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# Linked-cluster series expansion for the spin-one Heisenberg model with easy-axis anisotropy: specific heat

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**Abstract.** The linked-cluster series expansion technique is used to calculate the specific heat series of the spin-one Heisenberg model with easy-axis anisotropy on the FCC lattice. Series coefficients through sixth order in the interaction parameter are obtained. Examples of the temperature dependence of the specific heat in both ferromagnetic and paramagnetic phase are given. Comparison is made with the mean-field approximation and with a Green function theory.

## 1. Introduction

Analysis of magnetic specific heat experiments can yield valuable information about a magnetic material including the energy level structure, estimates of model interaction parameters, and the existence of magnetic phase transitions. For systems with many single-ion energy levels and complicated interactions the main theoretical tool for analysing the specific heat is the mean-field approximation, which in the paramagnetic phase will be simply the Schottky anomalies of the single-ion energy levels. Use of this approximation will be problematic whenever fluctuation correlations or dispersion in the energy levels become significant. It is desirable to have a method of assessing the validity of the mean-field approximation for the specific heat and to provide an improvement.

The equation of motion Green function method in the random-phase approximation has shown some improvement of mean-field results for the isotropic Heisenberg model in the ordered phase. In the disordered phase or in the situation of high anisotropy this RPA Green function approach will yield results which are similar to the mean-field approximation. In fact there are physical inconsistencies in the RPA Green function method for the Heisenberg model with easy-axis single-ion anisotropy (Yang and Wang 1975) and it does not give a good result for the dependence of Curie temperature on single-ion anisotropy (Lines 1975). One method of systematically improving mean-field theory is the linked-cluster series expansion method for treating quantum spin systems (Wentworth *et al* 1987). As an example of how to use this method for calculating the specific heat we present in this paper the linked-cluster series expansion of the specific heat for the spin-one isotropic Heisenberg model with an easy-axis single-ion potential on the FCC lattice. We show how to analyse the series using Padé approximates to obtain the specific heat in both ordered and paramagnetic phases. Comparisons with

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the mean-field approximation and the zeroth order contribution of the $1/z$ expansion for the temperature Green functions are given.

The Hamiltonian for the model under consideration is given in equation (1) where $S = 1$ is considered.

$$\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_1 \tag{1}$$

$$\mathscr{H}_0 = \sum_i [-(h + 2JzM)S_i^z - D(S_i^z)^2 + JzM^2] \tag{2}$$

$$\mathscr{H}_1 = -\sum_{i,j} J_{ij}[S_i^+ S_j^- + (S_i^z - M)(S_j^z - M)]. \tag{3}$$

The exchange parameter $J_{ij}$ is taken to be $J > 0$ for nearest-neighbours $i$ and $j$ and zero otherwise; $D > 0$ specifies the strength of the single-ion potential; $M$ is a free parameter which is set equal to the magnetisation $\langle S^z \rangle$, a choice which minimises the finite-order perturbatively calculated free energy described below (Wentworth 1986, Horwitz and Callen 1961); $h$ is an external magnetic field. $\mathscr{H}_0$ represents the unperturbed Hamiltonian of mean-field type and $\mathscr{H}_1$ is a perturbation representing the effects of fluctuation correlations.

The linked-cluster expansion method used in this paper in calculating the thermodynamic properties of the model is a many-body perturbation expansion for either the free energy or the temperature Green functions (Wang and Lee 1977, Yang and Wang 1975, Wortis 1974). The free energy and temperature Green functions can be expressed in terms of the temperature scattering operator $S(\beta)$.

$$S(\beta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n T_\tau [H_1(\tau_1) \ldots H_1(\tau_n)]. \tag{4}$$

The free energy is given by

$$-\beta F = -\beta F_0 + \ln \langle S(\beta) \rangle_0 \tag{5}$$

and the temperature Green function of spin operators $O_1$ and $O_2$ is

$$\langle T_\tau [O_1(\tau) O_2(0)] \rangle = \langle T_\tau [O_1(\tau) O_2(0) S(\beta)] \rangle_0 / \langle S(\beta) \rangle_0. \tag{6}$$

The operators in these equations are written in the interaction picture, and $T_\tau$ is the Dyson $\tau$-ordering operator which orders $\tau$ in decreasing order from left to the right. The expectation value $\langle \ldots \rangle_0$ is a thermal average evaluated using the $H_0$ ensemble.

The expansions of both the free energy and the temperature Green function in equations (5) and (6) can be shown to be sums of only linked graphs after thermal averages have been expressed in terms of semi-invariants (cumulants). This expansion for the fluctuation correlation part of the free energy can be represented by

$$\ln \langle S(\beta) \rangle_0 = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \langle T_\tau [H_1(\tau_1) \ldots H_1(\tau_n)] \rangle_L \tag{7}$$

where the subscript $L$ means linked graphs only are considered. The temperature Green function of equation (6) can be represented similarly as

$$\langle T_\tau [O_1(\tau) O_2(0)] \rangle = \sum_{n=0}^{\infty} \frac{(-1)}{n!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \langle T_\tau [O_1(\tau) O_2(0) H_1(\tau_1) \ldots H_1(\tau_n)] \rangle_L \tag{8}$$

The linked-cluster series expansion for the free energy is obtained from equation (7) by evaluating all terms to a given finite order in $H_1$. A summary of how this free energy series is calculated for the model of equation (1) is given in Wentworth *et al* (1987) and in Wentworth and Wang (1987).

After evaluating the integrals present in equation (5) the free energy series takes the form

$$-\beta F = -\beta F_0 + \sum_{n=2}^{N} f_n(x,y)(\beta J)^n \tag{9}$$

$$-\beta F_0 = \ln[1 + \exp(x+y) + \exp(x-y)] - \beta J z M^2 \tag{10}$$

$$x = \beta D \tag{11}$$

$$y = \beta(h + 2JzM). \tag{12}$$

The coefficients $f_n(x,y)$ can be expressed as polynomials in the variables $p$, $q$ and $(\beta D)^{-1}$ where $p$ and $q$ are the functions of $x$ and $y$ given by (Wentworth and Wang 1987)

$$p = \exp(x)[\exp(y) - \exp(-y)]/Z_0 \tag{13}$$

$$q = \exp(x)[\exp(y) + \exp(-y)]/Z_0 \tag{14}$$

$$Z_0 = 1 + \exp(x)[\exp(y) + \exp(-y)]. \tag{15}$$

## 2. Green function formalism

For comparison with the series expansion derived from the free energy we will give the specific heat obtained by summing the chain diagrams in equation (6) for the temperature Green functions. This approximation has been considered by Yang and Wang (1975). In this paper we calculate only the zeroth-order contribution to the Green functions in the $1/Z$ classification of terms. Two Green functions are required for calculating the internal energy: the Green functions for the pair $S_i^+$ and $S_j^-$ and the pair $(S_i^z - \langle S_i^z\rangle)$ and $(S_j^z - \langle S_j^z\rangle)$. These Green functions are (Yang and Wang 1975)

$$\langle T_\tau[S_i^+(\tau)S_j^-(0)]\rangle_{q,\omega_n} = -\frac{2}{\beta}\frac{D_{1\bar{1}}(\mathrm{i}\omega_n - 2J(0)\langle S^z\rangle) + D(D_{10} - D_{0\bar{1}})}{(\mathrm{i}\omega_n - \omega_q^+)(\mathrm{i}\omega_n - \omega_q^-)} \tag{16}$$

and

$$\langle T_\tau[(S_i^z(\tau) - \langle S^z\rangle)(S_j^z(0) - \langle S^z\rangle)]\rangle_q = \frac{\langle (S^z)^2\rangle_0 - \langle S^z\rangle_0^2}{1 - 2\beta J(q)[\langle (S^2)^2\rangle_0 - \langle S^z\rangle^2]} \tag{17}$$

The excitation energies $\omega_q^\pm$ are given by

$$\omega_q^\pm = \langle S^z\rangle_0(2J(0) - J(q)) \pm \{D^2 - 2DJ(q)[3\langle (S^z)^2\rangle_0 - 2] + [\langle S^z\rangle_0 J(q)]^2\}^{1/2}. \tag{18}$$

In these equations the Fourier transforms have been defined by

$$f(r_i - r_j) = \frac{1}{N}\sum_q \exp[-\mathrm{i}q\cdot(r_i - r_j)]\tilde{f}(q) \tag{19}$$

and

$$g(\tau) = \sum_n \exp(-i\omega_n\tau)\tilde{g}(\omega_n) \tag{20}$$

where

$$\omega_n = 2n\pi/\beta \qquad n = 0, \pm 1, \pm 2, \ldots \tag{21}$$

The factors $D_{ij}$ in equation (16) are defined by

$$D_{ij} = D_i - D_j \tag{22}$$

with

$$D_1 = \tfrac{1}{2}(p+q) \tag{23}$$
$$D_0 = 1 - q \tag{24}$$
$$D_{\bar{1}} = \tfrac{1}{2}(q-p). \tag{25}$$

The Green function $\langle T_\tau[S_i^+(\tau)S_j^-(o)]\rangle_{q,\omega_n}$ can be Fourier transformed back to $\tau$ space to give the transverse correlation function in momentum space.

$$\langle S_i^+ S_j^-\rangle_q = \frac{2}{(\omega_q^+ - \omega_q^-)}[D_{1\bar{1}}(\omega_q^+ - 2J(0)\langle S^z\rangle)f(\omega_q^+) - D_{1\bar{1}}(\omega_q^- - 2J(0)\langle S^z\rangle)f(\omega_q^-) + D(D_{10} - D_{0\bar{1}})(f(\omega_q^+) - f(\omega_q^-))]. \tag{26}$$

In this equation $f(\omega)$ is the Bose distribution function

$$f(\omega) = (e^{\beta\omega} - 1)^{-1}. \tag{27}$$

From the correlation functions given by equations (17) and (26) the internal energy can be calculated

$$U = \langle H_0\rangle - \sum_q J(-q)[\langle S_i^+ S_j^-\rangle_q + \langle (S_i^z - \langle S^z\rangle)(S_j^z - \langle S^z\rangle)\rangle_q] \tag{28}$$

and the specific heat can be obtained by differentiation.

## 3. The linked-cluster specific heat series

Calculation of the magnetisation and susceptibility linked-cluster series expansions has been described previously (Wentworth *et al* 1987). Here we discuss calculation of the specific heat series. The specific heat is the second derivative of the free energy with respect to temperature in fixed field. In dimensionless form it is obtained by differentiating the free energy with respect to $x$

$$C_h R^{-1} = x^2 \frac{\partial^2(-\beta F)}{\partial x^2} = g_0(x,y) + \sum_{n=2}^{\infty} g_n(x,y)(\beta J)^n. \tag{29}$$

A formula for the coefficient $g_n$ in terms of derivatives of the free energy coefficients is given by

$$g_n(x, y) = x^2\left(\frac{\partial^2 f_n}{\partial x^2}\right) + 2nx\left(\frac{\partial f_n}{\partial x}\right) + n(n-1)f_n. \tag{30}$$

To obtain a specific heat series valid in the ordered phase the temperature dependence of the magnetisation must be considered. We have chosen to obtain series coefficients with $\partial y/\partial x$ and $\partial^2 y/\partial x^2$ expressed explicitly, and when numerical values for $g_n$ are needed these derivatives are evaluated numerically from the magnetisation series. Therefore the coefficients $g_n$ evaluated from equation (30) will be polynomials in the variables $p$, $q$, $(\beta D)^{-1}$, $\partial y/\partial x$ and $\partial^2 y/\partial x^2$. The form is expressed by

$$g_n = \sum_{ijklm} C^n_{ijklm} p^i q^j (\beta D)^{-k}\left(\frac{\partial y}{\partial x}\right)^l\left(\frac{\partial^2 y}{\partial x^2}\right)^m. \tag{31}$$

Table 1† gives the coefficient $C^n_{ijklm}$ for $n = 0$–6 for the FCC lattice.

## 4. Analysis of the series

To obtain the best estimate of the actual specific heat of the model from the linked-cluster series expansion requires that an extrapolation procedure be done on the finite number of terms obtained. Padé approximants (Baker and Graves-Morris 1981) have been used as the extrapolation method for the specific heat series.

Extrapolations are done for fixed $D/2Jz$ and fixed $kT/2Jz$. The procedure is to evaluate $x$, $y$, $\partial y/\partial x$ and $\partial^2 y/\partial x^2$ for the fixed values of $D/2Jz$ and $kT/2Jz$; then the coefficients $g_n$ are evaluated using equation (31). With numerical values of $g_n$ obtained, equation (29) can be regarded as a power series in $(\beta J)$ for the specific heat to be evaluated at the chosen temperature. A new series is formed which excludes the $g_o$ and $g_1$ terms as indicated in equation (32)

$$\bar{C} = (C_h R^{-1} - g_0)/(\beta J)^2 = \sum_{n=2}^{\infty} g_n(\beta J)^{n-2} = \sum_{m=0}^{\infty} h_m(\beta J)^m \tag{32}$$

$$h_m = g_{m+2} \tag{33}$$

Padé approximants $[L/M]$ to the series expansion for $\bar{C}$ are defined by

$$[L/M] = \frac{n_0 + n_1(\beta J) + \ldots + n_L(\beta J)^L}{1 + d_1(\beta J) + \ldots + d_M(\beta J)^M} \tag{34}$$

All approximants to $\bar{C}$ with $(L + M) \leq 4$ are calculated at the chosen value of $(\beta J)$ and an average of selected approximants is done to obtain the estimate of $\bar{C}$ at the selected temperature, which in turn gives a value $C_h R^{-1}$ from equation (32).

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The method by which $y$ is calculated needs to be discussed. The external field $h$ is taken to be zero in this discussion so that $y$ is $2\beta Jz\langle S^z\rangle$. The series expansion for $\langle S^z\rangle$ has been presented previously (Wentworth *et al* 1987). To obtain a numerical value of $\langle S^z\rangle$ for the chosen values of $D/2Jz$ and $kT/2Jz$ an extrapolation procedure on the magnetisation series must be used. The extrapolation must yield a function which varies smoothly with temperature so that meaningful numerical derivatives $\partial y/\partial x$ and $\partial^2 y/\partial x^2$ can be taken. We have chosen a ratio method for estimating the extrapolated value of $\langle S^z\rangle$ (and therefore $y$). A series $\bar{S}$ defined in equation (36) is calculated from the magnetisation series written

$$\langle S^z\rangle = -\frac{\partial(\beta F)}{\partial y} = \sum_{n=0}^{\infty} m_n(x, y)(\beta J)^n \tag{35}$$

$$\bar{S} = \frac{2z\sum m_n(\beta J)^{n+1}}{y - 2z\sum m_n(\beta J)^{n+1}} = \sum_{m=0}^{\infty} \sigma_m(\beta J)^m. \tag{36}$$

The series for $\langle S^z\rangle$ and $\bar{S}$ have been obtained through sixth order. If the correct self-consistently determined value of $y$ has been chosen then $\bar{S}$ should diverge, therefore for a given $y$ an estimate of the $\beta J$ which produces a divergence in $\bar{S}$ can be obtained by the ratio test given by

$$(\beta J)^{-1} = nr_n - (n-1)r_{n-1} \tag{37}$$

$$r_n = \sigma_n/\sigma_{n-1}. \tag{38}$$

If this estimate for $\beta J$ is not equal to the chosen $\beta J$ then $y$ is adjusted and the ratio method extrapolation is repeated until self-consistency is obtained.

By using the procedure outlined above the specific heat as a function of $kT/2Jz$ can be obtained for particular values of the parameter $D/2Jz$. Examples of such specific heat calculations are presented in figures 1 and 2 along with the mean-field approximation and the chain-diagram Green function theory for comparison. The linked-cluster curve is the result of averaging over the [1/2], [1/3], [2/1], [2/2] and [3/1] approximants, except that when an approximant gives a clearly unphysical result it is excluded. Such is the case for the [2/1] approximant in the region around the phase transition when $D/2Jz$ is equal to 0.1.

Some trends in the convergence properties of the Padé approximants to the specific heat series are observed. For a particular $D/2Jz$ the apparent convergence of the approximants as a function of temperature depends on the value of $D/2Jz$. For $D/2Jz \gtrsim 2$ the approximants show good convergence. For $kT/2Jz < 0.35$ the difference between the series expansion estimate and the mean-field approximation are less than one per cent. It is obvious that both transverse and longitudinal spin fluctuation correlation functions are weak in their temperature dependence because of the large energy gap for the excitations and because the magnetisation is nearly saturated in this region. The poorest convergence is expected near the phase transition temperature where the rapid changes of spin fluctuation correlation functions occur. The specific heat shows a tendency to diverge, while the mean-field approximation gives a finite value. The convergence of the Padé approximants at low temperatures is worse

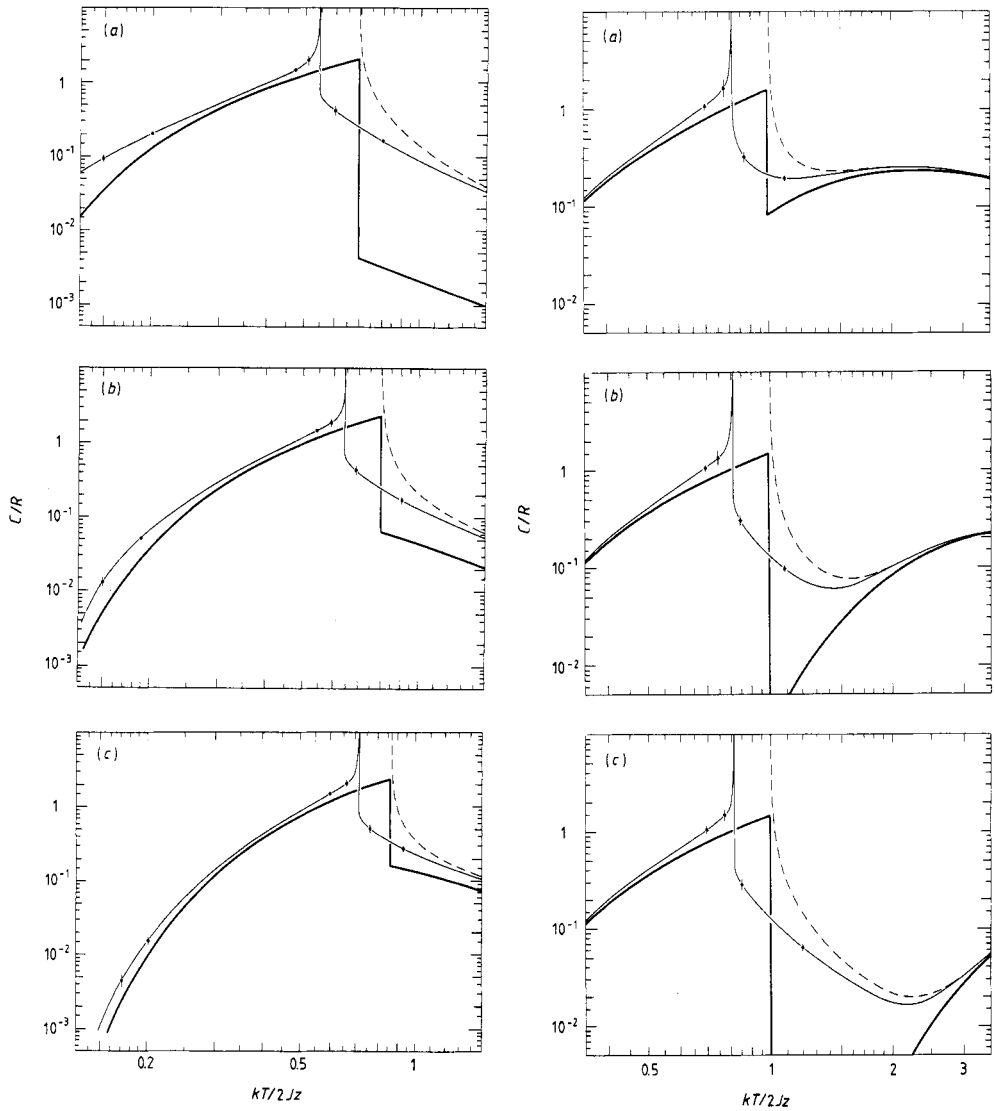


**Figure 1.** Specific heat estimates for values of $D/2Jz$ for which the Schottky anomaly occurs in the ordered phase. The full curve is the series expansion estimate with uncertainty bars drawn for selected temperatures. The bold curve is the mean-field approximation. The dotted curve is the Green function theory. (*a*) $D/Jz = 0.1$; (*b*) $D/2Jz = 0.5$; (*c*) $D/2Jz = 1.0$.

**Figure 2.** Specific heat estimates for values of $D/2Jz$ for which the Schottky anomaly peak occurs in the paramagnetic phase. The full curve is the series expansion estimate with uncertainty bars drawn for selected temperatures. The bold curve is the mean-field approximation. The dotted curve is the Green function theory. (*a*) $D/2Jz = 5.0$; (*b*) $D/2Jz = 10.0$; (*c*) $D/2Jz = 20.0$.

**Table 2.** $C_h R^{-1} = C_0 + (\beta J)^2 [L/M]$ for $D/2Jz = 0.1$.

| $kT/2Jz$ | [1/1] | [1/2] | [1/3] | [2/1] | [2/2] | [3/1] |
|---|---|---|---|---|---|---|
| 0.14 | 0.3071 | 0.08617 | 0.08288 | 0.07015 | 0.08305 | 0.07485 |
| 0.16 | 0.1358 | 0.1194 | 0.1131 | 0.1114 | 0.1141 | 0.1132 |
| 0.18 | 0.1602 | 0.1582 | 0.1483 | 0.1533 | 0.1507 | 0.1489 |
| 0.20 | 0.2015 | 0.2055 | 0.1915 | 0.1999 | 0.1944 | 0.1871 |
| 0.22 | 0.2516 | 0.2724 | 0.2428 | 0.2532 | 0.2448 | 0.2393 |
| 0.24 | 0.3083 | 0.2824 | 0.3013 | 0.3152 | 0.3023 | 0.2997 |
| 0.26 | 0.3705 | 0.3616 | 0.3657 | 0.4434 | 0.3662 | 0.3651 |
| 0.28 | 0.4377 | 0.4377 | 0.4353 | 0.4283 | 0.4356 | 0.4352 |
| 0.30 | 0.5099 | 0.5092 | 0.5095 | 0.5088 | 0.5097 | 0.5096 |
| 0.34 | 0.6732 | 0.6777 | 0.6780 | 0.6771 | 0.6780 | 0.6779 |
| 0.38 | 0.8662 | 0.8671 | 0.8638 | 0.8671 | 0.8663 | 0.8643 |
| 0.42 | 1.083 | 1.093 | 1.082 | 1.092 | 1.086 | 1.080 |
| 0.46 | 1.333 | 1.225 | 1.350 | 1.388 | 1.353 | 1.344 |
| 0.50 | 1.722 | 1.750 | 1.728 | 1.723 | 1.735 | 1.734 |
| 0.51 | 1.977 | 1.917 | 1.863 | 1.865 | 2.133 | 2.088 |
| 0.52 | 2.663 | 2.176 | 2.068 | 1.421 | 1.850 | 1.833 |
| 0.53 | 5.039 | 2.955 | 2.777 | −2.092 | 2.366 | 1.942 |
| 0.54 | 8.922 | 5.854 | 5.561 | −17.72 | 3.746 | 1.416 |
| 0.55 | 0.5161 | 0.5433 | 0.5900 | 0.5540 | 0.7209 | 0.5929 |
| 0.58 | 0.4290 | 0.4468 | 0.4739 | 0.4532 | 0.5268 | 0.4753 |
| 0.62 | 0.3445 | 0.3553 | 0.3696 | 0.3588 | 0.3899 | 0.3702 |
| 0.66 | 0.2833 | 0.2902 | 0.2984 | 0.2923 | 0.3075 | 0.2987 |
| 0.70 | 0.2375 | 0.2421 | 0.2471 | 0.2434 | 0.2516 | 0.2472 |
| 0.76 | 0.1875 | 0.1901 | 0.1927 | 0.1908 | 0.1945 | 0.1927 |
| 0.82 | 0.1519 | 0.1536 | 0.1550 | 0.1539 | 0.1555 | 0.1550 |
| 0.88 | 0.1258 | 0.1268 | 0.1276 | 0.1270 | 0.1281 | 0.1276 |
| 0.96 | 0.1003 | 0.1009 | 0.1013 | 0.1010 | 0.1015 | 0.1013 |
| 1.04 | 0.08188 | 0.08226 | 0.08251 | 0.08233 | 0.08260 | 0.08251 |

for smaller values of $D/2Jz$. When $D/2Jz = 0.1$ the approximants show essentially no convergence for $kT/2Jz < 0.14$ or so. This is illustrated in table 2 where the Padé approximants for $D/2Jz = 0.1$ are listed for several temperatures. In this case the apparent convergence gets better as the temperature increases, except in the immediate region of the phase transition.

There is no mathematically rigorous way to estimate an uncertainty in the series estimate, but an apparent uncertainty is indicated for selected temperatures by plotting an error bar of length $2\Delta C R^{-1}$, where $\Delta C$ is calculated by taking the difference between the largest and smallest approximant to equation (32) used in forming the average.

Figure 1 shows the temperature dependence of the specific heat for three values of $D/2Jz$ where the Schottky anomaly occurs within the ordered region. The case of $D/2Jz = 0.1$ is especially interesting. The series expansion result in the paramagnetic phase is an order of magnitude larger than the mean-field approximation. This is not surprising since above $T_c$ only the high-temperature tail from the Schottky anomaly is present in the mean-field result. The difference between the series expansion and mean-field approximation is even more dramatic in the ordered phase where figure 1(*a*) shows clearly that the functional form of the series expansion result is almost a power-law behaviour over much of the temperature range.

Figure 2 shows the temperature dependence of the specific heat for three values of $D/2Jz$ where the Schottky anomaly occurs above the transition temperature. For

such large values of $D/2Jz$ the system behaves very nearly as an Ising system in the ordered phase. The specific heat is almost independent of the parameter $D/2Jz$. The mean-field approximation produces rather good results for the specific heat at temperatures below $\frac{1}{2}T_c$. In the disordered phase the specific heat dependence on the value of $D$ is obvious. Since the mean-field approximation ignores the correlation of spin fluctuations the specific heat drops tremendously. The differences between series expansion values and those of the mean-field approximation are dramatic in this case. The zeroth order diagrammatic Green function results for the disordered phase are also shown in figures 1 and 2. It includes the perturbation contributions of the spin fluctuation correlation functions based on the mean-field approximation. In the region of temperatures around $T_c$ the contribution from the spin fluctuation correlation functions is very large. Below the transition temperature the Green function calculation yields a result which is smaller than the mean-field approximation. For most temperatures this is a physically reasonable result. In a real system one usually finds the mean-field approximation in the ordered phase to lie above the experiment when one fixes the exchange parameter by the transition temperature. Close to the transition temperature the zeroth-order Green function calculation yields a negative specific heat instead of a positive divergence as expected. This is evidently an artifact of the chain-diagram approximation as the series analysis shows.

## 5. Conclusion

The calculations presented in this paper show that the linked-cluster series expansion method can give reliable estimates for the specific heat of the model given by equation (1) on the FCC lattice for most temperatures in both ordered and paramagnetic phases. The exception to this conclusion is the low-temperature region ($kT/2Jz \lesssim 0.15$) for small values of $D/2Jz$.

One consequence of these series expansion estimates is an indication of the reliability of mean-field theory. For $D/2Jz \gtrsim 2$ the mean-field approximation can be trusted at high and low temperatures with problems arising in the vicinity of the phase transition. For smaller values of $D/2Jz$ the mean-field approximation fails to give the correct behaviour in the ordered phase. In general the effects of spin fluctuation correlations yield the major contributions to the specific heat in the vicinity of the phase transition. When the single-ion anisotropy is small their contribution at low temperatures is also significant.

Comparison of the series expansion results and the chain-diagram Green function calculation shows the latter gives a reasonable result in the paramagnetic phase although no shift in transition temperature is obtained. In the ordered phase use of the Green function calculation is problematic because of some unphysical features introduced by the chain-diagram approximation even though good results are produced at low temperatures. A higher order Green function calculation has shown much improvement: the critical temperatures are consistent with the present linked-cluster series expansion values; however, calculation of the specific heat is more complicated (Yang and Wang 1975).

The specific heat series presented here might be helpful in data fitting. If this is done care should be taken in choosing which Padé approximants to average over since for certain values of $D/2Jz$ and $kT/2Jz$ some approximants give clearly wrong estimates. The procedure should be first check that the magnetisation extrapolation

can be done over the range of temperature and model parameter values in which there is interest, then a similar check on the Padé approximants should be done.

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## References

Baker G A and Graves-Morris P 1981 *Pade Approximants, Encyclopedia of Mathematics and its Applications* vol 13 and 14 (London: Addison-Wesley)
Horwitz G and Callen H B 1961 *Phys. Rev.* **124** 1757
Lines M E 1975 *Phys. Rev.* B **12** 3766
Wang Y-L and Lee F 1977 *Phys. Rev. Lett.* **38** 912
Wentworth C D 1986 *Dissertation* Florida State University (unpublished)
Wentworth C and Wang Y-L 1987 *Phys. Rev.* B **36** 8687
Wentworth C, Wang Y-L and Westwanski B 1987 *J. Phys. C: Solid State Phys.* **20** 6255
Wortis M 1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) p 114
Yang D H and Wang Y-L 1975 *Phys. Rev.* B **12** 1057