Differential approximants: An accurate interpolation from high-temperature series expansions to low-temperature behavior in two-dimensional ferromagnets

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We introduce *biased* differential approximants to high-temperature series expansions of the susceptibility in two-dimensional Heisenberg ferromagnets, taking into account the exponential divergence at low temperature. They provide a remarkable continuous description of the susceptibility from high temperature down to the low-temperature regime. [S0163-1829(98)06637-5]

Padé approximants have been extensively used for the analysis of high-temperature series expansions.[1] A $[L,M]$ Padé approximant to a series $f(x)=\Sigma_{n=0}^{N}a_n x^n$ is a rational fraction $P_L(x)/Q_M(x)$, with P_L and Q_M polynomials of order L and M, such that $f(x)=P_L(x)/Q_M(x)+O(x^{L+M+1})$.

Close to a second-order transition at finite temperature x_c^{-1} from a paramagnetic to an ordered state, thermodynamic quantities generally diverge as

$$f(x)_{x\to x_c}\sim A(x_c-x)^{-\gamma} \tag{1}$$

and Padé approximants to the logarithmic derivative $x d\ln f(x)/dx$ are most relevant.[1] They satisfy, up to order N the following relation:

$$xQ_M(x)f'(x)-P_L(x)f(x)=0. \tag{2}$$

We thus obtain a linear homogeneous *ordinary differential equation* of first order.

A natural generalization is to add an inhomogeneous term to Eq. (2) in the form of a polynomial R_K of degree K:

$$xQ_M(x)f'(x)-P_L(x)f(x)=R_K(x). \tag{3}$$

Further generalizations consider a nth-order differential equation:[2]

$$\sum_{i=0}^{n} Q_i(x)\mathcal{D}^i f(x)=R(x) \quad \text{with} \quad \mathcal{D}=x\frac{d}{dx}, \tag{4}$$

where $R(x)$ is a polynomial of degree K and $Q_i(x)$ are polynomials of degree M_i. The solution of this differential inhomogeneous nth-order linear differential equation is a ''*differential approximant,*'' usually noted $[K/M_0;M_1;\ldots;M_n]$. In this report, we shall only consider the simplest case $n=1$, i.e., $[K/L;M]$, a differential approximant defined by Eq. (3).

The method of differential approximants is one of the most efficient tools in series analysis.[2] It is particularly relevant if Eq. (1) does not hold. It is well known from the Mermin-Wagner theorem[3] that there is no ordering at finite temperature for the Heisenberg model in one or two dimensions.

$$\mathcal{H}=-\frac{J}{2}\sum_{i<j}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j \tag{5}$$

($\boldsymbol{\sigma}_i$ represent Pauli operators and the sum is over all distinct first-neighbor pairs). In two dimensions, the correlation length $\xi(T)$ and zero-field susceptibility $\chi(T)$ diverge exponentially at low temperature.[4–6] More precisely renormalization group techniques have proven that the susceptibility behaves as[6]

$$T\chi(T)=C\beta^{-3}\exp(\lambda\beta) \tag{6}$$

with $\beta=J/T$ $(k_B=1)$. Moreover, there is an intermediate temperature range ($0.7J\lesssim T\lesssim J$ for the square lattice) where both a high-temperature series and Eq. (6) are expected to describe the correct behavior. We use this information to introduce *biased* $[K/L;M]$ differential approximants that satisfy the functional form of Eq. (6) at low temperature.

In series approximations, Euler transformations on the expansion variable are frequently used to accelerate the convergence. They leave diagonal $[L,L]$ Padé approximants invariant but may improve the convergence of other type of approximants. We consider here the high-temperature series expansion of $T\chi(T)$ after an Euler transformation on the expansion variable β:

$$\beta=z/(1-az). \tag{7}$$

The lowest-degree polynomials $P_L(z)$ and $Q_M(z)$ that lead to a biased $[K/L;M]$ differential approximant approaching the correct limit [Eq. (6)] at $T\to 0$ [i.e., $z\to(1/a)^-$] are

$$Q_M(z)=(1-az)^2, \quad P_L(z)=(\lambda_K+3a)z-3. \tag{8}$$

The solution $[K/1;2]$ of the corresponding first-order linear differential equation will be now more shortly noted $DA[K+1]$. The $(K+1)$ coefficients of the polynomial R_K and the parameter λ_K are determined from the $(K+2)$ first coefficients of the high-temperature series expansion by writing that Eq. (3) is verified up to order $(K+1)$. This requires the knowledge of the susceptibility series up to order $(K+1)$ in β. The limit $\lambda_{K\to\infty}=\lambda$ represents the exponent in Eq. (6). The value of a in the Euler transformation will be optimized to obtain a good convergence of a sequence of differential approximants $DA[N]$. The general solution of the first-order linear differential equation (3) with $P_L(z)$ and $Q_M(z)$ given by Eq. (8) is

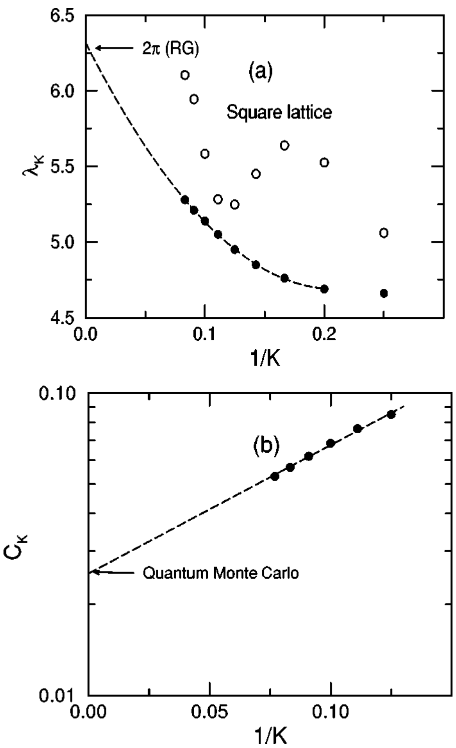

FIG. 1. Square lattice. Parameters λ_K and C_K corresponding to differential approximants $DA[K+1]$. The open circles represent the results obtained after the Euler transformation: $\beta \rightarrow z/(1-z)$. A better convergence is obtained after the Euler transformation $\beta \rightarrow z/(1-4z)$ (filled circles). Extrapolations (dashed lines) based on a quadratic least-squares fit of λ_K and linear fit of $\ln(C_K)$ give the following: $\lambda_\infty \approx 6.32$, in excellent agreement with the renormalization-group expectation $\lambda = 2\pi$, and $C_\infty \approx 0.25$, in good agreement with the estimate $C \approx 0.26$ from quantum Monte Carlo calculations (Ref. 6).

$$F(z) = A(z)\left[\frac{(1-az)}{z}\right]^3 \exp\left[\lambda \frac{z}{(1-az)}\right] \tag{9}$$

with

$$\frac{dA(z)}{dz} = \frac{R_K(z) z^2}{(1-az)^5} \exp\left[-\lambda \frac{z}{(1-az)}\right]. \tag{10}$$

The integration of the left-hand side of Eq. (10) can be done algebraically. It involves exponential functions and products of an exponential with the *exponential integral* function[7] $\mathrm{Ei}(u)$. The MATHEMATICA software[8] was used in this tedious task. $T\chi(T)$ is normalized to 1 at $T \rightarrow \infty$. The integration constant C_K is determined by choosing the particular solution $DA[K+1] = F^1(z)$ that tends to 1 for $z \rightarrow 0$. The limit $C_{K\rightarrow\infty} = C$ corresponds to the prefactor in Eq. (6).

We considered high-temperature series expansions of $T\chi(T)$ for the Heisenberg model on the square and triangular lattice calculated up to tenth order in β a long time ago[1] and recently extended up to 13th order[9,10] using modern computers.

1. Square lattice. We first examine the convergence of our *biased differential approximants* $DA[N]$ as a function of the parameter a in the Euler transformation [Eq. (7)]. Figure 1(a) represents for different values of a in the Euler transformation the variation of λ_K as a function of $1/K$. The convergence is poor for $a \ll 1$. Large oscillations remain up to $a \approx 1$ (see open circles). An optimum is obtained around $a = 4$ (filled circles). We choose this value. Figure 1(b) represents the corresponding prefactor C_K. A quadratic least-squares fit of λ_K for $K > 6$ extrapolates to $\lambda \approx 6.32$ for $K \rightarrow \infty$. This value is remarkably close to that expected from renormalization-group calculations: $\lambda = 2\pi$. A linear extrapolation of $\ln C_K$ as a function of $1/K$ gives $C \approx 0.025$ for $K \rightarrow \infty$. This is also in excellent agreement with the value $C \approx 0.026$ estimated from quantum Monte Carlo calculations.[6]

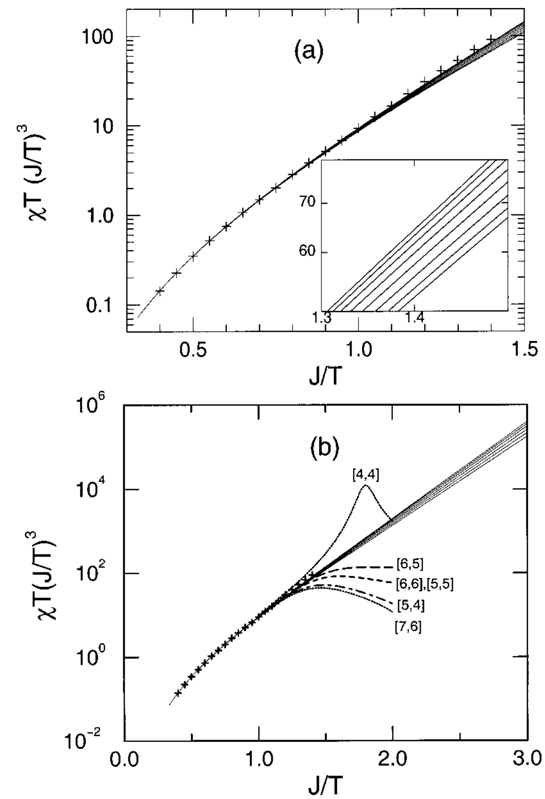

FIG. 2. Square lattice. (a) Differential approximants $DA[6]$ to $DA[13]$ (solid lines) are compared to the results of the quantum Monte Carlo calculations (+) by Kopietz *et al.* (Ref. 6). The inset represents a zooming of the upper part. From bottom to top, the solid lines represents $DA[6]$ to $DA[13]$. (b) Differential approximants $DA[8]$ to $DA[13]$ are compared to various Padé approximants $[L,M]$, with $8 \leqslant L+M \leqslant 13$.

Differential approximants $DA[N]$ are compared in Fig. 2(a) to quantum Monte Carlo simulations.[6] There is a remarkable monotonous convergence of the differential approximants $DA[6]$ to $DA[13]$. Differential approximants of relatively low order ($N=6$) already give an excellent approximation of the susceptibility down to $T/J = 0.8$. We have also compared differential approximants to usual Padé approximants to $T\chi$ in Fig. 2(b). While Padé approximants diverge at $T/J < 0.8$, differential approximants give a reliable estimate of the susceptibility down to $T/J \approx 0.4$.

2. Triangular lattice. We apply the same analysis to the susceptibility series of the triangular lattice.[10] An optimal convergence is obtained after the Euler transformation: $\beta = z/(1-3z)$. The parameters λ_K and C_K are represented in Fig. 3. A quadratic extrapolation of λ_K at $K \rightarrow \infty$ gives $\lambda \approx 12.5$, a value 15% higher than that expected from

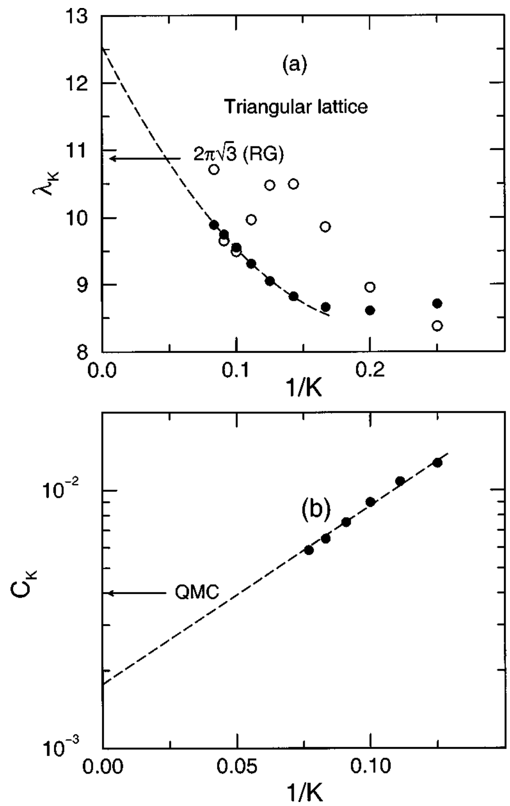

FIG. 3. Triangular lattice. Parameters λ_K and C_K corresponding to differential approximants $DA[K+1]$. The open circles represent the results obtained after the Euler transformation: $\beta\to z/(1-z)$. A better convergence is obtained after the Euler transformation $\beta\to z/(1-3z)$ (filled circles). An extrapolation (dashed lines) based on a quadratic least-squares fit of λ_K gives $\lambda=12.5$ at $K\to\infty$, a value 15% higher than that expected from renormalization-group calculations (see arrow). Consequently, the extrapolated value of C_K also differs from the value estimated through quantum Monte Carlo (QMC) calculations (Ref. 6).

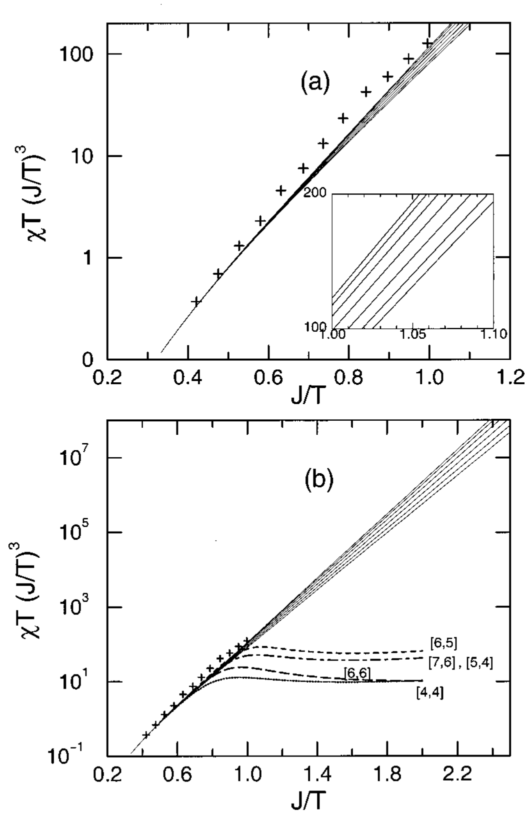

FIG. 4. Triangular lattice. (a) Differential approximants $DA[7]$ to $DA[13]$ (solid lines) are compared to the results of the quantum Monte Carlo calculations $(+)$ by Kopietz *et al.* (Ref. 6). The inset represent a zooming of the upper part. From bottom to top, the solid lines represents $DA[7]$ to $DA[13]$. (b) Differential approximants $DA[8]$ to $DA[13]$ are compared to various Padé approximants $[L,M]$ with $8\leq L+M\leq 13$.

renormalization-group calculations: $\lambda=2\pi\sqrt{3}$ [see Fig. 3(a)]. This difference might be due to the uncertainty in the extrapolation. The extrapolated prefactor C_K is a factor of 2 smaller than the value estimated from quantum Monte Carlo calculations[6] [see Fig. 3(b)]. A remarkable monotonous convergence of the differential approximants $DA[7]$ to $DA[13]$ is observed in Fig. 4(a). There is a discrepancy with quantum Monte Carlo calculations[6] that is maximum at $J/T\approx 0.8$. Since in this range both differential approximants and usual Padé approximants converge accurately to the same value, we believe that this discrepancy is due to large uncertainties in the quantum Monte Carlo calculation for the triangular lattice.

We have also considered more complicated biased differential approximants with polynomials P_L and Q_M of higher degrees. We have not observed a substantial improvement of the convergence.

We have recently extended this analysis to the susceptibility series of a generalized Heisenberg Hamiltonian including four-spin exchange interactions. It has proved to be very useful in the analysis of the experimental susceptibility of ferromagnetic solid ^{3}He films.[11]

Differential Padé approximants are already known as one of the most powerful general tools in series analysis. We have introduced biased differential approximants to the susceptibility series of the two-dimensional ferromagnetic Heisenberg models that satisfy, at low temperature, the correct functional form known from renormalization-group calculations. They provide a remarkable continuous description of the susceptibility over the whole temperature range.

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