Specific heats of classical spin systems and inhomogeneous differential approximants

1981 J. Phys. A: Math. Gen. 14 2553

(http://iopscience.iop.org/0305-4470/14/10/011)

J. Phys. A: Math. Gen. **14** (1981) 2553–2566. Printed in Great Britain

Specific heats of classical spin systems and inhomogeneous differential approximants

Jing-Huei Chen and Michael E Fisher
Baker Laboratory, Cornell University, Ithaca, New York 14853, USA

Received 19 February 1981

Abstract. We derive accurate compact expressions for the high-temperature specific heats of classical ($S=\infty$, 3-vector) spin systems on the FCC, BCC and SC lattices for pure Heisenberg, XY and Ising-like couplings, respectively. The analysis of the appropriate series expansions demonstrates the utility of inhomogeneous differential approximants and supports the estimate $\alpha_H = -0.21 \bullet 0.04$.

1. Introduction

At a bicritical point (see e.g. Fisher 1974), such as is exhibited by the antiferromagnet MnF_2 in a magnetic field, two critical lines of distinct character, typically Ising-like (or $n_\parallel = 1$-component) and XY-like ($n_\perp = 2$-component), meet: the bicritical point itself is then characterised by critical exponents of Heisenberg (or $n = n_\parallel + n_\perp = 3$) type. To describe the subtle changes in critical behaviour from Ising-like to Heisenberg-like to XY-like observed in the vicinity of a bicritical point one must determine the crossover scaling functions. These scaling functions are expected, on renormalisation group grounds (Kosterlitz *et al* 1976), to be universal: hence they may be studied conveniently in the context of a classical ($S=\infty$) spin model with three-component spins, $\boldsymbol{s} = (s^x, s^y, s^z)$, $|\boldsymbol{s}| = 1$, on a regular lattice coupled via the anisotropic nearest-neighbour interaction

$$\Delta\mathcal{H}_{ij} = -J_\perp(s_i^x s_j^x + s_i^y s_j^y) - J_\parallel s_i^z s_j^z \tag{1.1}$$

(Pfeuty *et al* 1974). When $J_\perp = J_\parallel = J$ this yields pure Heisenberg coupling; $J_\perp = 0$, $J_\parallel = J$ corresponds to the pure Ising-like case (but note that the components s_i^x and s_i^y still enter in determining statistical weights); $J_\perp = J$, $J_\parallel = 0$ describes pure XY-like coupling.

High-temperature series expansions, in powers of $x = J_\perp/k_B T$ and $y = J_\parallel/k_B T$, for the models described by (1.1) may be used as a basis for studying the bicritical region, $g \propto (J_\parallel - J_\perp)$ small. An initial study utilised well-established single-variable methods of series analysis (ratio extrapolation and Padé approximants) to examine the ordering susceptibilities, $\chi_\parallel(T, g)$ and $\chi_\perp(T, g)$ (Pfeuty *et al* 1974), and the specific heats, $C(T, g)$, and non-ordering susceptibilities, $\tilde{\chi}_\parallel(T, g)$ and $\tilde{\chi}_\perp(T, g)$ (Gerber and Fisher 1976). However, single-variable techniques cannot be used directly or reliably in the immediate bicritical region, which is what is really needed to find the crossover scaling functions, because of the discontinuous changes in critical exponents occurring at the bicritical point. These difficulties can be overcome by using the recently devised partial differential approximant techniques (Fisher 1977, Fisher and Kerr 1977) to analyse

0305-4470/81/102553+14\$01.50

directly the double series in x and y together. This two-variable approach has, in particular, been successful in estimating precisely the ratio, Q, which determines the relative rapidity with which the two critical lines approach the bicritical point (Fisher *et al* 1980).

Now the calculation of crossover scaling functions via partial differential approximants involves integrating the coupled ordinary differential equations for the 'trajectories' using appropriate initial or boundary values specified on particular loci in the (x, y) (or (T, g)) plane. Convenient choices are the axes $x = 0$ and $y = 0$ corresponding to the pure XY-like and pure Ising-like models (Fisher and Kerr 1977, Fisher *et al* 1980). Thus to determine the crossover behaviour of the specific heat which, unlike the ordering susceptibilities $\chi_{\parallel}$ and $\chi_{\perp}$, is directly susceptible to thermodynamic measurements in real antiferromagnets, one needs easily computable approximants for the specific heats of the pure Ising-like and pure XY-like models: the desired approximants should be accurate in the critical region and, in particular, must embody the correct type of singular behaviour. Corresponding knowledge of the pure Heisenberg models serves to crosscheck the two-variable calculations.

Accordingly in this note we address the problem of producing compact, reliable approximate formulae for the specific heats of the pure Heisenberg ($n = 3$), XY-like ($n = 2$) and Ising-like ($n = 1$) spin-∞ models on the three standard cubic lattices, FCC, BCC and SC. Since the specific heat exponents $\alpha_{\rm I}$, $\alpha_{\rm XY}$ and $\alpha_{\rm H}$ (for $n = 1, 2, 3$) are known to be small, and since the last two are negative, normal Padé approximant techniques are unsuited to the task. Instead we have utilised *inhomogeneous differential approximants* as explored recently by Fisher and Au-Yang (1979) and Hunter and Baker (1979). (See also Guttmann and Joyce (1972) and Rehr *et al* (1980).) We have, of course, taken advantage of the longest series currently available: in particular for the Heisenberg model we have used the 13th-order series for the FCC lattice recently published by English *et al* (1979). It transpires, however, that the inhomogeneous approximants are sufficiently powerful that, in combination with the susceptibility series, they already yield comparable results at 11th and 12th order. In particular we conclude, for spin ∞, that the specific heat is described by $\alpha_{\rm H} = -0.21 \pm 4$ (all uncertainties quoted, here and below, referring to the last decimal place), which is significantly lower than the original estimate of Ferer *et al* (1971) of $\alpha_{\rm H} = -0.14 \pm 6$, but not inconsistent with the ratio analysis of English *et al* (although we do not feel especially sensitive to their expressed need for longer susceptibility series). Our estimate for $\alpha_{\rm H}$ is also considerably lower than that obtained by renormalised field theory perturbation techniques applied in three dimensions which yield $\alpha_{\rm H} = -0.115 \pm 15$ (Baker *et al* 1978; see also Le Guillou and Zinn-Justin 1977). (However, the estimates for the susceptibility exponents, γ, are in satisfactory agreement.) It is unclear whether this discrepancy in α, like similar ones seen in comparisons with spin-$\frac{1}{2}$ Ising model series, is to be explained as due simply to the inadequate length of the present 13th-order series and the neglect of specific allowance for confluent corrections to the critical singularities (see further below), or as indicating that the fixed-length spin models belong to a distinct universality class, as argued by Baker and Kincaid (1979) for the standard Ising model. In either situation we believe that the explicit approximants presented below will provide very good numerical representations of the specific heats of the classical spin models close in to the critical point even if the analytic forms are not precisely correct. Certainly our forms should be more than adequate for the purpose of obtaining good estimates for the crossover scaling function for the bicritical specific heat.

2. Inhomogeneous differential approximants

Given a function f defined via its power series as

$$f(x)=\sum_{i=0}^{\infty} f_i x^i, \tag{2.1}$$

the inhomogeneous differential approximant (or 'U/PQ approximant') $F_{J/L;M}(x)\equiv [J/L;M]_f$ is defined as the solution of the differential equation

$$U_J(x)+P_L(x)F(x)=Q_M(x)(\mathrm{d}F/\mathrm{d}x) \tag{2.2}$$

satisfying the initial condition $F(0)=f(0)=f_0$, where the polynomial coefficients $U_J(x)=\Sigma_{j=0}^{J} u_j x^j$, $P_L(x)$ with $P_L(0)=p_0=1$, and $Q_M(x)$ are chosen so that the formal power series expansion of the solution function, $F(x)$, reproduces the known series for $f(x)$ at least to order x^N, where $N=J+L+M+2$ (Fisher and Au-Yang 1979). In the case $J\equiv\varnothing$, meaning the coefficient $U_J(x)$ is absent or identically zero, the inhomogeneous approximant reduces to an ordinary Dlog Padé approximant (e.g. Baker 1975), and one should set $J=-1$ in the expression for N.

Inhomogeneous differential approximants are particularly useful in representing functions with critical behaviour, as $x\to x_c^-$, resembling

$$f(x)=A(x)[1-(x/x_c)]^{-\alpha}+B(x), \tag{2.3}$$

where $A(x)$ and $B(x)$ are smooth in the critical region and where the exponent α is relatively small (or negative) or where the 'background', $B(x)$, is relatively large near x_c. Estimates for the critical point x_c are then obtained by finding the appropriate root of the equation

$$Q_M(x_c)=0. \tag{2.4}$$

If a prime denotes differentiation, one also has the estimates

$$\alpha=-P_L(x_c)/Q'_M(x_c), \qquad B_c=B(x_c)=-U_J(x_c)/P_L(x_c) \tag{2.5}$$

and similarly for $B'(x_c)$. With the amplitude function

$$A(x)=A_c[1+a_1(x-x_c)+\dots], \tag{2.6}$$

one further has

$$a_1=[P'_L(x_c)+\tfrac{1}{2}\alpha Q''_M(x_c)]/Q'_M(x_c), \tag{2.7}$$

while the leading amplitude may, in the present cases of small α, be calculated conveniently by integrating (2.2), taking appropriate precautions as to accuracy, and using

$$A_c=\lim_{x\to x_c^-}[1-(x/x_c)]^{\alpha}[F(x)-B_c]. \tag{2.8}$$

(See also Fisher and Au-Yang (1979) and Hunter and Baker (1979).)

Since the equations determining U_J, P_L and Q_M are merely linear and algebraic, it is straightforward to *bias* the approximants by imposing specified values of (i) x_c, or (ii) x_c and α, or (iii) x_c and B_c, or (iv) x_c, α and B_c. As in standard Padé approximant techniques, this may be useful if x_c is known more reliably from, say, strongly divergent functions like the susceptibility.

The approximants $[J/L; M]$ do not explicitly allow for confluent critical singularities of the sort suggested by current renormalisation group theory (Wegner 1972), which would insert a term $a_\theta(x_c - x)^\theta$ with $\theta \simeq 0.5$ before the a_1 term in the amplitude factor in (2.6). (But see Rehr *et al* (1980) for more general methods.) While there is little reason to doubt the presence of such terms, they will be strongly dominated by the effects of the background term, $B(x)$, in the case of the specific heat series where $\alpha \lesssim 0.15$. Conversely for the strongly divergent susceptibility series, on which we rely for the optimal estimates of x_c, the confluent singularities are more important than the background. However, it transpires that, to within the precision that concerns us here, allowance for such confluent singularities in the susceptibility has an insignificant effect on the estimates for x_c. To be explicit, Rogiers *et al* (1979) have studied the XY model on the FCC lattice and, allowing for a confluent singularity, found $x_c \simeq 0.29932$ if $\gamma = 1.333$ is assumed, but $x_c \simeq 0.29922$ if $\gamma = 1.316$: on the other hand a naïve Dlog (or inhomogeneous differential) approximant analysis indicates $x_c \simeq 0.2993 \pm 1$ and $\gamma \simeq 1.315 \pm 20$. It may also be remarked here that the naïve estimates for γ for the classical spin models with $n = 1$, 2 and 3 are in rather satisfactory agreement with the field theoretic perturbation estimates for $d = 3$ (Baker *et al* 1978, Le Guillou and Zinn-Justin 1977).

3. Heisenberg model on the face-centred cubic lattice

We discuss first some details of the analysis of the specific heat series for the FCC lattice with pure Heisenberg coupling. This case is interesting because the value of the exponent α_H is still not well established. Furthermore, for the FCC lattice terms to 13th order are now available (English *et al* 1979) and, unlike the BCC and SC series, the coefficients of all powers are non-vanishing (except those of x^0 and x which are zero for all lattices). Finally, this case will amply illustrate the nature and power of the methods of analysis as they apply equally to the other lattices and types of coupling.

Figure 1 shows a correlation plot of α_H estimates versus the corresponding x_c estimates for a range of $[J/L; M]$ approximants with $J = 1$ to 5 using coefficients up to orders $N = 9$ to 13. Note that we always count the series as starting with the constant term, namely

$$C(T)/k_B = \sum_{n=0}^{\infty} c_n x^n = 0 + 0x + x^2 + c_3 x^3 + \dots, \tag{3.1}$$

where the normalisation of $C(T)$ is chosen to make the coefficient of x^2 equal to unity. Already at 11th order (full symbols in the figure) a well-defined linear correlation is established between the estimates: this can be represented by

$$\alpha_H \simeq -0.200 + 65(x_c - 0.3150) \pm 0.040. \tag{3.2}$$

Inclusion of the 12th-order terms merely reinforces this correlation through to $x_c \lesssim 0.3150$; the 13th-order terms add essentially nothing new. This same correlation is also reproduced in biased approximants in which the value of x_c is imposed. Specifically, with x_c set equal to 0.31470 (the central estimate of Ritchie and Fisher (1972)), approximants with $J = 1$ and 2 yield $\alpha_H \simeq -0.18$ to -0.25 for $N = 10$, -0.19 to -0.24 for $N = 11$, -0.20 to -0.24 for $N = 12$, and -0.22 to -0.25 for $N = 13$: the values are consistent with (3.2) which yields $\alpha_H \simeq -0.22 \pm 4$.

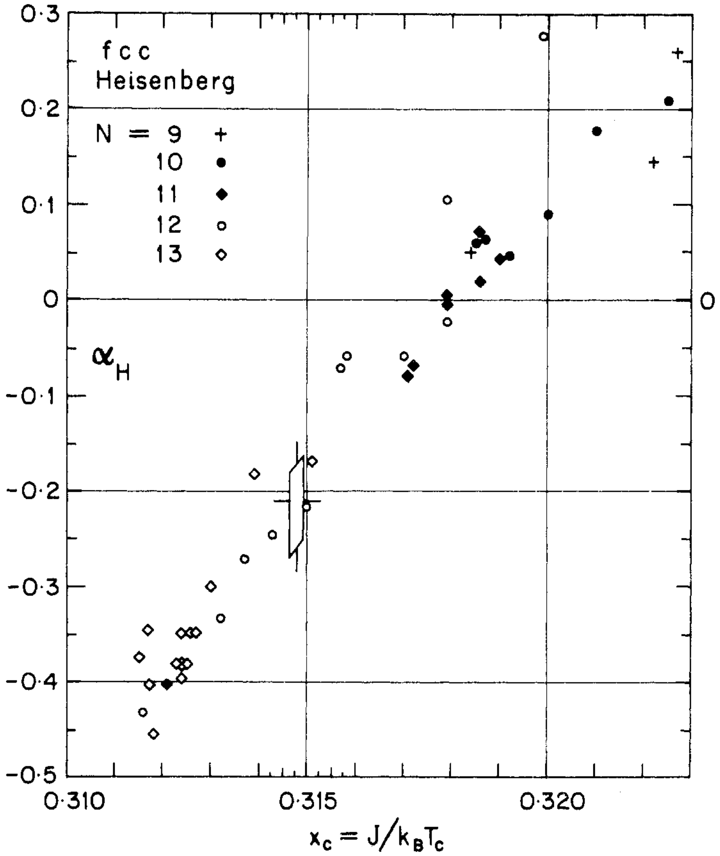

Figure 1. Unbiased estimates of the specific heat exponent, α, for the FCC classical Heisenberg model versus corresponding estimates for the critical point, from inhomogeneous differential approximants using the series coefficients up to the orders N indicated by the symbols.

It is clear from these results that it is more important to have a reliable independent estimate for x_c than to have the last term or two in the specific heat series. Ritchie and Fisher (1972) based their estimate of $x_c = 0.3147 \pm 1$ mainly on the Dlog Padé table for the susceptibility series to 10th order. Bowers and Woolf (1969), using only the 8th-order series, had earlier claimed $x_c = 0.314450 \pm 7$, but their apparent precision is illusory. On the other hand, Ferer *et al* (1971), using the 10th-order series and ratio and related extrapolation techniques, concluded $x_c = 0.3149_3 \pm 2$, which is essentially consistent with the Ritchie–Fisher estimate. English *et al* (1979), on the basis of the same data, have recently suggested that x_c might be as large as 0.3157; but this does not seem plausible to us even, in the light of the comments in the previous section, if allowance is made for confluent singularities. However, to supplement the Ritchie–Fisher Dlog Padé analysis (corresponding to $U_J \equiv 0$ or $J = \varnothing$) we have computed the inhomogeneous approximant tables for $J = 0, 1, 2$ and 3. For $J = 1$ and 2 and $N = 9$ and 10 the tables seem quite well converged: over all we are led to the estimate

$$x_c = 0.31480 \pm 15, \tag{3.3}$$

which encompasses the central estimates of both Ferer *et al* (1971) and Ritchie and Fisher (1972).

If (3.3) is accepted and we examine the corresponding sets of biased estimates for α, which confirm (3.2) and show essentially no variation for $N = 10, 11, 12$ and 13, we are led to conclude that the Heisenberg specific heat exponent for $S = \infty$ is

$$\alpha_{\rm H} = -0.21 \pm 4 \tag{3.4}$$

(see the 'box' in figure 1). It is interesting that this agrees closely with the long-standing estimate of Baker *et al* (1967) of $\alpha_{\rm H} = -0.20 \pm 4$ for the spin-$\frac{1}{2}$ Heisenberg model.

Incidentally, the specific results reported by English *et al* (1979) are also consistent with the correlation (3.2): thus they concluded $\alpha_{\rm H} \simeq -0.204$ if the Ferer *et al* estimate for $x_{\rm c}$ were accepted. Ferer *et al* themselves, using graphical methods and the shorter series, had concluded $\alpha_{\rm H} = -0.14 \pm 6$. Gerber and Fisher (1976; see also Ritchie and Fisher 1972) adopted $\alpha_{\rm H} \simeq -0.10$, in the upper part of this range, for their study of bicriticality.

In our subsequent calculations of approximants for the specific heat we employ the two explicit values (i) $x_{\rm c} \simeq 0.31470$ (with $\alpha_{\rm H} \simeq -0.22$) and (ii) $x_{\rm c} = 0.31485$ (with $\alpha_{\rm H} \simeq -0.21$). Both these are within the range (3.3): the former, Ritchie–Fisher value is adopted for consistency with previous and current calculations of bicritical behaviour (Fisher and Kerr 1977, Fisher *et al* 1980, etc); the latter is closer to the central value of Ferer *et al.*

The next step is the estimation of the background term, $B_{\rm c} = B(x_{\rm c})$, which, since $\alpha_{\rm H}$ is negative, is here equal to the critical point value, $C_{\rm c}/k_{\rm B}$, of the specific heat itself. To this end it is appropriate to use biased approximants with the value of $x_{\rm c}$ imposed. The assignment (ii), namely $x_{\rm c} = 0.31485$, yields estimates of $\alpha_{\rm H}$ strongly concentrated in the interval (3.4), but with a few outlyers reaching to around -0.07 and -0.33. However, the various estimates for $B_{\rm c}$ obey the correlation relation

$$B_{\rm c}(\alpha) \simeq -0.2521\alpha^{-1} + 0.7604 - 0.280\alpha \pm 0.02. \tag{3.5}$$

The central estimate, $\alpha_{\rm H} = -0.21$, thence yields $B_{\rm c} = C_{\rm c}/k_{\rm B} = 2.02 \pm 2$, which is adopted for subsequent fitting. Likewise for the assignment (i), $x_{\rm c} = 0.31470$, the value $\alpha_{\rm H} = -0.22$ yields $B_{\rm c} = C_{\rm c}/k_{\rm B} = 1.94_5 \pm 2$. However, the assumption $\alpha_{\rm H} = -0.10$, adopted by Gerber and Fisher (1976), yields $B_{\rm c} = 3.31 \pm 4$, which actually compares quite satisfactorily with the Gerber–Fisher estimate of 3.37 ± 7 based on the shorter, 11th-order series.

As is evidently to be anticipated, there are also strong correlations between the estimated values of $B_{\rm c}$ and amplitude estimates $A_{\rm c}$. For both assignments (i) and (ii) one finds $\delta A_{\rm c}/\delta B_{\rm c} \simeq 2.7$, the correlation being quite linear over the relevant range of 1% or so in $B_{\rm c}$. The central values for $B_{\rm c}$ then yield (i) $A_{\rm c} = -2.951 \pm 1$ and (ii) $A_{\rm c} = -3.003 \pm 1$, where the uncertainties quoted take *no account* of the original uncertainties in $B_{\rm c}$. Quite consistent but even more precise estimates for $A_{\rm c}$ are obtained from approximants in which the value of $B_{\rm c}$ is also specified. Notice that the negative sign for $A_{\rm c}$ merely reflects the negative sign of $\alpha_{\rm H}$. We also find that the Gerber–Fisher estimate of $B_{\rm c} \simeq 3.37$ yields $A_{\rm c} \simeq -3.89$, which agrees well with their corresponding estimate. The central estimates for α, $B_{\rm c}$ and $A_{\rm c}$ are collected in table 1.

It is instructive to compare these inhomogeneous differential amplitude estimates with the amplitudes that would be estimated by ratio techniques (see e.g. Fisher 1967). If c_n are the expansion coefficients to order n, and $x_{\rm c}$ and α are good critical point and

Table 1. Estimates for critical points, exponents, amplitudes and backgrounds of the classical ($S = \infty$) spin models with pure couplings of different symmetry. The uncertainties to be attached to these estimates are discussed in the text.

Symmetry	Lattice	$x_c = J/k_BT_c$	α	A_c	B_c
Heisenberg	FCC (i)	0.31470	−0.22	−2.951	1.945
($n = 3$)	(ii)	0.31485	−0.21	−3.003	2.023
	BCC	0.48635	−0.22	−4.29	2.88
	SC	0.69160	−0.22	−4.910	3.615
XY	FCC	0.29930	−0.02	−20.8736	20.16
($n = 2$)	BCC	0.45977		−31.4033	30.375
	SC	0.64430		−41.620	40.5
Ising	FCC	0.28503	0.125	2.6333	−3.30
($n = 1$)	BCC	0.43510		4.214	−5.31
	SC	0.60090		6.027	−7.35

exponent estimates, one may compute A_c by extrapolating the sequence

$$A_{c,n} = c_n(-x_c)^n \bigg/ \binom{-\alpha}{n}, \tag{3.6}$$

to $n = \infty$ as illustrated in figure 2. Evidently the plot for the assignment $x_c = 0.31470$ and $\alpha_H = -0.22$ is fairly linear in $1/n$ and would be extrapolated to a value rather close to the differential approximant estimate marked by an arrow labelled $[J/L; M]$. The assignment $\alpha = -0.10$ (of Gerber and Fisher) yields a distinctly curved plot which goes through a minimum where $A_c \simeq -3.84$, but a naïve extrapolation would agree within 2 or 3% with the differential approximant estimate $A_c \simeq -3.89$: of course, the curvature and minimum suggest strongly that $\alpha_H \simeq -0.10$ is not an optimal estimate.

Finally, values of the specific heat itself can be found by integrating the defining equation for optimal biased approximants with, say, x_c, α and B_c specified. Explicitly in case (i) the [3/5; 6], [3/3; 8] and [3/4; 7] approximants, among others, prove quite satisfactory. However, such a representation is not very convenient for subsequent applications in which a simple, rapid evaluation is desirable. Accordingly, we approximate the specific heats by the expression

$$C(T)/k_B \simeq A_c[(1-\bar{x})^{-\alpha} - 1 - \alpha\bar{x}] + A_c'[(1-\bar{x})^{1-\alpha} - 1 - (\alpha-1)\bar{x}] + \sum_{n=2}^{N} b_n\bar{x}^n + \bar{b}\bar{x}^{N+1}(1-\bar{c}\bar{x})^{-1}, \tag{3.7}$$

in which $\bar{x} = x/x_c = T_c/T$, while A_c is taken from (2.8) for an optimal approximant of highest order N with specified x_c, α and B_c, and $A_c' = -a_1x_cA_c$ where a_1 is given by (2.7). The polynomial coefficients are defined by

$$b_n = c_nx_c^n - (-)^n\left[A_c\binom{-\alpha}{n} + A_c'\binom{1-\alpha}{n}\right], \tag{3.8}$$

in which the c_n are the expansion coefficients for the specific heat (see (3.1)). The remainder amplitude, $\bar{b}$, is taken as a reasonable extrapolant for b_{N+1}, while $\bar{c}$ is chosen

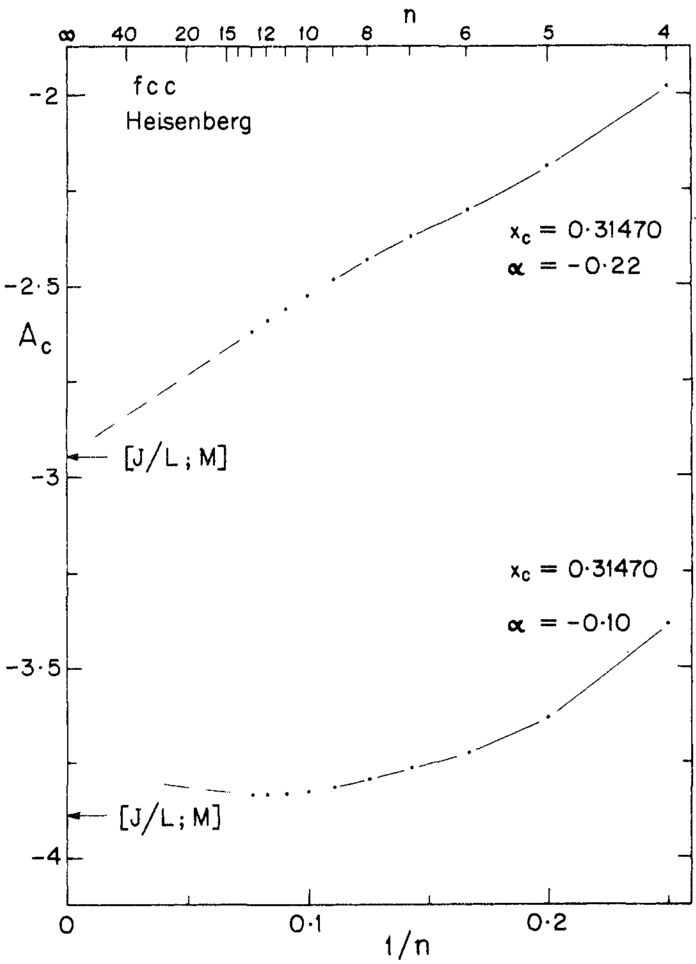

Figure 2. Estimation of the critical point amplitude, A_c, by extrapolation versus $1/n$ using (3.6) with specified x_c and α, in comparison with the corresponding inhomogeneous differential approximant results (labelled $[J/L; M]$).

to give the appropriate background value through

$$B_c = -A_c(1+\alpha) - \alpha A_c' + \sum_{n=2}^{N} b_n + \frac{\bar{b}}{1-\bar{c}}. \tag{3.9}$$

Clearly, the overall approximant (3.7) embodies all the known exact expansion coefficients as well as the preferred estimates for x_c, α and B_c. Furthermore, it is found that, within the errors of the numerical integration, an expression such as (3.7) will agree precisely through the whole range of $x \leqslant x_c$, not only with a particular, good differential approximant, but also with all other approximants yielding comparable values of A_c. (It may be remarked that inclusion of the term with coefficient A_c' is essential for this agreement.) For the central values of x_c, α and B_c given in table 1, the parameters N, A_c, A_c', $\bar{b}$ and $\bar{c}$ are listed in table 2, while the coefficients b_n are collected

Table 2. Parameters for evaluating the specific heat approximant (3.7) for optimal inhomogeneous differential approximants $[J/L; M]$ with values of x_c and α listed in table 1.

Symmetry	Lattice	N	$[J/L; M]$	A_c	A_c'/A_c	$\bar{b}$	$\bar{c}$
Heisenberg	FCC (i)	13	[3/3; 8]	−2.95075	1.25848	0.00034	0.850876
($n = 3$)	(ii)	13	[3/4; 7]	−3.00303	1.28638	0.00038	0.847838
	BCC	10	[3/5; 4]	−4.29102	1.18590	0.00525	0.386504
	SC	10	[3/6; 3]	−4.91233	0.547764	0.00400	0.409802
XY	FCC	11	[1/4; 7]	−20.8734	0.863705	0.000045	0.879796
($n = 2$)	BCC	12	[3/5; 6]	−31.4033	0.717188	0.00027	0.732539
	SC	12	[2/4; 8]	−41.6204	0.524960	0.00150	0.729970
Ising	FCC	9	[1/4; 6]	2.63339	1.28483	0.00015	0.888881
($n = 1$)	BCC	10	[2/3; 7]	4.21182	1.90733	0.006075	0.720188
	SC	10	[1/6; 5]	6.02739	1.28946	0.00540	0.781661

in table 3. The precision is 1 in 10^4 or better or, more generally, a fraction of $\bar{b}$. The corresponding plot of the specific heat is presented in figure 3 which, for comparison, includes also the specific heats for pure XY and pure Ising coupling on the FCC lattice.

4. XY and Ising models

Our analysis of the pure XY and Ising limits on the FCC lattice proceeds in a completely parallel manner. The series for the XY model on the FCC lattice have been given to order 11 by Ferer *et al* (1973), and for the Ising case to order 10 by Gerber (1975). The estimates adopted for x_c, on the basis of analysis of the susceptibility series, are listed in table 1: they agree or are quite consistent with other estimates in the literature (Moore *et al* 1974, Pfeuty *et al* 1974, Gerber and Fisher 1976). The XY estimate is of comparable precision to that for the Heisenberg case; analyses of the Ising series suggest somewhat higher precision. Plots of α versus x_c for unbiased approximants again reveal strong correlation and, on accepting the x_c estimates, yield the conclusions

$$\alpha_{XY} = -0.02 \pm 3, \qquad \alpha_I = 0.125 \pm 25. \tag{4.1}$$

These add nothing to results already in the literature (Ferer *et al* 1973) and are consistent with estimates for the spin-$\frac{1}{2}$ models (Betts and Lothian 1973, Sykes *et al* 1972), and, owing to the comparatively low precision, cannot be distinguished from the field theoretic estimates for three dimensions (Baker *et al* 1978, Le Guillou and Zinn-Justin 1977).

The correlation between B_c and α for approximants with the value of x_c specified is strong and, for the XY case, similar to (3.5). Accepting the central estimates for α_{XY} and α_I yields $B_c = 20.2 \pm 3$ and -3.30 ± 10, respectively, but it must be noted that, since the correlation yields $B_c \approx -0.41/\alpha$, the value $B_c \equiv C_c/k_B$ for the XY model is very sensitive to the precise assignment of α_{XY}.

Granted the values of x_c, α and B_c, the critical point amplitudes A_c are determined (see table 1) to within a precision of about 3 parts in 10^4; however, the correlation coefficients, $\delta A_c/\delta B_c$, are −1.10 and −0.060 for the XY and Ising cases, respectively.

Table 3. Polynomial coefficients for evaluating the FCC specific heat approximants (3.7) in conjunction with the parameters given in tables 1 and 2. (The figure in parentheses after each entry denotes the power of 10 by which the entry should be multiplied to yield b_n.)

Symmetry	b_2	b_3	b_4	b_5	b_6	b_7
Heisenberg (i)	3.44208(−1)	6.24645(−2)	2.32229(−2)	1.16630(−2)	6.32970(−3)	3.63978(−3)
(ii)	3.40828(−1)	6.38430(−2)	2.42651(−2)	1.23623(−2)	6.80300(−3)	3.96678(−3)
XY	6.89114(−2)	−3.44115(−3)	−9.78683(−4)	−2.86101(−4)	−1.30390(−4)	3.18086(−5)
Ising	8.11148(−1)	−1.72208(−5)	2.24804(−3)	4.39539(−5)	1.05941(−4)	1.49492(−4)

Symmetry	b_8	b_9	b_{10}	b_{11}	b_{12}	b_{13}
Heisenberg (i)	2.25804(−3)	1.50135(−3)	1.05045(−3)	7.61630(−4)	5.67220(−4)	4.23705(−4)
(ii)	2.48833(−3)	1.66590(−3)	1.16915(−3)	8.47655(−4)	6.29585(−4)	4.77735(−4)
XY	4.01747(−5)	4.86138(−5)	4.93455(−5)	4.63787(−5)		
Ising	1.63391(−4)	1.69440(−4)	1.61940(−4)			

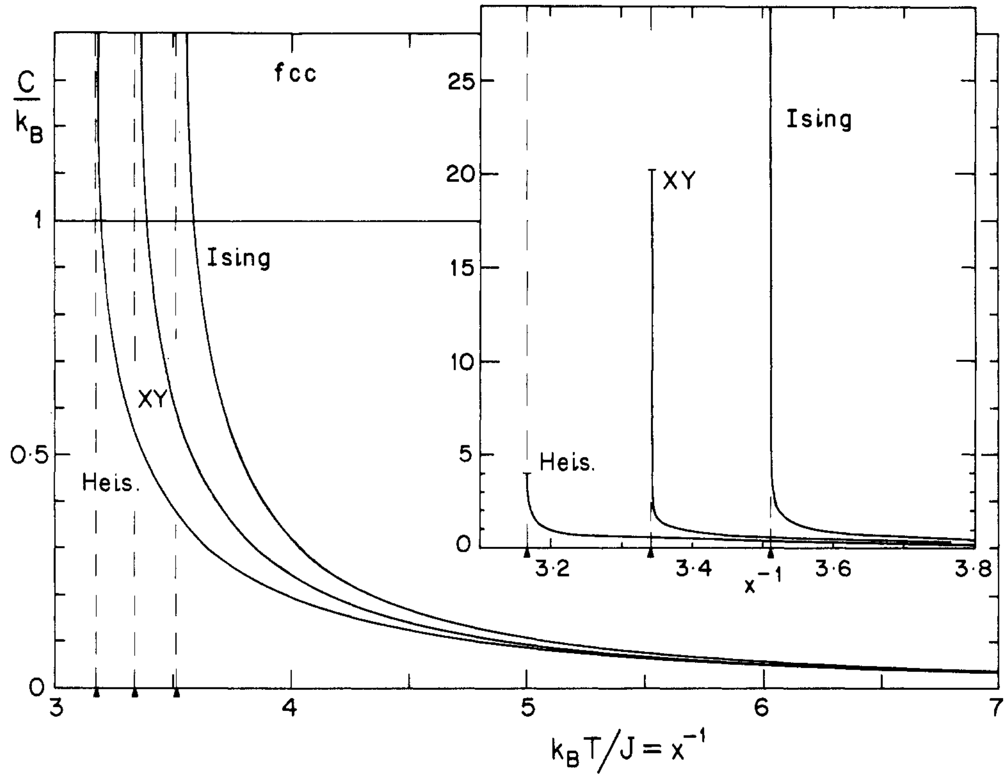

Figure 3. Variation of the specific heats of the classical Heisenberg, XY and Ising models on the FCC lattice above T_c with $k_B T/J$. Note that the specific heats are normalised so that $C(T)/k_B \approx (J/k_B T)^2$ as $T \to \infty$.

Lastly, the specific heats may be fitted to the form (3.7). Appropriate parameters, consistent with the data in table 1, are listed in tables 2 and 3, and the corresponding plots are presented in figure 3.

5. Other lattices

The specific heat series for the BCC and SC lattices may be obtained to 10th order from the work of Gerber (1975) for all anisotropies; for the pure Heisenberg model they are also given by Rushbrooke *et al* (1974). For the XY case Ferer *et al* (1973) give series to order 12. Since the lattices are loose packed, the specific heats are all even functions of x and hence alternate coefficients vanish identically. For this reason it is not worthwhile attempting independent estimates for α_H, α_{XY} or α_I. Instead, as indicated in table 1, we adopt the estimates derived for the FCC lattice. As regards the critical points, x_c, the values adopted (see table 1) are taken from Ritchie and Fisher (1972) for the Heisenberg model, from Pfeuty *et al* (1974) and Ferer *et al* (1973) for the XY case, and from our own analyses for the pure Ising-like limit.

In order to estimate the critical point background, B_c, and study its correlation with the amplitude, A_c, we have computed a range of differential approximants, with specified x_c and α, but using the specific heat series *in powers of x with zero coefficients*

Table 4. Polynomial coefficients for evaluating the specific heats for the BCC and SC lattices through (5.1) and the data in tables 1 and 2. (The figure in parentheses after each entry denotes the power of 10 by which the entry should be multiplied to yield b_{2m}.)

Symmetry	Lattice	b_2	b_4	b_6	b_8	b_{10}	b_{12}
Heisenberg	BCC	−3.23906(0)	1.89670(−1)	3.51554(−2)	1.17609(−2)	5.29504(−3)	
($n = 3$)	SC	−1.85879(0)	5.24349(−2)	2.90139(−2)	8.13225(−3)	4.76156(−3)	
XY	BCC	−1.17361(2)	2.60418(−2)	4.47166(−3)	1.57431(−3)	7.33322(−4)	4.06620(−4)
($n = 2$)	SC	−1.13954(2)	3.62015(−2)	1.56665(−2)	9.22952(−3)	4.66725(−3)	2.63675(−3)
Ising	BCC	3.44786(0)	1.27329(−1)	3.86714(−2)	1.78901(−2)	9.76210(−3)	
($n = 1$)	SC	3.24750(0)	1.19011(−1)	3.92298(−2)	1.96974(−2)	1.04984(−2)	

specified. The resulting approximants do not, of course, preserve exactly the true symmetry $x \Leftrightarrow -x$: however, many more approximants are thence available for inspection and, in fact, the values for $x < 0$, although not utilised, turn out to mirror the values for $x > 0$ quite accurately. The values for B_c and A_c thus estimated are collected in table 1: for the Heisenberg, XY and Ising cases the precision of the B_c estimates is roughly $\frac{1}{2}$–1%, 2% and 2–3%, respectively. The corresponding correlation coefficients, $\delta A_c/\delta B_c$, are likewise −2.65, −1.09 and −0.608 for the BCC lattice, and −4.00, −1.075 and −0.620 for the SC lattice.

Finally, it is desirable to have easily computable approximants which respect the loose-packed symmetry in x. Accordingly, in place of (3.7), we summarise our findings for the BCC and SC lattices by fitting to the expression

$$\frac{C(T)}{k_B} \simeq 2^{\alpha} A_c[(1-\bar{x}^2)^{-\alpha} - 1] + 2^{\alpha-1} A_c'[(1-\bar{x}^2)^{1-\alpha} - 1] + \sum_{m=1}^{N/2} b_{2m}\bar{x}^{2m} + \bar{b}\bar{x}^{N+2}(1-\bar{c}\bar{x}^2)^{-1}, \quad (5.1)$$

where $\bar{x} = x/x_c = T_c/T$ and $A_c' = -(a_1 x_c + \frac{1}{2}\alpha)A_c$, while A_c and a_1 are defined as before. The polynomial coefficients are now given by

$$b_{2m} = c_{2m} x_c^{2m} - (-)^{2m} 2^{\alpha}\left[A_c\binom{-\alpha}{m} + \tfrac{1}{2}A_c'\binom{1-\alpha}{m}\right], \quad (5.2)$$

while $\bar{b}$ is a reasonable extrapolant for b_{N+2} and $\bar{c}$ is chosen to satisfy

$$B_c = -2^{\alpha}A_c - 2^{\alpha-1}A_c' + \sum_{m=1}^{N/2} b_{2m} + \frac{\bar{b}}{1-\bar{c}}. \quad (5.3)$$

As previously, the approximant (5.1) will reproduce all the known specific heat coefficients and will embody precisely the preferred estimates for x_c, α and B_c. The required parameters, N, A_c, A_c', $\bar{b}$ and $\bar{c}$, are presented in table 2, while the coefficients b_{2m} are in table 4. We find, however, that (5.1) is not quite so successful in matching the differential approximant predictions for the BCC and SC lattices as is (3.7) for the FCC lattice. Nevertheless, the maximum deviations, which occur around $T/T_c \simeq 1.10$, amount to only a few parts in 10^4 and are less than 1 in 10^3 even in the worst case.

Acknowledgments

We are grateful for the support of the National Science Foundation through the Applied Mathematics Program, and for some supplementary assistance through the Materials Science Center at Cornell University.

References

Baker G A Jr 1975 *Essentials of Padé Approximants* (New York: Academic)
Baker G A Jr, Gilbert H E, Eve J and Rushbrooke G S 1967 *Phys. Rev.* **164** 800–17
Baker G A Jr and Kincaid J M 1979 *Phys. Rev. Lett.* **42** 1431–4
Baker G A Jr, Nickel B G and Meiron D I 1978 *Phys. Rev.* B **17** 1365–74
Betts D D and Lothian J R 1973 *Can. J. Phys.* **51** 2249–59

Bowers R G and Woolf M E 1969 *Phys. Rev.* **177** 917–32
English P S, Hunter D L and Domb C 1979 *J. Phys. A: Math. Gen.* **12** 2111–30
Ferer M, Moore M A and Wortis M 1971 *Phys. Rev.* B **4** 3954–63
—— 1973 *Phys. Rev.* B **8** 5205–12
Fisher M E 1967 *Rep. Prog. Phys.* **30** 615–731
—— 1974 *AIP Conf. Proc.* **24** 273–80
—— 1977 *Physica* **86–88** 590–2
Fisher M E and Au-Yang H 1979 *J. Phys. A: Math. Gen.* **12** 1677–92, **13** 1517 (corrigendum)
Fisher M E, Chen J-H and Au-Yang H 1980 *J. Phys. C: Solid State Phys.* **13** L459–64
Fisher M E and Kerr R M 1977 *Phys. Rev. Lett.* **39** 667–70
Gerber P R 1975 *J. Phys. A: Math. Gen.* **8** 1788–96
Gerber P R and Fisher M E 1976 *Phys. Rev.* B **13** 5042–53
Guttmann A J and Joyce G S 1972 *J. Phys. A: Gen. Phys.* **5** L81–4
Hunter D L and Baker G A Jr 1979 *Phys. Rev.* **19** 3808–21
Kosterlitz J M, Nelson D R and Fisher M E 1976 *Phys. Rev.* B **13** 412–32
Le Guillou J C and Zinn-Justin J 1977 *Phys. Rev. Lett.* **39** 95–8
Moore M A, Saul D M and Wortis M 1974 *J. Phys. C: Solid State Phys.* **7** 162–7
Pfeuty P, Jasnow D and Fisher M E 1974 *Phys. Rev.* B **10** 2088–112
Rehr J J, Joyce G S and Guttmann A J 1980 *J. Phys. A: Math. Gen.* **13** 1587–602
Ritchie D S and Fisher M E 1972 *Phys. Rev.* B **5** 2668–92
Rogiers J, Ferer M and Scaggs E R 1979 *Phys. Rev.* B **19** 1644–50
Rushbrooke G S, Baker G A Jr and Wood P J 1974 in *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) pp 245–356
Sykes M F, Hunter D L, McKenzie D S and Heap B R 1972 *J. Phys. A: Gen. Phys.* **5** 667–73
Wegner F J 1972 *Phys. Rev.* B **5** 4529–41