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Two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet at finite temperature

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We analyzed the high-temperature series of the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet using a variant of the Padé approximant method. Our analysis agrees very well with the Monte Carlo simulation result. Specifically, the agreement is very good for the internal energy per spin at $T > 0.3J$, for the specific heat and for the uniform susceptibility at $T > 0.5J$ on a square lattice. We also analyzed the internal-energy series on a triangular lattice. The ground-state energy per spin at zero temperature is found to be $E_g/N = -0.524$, which is in good agreement with the values obtained by simulations and spin-wave theory.

Since the discovery of high-T_c superconductors, the two-dimensional (2D) Heisenberg antiferromagnet has been studied extensively.[1] To calculate the thermodynamic properties such as the internal energy $E(T)$, the specific heat $C_v(T)$, and the uniform susceptibility $\chi(T)$, one uses methods such as spin-wave theory, quantum Monte Carlo simulation, and high-temperature series expansion. At very low temperature, spin-wave theory[2] works very well. In the intermediate-temperature regime, one uses quantum Monte Carlo simulation. The recent quantum Monte Carlo simulations[3] were done in the temperature range from $T = 2.5J$ to $T = 0.25J$ but the simulation is very time consuming at low temperature due to thermalization problems. The high-temperature series expansion,[4] unfortunately, converges only at high temperature since the expansion parameter is J/T. So this method is not useful unless we have a way of extrapolating the series to the low-temperature regime. In this paper, we apply a variant of the Padé approximant[5,6] to analyze the existing series.[4] Our analysis of the low-temperature behavior agrees very well with Monte Carlo simulation.[3]

The series for the 2D spin-$\frac{1}{2}$ Heisenberg antiferromagnet was calculated 20 years ago. The high-temperature series on a square lattice for $E(T)$ up to ninth order,

$$E/N = -0.5J(\,1.5x + 0.75x^2 - 0.875x^3 - 1.5625x^4 + 0.406\,25x^5 + 2.705\,208x^6 + 0.713\,764\,9x^7 - 4.179\,204x^8 - 3.315\,586x^9), \tag{1}$$

where $x = J/(2T)$. For $C_v(T)$ up to tenth order,

$$C_v = 1.5x^2(\,1 + x - 1.75x^2 - 4.16\dot{6}x^3 + 1.354\,16\dot{6}x^4 + 10.820\,833x^5 + 3.330\,902\,3x^6 - 22.289\,087x^7 - 19.893\,514x^8). \tag{2}$$

For $\chi(T)$ up to 11th order,

$$\chi = 0.5x(\,1 - 2x + 2x^2 - 1.\dot{3}x^3 + 1.08\dot{3}x^4 - 1.18\dot{3}x^5 + 0.509\,722\,2x^6 + 0.321\,825\,4x^7 + 0.407\,390\,9x^8 - 1.067\,28x^9 - 0.692\,818\,8x^{10}). \tag{3}$$

In order to extrapolate to the low-temperature limit, we take the derivative of E with respect to x and then make the Padé approximant[7] of $dE(x)/dx$ so that we have

$$\frac{dE(x)}{dx} = \frac{G_N}{F_M} \equiv [N, M], \tag{4}$$

where

$$G_N(x) = \sum_{n=0}^{N} g_n x^n \tag{5}$$

and

$$F_M(x) = \sum_{n=0}^{M} f_n x^n. \tag{6}$$

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

$$E(T) = \int_0^{J/2T} \frac{G_N(x)}{F_M(x)} dx. \tag{7}$$

Using the series coefficients in Eqs. [1]–[3], we can

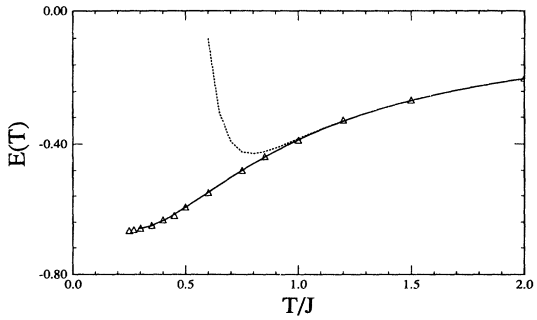

FIG. 1. The internal energy $E(T)$ vs temperature T/J. Here the triangle is the data of Makivi and Ding, the dotted line is the direct estimate of the high-temperature series, and the solid line is from our analysis. In the plot, we used the Padé approximant of [4,4].

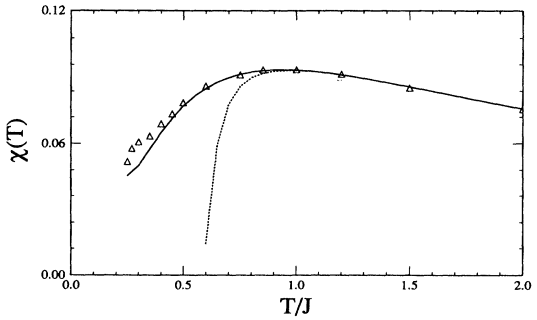

FIG. 3. The uniform susceptibility $\chi(T)$ vs temperature T/J. Here we used the Padé approximant of [5,5]. Symbols are as in Fig. 1.

easily compute Eq. (7) at a given temperature. In Figs. 1–3, we plot the quantities $E(T)$, $C_v(T)$, and $\chi(T)$ versus temperature T/J, respectively. For comparison, we also plot the Monte Carlo simulation results[3] and the direct estimates from Eqs. (1)–(3). We see that the agreement between our result and that of Monte Carlo simulation is excellent for internal energy at temperature as low as $T = 0.3J$. Below that this method does not apply. This is because the internal energy is a monotonic function of the temperature so that the point where the Padé approximant changes sign indicates the breakdown of the method. For $C_v(T)$ and $\chi(T)$ such a problem does not exist but unfortunately the agreement is not as good as for $E(T)$. Here the agreement is good at temperature down to $T = 0.5J$. Finally, we analyzed the series for internal energy on a triangular lattice. The series has been calculated[4] up to tenth order,

$$E/N = -1.125J(\,x - 0.5x^2 - 1.416\dot{6}x^3 + 1.875x^4 + 2.845\,83\dot{x}^5 - 7.072\,916\,6x^6 - 4.693\,700\,2x^7 + 25.246\,552x^8 + 0.090\,011\,8x^9). \quad (8)$$

In Fig. 4, only $E(T)$ versus T/J and the direct estimate of the above equation are plotted since we are not aware of any other calculation at finite temperature on the triangular lattice. For the triangular lattice, the internal energy can be extrapolated down to zero temperature. This is not surprising because usually the series for the triangular lattice behaves better than that of the square lattice up to the same order. Our estimate for the ground-state energy per spin is $E_g/N = -0.524$ or per bond, $E_g/N_b = -0.175$, which is compared with the results obtained by other methods: $E_g/N_b = -0.1789$ obtained[8] by the variational method for small lattices; $E_g/N_b = -0.183$ obtained[9] from exact diagonalization of small clusters; and $E_g/N_b = -0.181$ obtained from a general spin-wave theory.[10] This method has also been used[11] in analyzing the series of thermodynamic properties of the 2D Heisenberg antiferromagnet on a square lattice generated by the finite-size expansion method.[12] In this case, the series suffers a similar divergence problem at low temperature by direct estimate. And this

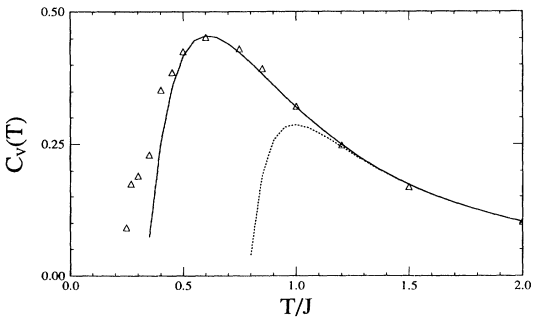

FIG. 2. The specific heat $C_v(T)$ vs temperature T/J. Here we used the Padé approximant of [4,4]. Symbols are as in Fig. 1.

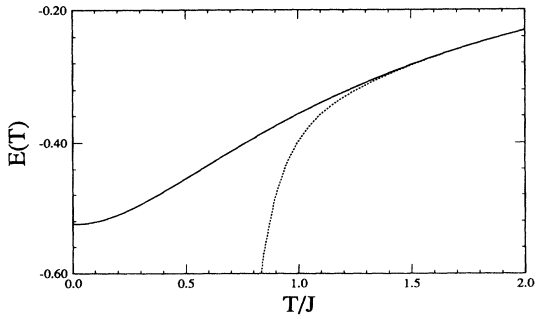

FIG. 4. The internal energy $E(T)$ vs temperature T/J on a triangular lattice. Here, we used the Padé approximant of [2,6]. Symbols are as in Fig. 1.

method works very well. In view of our result the high-temperature series of higher order is clearly desired.

In summary, we have applied a variant of the Padé approximant to analyze the high-temperature series of the 2D spin-$\frac{1}{2}$ Heisenberg antiferromagnet. Our results agree very well with Monte Carlo simulation results.

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