Thermodynamic properties of the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet at finite temperature: A finite-cluster-expansion approach

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(Received 5 August 1991)

We have calculated the series for the internal energy and the specific heat of a two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet at finite temperature on a square lattice using a finite-cluster-expansion method. The series are analyzed using a variant of Padé approximants. Our analysis agrees very well with the Monte Carlo simulation result for the internal energy per spin at $T > 0.3J$ and the specific heat at $T > 0.4J$.

Recently, Narayanan and Singh[1] have calculated the thermal properties of spin-$\frac{1}{2}$ and spin-1 antiferromagnetic Heisenberg spin chains by an expansion in finite lattice. For one-dimensional spin chains the series shows excellent convergence for $T > 0.25J$ for $s = \frac{1}{2}$ and $T > 0.35J$ for $s = 1$. At lower temperature, they also estimated the correlation length ξ and obtained good estimates for ξ down to $T = 0.06J$ for $s = \frac{1}{2}$ and $T = 0.02J$ for $s = 1$. In this paper, we present a finite-cluster-expansion calculation of the series for the internal energy and the specific heat of two-dimensional (2D) spin-$\frac{1}{2}$ Heisenberg antiferromagnets at finite temperature on a square lattice. Unlike the one-dimensional case, our series is divergent at the low-temperature regime. Using a variant of the Padé approximant,[2–4] we obtained very good agreement with the Monte Carlo simulation.[5]

The thermodynamic properties, such as internal energy E, of an infinite system can be obtained by finite-cluster expansion. The basic idea is to obtain a systematic expansion of the internal energy E in powers of the coupling constants. The physical basis for this expansion is that we want to collect all terms which include n-spin effects as our nth-order term. This is easily done via the cumulant. The cumulant of a n-spin configuration Γ is defined recursively as

$$E^c(\Gamma) = E(\Gamma) - \sum_{\gamma \subset \Gamma} E^c(\gamma), \tag{1}$$

and we refer to E and E^c, respectively, as the "bare" and "cumulant" values of E. In this definition, we sum over all subsets γ which are contained in Γ, excluding Γ itself. If Γ consists of a single bond connecting a pair of nearest-neighbor spins, then it has no subsets and for this case we have that the bare and cumulant values of Γ are the same. If Γ contains n bonds, then it has $(2^n - 1)$ different subsets γ. However, it is only necessary to sum over subsets which are connected, since $E^c(\gamma)$ vanishes if γ is not connected. Once we have constructed all the cumulant values of E, we may write

$$E(\Gamma) = \sum_{\gamma \subset \Gamma} E^c(\gamma), \tag{2}$$

where now we sum γ over all sets equal to or included in Γ. Denoting E_n^c the contribution of all n-spin configurations, we express the internal energy as a sum over cumulants corresponding to an ever increasing number of spins:

$$E = \sum_n E_n^c. \tag{3}$$

The internal energy for a given spin configuration (bare value of E) is defined as

$$E = \frac{\mathrm{Tr} H \exp(-\beta H)}{\mathrm{Tr} \exp(-\beta H)} = \frac{\sum_i E_i \exp(-\beta E_i)}{\sum_i \exp(-\beta E_i)}. \tag{4}$$

where H is the Hamiltonian given by

$$H = J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{5}$$

with positive coupling constant J.

Thus we diagonalize the Hamiltonian, find all the eigenvalues, and use Eq. (4) to calculate the bare value of E for a given n-spin configuration. Notice that two topological equivalent configurations give the same value E. Hence we only need to generate the topological inequivalent configurations. Once the configurations are generated we calculate the bare value of E and then use an embedding program to calculate the cumulant. The specific heat can be defined and calculated in a similar fashion. Comparing with the high-temperature series expansion method,[6] this calculation is simpler and more straightforward. But the quantity of interest has to be computed at each temperature.

We have calculated the internal energy $E(T)$ and the specific heat $C_v(T)$ at temperatures ranging from $0.01J$ to $2.00J$ on a square lattice up to 11 spins. In Tables I and II, the series coefficients for $E(T)$ and $C_v(T)$ are listed for selected temperatures. As shown in Figs. 1 and 2, the series (dash-dotted line) agrees with the simulation (triangles) very well at high temperature. At temperatures down to $T = 0.7J$ for $E(T)$ and $T = 0.8J$ for $C_v(T)$ the series starts to deviate from the expected value. This

TABLE I. The series for $E(T)$ at selected temperatures.

n	$T=0.4J$	$T=0.6J$	$T=0.8J$	$T=1.0J$
2	−1.1048	−0.7766	−0.5756	−0.4507
3	1.4400	0.5893	0.2649	0.1350
4	−2.3467	−0.6691	−0.2302	−0.0979
5	3.5502	0.6352	0.1469	0.0444
6	−5.4946	−0.6276	−0.1055	−0.0257
7	8.5064	0.6073	0.0704	0.0127
8	−13.2098	−0.6029	−0.0513	−0.0076
9	20.4933	0.5950	0.0361	0.0041
10	−31.8311	−0.5944	−0.0269	−0.0026
11	49.4763	0.5954	0.0198	0.0015

TABLE II. The series for $C_v(T)$ at selected temperatures.

n	$T=0.4J$	$T=0.6J$	$T=0.8J$	$T=1.0J$
2	1.9819	1.2826	0.7768	0.4988
3	−6.3357	−2.5428	−0.9727	−0.4167
4	14.9839	3.9465	1.0985	0.3737
5	−31.6241	−5.1091	−0.9712	−0.2404
6	63.0166	6.2476	0.8349	0.1615
7	−119.6771	−7.3139	−0.6739	−0.0973
8	219.5214	8.4012	0.5537	0.0642
9	−392.9839	−9.4527	−0.4430	−0.0397
10	691.4413	10.5329	0.3607	0.0264
11	−1200.3792	−11.6407	−0.2917	−0.0170

should be compared with the high-temperature series where a direct estimate gives good result at temperature down to $T=J$ for $E(T)$ and $T=1.2J$ for $C_v(T)$. At the low-temperature regime our series is divergent similar to the high-temperature series. In order to extrapolate to the low-temperature limit, we make an auxiliary function:

$$E(x)=\sum_n E_n^c x^n \ . \tag{6}$$

So the internal energy E can be obtained by letting $x=1$, i.e., $E=E(x)|_{x=1}$. Equation (6) can also be evaluated using Padé approximants as follows:[4] we take the derivative of $E(x)$ with respect to x and then make a Padé approximant[7] of $dE(x)/dx$,

$$\frac{dE(x)}{dx}=\frac{G_N}{F_M} \ , \tag{7}$$

where

$$G_N(x)=\sum_{n=0}^{N} g_n x^n \tag{8}$$

and

$$F_M(x)=\sum_{n=0}^{M} f_n x^n \ . \tag{9}$$

After integrating $dE(x)/dx$ we obtain

$$E(x)|_{x=1}=\int_0^1 \frac{G_N(x)}{F_M(x)}dx \ . \tag{10}$$

Using the series coefficients obtained by our finite-cluster-expansion method, we can easily compute Eq. (10) at given temperatures. In Figs. 1 and 2, we plot the quantities $E(T)$ and $C_v(T)$ versus temperature T/J. For comparison, we also plot the Monte Carlo simulation results[5] and the direct estimates from Eq. (6). We see

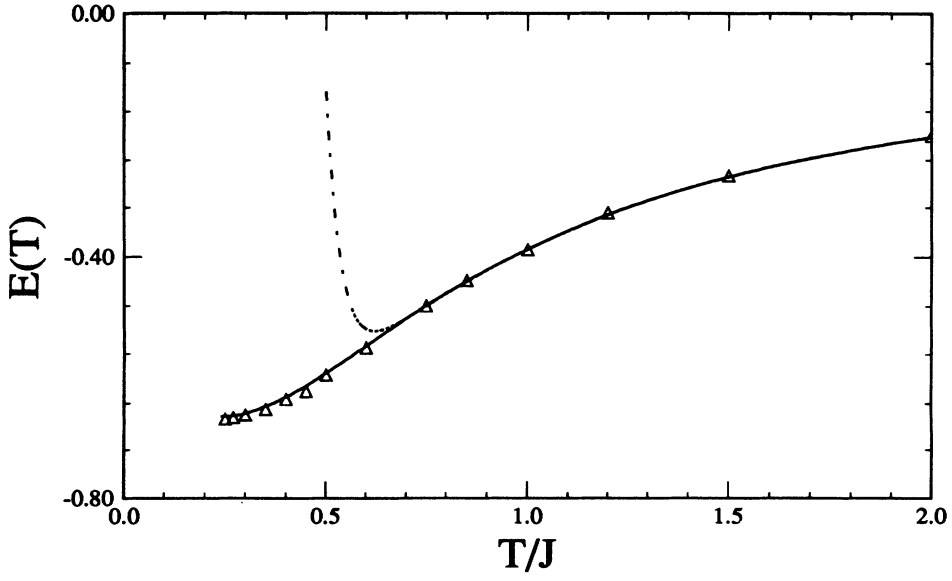

FIG. 1. The internal energy $E(T)$ vs temperature T/J. Here the triangle is the data of Makivi and Ding, the dash-dotted line is the direct estimate of the high-temperature series, and the solid line is from our analysis.

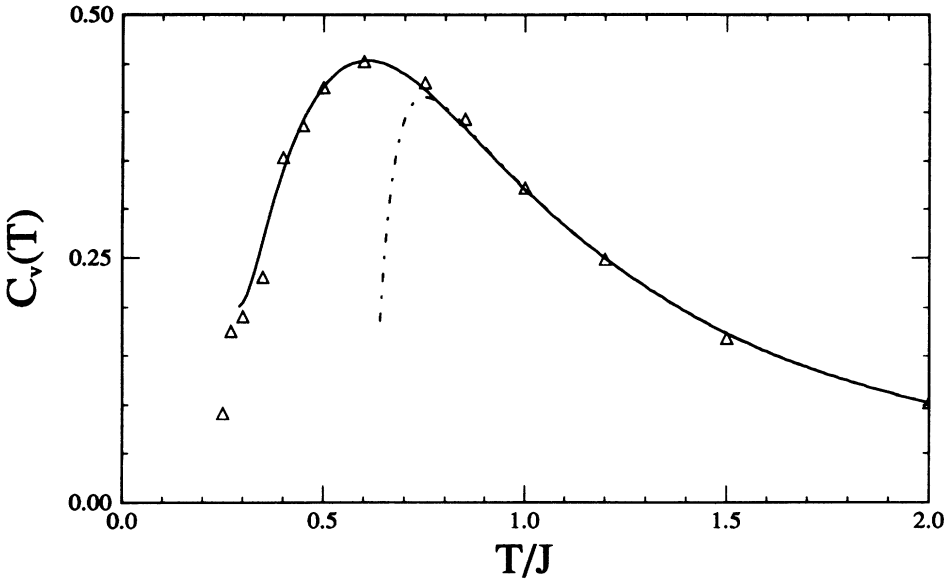

FIG. 2. The specific heat $C_v(T)$ vs temperature T/J. Symbols are as in Fig. 1.

that the agreement between our result and that of Monte Carlo simulation is excellent for internal energy at temperatures as low as $T = 0.3J$. For $C_v(T)$ the agreement is good at temperatures down to $T = 0.4J$.

The internal energy and the specific heat of 2D spin-1 Heisenberg antiferromagnets is also calculated up to eight spins on the square lattice. Due to the shortness of the series, the Padé method which we used to analyze the spin-$\frac{1}{2}$ series does not work as well. At present it is very hard to extend the series for the spin-1 case because even for the eight-spin configuration we have to diagonalize a 1200 by 1200 matrix and there are about 50 eight-spin configurations. Since at low temperature the thermodynamic properties are dominated by the first few eigenvalues, one may calculate the thermodynamic properties such as internal energy using only the first few eigenvalues to speed up the calculation and hence to improve the low-temperature behavior of the series.

In summary, we have calculated the internal energy and the specific heat of 2D spin-$\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice using a finite-cluster-expansion method. A variant of the Padé approximant is employed to analyze the series, and our results agree very well with those of the Monte Carlo simulation.

This work was supported by the Natural Sciences and Engineering Research Council of Canada and le Fonds pour la Formation de Chercheurs et l'Aide à la Recherche de la Province du Québec.

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