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PADÉ APPROXIMANT CALCULATION OF THE SINGULARITY IN THE MAGNETIC SUSCEPTIBILITY OF AN ISING SQUARE LATTICE

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SUMMARY

The Padé approximant method was applied to Clapp's spin-spin correlation formulation for the magnetic susceptibility in an Ising square lattice, in order to investigate the nature of the critical point. For the exact cluster formulation it is found that as the cluster size increases, the critical point, namely the point at which the susceptibility has a singularity, approaches Onsager's exact value of 0.414, and that $\chi(t) \sim 1/(t - t_c)$. For the self-consistent formulation, twenty Padé approximants were calculated. The value of the critical point converged very rapidly to 0.41862770 and it was found that $\chi(t) \sim 1/(t - t_c)$.

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PADÉ APPROXIMANT CALCULATION OF THE SINGULARITY IN THE MAGNETIC SUSCEPTIBILITY OF AN ISING SQUARE LATTICE*

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INTRODUCTION

In this work the Padé approximant method is applied to the formula given by Clapp† for the magnetic susceptibility of an Ising square lattice, in order to determine the location and nature of the critical point. Utilizing spin-spin correlation functions and on the basis of a cluster theory, Clapp has developed an exact method and a self-consistent method for performing the cluster calculations. For a detailed exposition on the derivation of these methods and their applications in describing the behavior of magnetic systems, reference may be made to his thesis (Reference 1).

THE MAGNETIC SUSCEPTIBILITY

Fisher (Reference 2) gives the following high temperature formula for the susceptibility:

$$\chi = \frac{N\mu^2}{kT} \sum_{n=0}^{N} \langle \sigma_0^z \sigma_n^z \rangle ; \qquad T > T_c , \tag{1}$$

where N is the number of spins in the system, μ the magnetic moment of each spin, k the Boltzmann constant, T the absolute temperature, $\sigma = 2S$ where $S = 1/2$ for the systems considered here, and $\langle \sigma_0^z \sigma_n^z \rangle$ is the correlation function for the z components of the spins. Equation 1 is rewritten in the form (Reference 1):

$$\frac{kT}{N\mu^2} \chi(t) = \frac{1}{3} \cdot \frac{3 + 4t^2 - 4t^4}{1 - \lambda(t)} ; \qquad \lambda(t) < 1 , \tag{2}$$

*This work was performed during a post doctoral appointment at Massachusetts Institute of Technology; and a preliminary report will appear in *Physics Letters,* 15(2): March 15, 1965.

†See also P. C. Clapp, "Self-Consistent Correlation Theory of ferromagnetism," *Phys. Rev.* 137(4A):A1295-A1305, 1965, which appeared while this work was in the process of being published.

where

$$\lambda(t) = 2\langle 01\rangle \Big/ \left(1 + 2t^2 - 2t^4\right) \quad , \tag{3}$$

$$\langle 01\rangle = (01)/Z \quad , \tag{4}$$

$t = \tanh(\beta J/2)$, $\beta = 1/kT$, and J is the exchange integral.

The correlation function $\langle 01\rangle$ is a ratio of two polynomials in t, (01) and the partition function Z, whose degree depends on the number of spins in the cluster. (01) and Z have been tabulated by Clapp for a number of two dimensional clusters.

PADÉ APPROXIMANTS

In solving physical problems, the answer often can be obtained completely in principle, but sometimes it cannot be expressed in a closed form. For instance, in the three dimensional Ising model, any finite number of terms in the power series expansion of the partition function can be computed. Knowing every term of the series is equivalent to knowing the function everywhere, and by analytic continuation it can be extended outside the region of convergence of the power series representation. However, in some cases it is unnecessary to compute the value of the function and then to continue it analytically.

What is done is to replace the infinite series (of which only the first few terms may be known) by a ratio of polynomials. Such a ratio is called a Padé approximant (Reference 3) and the zeros of the numerator and denominator represent the zeros and poles of the function which is being approximated. Clearly, the more terms known in the series representation, the higher will be the degree of the Padé approximants that can be computed, and the more closely will the "true" function be represented. However, the question "When is the Padé approximant method applicable?" is difficult to answer (Reference 4).

An (N, M) Padé approximant, $P^{(M)}(\chi)/Q^{(N)}(\chi)$, has polynomials of degree M and N in the numerator and denominator respectively. In general it is sufficient to deal with the (N, N) approximants as they usually converge very rapidly (Reference 3). It will be seen later, that the degree of the numerator and of the denominator together cannot exceed the degree of the last term known in the series from which the approximants are being computed.

The Padé method enables the real pole of a function to be found even if it lies outside the circle of convergence of the power series from which the approximant was obtained. For example, if a function which has a known power series representation has poles in the complex plane inside a certain region, then by taking enough terms to represent these poles on the boundary of the circle of convergence, the Padé approximants can be computed. The real and complex poles of the function outside this region are given by the zeros of the Padé denominator. Baker (Reference 3) explains this in detail and reference may be made to his work.

A further advantage of the Padé method is that it enables the power with which a function diverges to be found. This is evident from the nature of the Padé polynomials. But what if, as in the case of the susceptibility, which near the critical point behaves as $1/(t - t_c)^a$, the pole is not a simple pole? In this case, forming the logarithmic derivative gives a function which has a simple pole:

$$\chi \sim \frac{1}{(t - t_c)^a} ; \qquad \frac{d}{dt} \ln \chi = \frac{-a}{(t - t_c)} ,$$

The power with which the susceptibility diverges at the critical point is obtained by evaluating the residue of the logarithmic derivative at the pole. For example, given the first few terms in the series expansion of the logarithmic derivative of the susceptibility,

$$\frac{d}{dt} \ln \chi(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + \cdots + a_M t^M + \cdots ,$$

let us try to locate the critical point t_c and a, where it is assumed that

$$\chi(t) \sim 1/(t - t_c)^a .$$

The series is first replaced by Padé approximants of the form

$$\frac{A^{(N)}(t)}{B^{(N)}(t)} = \frac{\sum_{n=0}^{N} A_n^{(N)} t^n}{\sum_{n=0}^{N} B_n^{(N)} t^n} ; \qquad N = 1, 2, 3, \cdots , M/2 .$$

The critical point in the Nth Padé approximation is the least real positive value of t for which $B^{(N)}(t)$ becomes zero. The value of a can then be found by calculating the residue of the approximant at the critical point.

$$-a = (t - t_c) \cdot \left. \frac{A^{(N)}(t)}{B^{(N)}(t)} \right|_{t=t_c}$$

This will become clearer by taking an example from Baker (Reference 3), who gives

$$\Theta(t) \equiv \frac{d}{dt} \ln \chi(t) = 3 + 3t + 9t^2 + 15t^3 + 33t^4 + \cdots ,$$

for the logarithmic derivative of the susceptibility of a plane hexagonal lattice. Let

$$B^{(1)}(t) = b_0^{(1)} + b_1^{(1)} t ,$$

$$A^{(1)}(t) = a_0^{(1)} + a_1^{(1)} t ,$$

$$\Theta(t) B^{(1)}(t) = 3b_0^{(1)} + \left(3b_0^{(1)} + 3b_1^{(1)}\right) t + \left(9b_0^{(1)} + 3b_1^{(1)}\right) t^2 + \cdots ,$$

And since $B^{(1)}(t)$ and $A^{(1)}(t)$ are each of degree 1, the following equalities may be made (Reference 4):

$$a_0^{(1)} = 3b_0^{(1)} , \tag{5}$$

$$a_1^{(1)} = 3b_0^{(1)} + 3b_1^{(1)} , \tag{6}$$

$$0 = 9b_0^{(1)} + 3b_1^{(1)} . \tag{7}$$

Inserting $b_1^{(1)}$ in terms of $b_0^{(1)}$ from Equation 7 into Equation 6 and eliminating $b_0^{(1)}$, we obtain the first Padé approximant:

$$\frac{A^{(1)}(t)}{B^{(1)}(t)} = \frac{2\left(t - \frac{1}{2}\right)}{t - \frac{1}{3}} .$$

And the residue is

$$\left(t - \frac{1}{3}\right) \frac{A^{(1)}(t)}{B^{(1)}(t)}\Bigg|_{t=1/3} = -\frac{1}{3} .$$

It is seen that the first Padé approximant locates the Curie point at $t_c = 1/3$ and indicates that the power with which the susceptibility diverges is 1/3. By calculating higher Padé approximants, these values are refined. For the example we have just described, the critical point occurs at $t_c = 0.577$ and the susceptibility behaves as $1/\left(t - t_c\right)^{1.75}$.

EXACT CLUSTER CALCULATIONS

By defining a reduced susceptibility,

$$\chi_R(t) = \frac{kT}{N\mu^2} \chi(t) ,$$

Equation 2 can be rewritten as

$$\chi_R(t) = F(t)/G(t) \ , \tag{8}$$

where

$$F(t) = A(t) \cdot Z \ , \tag{9}$$

$$A(t) = \left(3 + 4t^2 - 4t^4\right) \ , \tag{10}$$

$$G(t) = C(t) \cdot Z - 2(01) \ , \tag{11}$$

$$C(t) = \left(1 + 2t^2 - 2t^4\right) \ . \tag{12}$$

The IBM 709 was used to evaluate the polynomials $F(t)$ and $G(t)$ and to locate the zeros of $G(t)$. The smallest real positive value of t for which $G(t)$ is zero is identified as the critical point t_c. Table 1 gives t_c for different clusters of increasing size.

Table 1

Location of Singularity.

Number of Spins in Cluster	6	9	20	25	30
t_c	0.521	0.473	0.442	*	0.431

*This value was obtained and later misplaced.

It is evident from these results that the susceptibility has a singularity at a point which is identified as the critical point, and that as the cluster size increases, the critical point occurs at lower values of t. It is possible that in a cluster of an infinite number of spins, the critical point would converge to Onsager's exact value (Reference 5) of 0.414.

The Padé method (Reference 3) is now applied to the problem of determining the power with which the susceptibility diverges. Now, if

$$\chi(t) \sim 1/\left(t - t_c\right)^a \ ,$$

then

$$a = -\left(t - t_c\right) \cdot d(\ln \chi)/dt\big|_{t=t_c} \ .$$

Hence, if the expression $\chi(t) = F(t)/G(t)$ behaves as $1/\left(t - t_c\right)^a$ in the neighborhood of the critical point, the power a should be obtainable by evaluating the residue of the logarithmic derivative of the susceptibility at the critical point. This was done on the IBM 709 and the residue was found to be exactly -1 for each cluster. This means that whenever the susceptibility is calculated from a finite cluster in the exact manner of Clapp, it will appear as a ratio of polynomials and thus will behave as $1/(t - t_c)$. This can easily be proven, for let

$$\chi(t) = \frac{E(t)}{(t - t_c)} ,$$

where

$$E(t) = \frac{F(t)}{\hat{G}(t)}$$

and

$$\hat{G}(t) = \frac{G(t)}{(t - t_c)} .$$

Then

$$\frac{d(\ln \chi)}{dt} = \frac{E'(t)}{E(t)} - \frac{1}{(t - t_c)}$$

and the residue is

$$(t - t_c) \cdot d(\ln \chi)/dt \Big|_{t=t_c} = (t - t_c) \cdot \left[\frac{E'(t)}{E(t)} - \frac{1}{(t - t_c)}\right]\Bigg|_{t=t_c} = -1 .$$

SELF-CONSISTENT METHOD CALCULATIONS

The self-consistent method (Reference 1) may be explained briefly by considering an example of a two dimensional cluster of six spins. The bonds in Figure 1 represent the exchange coupling between spins located on the numbered sites. Unlike the usual cluster theory where all exchange couplings have the constant value J, in the self-consistent method only the coupling between spins 1 and 4 is assumed to have the value J. All other couplings are assumed to have a temperature dependent value $J_1(\beta)$ which is to be determined by requiring that at all temperatures the correlations between spins 1 and 4 and between spins 1 and 2 (or any outside nearest neighbor pair) be equal.

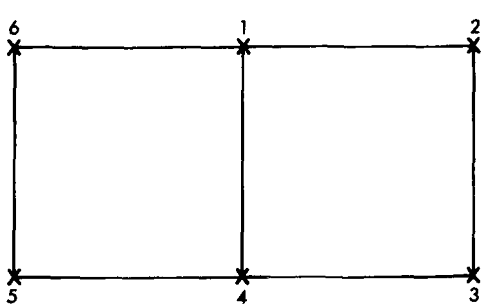

Figure 1—Spin cluster used for two-dimensional lattices.

The physical reasoning for this is that in an infinite lattice of which this cluster is a part, a spin pair like 1 and 2 for instance, will have, in addition to the coupling paths in the cluster, other paths in the rest of the lattice. If this temperature dependent additional coupling be represented by $J'(\beta)$, then the effective coupling between this spin pair will be given by $J_1(\beta)$, that is by the constant coupling J plus $J'(\beta)$. In the case of the pair 1-4, it is assumed that the coupling from the rest of the lattice is accounted for by the augmented coupling between spins on the perimeter of the cluster, thus enabling the coupling to be kept at the constant value J.

The correlation function $\langle 01 \rangle$, a function of J and J_1, now appears as a ratio of polynomials in t and t_1, where $t_1 = \tanh(\beta J/\sqrt{2})$. The requirement that in an infinite crystal all nearest neighbor correlations must be equal, leads to the self-consistency relation (Reference 1):

$$t_1 = \frac{1 - \sqrt{1 - 4t^2}}{2t}; \qquad t < \frac{1}{2} .$$

Thus in the self-consistent method calculation, the susceptibility

$$\chi_R(t) = \frac{1}{3}\,\frac{3 + 4t^2 - 4t^4}{1 - \lambda}, \qquad \lambda < 1 ,$$

can be put into the form

$$\chi_R(t) = \sum_{n=0} Q_n t^n , \tag{13}$$

where

$$\sum_{n=0} Q_n t^n = \frac{\sum_{n=0} F_n t^n}{\sum_{n=0} G_n t^n}, \tag{14}$$

$$\sum_{n=0} F_n\, t^n = A(t)\, C(t) \sum_{n=0} E_n\, t^n \;,$$

$$\sum_{n=0} G_n\, t^n = C(t) \sum_{n=0} E_n\, t^n - 2 \sum_{n=0} D_n\, t^n \;,$$

$$A(t) = \left(3 + 4t^2 - 4t^4\right) \;,$$

$$C(t) = \left(1 + 2t^2 - 2t^4\right) \;,$$

$$\sum_{n=0} D_n\, t^n = t + 2\left(\sum_{n=0} \tau_n\, t^n\right)^3 + t\left(\sum_{n=0} \tau_n\, t^n\right)^6 \;,$$

$$\sum_{n=0} E_n\, t^n = 1 + 2t\left(\sum_{n=0} \tau_n\, t^n\right)^3 + \left(\sum_{n=0} \tau_n\, t^n\right)^6 \;,$$

$$t_1 = \sum_{n=0} \tau_n\, t^n = \frac{1 - \sqrt{1 - 4t^2}}{2t} \;, \qquad t < \frac{1}{2} \;. \tag{15}$$

The logarithmic derivative of the susceptibility is

$$\frac{d(\ln \chi)}{dt} = \sum_{n=0} T_n\, t^n \;, \tag{16}$$

where

$$\sum_{n=0} T_n\, t^n = \frac{\sum_{n=0} \dot{Q}_n\, t^n}{\sum_{n=0} Q_n\, t^n}$$

and

$$\dot{Q}_n = (n+1)\, Q_{n+1} \;, \qquad n = 0, 1, 2, \cdots \;.$$

The IBM 709 was used to generate 41 terms in the power series expansion of t_1 and to compute the first 40 coefficients D_n, E_n, F_n, G_n, Q_n, $\dot{Q}_n$ and T_n. In Appendix A the series representation for the susceptibility and its logarithmic derivative are given. For comparison the poles of the susceptibility as given by Equation 14 were located. It was found that the only real value for which there is a pole is at $t = 0.41862991$.

The first 20 Padé approximants were then computed and their poles located. The critical point is identified as the smallest positive real value of t for which the approximant has a pole. At this point t_c, the residue was calculated and the results are tabulated in Table 2.

The fifth approximant locates t_c at 0.4151549 which is in excellent agreement with Onsager's exact value of 0.414. The sixth approximant behaves strangely with t_c at 3.4049675 and a residue of 33.771. This result seems spurious though it is not clear why it appears. The next fourteen approximants behave well and t_c converges rapidly to 0.41862770 with a slight oscillation in the last two decimal places. The residue rapidly becomes -1. It is interesting to observe that direct calculation of the singularity in the susceptibility locates t_c at 0.41862991.

Table 2

Results derived from $d(\ln \chi)/dt = \dfrac{\sum \dot{Q}_n t^n}{\sum Q_n t^n} = \sum T_n t^n$.

N	location of t_c	residue	N	location of t_c	residue
1	0.83333333	- 4.61	12	0.41862779	- 1.00000
2	0.8259	- 3.59	13	0.41862779	- 1.00000
3	0.34672120	- 0.336211	14	0.41862778	- 1.00000
4	0.4072426	- 0.793024		(0.21132568*	-11.3767×10^{-7})
5	0.4151549	- 0.915533	15	0.41862864	- 1.00000
6	3.4049675	33.771	16	0.41862795	- 1.00004
7	0.41884024	- 1.00726	17	0.41862788	- 1.00001
8	0.41859223	- 0.998611	18	0.41862784	- 1.00001
9	0.41862295	- 0.999777	19	0.41862816	- 1.00001
10	0.41862277	- 0.999769	20	0.41862770	- 1.00002
11	0.41862652	- 0.999937			

*The first real pole occurs at this value.

DISCUSSION AND CONCLUSIONS

For the exact cluster calculations the value of the critical point appeared to converge to the exact value as the size of the cluster increased, and the susceptibility behaves as $1/(t - t_c)$.

For the self-consistent calculations, twenty Padé approximants were calculated and the critical point was found to converge rapidly to 0.41862770 which is in excellent agreement with the value 0.41862991 obtained by directly calculating the location of the singularity in the susceptibility. Here, as well, the susceptibility behaves as $1/(t - t_c)$ which is consistent with the result of the exact cluster calculation.

Although the behavior of the susceptibility at the critical point is not predicted accurately by the self-consistent method of Clapp, the critical point itself is located with excellent accuracy. Insofar as this is obtained by using the smallest cluster, the self-consistent formulation seems a useful one. It is proposed to investigate, in a similar manner, the singularity in the susceptibility and in the specific heat of a Heisenberg lattice.

ACKNOWLEDGMENTS

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Appendix A

SERIES REPRESENTATION FOR THE SELF-CONSISTENT CLUSTER METHOD SUSCEPTIBILITY OF AN ISING SQUARE LATTICE

$$
\begin{aligned}
\chi(t) = {} & 3 + 6t + 16t^2 + 32t^3 + 60t^4 + 156t^5 + 384t^6 + 936t^7 \\
& + 2208t^8 + 5224t^9 + 12496t^{10} + 29984t^{11} + 71677t^{12} \\
& + 170960t^{13} + 408064t^{14} + 975136t^{15} + 2330368t^{16} \\
& + 5566560t^{17} + 13294784t^{18} + 31756544t^{19} \\
& + 75863039t^{20} + 181224890t^{21} + 432897020t^{22} \\
& + 1034067100t^{23} + 2470133200t^{24} + 5900589300t^{25} \\
& + 14095108000t^{26} + 33.669717 \times 10^9\, t^{27} + 80.428637t^{28} \\
& + 19.212452 \times 10^{10}\, t^{29} + 45.893912 \times 10^{10}\, t^{30} + 10.962941 \times 10^{11}\, t^{31} \\
& + 26.187793 \times 10^{11}\, t^{32} + 62.556262 \times 10^{11}\, t^{33} + 14.943172 \times 10^{12}\, t^{34} \\
& + 35.695605 \times 10^{12}\, t^{35} + 85.268115 \times 10^{12}\, t^{36} + 20.368479 \times 10^{13}\, t^{37} \\
& + 48.655348 \times 10^{13}\, t^{38} + 11.622579 \times 10^{14}\, t^{39} + 27.763514 \times 10^{14}\, t^{40}
\end{aligned}
$$

SERIES REPRESENTATION FOR THE LOGARITHMIC DERIVATIVE OF THE SUSCEPTIBILITY

$$
\begin{aligned}
\frac{d}{dt} \ln \chi(t) = {} & 2 + 6.666666t + 8t^2 + 70.111114t^3 + 92t^4 + 223.4074t^5 + 408t^6 \\
& + 863.60496t^7 + 2600t^8 + 6447.7359t^9 + 14368t^{10} \\
& + 33151.827t^{11} + 82448t^{12} + 199871.87t^{13} + 471008.05t^{14} \\
& + 1115647.7t^{15} + 2682975.8t^{16} + 6431553t^{17} + 15325437t^{18} \\
& + 36547323t^{19} + 87409346t^{20} + 20894122t^{21} \\
& + 49.885005 \times 10^7\, t^{22} + 11.912655 \times 10^8\, t^{23} + 28.464097 \times 10^8\, t^{24} \\
& + 68.002609 \times 10^8\, t^{25} + 16.242093 \times 10^9\, t^{26} + 38.795986 \times 10^{10}\, t^{27} \\
& + 92.680261 \times 10^{10}\, t^{28} + 22.139729 \times 10^{10}\, t^{29} + 52.884728 \times 10^{10}\, t^{30} \\
& + 12.632670 \times 10^{10}\, t^{31} + 30.176868 \times 10^{11}\, t^{32} + 72.085836 \times 10^{11}\, t^{33} \\
& + 17.219383 \times 10^{12}\, t^{34} + 41.132729 \times 10^{12}\, t^{35} + 98.256681 \times 10^{12}\, t^{36} \\
& + 23.471224 \times 10^{13}\, t^{37} + 56.066712 \times 10^{13}\, t^{38} + 13.372948 \times 10^{14}\, t^{39}
\end{aligned}
$$

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