Further Applications of the Padé Approximant Method to the Ising and Heisenberg Models*

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(Received 3 August 1962)

We use the Padé approximant method to investigate the nature of the singularity in the specific heat for some three-dimensional Ising model lattices and to investigate the nature and location of the singularity in the magnetic susceptibility for some three-dimensional Heisenberg model lattices. We find that the three-dimensional Ising model specific heat becomes singular like $\log|T\text{-}T_c|$ with a different coefficient above and below the singular point. For the Heisenberg model we find that the magnetic susceptibility does not behave like the Curie-Weiss law, but tends to infinity more rapidly than $1/(T\text{-}T_c)$.

1. INTRODUCTION AND SUMMARY

THE purpose of this paper is to investigate the nature of the singularity in the specific heat for the three-dimensional Ising model and to try to locate the critical point and determine the nature of the singularity in the magnetic susceptibility for the three-dimensional Heisenberg model. To this end we employ the Padé approximant method which has recently been investigated and successfully applied to a number of problems.[1–4] This method may be thought of as a procedure for obtaining the analytic continuation of a function defined by a Taylor series into almost all of the complex plane—in particular, for finding it beyond the radius of convergence of the Taylor series. In general, a Padé approximant is of the form of one polynomial divided by another polynomial. In the $[N,M]$ Padé approximant the numerator has degree M and the denominator degree N. The coefficients are determined by equating like powers of z in the following equations:

$$f(z)Q(z)-P(z)=Az^{M+N+1}+Bz^{M+N+2}+\dots,$$
$$Q(0)=1.0,$$

where $P(z)/Q(z)$ is the $[N,M]$ Padé approximant to $f(z)$. The Padé approximant method consists of approximating $f(z)$ by the sequence of $[N,N]$ approximants. For a fuller discussion of the method, see references 1 and 2 and the references given therein.

Although the full range of convergence of the $[N,N]$ Padé approximants is not known, the method is as reliable as the familiar one of summing a presumably convergent Taylor series and justifying the procedure *a posteriori* by the apparent convergence of the first several terms. One can easily prove, following arguments analogous to those of Wall,[5] that the Padé approximant method never converges to the wrong answer. More precisely, if at least a subsequence of the $[N,N]$ Padé approximants converge uniformly for $|z|\leq M$, then the power series has a radius of convergence of at least M and the sum of the series is equal to $\lim_{N\to\infty}[N,N]$. By means of the transformations given in reference 2 and analytic continuation the domain of the z plane involved may be greatly extended. We remark that we have never yet found an example in which at least a subsequence of Padé approximants failed to converge everywhere except at singularities, outside natural boundaries, or on branch cuts.

We find that the specific heat for the Ising model for several three-dimensional lattices is proportional to $\log(1-T/T_c)$ for $T<T_c$. This behavior is the same as for the two-dimensional Ising model.[6] There are not sufficient Taylor series coefficients known in the high-temperature expansion to make as definite a statement about the behavior in the disordered region. However, the coefficients are not inconsistent with the conclusion that here again the specific heat is proportional to $\log(1-T_c/T)$. In three dimensions the coefficient of the log is about 0.3 in the disorder region times that in the ordered region, in contrast to the equality found in two dimensions.[6] This conclusion is in accord with the conclusions of Domb[7] based on entropy calculations.

Our results on the magnetic susceptibility of the Heisenberg model for several three-dimensional lattices are not as accurate as our previous results[3] for the Ising model. Since the Taylor series coefficients are harder to calculate, there are fewer of them available to form Padé approximants from. We find for the Heisenberg model that the magnetic susceptibility is proportional to $(1-T_c/T)^{-\alpha}$, where α is about $\frac{4}{3}$ for the loose-packed lattices, simple cubic and body-centered cubic, and $\frac{3}{2}$ for the close-packed lattice, face-centered cubic. The values of α are not too well defined, but are definitely greater than $\alpha=1$—the Curie-Weiss law. That the

* Work supported in part by the U. S. Atomic Energy Commission.
† On leave of absence from Los Alamos Scientific Laboratory, 1961–62.
[1] G. A. Baker, Jr., and J. L. Gammel, J. Math. and Applications 2, 21 (1961).
[2] G. A. Baker, Jr., J. L. Gammel, J. G. Wills, J. Math. Anal. and Applications 2, 405 (1961).
[3] G. A. Baker, Jr., Phys. Rev. 124, 768 (1961).
[4] C. Domb and C. Isenberg, Proc. Phys. Soc. (London) 79, 659 (1962).
[5] H. S. Wall, *Analytic Theory of Continued Fractions* (D. Van Nostrand Company, Inc., Princton, New Jersey, 1948), Theorem 54.1.
[6] L. Onsager, Phys. Rev. 65, 117 (1944).
[7] C. Domb, Phil. Mag. Suppl. 9, 149 (1960). See Sec. 4.7.2, pp. 287–9.

Heisenberg model should fail to give the Curie-Weiss law does not necessarily disagree with experiments, but even if it did, differences might arise from the approximate nature of the Heisenberg Hamiltonian[8] and the neglect of such effects as lattice compressibility.

2. SPECIFIC HEAT FOR THE ISING MODEL FOR SOME THREE-DIMENSIONAL LATTICES

Previous work by Domb and Sykes[7] has indicated for the disordered region for the face-centered cubic lattice that the specific heat, C_v, varies approximately as $(1-T_c/T)^{-1/b}$, where $b\geq 4$. The specific heat is also found to diverge at T_c in the ordered region.[7]

To investigate the behavior of C_v near the critical point, we first calculated the $[N,N]$ Padé approximants ($N=3-7$) to the low-temperature, simple-cubic-lattice series for $(kT/J)^2C_v(u)$, where $u=\exp(-4J/kT)$. For the convenience of the reader we have listed in the Appendix the coefficients of the series we have used. They are taken from Newell and Montroll,[9] and Domb and Sykes.[7,10] Convergence was not obtained, but the value at the critical point (known approximately from reference 3), as expected, seemed to be tending to infinity. Next we computed the $[N,N]$ Padé approximants ($N=2-5$) to the logarithmic derivative of $(kT/J)^2C_v$. If C_v were proportional to some power of $(1-T/T_c)$, then the logarithmic derivative would have a simple pole at T_c. No such simple pole appeared. If the behavior near the critical point were describable by a simple pole, our experience[3] with the Padé approximant method leads us to expect to have obtained a better result by this degree of approximation. Therefore, C_v probably does not behave like $(1-T/T_c)^{-\alpha}$ for any α.

To pursue the question further, with particular emphasis on the possibility that C_v may be proportional to some power of $\log|1-T/T_c|$, we expanded the neighborhood of the critical point into the neighborhood of infinity by means of the transformation $u=u_c(1-e^{-x})$, where u_c is the critical value of u. We have taken this value from reference 3. Since this work was begun, an erratum[11] appeared modifying one of the coefficients used in reference 3 to estimate u_v for the simple cubic lattice. As the corrected coefficient modifies the value of u_c in the sixth figure, which was thought to be uncertain anyway, we have not redone these calculations but use the value of reference 3 consistently throughout. We mention that the Padé approximants computed in this paper were done on a CDC 1604 and about 21 decimal places were carried to insure accuracy. After making this transformation, we computed the $[N,N]$, $[N,N+1]$, and $[N,N+2]$ Padé approximants to $(kT/J)^2C_v[u_c(1-e^{-x})]$, which are appropriate[1] to $C_v\sim x^0$, x^1, x^2 as $x\rightarrow+\infty$. All three series converged to graphing accuracy out as far as $x\simeq 3.3$ although the $[N,N+1]$ converged the best. In Fig. 1 we have graphed $(kT/J)^2C_v(u)/[\log_e(1-u/u_c)]$ based on these results. It is to be noted that the resultant plot is reasonably well behaved near the critical point. On this basis we adopt the tentative hypothesis that C_v is proportional to the first power of $\log(1-u/u_c)$ in three dimensions, just as in two dimensions.[6] We mention that this is not necessarily in conflict with Domb and Sykes[7] as $b\rightarrow\infty$ corresponds in some sense to a logarithmic singularity.

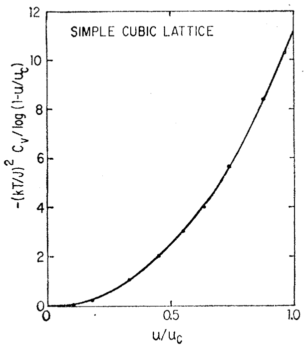

FIG. 1. $C_v/\log_e(1-u/u_c)$ as a function of u/u_c taken from the [7,7] Padé approximant for the simple cubic lattice.

In order to confirm (or negate) this hypothesis, we have computed $[N,N]$ Padé approximants to $-(kT/J)^2C_v(u)/[\log_e(1-u/u_c)]$. The Padé approximants evaluated at u_c are given in Table I for the simple cubic lattice (sc), the body-centered cubic lattice (bcc), the face centered cubic lattice (fcc), the two-dimensional simple quadratic lattice (sq), and the function $-x/[\log_e(1-x)]$. The values of u_c used in the preparation of this table are:

sq,	0.17157287525;
sc,	0.411940;
bcc,	0.5326607;
fcc,	0.664658.

The first thing one can note from Table I is that in the simple quadratic case where the tabulated quantity is known[6] to tend to $8/\pi$ we see apparent rapid convergence to a value about one percent smaller than the true value. Several remarks can be made about this. First, the difference between the [5,5] and the [4,4] approximants is abnormally small and is caused by the pole of very small residue between 0 and u_c. This phenomenon is quite common and has been discussed elsewhere.[1–3] It invariably slows the convergence by causing the very near equality of two successive approximants. Leaving the [5,5] aside, it still appears that the Padé approximant is not converging to the right value. (That it should converge to the wrong value is precluded by the theorem mentioned in Sec. 1.) To investigate what sort of rate of convergence we would expect we note that there will be terms which tend to zero inversely as $\log(1-u/u_c)$. This observation suggests considering the

[8] T. Arai, Phys. Rev. **126**, 471 (1962).
[9] G. F. Newell and E. W. Montroll, Revs. Modern Phys. **25**, 353 (1953).
[10] C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A235**, 247 (1956).
[11] C. Domb and M. F. Sykes, J. Math. Phys. **3**, 586 (1962).

convergence of $-x/[\log(1-x)]$ at $x=1$. The convergence of the $[N,N]$ Padé approximants to this function has been shown by Luke[12] to be exponential everywhere in the complex plane except on the cut $1\leq x\leq\infty$. At $x=1$ Luke's arguments break down. We have listed in Table I the values of the $[N,N]$ Padé approximants at $x=1$ for $N=1-12$. We find that $\log(N+1)$ times this sequence forms a monotonically increasing sequence and $\log(N+3)$ times this sequence forms a monotonically decreasing sequence. Thus the Padé approximants at $x=1$ apparently converge inversely as $\log(N)$. This rate is the slowest we have so far observed. Of all functions studied previously,[2] the slowest had converged at least as fast as $(N)^{-1/2}$. This very slow rate of convergence must be expected for all the lattices listed in Table I. Thus we see why the value obtained for the simple quadratic lattice is less accurate than might be expected in view of the closeness of successive approximants. We remark that the same slowness of convergence appears in the Taylor series expansion for

$$-\frac{\log_e(1-x)}{x}=1+\tfrac{1}{2}x+\tfrac{1}{3}x^2+\cdots.$$

The partial sums here for $x=1$ are only proportional to $\log(N)$.

The slow rate of convergence precludes the precise determination of the coefficient of $\log(1-u/u_c)$. However, judging by the reasonably accurate results obtained for the simple quadratic lattice and the agreement with the graphical extrapolation for the simple cubic lattice we feel that the conclusion that C_v is proportional to $\log(1-u/u_c)$ at u_c is confirmed and that the coefficients given by the last entry in Table I are more accurate than 10%.

The high-temperature expansion of $(kT/J)^2C_v$ is in terms of w^2 for the loose-packed lattices, simple cubic and body-centered cubic and w for the close-packed lattice, face-centered cubic, where $w=\tanh(J/kT)$. We have again listed the series expansions used in the

Table I. Results derived from $(kT/J)^2C_v(u)/[\log_e(1-u/u_c)]$.

N	$-x/[\log_e(1-x)]$	sq	sc	bcc	fcc
1	0.4	2.58817	...	...	...
2	0.3	2.51469	2.4012	...	...
3	0.2553	2.51857	12.0669	8.8835	...
4	0.2290	2.51576	12.1906	14.7564	...
5	0.2113	2.51567[a]	11.6193	20.2049	−299.28
6	0.1983		11.6207	21.6414	33.4795
7	0.1883			20.7962	33.2534
8	0.1803			20.3615	44.6989
9	0.1737				42.2747
10	0.1681				43.0475
11	0.1633				43.0834
12	0.1592				
∞	0.0	2.54648			

[a] Pole at 0.10405212 with residue of -2.09×10^{-8}.

[12] Y. L. Luke, J. Math. and Phys. **37**, 110 (1958).

Table II. Results derived from $(kT/J)^2C_v(w)w^\gamma/\log_e[1-(w/w_c)^\gamma]$.

N	sc	bcc	fcc
1	2.9714	5.9203	10.5072
2	3.3294	6.7303	11.3066
3	3.7769		−0.2030[a]
4			(12.9526)[b]

[a] Pole at $0.979w_c$.
[b] "[3.5,3.5]" = ([3,4]×[4,3])$^{1/2}$.

Appendix. They are derived from the results quoted by Domb[13] and Rushbrooke and Eve.[14] We first computed the $[N,N]$ Padé approximants to C_v and while the series were short the appearance of poles and zeros on the real axis directly beyond the critical point indicates[1] that it is likely to be a branch point. The Padé approximant method simulates a cut as a line of poles and zeros. We next computed the $[N,N]$ to $w^\gamma C_v(w)/\log_e[1-(w/w_c)^\gamma]$, where γ is 2 for loose-packed lattices and γ is 1 for close-packed ones. The values of the $[N,N]$ approximants at w_c divided by w_c^γ to $w^\gamma C_v(w)/\log_e[1-(w/w_c)^\gamma]$ are given in Table II. At the present time one may only say that the behavior is consistent with the hypothesis that there is a logarithmic singularity on the high-temperature side as well as the low-temperature side. The best results of Table II are remarkably close to 0.3 times thta for the corresponding low-temperature result. This is remarkable in that one cannot reasonably ascribe an accuracy of better than twenty percent to the results of Table II.

3. HEISENBERG MODEL MAGNETIC SUSCEPTIBILITY

Since the Heisenberg model for ferromagnetism is widely considered to be a good approximation to a real ferromagnet and some of its predictions, especially at low temperature, seem to be in agreement with experimental results, it is natural to ask if the Curie-Weiss law for magnetic susceptibility can be obtained as a consequence of the Heisenberg model for a three-dimensional lattice. If, in fact, the Heisenberg model did predict that the magnetic susceptibility became infinite in a manner inversely proportional to $(T-T_c)$ as required by Curie-Weiss law, then the magnetic susceptibility series should be easily summed by the method of Padé approximants. We have used the coefficients as given by Domb[15] from the work of Sykes,[16] Rushbrooke and Wood[17] and we have tabulated them in the Appendix for the convenience of the reader.

We computed the $[N,N]$ Padé approximants ($N=1-3$) for sc, bcc, and fcc lattices to the magnetic susceptibility, χ (actually the reduced susceptibility,

[13] Reference 7, p. 276.
[14] G. S. Rushbrooke and J. Eve, J. Math. Phys. **3**, 185 (1962).
[15] Reference 7, p. 329.
[16] M. F. Sykes, Oxford thesis, 1956 (unpublished).
[17] G. S. Rushbrooke and P. J. Wood, Mol. Phys. **1**, 257 (1958).

TABLE III. Location of the first pole of the $[N,N]$ Padé approximant to $\chi^m(K)$.

N	sc	bcc	fcc
1	0.61538	0.4	0.25
2	0.61541[a]	0.39109	0.25466
3	0.59359	0.39154	0.25134

[a] Pole at -0.013986 with residue 4.3×10^{-10}.

$\chi=kT\chi_0/m^2$). The hoped-for rapid convergence was not obtained and although the series of approximants was short, there seemed to be evidence, as explained above and in reference 1, that the critical point was a branch point. To investigate the nature of this branch point, and to obtain evidence from a viewpoint independent of the Padé approximant method such as was provided for the Ising model case by the work of Domb and Sykes[18] we have proceeded as follows. If χ is proportional to some power, $-(1+g)$, of $(T-T_c)$ at T_c then[18]

$$a_n/a_{n-1}\simeq(1+g/n)/K_c, \tag{3.1}$$

if the a_n are the coefficients in the series expansion of χ as a function of $K=J/kT$ and K_c is the critical value of K.

We have used (3.1) by fitting a_n/a_{n-1} to a straight line in $(1/n)$ by the usual method of least squares.[19] We obtained for K_c and g

$$\text{sc:}\quad K_c=0.581\pm0.011,\quad g=0.301\pm0.133, \tag{3.2a}$$

$$\text{bcc:}\quad K_c=0.392\pm0.002,\quad g=0.362\pm0.034, \tag{3.2b}$$

$$\text{fcc:}\quad K_c=0.255\pm0.001,\quad g=0.541\pm0.027. \tag{3.2c}$$

The errors quoted are the standard statistical ones for the errors in the coefficients of a fit. It is to be noted that the result for the simple cubic lattice is much more inaccurate than for the other two lattices. From (3.2) it looks likely that $g=\frac{1}{3}$ for the loose-packed lattices and $g=\frac{1}{2}$ for the close-packed one. We have, therefore, computed the $[N,N]$ Padé approximants to χ^m where $m=\frac{3}{4}$ for sc and bcc and $m=\frac{2}{3}$ for fcc. The agreement between the results of Table III and Eq. (3.2) is quite good. We consider, therefore, since we have consistent evidence from two points of view, that the exact power series coefficients definitely do *not* support the conclusion that the Heisenberg model implies the Curie-Weiss law. They also seem to imply that for the Heisenberg model, in contrast to the Ising model, the lattice structure may be important in determining the nature of the transition.

[18] C. Domb and M. F. Sykes, J. Math. Phys. **2**, 63 (1962).
[19] See, for instance, R. L. Anderson and T. A. Bancroft, *Statistical Theory in Research* (McGraw-Hill Book Company, Inc., New York, 1952).

APPENDIX

$(kT/J)^2C_v(u)$, Ising Model, Low Temperature

sq: $64u^2+288u^3+1152u^4+4800u^5+21504u^6+101920u^7+502016u^8+2538432u^9+13078720u^{10}+68344496u^{11}$,

sc: $144u^3+1200u^5-2016u^6+11760u^7-33792u^8+135216u^9-448800u^{10}+1643664u^{11}-5671872u^{12}+20239440u^{13}-70668192u^{14}$,

bcc: $256u^4+3136u^7-4608u^8+44800u^{10}-123904u^{11}+111360u^{12}+551616u^{13}-2464896u^{14}+4190400u^{15}+3779584u^{16}-40506240u^{17}$,

fcc: $576u^6+11616u^{11}-14976u^{12}+28800u^{15}+172032u^{16}-554880u^{17}+374976u^{18}+138624u^{19}+787200u^{20}+889056u^{21}-12568512u^{22}+20465952u^{23}-4564224u^{24}$.

$(kT/J)^2C_v(w)$, Ising Model, High Temperature

sc: $3+33w^2+564w^4+8976w^6+155124w^8+2791300w^{10}+51395172w^{12}$,

bcc: $4+140w^2+4056w^4+129360w^6+4381848w^8$,

fcc: $6+48w+390w^2+3216w^3+26844w^4+229584w^5+2006736w^6+17809008w^7$.

$\chi(K)$, Heisenberg Model, High Temperature

sc: $1+3K+6K^2+11K^3+\frac{165}{8}K^4+\frac{1561}{40}K^5+\frac{33013}{480}K^6$,

bcc: $1+4K+12K^2+\frac{104}{3}K^3+\frac{575}{6}K^4+\frac{2627}{10}K^5+\frac{16993}{24}K^6$,

fcc: $1+6K+30K^2+138K^3+\frac{2445}{4}K^4+\frac{53171}{20}K^5+\frac{914601}{80}K^6$.