \sim 0.1$.

We also looked at the order dependence of the specific heat curves. For a given value of the ground-state energy some approximants give similar curves for $c_v(T)$ while some other are “isolated”. The later ones can be recognized as isolated curves in Fig. 3. According to our experience with this method, those isolated approximants do not reflect the convergence to the true function. We obtained the results of Fig. 3 by keeping only the approximants which value of $c_0(T)$ is at less than $3 \times 10^{-3}$ from the $c_0$ of another approximant. This selection was repeated from orders $\beta^{13}$ to $\beta^{17}$ for the six combinations of ground-state energies and low-temperature behaviors used before. As one can see, the low-temperature structure appears to be a robust feature, although a convergence of the full curve is not reached for $T \lesssim 0.6$. Still, a better convergence as a function of the order of the series (and a larger number of physical Padé approximants) is obtained when the ground-state energy is low ($e_0 = -0.89$ or $e_0 = -0.88$). This suggests that the actual value of $e_0$ may be lower than $-0.865$, although $e_0 = -0.89$ is probably too low (compared to the available estimates).

For $N = 18$ spins, exact diagonalizations gave a low-temperature peak of the specific heat at $T \simeq 0.2$ and $c_v \simeq 0.17$. An hybrid method based on exact diagonalizations and high-temperature series expansion gave a peak at $T \simeq 0.2$ and $c_v \simeq 0.17$ for $N = 36$ (see also Ref. 6). Quantum Monte-Carlo simulations for $N = 72$ spins indicated that a peak may exist below $T \simeq 0.3$ for this system. Those results obtained for small systems are qualitatively consistent with those of Fig. 3 but our peak is located at a lower temperature by at least a factor of two. We think that this discrepancy is likely to be due to finite-size effects in previous studies.

FIG. 4: (color online) Specific heat computed at order $\beta^{17}$ with the ground-state energies $e_0 = -0.89$ (top), $e_0 = -0.88$ (center) and and $e_0 = -0.865$ (bottom). Left: $c_v \sim T$. Right: $c_v \sim T^2$. The different curves correspond to all the physical Padé approximants. The degree $u$ of the numerator is indicated (the denominator has degree $d = 17 - u$).
FIG. 5: (color online) Specific heat curves from order $\beta^{13}$ to $\beta^{17}$ with $e_0 = -0.89$ (top), $e_0 = -0.88$ (center) and $e_0 = -0.865$ (bottom). The degree of the numerator of each approximant is indicated and each column corresponds to a given order ($\beta^n$) of the series ($n = 13, 14, 15, 16$ and $17$ from left to right). Left panels: $c_v \sim T$. Right panels: $c_v \sim T^2$. In all cases the specific heat shows a maximum around $T \simeq 1.3$ (corresponding to $e(T) \simeq -0.7$, see Fig. 3) and a low-temperature peak (or shoulder).

IV. CONCLUSIONS

By means of a detailed high-temperature series analysis we provided quantitative estimates for the specific heat curve of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the kagome lattice. Those results show a low-temperature peak in the specific heat of the model for $T \lesssim 0.1$, although its precise location cannot be determined due to uncertainties on the ground-state energy. The corresponding degrees of freedom are also responsible for the large density of singlet states observed in exact diagonalization studies but their nature, as well as the nature of the ground state itself, remains to be explained.

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Bernhard et al. used a mean-field decoupling on correlation functions to compute the specific heat of this system. Their result are qualitatively similar and also shows a large entropy deficit (46% of log(2)).

Eq. 6 is slightly different from the original choice made in Ref. 17.

See Ref. 13 for a related model where this property is explicitly demonstrated. This, however, requires some fine tuning of the Hamiltonian and there is no reason to think that the kagome Heisenberg model may have such very special property. From finite-size spectra it can however be difficult to resolve the difference between a model with an extensive entropy at $T = 0$ and a system with vanishing entropy at $T = 0$ but a large low-temperature peak in the specific heat for $T \ll J$. We stress that the $T = 0$ entropy that follows from $\rho \sim 1.15^N$ is consistent with that of the low-temperature peak predicted by the present method: about 20%-25% of log(2).

The possibility of having a gapped spectrum with a (very) small gap cannot be excluded. This would be the case if the system realizes a $\mathbb{Z}_2$ spin-liquid, as predicted in large-$N$ approaches or if the ground-state has some valence-bond long-ranged order. A thermally activated behavior $c_v \sim \exp(-\Delta/T)$ can be treated within the entropy method and we applied it to the present model. The gaps we obtained are rather large (of order 1) but the specific-heat curves also exhibited a low-temperature peak consistent with the $c_v \sim T^\alpha$ results discussed below.

The expectation value of the Hamiltonian in any first-neighbor valence-bond covering is $e = -0.75$. By optimizing the wave-function in the vicinity of each triangle without any dimer, Elser obtained a variational state with energy $e = -0.333$. This rigorous upper bound was refined by Pierre who used an improved variational state to prove that $e_0 \leq -0.84267$. And exact lower bound can be obtained by remarking that the ground-state energy per triangle in the kagome AF is necessarily larger than the ground-state energy of an isolated triangle. This gives $e_0 \geq -1$. By extending this reasoning to larger clusters we can improve this lower bound. We can prove that $e_0 \geq -0.909952$ by exactly diagonalizing a 24-site cluster with open boundary conditions. Farnell, et al. used a coupled cluster method and predicted $e_0 \approx -0.8504$. They recently improved their calculation and obtained $e_0 \approx -0.86208$ by fitting their $n^{th}$-order results by $1/n^2$ corrections. We observed that their bare data are better described by $1/n$ corrections. In that case a fit gives $e_0 \approx -0.875$.

The physical meaning of this observation is that if two specific heat curves have i) the high-temperature expansion up to some relatively high order ii) the same ground-state energy, iii) the same entropy and iv) the same $c_v \sim (T/c_0)^\alpha$ limit at low temperature they must be very “similar”.

For lower energies the curves gets closer but the number of physical Padé approximants actually gets smaller and smaller, as can be seen in the lower panels of Fig. 3.