Finite-size effects in Heisenberg antiferromagnetic films with a body-centered cubic lattice

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High-temperature series expansions of the zero-field free energy and staggered susceptibility are calculated for spin-$\frac{1}{2}$ Heisenberg antiferromagnetic bcc lattice films consisting of $m=2$, 3, 4, 5, and 6 interacting layers. Sixth order series in $x=J/k_BT$ have been obtained for free-surface boundary conditions. The staggered susceptibility series is analyzed by using the ratio and Padé approximant techniques. The critical temperatures $T_N(m)$ as a function of the number of m spin layers in the films are obtained. The shifts of the critical temperatures from the bulk value $[1-T_N(m)/T_N(\infty)]$ can be described by a power law $m^{-\lambda}$ with $\lambda \simeq 1.31$, where λ is the inverse of the correlation length exponent. A comparison is made with related works.

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I. INTRODUCTION

It is well established that the dimensionality of a system plays an important role in determining the critical behavior of the magnetic system.[1] The magnetic properties of magnetic thin film multilayers systems have been the subject of intense research in recent years.[2–5] The size in the lateral directions are of infinite extent in thin layers, but restricted by the layer thickness in the third direction. Since the correlation length in the third direction is terminated by the layer thickness,[6] thin layers are ideal media for the studies of finite-size effects on the critical behavior. The magnetic properties of the Ising and Heisenberg ferromagnetic films have been extensively investigated by various authors.[7–9] There have been some theoretical studies on phase transitions in Heisenberg antiferromagnetic thin films using a mean-field approach[10] and a Green's-function technique.[11] In this work, we present the finite-size effects on critical behavior of spin-$\frac{1}{2}$ Heisenberg antiferromagnetic cubic lattice films. The staggered susceptibilities of Heisenberg antiferromagnetic films are studied theoretically by the exact high-temperature series expansions. The method has been extensively used for the study of phase transition and critical phenomena in spin systems.[12]

We consider $\infty \times \infty \times m$ cubic lattice films formed of magnetic spins localized on the sites of cubic lattice which are infinite in two of its dimensions but of m finite layers in the third dimension[7,8] (z direction). We impose free-surface boundary[7,8] condition, in which each surface spin lacks one nearest neighboring spin on the simple cubic (sc) lattice and four nearest neighboring spins on the body-centered cubic (bcc) lattice.

The Hamiltonian of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet is given as

$$H=\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j-h_s\sum_{i\in A} S_i^z+h_s\sum_{j\in B} S_j^z, \qquad (1)$$

where i and j refer to the sites of two distinct interpenetrating sublattice and the pair interaction parameter $J_{i,j}$ is taken to be $J>0$ when i and j are nearest neighbors and zero otherwise. h_s in the Zeeman energy term are staggered magnetic fields on two sublattices A and B for calculating the sublattice magnetization and staggered susceptibility. The lattice has been divided into two distinct interpenetrating sublattices. High-temperature series expansions of the free energy and the staggered susceptibility series (up to the sixth-order series for the bcc lattice and to the seventh-order series for the sc lattice) are obtained. We report in this paper the numerical results of a high-temperature series expansion study on the bcc lattice film. The series are analyzed using the standard extrapolation techniques.[13] The dependence of the Néel temperature on the number of layers m of the bcc lattice film is investigated from the sixth-order series. The results obtained are consistent with the conjecture that the shift of the critical temperatures from the bulk value $[1-T_N(m)/T_N(\infty)]$ varies with thickness m, as $m^{-\lambda}$ with $\lambda \simeq 1.31$.

Unlike the bcc lattice film, the spin-$\frac{1}{2}$ staggered susceptibility series for the sc lattice film behaves irregularly. The series for lattices with lower coordination number and lower spin quantum number S usually have a slower convergence. The ratio and Padé approximant analysis do not show clear signs of convergence. Analysis of such series becomes difficult because nonphysical singularities exist near the circle of convergence. The interference by the nonphysical singularities makes the results of ratio and Padé analysis less reliable and less consistent. In such situations transformation methods[14,15] can be effectively used to analyze the series. We had applied a transformation method to analyze the series. For the sc lattice film, the estimate of the inverse of the correlation length exponent $\lambda \simeq 1.24$ is obtained using the transformation method. The complete series and further details of the transformation method and the analysis for the sc lattice film will be given in a future publication.[16]

A brief outline of the paper is as follows. In Sec. II we discuss the linked-cluster series expansion method to obtain high-temperatures series for the free energy and the staggered susceptibility in Heisenberg antiferromagnetic cubic layers. The results of the calculation and the analysis of series are presented in Sec. III. A summary is given in Sec. IV.

II. DERIVATION OF THE SERIES

The Hamiltonian is divided into two parts, the mean-field Hamiltonian

$$H_0=-\sum_{i\in A}[J_zM^+ +h_s]S_i^z+\sum_{j\in B}[J_zM^+ +h_s]S_j^z+\frac{1}{2}NJ_z(M^+)^2 \quad (2)$$

and the perturbation Hamiltonian

$$H_1=J\sum_{\langle i,j\rangle}[S_i^z-M^+][S_j^z+M^+]+\frac{J}{2}\sum_{\langle i,j\rangle}[S_i^+S_j^-+S_i^-S_j^+], \quad (3)$$

where z is the number of nearest neighbors and N is the total number of spins in a thin film. M^+ is the sublattice magnetization which minimizes the free energy of the system.[14]

The staggered susceptibility series for a thin film of m spin layers is obtained from the free energy F by the relation

$$\chi_m^s=\frac{1}{\beta}\frac{\partial^2(-\beta F)}{\partial h_s^2}=N_2\frac{1}{\beta}\int_0^\beta d\tau_k\int_0^\beta d\tau_l\left\langle T_\tau\left\{\sum_{k\in A}(S_k^z)\sum_{l\in B}(-S_l^z)S(\beta)\right\}\right\rangle_c, \quad (4)$$

where

$$S(\beta)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\cdots\int_0^\beta d\tau_n T_\tau\times[H_1(\tau_1)H_1(\tau_2)\cdots H_1(\tau_n)] \quad (5)$$

and N_2 is the number of lattice sites in each spin layer. The subscript c denotes that all connected diagrams have to be considered. It is noted that the summation over all nearest-neighbor spin pairs of Eq. (4) has to be summed over all sites in the z direction of m layer films.

The staggered susceptibility diagrams are therefore two-rooted diagrams[12] with two operators S_A^z and $-S_B^z$ placed together on one of the sites of the free energy diagrams. The contribution of a two-rooted diagram is composed of the product of the cumulants in the diagram, the weight factor, and the lattice constants which depend on the lattice structure. The calculations of all possible two-rooted connected graphs, the corresponding weight factors and the lattice constants are the most time consuming part of the computation. The connected graphs and the weights of the graphs are produced from the Ising graphs, which contain longitudinal interaction lines only $(S_i^z-M^+)(S_j^z+M^+)$, by an algorithm which has been implemented on a computer.

In a finite layer of bcc lattice each surface spin lacks four nearest neighboring spin. Since translational symmetry is lost in the direction of the layer thickness, the conventional lattice constants for a bulk lattice cannot be used. Computer programs have been developed to calculate the lattice constants of all connected graphs in a finite layer lattice. A graph with l interaction lines is generated by the sets of nearest-neighbor vectors (6 for the sc lattice and 8 for the bcc lattice) in a finite layer lattice. For a given layer thickness and given graph with l interaction lines, the program then generates all topologically equivalent graphs embedded in the layer lattice by adding independently l nearest neighboring vectors for each nonequivalent lattice sites of surface and interior layers. In order to reduce the computational time for enumerating lattice constants of thicker layers, the computer calculation is proceeded by dividing the free-surface films into even and odd number layers in which a graph is embedded. For even m layer only $\frac{1}{2}m$ in-layer lines need to be considered for counting by symmetry; for odd m layer extra counting for the $\frac{1}{2}(m+1)$th layer is also needed. The lattice constants obtained for the finite layer lattice are checked by comparing the ferromagnetic susceptibility series of an m-layer simple cubic lattice films with free surfaces. Our results to seventh order agree with those of the high-temperature series expansions for the susceptibility of spin-$\frac{1}{2}$ ferromagnetic Heisenberg simple cubic lattice films.[8] The multiple integrals containing τ-ordered products of spin operators in each connected diagram of the staggered susceptibility series are calculated by using the multiple-site Wick reduction theorem and the standard basis operators.[14,17] In Table I we show the low-order of Ising susceptibility diagrams, the corresponding weight factors, and lattice constants through fifth order. The corresponding lattice constants in terms of weak embedded lattice constants for the Ising graphs in a finite layer of bcc lattice are shown in Table II. Sixth order diagrams are available upon request.

The zero-field $(h_s=0)$ high-temperature series for the staggered susceptibility series of m-layer lattice with free surface is obtained as a series in $x=\beta J$,

$$\beta^{-1}\chi_m^s=\frac{1}{4}+\sum_{l=1}^{\infty}a_l^m x^l. \quad (6)$$

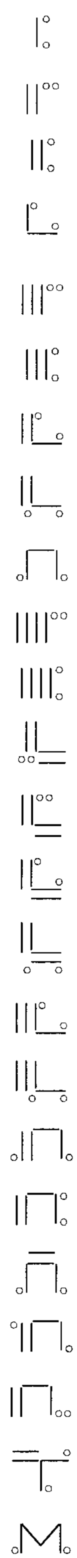
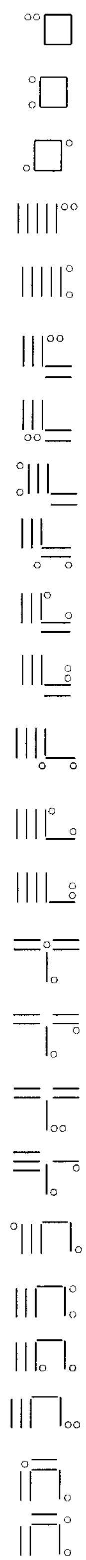
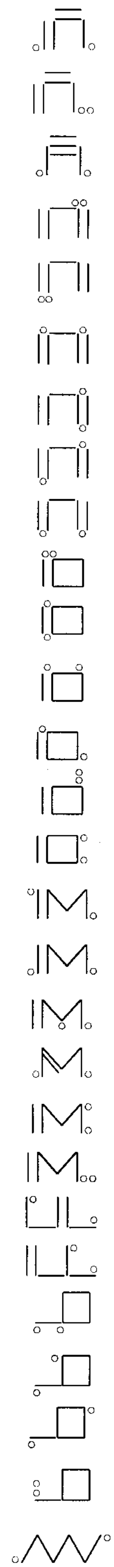
The coefficients a_l^m of an m layer for free surface for $m=2$, 3, 4, 5, and 6 layers are tabulated in Table III.

The staggered susceptibility series obtained in the present calculation is directly evaluated from the two rooted diagrams. The staggered susceptibility series could also be evaluated from the free energy to second order in h_s and take the derivative of the result twice with respect to the field. Both ways must yield the same result. For the bulk $(m=\infty)$ spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on both bcc and sc lattice, the results of the present calculation agree completely with previous results.[14,18] This is an independent check on the correctness of cumulants expansions, the corresponding weights and the value of the nth-order τ integral of the rooted diagrams. When $m=2$, we recover the high-temperature series expansions of spin-$\frac{1}{2}$ Heisenberg model for the square lattice.[14,19,20]

III. ANALYSIS OF THE SERIES

To estimate the Néel temperatures $T_N(m)$ for the m-layer films, we have used the well-known ratio and Padé approximant techniques. Since the ratio plot for a_l^m/a_{l-1}^m versus $1/l$ show oscillatory behavior, we have utilized[21] the ratio plot for $(a_l^m/a_{l-1}^m)^{1/2}$ versus $\{l(l-1)\}^{-1/2}$. The plot of $(a_l^m/a_{l-1}^m)^{1/2}$ versus $\{l(l-1)\}^{-1/2}$ for m-layer films with the free surface is shown in Fig. 1.

TABLE I. List of susceptibility diagrams through fifth order which contain longitudinal interaction lines only.

Graph	Weight	Lattice constant	Graph	Weight	Lattice constant	Graph	Weight	Lattice constant
	2	LC(1)		192	LC(5)		1920	LC(3)
	4	LC(1)		384	LC(5)		960	LC(3)
	4	LC(1)		192	LC(5)		640	LC(3)
	8	LC(2)		32	LC(1)		960	LC(3)
	8	LC(1)		32	LC(1)		960	LC(3)
	8	LC(1)		320	LC(2)		960	LC(3)
	24	LC(2)		320	LC(2)		1920	LC(3)
	48	LC(2)		640	LC(2)		1920	LC(3)
	48	LC(3)		640	LC(2)		960	LC(3)
	16	LC(1)		640	LC(2)		1920	LC(5)
	16	LC(1)		320	LC(2)		1920	LC(5)
	48	LC(2)		320	LC(2)		3840	LC(5)
	96	LC(2)		320	LC(2)		3840	LC(5)
	96	LC(2)		160	LC(2)		1920	LC(5)
	192	LC(2)		960	LC(4)		1920	LC(5)
	128	LC(2)		1920	LC(4)		3840	LC(7)
	128	LC(2)		480	LC(4)		3840	LC(7)
	384	LC(3)		640	LC(4)		3840	LC(7)
	384	LC(3)		1280	LC(3)		3840	LC(7)
	192	LC(3)		1280	LC(3)		3840	LC(7)
	384	LC(3)		1280	LC(3)		1920	LC(7)
	192	LC(3)		640	LC(3)		3840	LC(8)
	384	LC(4)		1920	LC(3)		1920	LC(8)
	384	LC(7)		1920	LC(3)		3840	LC(6)
							7680	LC(6)
							3840	LC(6)
							1920	LC(6)
							3840	LC(9)

TABLE II. The nonzero lattice constants in terms of weak embedded lattice constants for the graphs in m finite layers of bcc lattice.

LC number	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$
LC(1)	2	$\frac{8}{3}$	3	$\frac{16}{5}$	$\frac{10}{3}$
LC(2)	8	16	20	$\frac{112}{5}$	$\frac{72}{3}$
LC(3)	32	$\frac{256}{3}$	128	$\frac{768}{5}$	$\frac{512}{3}$
LC(4)	32	$\frac{320}{3}$	144	$\frac{832}{5}$	$\frac{544}{3}$
LC(5)	18	$\frac{144}{3}$	63	72	78
LC(6)	72	$\frac{864}{3}$	432	$\frac{2592}{5}$	576
LC(7)	128	$\frac{1536}{3}$	832	$\frac{5376}{5}$	$\frac{3712}{3}$
LC(8)	128	$\frac{1536}{3}$	896	$\frac{5632}{5}$	1280
LC(9)	512	$\frac{8192}{3}$	5376	$\frac{36864}{5}$	$\frac{26624}{3}$

In this plot, a straight line can be drawn through the points except those of the lower-order terms. The inverse Néel temperature is estimated from extrapolating the straight line to the asymptotic limit (value of the intercept at $\{l(l-1)\}^{-1/2}=0$), then the exponent γ can be determined from the slope of this line. The deviations of the points from being a straight line provide a measure of the uncertainty in the value of the critical temperature so obtained. From the longer series of three-dimensional staggered susceptibility, the critical temperature for the bulk is estimated to be $T_N=1.38$ (Ref. 14) with the exponent $\gamma=1.41$.[22] The estimated value of the critical exponent for ferromagnetic Heisenberg model is $\gamma=1.42$.[20,23] It is worth pointing out that the estimated values of γ for both systems agree with each other and this result is consistent with the conjecture[24] that the two systems belong to the same universality class. For the films with $m=4$, 5, and 6 layers, the estimates of exponent γ_2 range from values of 2.8 to 3.5 which are consistent with the estimate of exponent, $\gamma_2\simeq 3.0\pm 0.5$, for ferromagnetic Heisenberg films reported by Ritchie and Fisher.[8] This result is also consistent with the basic assumptions of scaling laws.[24] For $m=3$ layers film, there is a drastic change of the critical exponent γ_2. This result is perhaps unexpected and longer series are essential in order to estimate the correct exponent.

We have also used the Padé approximant analysis of the series to estimate the Néel temperature. Néel temperature is estimated from the poles of direct Padé approximants to the series $\{\chi_m^s\}^{1/\gamma_2}$. $\gamma_2=3.0$ is assumed for all finite thickness films. In Table IV we list the poles of Padé approximants to $\{\chi_m^s\}^{1/\gamma_2}$ for $m=4$, 5, and 6 layers. In general, the results of Padé approximants analysis of the series are consistent with those obtained from the ratio method except the results of $m=3$ layers film. The convergence of the present high-temperature series expansion for $m=3$ layers film is slow that the results of Padé analysis are too scattered to be conclusive. The estimates of Néel temperatures from the ratio method are compared with the corresponding estimates obtained from the average of $[\frac{2}{3}]$, $[\frac{2}{4}]$, $[\frac{3}{2}]$, $[\frac{3}{3}]$, and $[\frac{4}{2}]$ Padé

TABLE III. Exact series coefficients for the high-temperature staggered susceptibility series of body-centered cubic lattices with m layers and free-surface boundary condition.

m	a_1^m	a_2^m	a_3^m	a_4^m	a_5^m	a_6^m
2	0.2500	0.1667	0.0833	0.0305	0.0100	0.0052
3	0.3333	0.3889	0.3333	0.2924	0.1786	0.1219
4	0.3750	0.5000	0.5833	0.6004	0.5775	0.5213
5	0.4000	0.5667	0.7333	0.8852	0.9669	1.0497
6	0.4167	0.6111	0.8333	1.0751	1.3098	1.5339
∞	0.5000	0.8333	1.3333	2.02448	3.0244	4.4548

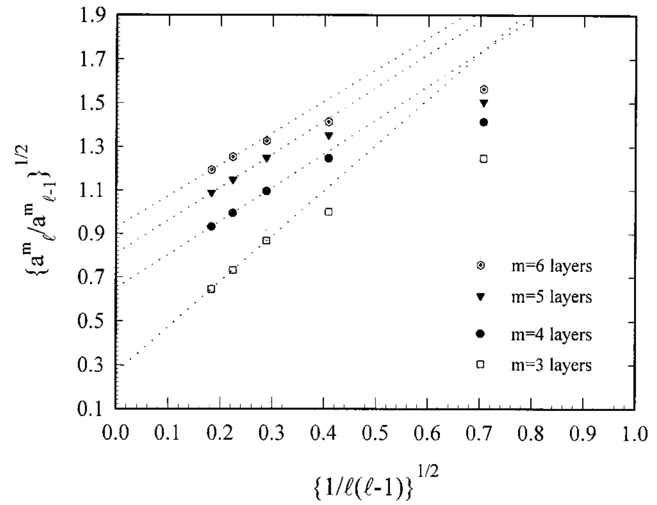


FIG. 1. Ratio plot of the high-temperature staggered susceptibility series $(a_l^m/a_{l-1}^m)^{1/2}$ versus $\{l(l-1)\}^{-1/2}$ for m-layer bcc lattice films with the free surfaces.

approximant for $m=4$, 5, and 6 layers films in Table V. c.c. denotes roots of a complex pair and a negative real root rather than a positive real root.

According to the finite-size scaling theory, the shift of the reduced Néel temperature $kT_N(m)/J$ from the three-dimensional bulk value $kT_N(\infty)/J$ for thicker layers m can be described by a power law of the form[8,25,26]

$$1-\frac{T_N(m)}{T_N(\infty)}\approx\frac{A}{m^\lambda}. \tag{7}$$

A log-log plot of $[1-T_N(m)/T_N(\infty)]$ versus m is shown in Fig. 2. The error bars represent the range of uncertainty for each value of m. The Néel temperature for $m=3$ layers film is obtained from the ratio plot. A good straight-line fit is obtained for the points through $3\leqslant m\leqslant 6$ with $\lambda\simeq 1.31$ and $\upsilon=1/\lambda\simeq 0.76$ according to the scaling prediction.[25,27] In the inset in Fig. 2 we show the variation of critical temperature shift with number of layers m for $\lambda\simeq 1.31$. This value is close to the shift exponent $\lambda=1.41$ ($\upsilon=0.71$) for ferromagnetic Heisenberg model by Monte Carlo[28] and high-temperature series expansion[29] methods. This results substantiates the general universality principles.[24]

TABLE IV. Estimates of Néel temperatures by Padé approximants. Poles of the Padé approximants to $\{\chi_m^s\}^{1/\gamma_2}$ with $\gamma_2=3.0$ are listed for a bcc lattice of $m=4$, 5, and 6 layers films.

m	M/L	2	3	4
	2	0.8745	0.6523	c.c.
4	3	0.6254	0.5929	
	4	0.6125		
	2	0.8588	0.8766	0.7968
5	3	0.8750	0.8467	
	4	0.7598		
	2	0.9405	0.9501	0.8853
6	3	0.9420	0.9056	
	4	0.8698		

TABLE V. Néel temperatures for the bcc lattices of m layers films. Estimates of $kT_N(m)/J$ are listed from (a) ratio estimate from $[\chi_m^s]$ and (b) Padé to $[\chi_m^s]^{1/3}$.

m	(a)	(b)	Average
4	0.62	0.62	0.62
5	0.81	0.83	0.82
6	0.93	0.91	0.92
∞	1.38	1.38	1.38

IV. CONCLUSIONS

In summary, we have studied the critical properties of spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on a m layers body-centered cubic lattice films for free-surface boundary condition by using the exact high-temperature series expansions. We have obtained the dependence of the Néel temperature on the number of layers with $m=3$, 4, 5, and 6. The Néel temperatures $T_N(m)$ for the m-layer films are estimated from the divergence of the staggered susceptibility with an exponent $\gamma_2\simeq 3.0\pm 0.5$, which is consistent with the basic assumptions of scaling laws. Our estimates for the shift exponent of the critical temperature, $\lambda\simeq 1.31$ and $\upsilon=1/\lambda\simeq 0.76$, and the exponent γ of bulk system, $\gamma=1.41$, are quite consistent with those for ferromagnetic Heisenberg model. This result is consistent with the conjecture that the

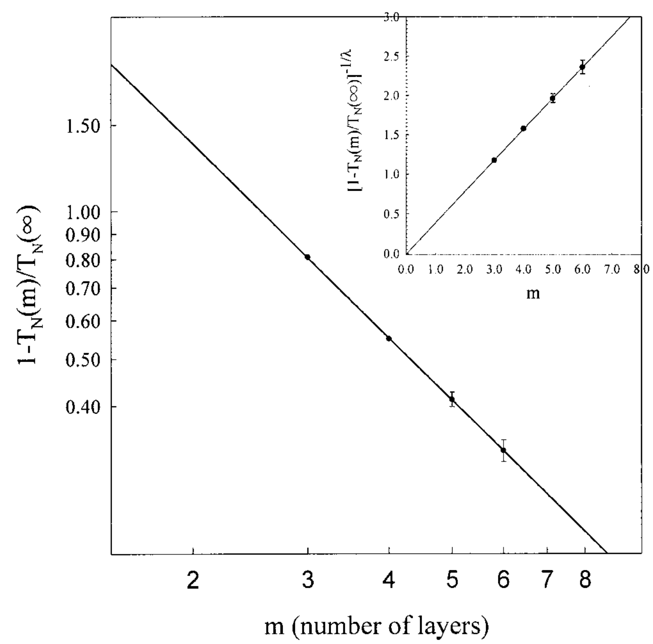


FIG. 2. Log-log plot of the shift of reduced critical temperature $[1-T_N(m)/T_N(\infty)]$ versus layers m. Slopes of the straight line yield the inverse of the correlation length exponent λ. In the inset we show the variation of critical temperature shift $[1-T_N(m)/T_N(\infty)]^{-1/\lambda}$ with number of layers m for $\lambda\simeq 1.31$. The error bars represent the range of uncertainty for each value of m.

two systems belong to the same universality class. However, the uncertainties in our numerical estimates, allowing for the scatter of the results in the ratio and Padé approximant analysis, leave small discrepancy between our estimates and those from Monte Carlo and high-temperature series. The lack of precision in the values of the critical temperatures and the limited number of layers due to the shortness of the series lead to the uncertainties in the estimates of the shift exponent of the critical temperature λ. Therefore, higher-order coefficients of the series are needed to obtain more precise estimates of the exponents.

We also hope to extend the present work to explore the question of the spin independence of the critical exponents. From the general universality principles, the critical exponents should be independent of spin quantum number S, and therefore the spin-1/2 and spin $>1/2$ models should have identical exponents.

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