

Application of the Padé Approximant Method to the Investigation of Some Magnetic Properties of the Ising Model*

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On the basis of the Padé approximant method we deduce from the exact series expansions for the Ising model that the reduced magnetic susceptibility behaves at the critical point as $\chi_{fcc} \approx [0.09923/(0.101767-w)]^{6/4}$, $\chi_{bcc} \approx [0.152773/(0.1561789-w)]^{6/4}$, $\chi_{sc} \approx [0.22138/(0.218156-w)]^{6/4}$, $\chi_t \approx [0.2432/(2-\sqrt{3}-w)]^{7/4}$, $\chi_{sq} \approx [0.35724/(\sqrt{2}-1-w)]^{7/4}$, and $\chi_h \approx [0.4506/(1/\sqrt{3}-w)]^{7/4}$, where $w = \tanh(J/kT)$ and the last figure quoted is somewhat uncertain. The spontaneous magnetization is found to behave as $(I_0/I_\infty)_{fcc} \approx [12.5(0.664658-z^2)]^{0.3}$, $(I_0/I_\infty)_{bcc} \approx [10.4(0.5326607-z^2)]^{0.3}$, $(I_0/I_\infty)_{sc} \approx [10.9(0.411940-z^2)]^{0.3}$, where $z = \exp(-2J/kT)$ and again the last place quoted is somewhat uncertain. The numbers 5/4 and 7/4 have an error of at most 10^{-3} , and 0.3 of at most 10^{-2} . The lattices referred to are fcc, face-centered cubic; bcc, body-centered cubic; sc, simple cubic; t, triangular; sq, simple quadratic; and h, honeycomb.

INTRODUCTION

IT is frequently the case in the solution of physical problems that one is unable to obtain a closed form for the answer. Yet one may, in principle, have completely solved the problem. Consider for example the three-dimensional Ising model. Methods have been developed¹ to compute any finite number of terms in the power series expansion of the partition function, both about infinite and zero temperature. From the theory of functions of a complex variable² we know that a knowledge of every term of the power series (convergent) is equivalent by analytic continuation to a knowledge of the function everywhere (as long as there are no "natural boundaries"). However, practically speaking the power series may converge so slowly as to be a most difficult way to evaluate the function. In fact, the power series may not even converge at all at the point of interest, even though the function considered is perfectly smooth and well behaved. [Consider, for example, $\tanh(10.0)$.] From the standard theory of analytic continuation, what one must do to continue the function beyond the circle of convergence of its power series is clear. We simply compute the value of the function and as many derivatives as necessary to as high a degree of accuracy as desired at some new point inside the circle of convergence but closer to the point of interest than our original origin. We obtain a new convergent series expansion for the function. By repeating this process sufficiently often we may finally obtain the value of the function at the point of interest (presumed non-singular).

In certain cases, all this work is not necessary. We may automatically obtain the analytic continuation by appropriate manipulations on the power series. Con-

sider, for example, a function $f(z)$ which has a singularity at $z = -1$ and all its other singularities within a circle of radius unity about $z = -2$. Suppose we wish to know $f(2)$ and $f(\infty)$. The change of variables $z = 3w/(1-2w)$ maps the exterior of the circle of radius unity about $z = -2$ in the z plane into the unit circle in the w plane. The points $z = 2$ and $z = \infty$ go into $w = 2/7$ and $1/2$, respectively. Since a power series converges out to the nearest singular point of the function it defines, the power series of $g(w) = f(3w/(1-2w))$ converges for all $|w| < 1$ and thus we may easily compute $f(2)$ and $f(\infty)$ from the power series expansion of $g(w)$. A case of very similar nature to the example just discussed is the spontaneous magnetization for the three-dimensional Ising model. The power series here is known *not* to converge at the critical point,¹ which makes the determination of its behavior near the critical point very difficult from the power series expansion. It is doubtless true that a trick similar to the one used in the example given above would enable one to compute the value of the spontaneous magnetization for every real temperature [the series expansions are given in terms of $\exp(-A/T)$] less than the critical temperature. The trouble is that one does not *a priori* know the location of all the singular points of the spontaneous magnetization. This trouble could be avoided if we could introduce a sequence of approximants to the function value which is invariant under the group³ of homographic transformations, $z = Aw/(1+Bw)$. One would expect such a sequence to converge at least as well as the best power series obtainable by any trick of the type described above. Such a sequence should automatically effect the analytic continuation to any point, not directly blocked off from the origin by singularities of the function under consideration.

The sequence of $[N, N]$ Padé approximants has the property that it is invariant under the above mentioned group of homographic transformations.⁴ In general a

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¹ C. Domb and M. F. Sykes, Proc. Roy. Soc. **A235**, 247 (1956) and references contained therein.

² See, for instance, E. T. Copson, *An Introduction to the Theory of Functions of a Complex Variable* (Oxford University Press, New York, 1948).

³ We shall actually consider only this subgroup of the full homographic group $z = (A+Bw)/(C+Dw)$.

⁴ G. A. Baker, Jr., J. L. Gammel, J. G. Wills, J. Math. Anal. and Applications **2**, 405 (1961).

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 full range of convergence of the sequence of $[N, N]$ Padé approximants is not known. For certain classes of functions their convergence has been proved and for many examples it has been shown to be quite rapid. For a fuller discussion of these questions the reader is referred to the work of Baker, Gammel, and Wills^{4,5} and the references quoted therein.

The purpose of this paper is to use the Padé approximant method (approximation by the sequence of $[N, N]$ approximants) to deduce relatively accurate values for the magnetic susceptibility and spontaneous magnetization for various three-dimensional Ising model lattices. We also consider the magnetic susceptibility for several two-dimensional lattices so that the value of the critical point deduced by this method may be compared with the exact value.^{6,7}

2. ESTIMATION OF THE NATURE AND LOCATION OF THE CRITICAL POINT FROM THE SERIES EXPANSIONS FOR THE MAGNETIC SUSCEPTIBILITY

The simplest assumption that one can make concerning the nature of the singularity of the magnetic susceptibility for a two- or three-dimensional Ising model lattice is that in the neighborhood of the critical point the magnetic susceptibility is proportional to $(1 - T_c/T)^{-1-\rho}$. The work of Sykes and Domb^{8,9} indicates that this assumption is very likely so. If it is so, then the logarithmic derivative of the magnetic susceptibility will have a simple pole at the critical point, and its residue will give the nature of the singularity. Since the Padé approximant is the ratio of two polynomials, a simple pole has the possibility of being exactly represented by the Padé approximant and hence one would expect convergence at this type of singularity to be particularly good. For this reason we have computed the $[N, N]$ Padé approximants to the logarithmic derivatives of the magnetic susceptibilities. We have used the series expansions given by Sykes and Domb.^{8,9} The logarithmic derivatives of the magnetic susceptibility,¹⁰ χ , are

⁵ G. A. Baker, Jr. and J. L. Gammel, *J. Math. Anal. and Applications* **2**, 21 (1961).

⁶ L. Onsager, *Phys. Rev.* **65**, 117 (1944).

⁷ R. M. F. Houtappel, *Physica* **16**, 425 (1950).

⁸ M. F. Sykes, *J. Math. Phys.* **2**, 52 (1961).

⁹ C. Domb and M. F. Sykes, *J. Math. Phys.* **2**, 63 (1961).

¹⁰ We are actually considering the reduced high-temperature susceptibility defined as $kT\chi_0/m^2$.

$$\begin{aligned} \frac{d \ln \chi_{fcc}}{dw} &= 12 + 120w + 1188w^2 + 11664w^3 + 114492w^4 \\ &\quad + 1124856w^5 + 11057268w^6 \\ &\quad + 108689568w^7 + \dots, \\ \frac{d \ln \chi_{bcc}}{dw} &= 8 + 48w + 344w^2 + 2016w^3 + 13928w^4 + 83376w^5 \\ &\quad + 567512w^6 + 3443136w^7 + 23173256w^8 + \dots, \\ \frac{d \ln \chi_{sc}}{dw} &= 6 + 24w + 126w^2 + 528w^3 + 2646w^4 + 11160w^5 \\ &\quad + 54942w^6 + 236448w^7 + 1147590w^8 \\ &\quad + 4995384w^9 + 23995758w^{10} + \dots, \\ \frac{d \ln \chi_t}{dw} &= 6 + 24w + 90w^2 + 336w^3 + 1266w^4 + 4752w^5 \\ &\quad + 17646w^6 + 65760w^7 + 245646w^8 + 917184w^9 \\ &\quad + 3422898w^{10} + 12773952w^{11} + \dots, \\ \frac{d \ln \chi_{sq}}{dw} &= 4 + 8w + 28w^2 + 48w^3 + 164w^4 + 296w^5 + 956w^6 \\ &\quad + 1760w^7 + 5428w^8 + 10568w^9 + 31068w^{10} \\ &\quad + 62640w^{11} + 179092w^{12} + 369160w^{13} \\ &\quad + 1034828w^{14} + \dots, \\ \frac{d \ln \chi_h}{dw} &= 3 + 3w + 9w^2 + 15w^3 + 33w^4 + 27w^5 + 87w^6 \\ &\quad + 159w^7 + 297w^8 + 243w^9 + 795w^{10} + 1503w^{11} \\ &\quad + 2499w^{12} + 2355w^{13} + 7209w^{14} + 13503w^{15} \\ &\quad + 21729w^{16} + 22707w^{17} + 64299w^{18} + 120975w^{19} \\ &\quad + 192411w^{20} + 214107w^{21} + 571461w^{22} \\ &\quad + 1086972w^{23} + \dots, \end{aligned}$$

where fcc stands for face-centered cubic lattice; bcc, body-centered cubic lattice; sc, simple cubic lattice; t, triangular lattice; sq, simple quadratic lattice; h, honeycomb lattice; and

$$w = \tanh J/kT, \quad J = \text{exchange integral.}$$

In Table I we have listed, except where otherwise noted, the location of and residue at the closest pole to the origin of the $[N, N]$ Padé approximant. By examination of the results listed in Table I it seems reasonable that, within an error of the order of a few thousandths, all the three-dimensional lattices have $g=0.25$ and all the two-dimensional lattices have $g=0.75$. These results confirm the previous observations of Domb and Sykes.⁹

It should be remarked that the poles in Table I which lie nearer than the one which corresponds to the ferromagnetic critical point always have a zero very close by and represent a severe perturbation of the function value over only a very small range. The occurrence of these perturbations is not clearly under-

TABLE I. Results derived from $d \ln \chi/dw$.

N	fcc		bcc		sc	
	location	residue	location	residue	location	residue
1	0.10101010	-1.2243648	0.13953488	-0.9345592	0.19047619	-0.8707483
2	0.10187683	-1.2564708	0.15593068	-1.242589	0.21510662	-1.2048243
3	0.10171078	-1.2451572	0.15618195	-1.2500231	0.21896751	-1.2808656
4			0.15601592	-1.2392262	0.21815114	-1.2505286
5					0.21818264	-1.2518014
					(-0.18387029	0.00068696)
N	t		sq		h	
	location	residue	location	residue	location	residue
1	0.26666667	-1.7066667	0.28571428	-0.6530612	0.33333333	-0.3333333
2	0.26705389	-1.7124366	0.41118648	-1.6545587	0.50000000	-1.0000000
3	(-0.12912285	0.00018936)				
4	0.26671401	-1.7055748	0.40926772	-1.6257290	no positive real pole	
5	0.26392285	-1.7516520	0.41644866	-1.7973526	0.56797947	-1.5308261
	(0.22948115	0.06541672)				
	0.26795019	-1.7495212	0.41216606	-1.6823402	0.56793836	-1.5302682
6			(-0.20919322	-0.00003223)	(-0.07395963	0.8×10^{-9})
7			0.41412464	-1.7458396	0.57301019	-1.6176357
8			0.41421058	-1.7496448	0.57266504	-1.6104612
9					(-0.09651947	-0.35×10^{-8})
10					0.57737042	-1.7512127
11					0.57739267	-1.7521167
					(-0.24445536	0.8×10^{-8})
					0.57736770	-1.7510165
					0.57737006	-1.7511293
∞	0.267949193		0.414213562		(-0.49713508	0.738×10^{-3})
					0.5773502692	

stood, but in the examples studied by Baker, Gammel, and Wills^{4,5} they have not impeded the convergence elsewhere.

To test the consistency of these results and obtain more accurate estimates of the location of the critical point we have raised the three-dimensional susceptibilities to the 4/5 power and the two-dimensional ones

to the 4/7 power. This operation has the effect of converting the ferromagnetic singularity into a simple pole. In Table II we list the location of the nearest pole and its residue for the $[N, N]$ Padé approximants to $[\chi(w)]^m$.

From looking at the results listed in Table II we see that the Padé approximants have converged to the

TABLE II. Results derived from $(\chi)^m$.

N	fcc		bcc		sc	
	location	residue	location	residue	location	residue
1	0.10204082	-0.09958349	0.16129032	-0.16649323	0.22727272	-0.24793388
2	0.10174095	-0.099113327	0.15627479	-0.15314145	0.21871837	-0.22349263
3	0.10177220	-0.099263130	0.15617854	-0.15277110	0.21804071	-0.22055930
4	0.10176345	-0.099202123	0.15617908	-0.15277365	0.21819754	-0.22169306
5					0.21814435	-0.22121910
N	t		sq		h	
	location	residue	location	residue	location	residue
1	0.26923077	-0.24852071	0.46666667	-0.49777778	0.73684211	-0.93074791
2	0.26837648	-0.24526609	0.41823005	-0.37414691	0.56866762	-0.42032321
3	0.27030309	-0.24664458	0.41404192	-0.35510985	0.56346843	-0.40380449
4	(0.21287916	-0.0023842)			(-0.14787515	-0.00000302)
	0.26784605	-0.24297979	0.41281162	-0.34657517	0.58226219	-0.47764838
5	0.26795882	-0.24383274	(-0.23886399	-0.00001166)		
6	0.26795969	-0.24383884	0.41421872	-0.35728803	0.57767633	-0.45254064
7	(0.12757395	-5.56×10^{-9})	0.41420612	-0.35719057	0.57719100	-0.44915654
			(-0.19136145	-0.9×10^{-8})		
			0.41421714	-0.35728743	0.57734619	-0.45052022
8					0.57734607	-0.45051897
9					(-0.01404287	-1.15×10^{-11})
10					0.57737434	-0.45082173
11					0.57734262	-0.45045917
12					(-0.54474770	-0.00015766)
					0.57734823	-0.45052893
					0.57735732	-0.45070361
∞	0.267949193		0.414213562		0.5773502692	

TABLE III. The $[N, N]$ Padé approximants to $(w-w_c)d \ln \chi/dw$ at w_c .

N	fcc	bcc	sc	t	sq	h
1	-1.2591654	-1.2211120	-1.2253865	-1.7320495	-1.5672233	-1.3660254
2	-1.2497759	-1.2507893	-1.3044557	-1.7320495 ^a	-1.7058387	0.0
3	-1.2497511	-1.2498902	-1.2501891	-1.7479548	-2.0000000	-1.6096621
4		-1.2493802	-1.2507423	-1.7508444	-1.7279384	-1.7179725
5			-1.2505479	-1.7494566	-1.7515982	-1.8376120
6					-1.7498932	-1.7409649
7					-1.7497973	-1.7542884
8						-1.7503526
9						-1.7501918
10						-1.7501958 ^b
11						-1.7500932

^a Pole at -0.562×10^{-6} with residue of -8.4×10^{-14} .

^b Pole at 0.11860601 with residue of -2.2×10^{-9} .

known answers for the location of the critical point within a few parts in the sixth place for the sq and h lattices and within a part in the fifth place for the triangular lattice. The rate of convergence for the three-dimensional lattices is such that about the same degree of accuracy is obtainable for them as was obtained for the two-dimensional cases. Furthermore they seem to show an oscillatory pattern of convergence (starting with $N=2$ for the loose packed lattices) which enables one to estimate the error. Using the rate of convergence as a guide to interpolate the last two approximants for each lattice, we estimate for the critical point

fcc	$w_c=0.101767$	Residue=0.09923
bcc	$w_c=0.1561789$	Residue=0.152773
sc	$w_c=0.218156$	Residue=0.22138

where the last place quoted must be considered rather uncertain. It is to be noted that these estimates are also consistent with those of Table I. They also round to the answers given by Domb and Sykes,⁹ except for the fcc which however differs by an amount which is less than their quoted error.

As an additional consistency check on our procedures we may now remove the simple pole in the logarithmic derivative which corresponds to the ferromagnetic critical point by multiplying the logarithmic derivative by $(w-w_c)$. We may then use Padé approximants to evaluate $(w-w_c)d \ln \chi/dw$ at w_c . Actually, for the close-packed lattices this refinement is not strictly necessary as the power series converges reasonably well at w_c . For the loose packed lattices χ goes to zero for a value of w somewhat smaller (algebraically) than $-w_c$, the antiferromagnetic critical point. This zero necessarily produces the maximum in χ_0 observed by Burley.¹¹ It also causes a singularity in $d \ln \chi/dw$ which slows the convergence of its power series so that the use of the Padé approximant method is necessary to obtain a reasonably accurate value at w_c from the terms available. We have listed the values of the $[N, N]$ Padé approximants to $(w-w_c)d \ln \chi(w_c)/dw_c$ in Table

III. They show consistency with the assumed values for g within an error of at most 10^{-3} . The exact values of w_c were used for the two-dimensional cases.

In Figs. 1 and 2 we have plotted the reduced magnetic susceptibility vs w/w_c . For loose-packed lattices this plot is carried over the whole disordered range from -1 to $+1$. The close-packed lattices are carried further in the negative direction as they have no antiferromagnetic state of order and hence no antiferromagnetic transition. We see that the magnetic susceptibility curves are differentiated almost entirely by the dimensionality of the lattice and the coordination number is relatively unimportant. These figures are based on the Padé approximants to $[\chi(w)]^m$. We have listed the coefficients for them in an Appendix.

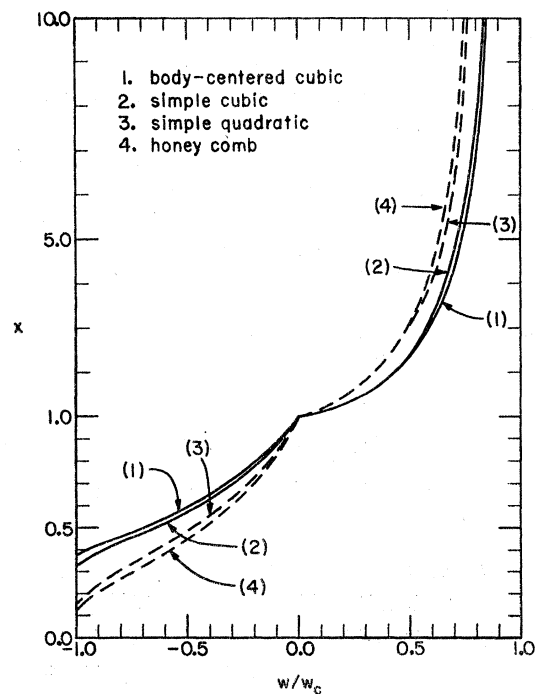


FIG. 1. Reduced magnetic susceptibility vs w/w_c for the loose-packed lattices. The discontinuity in the vertical scale at 1.0 should be noted.

¹¹ D. M. Burley, Phil. Mag. 5, 909 (1960).

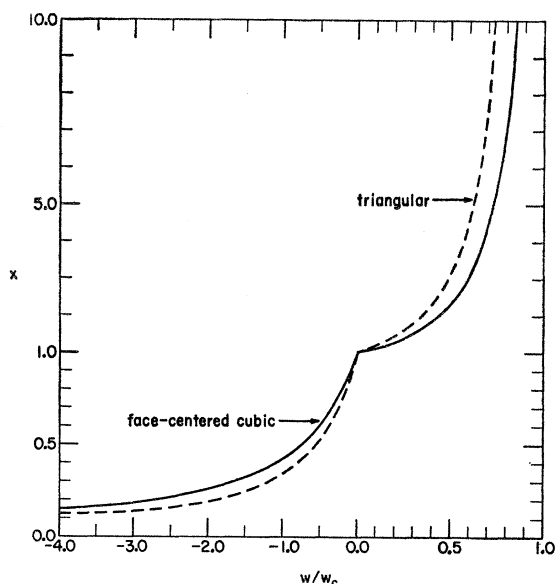


FIG. 2. Reduced magnetic susceptibility vs w/w_c for the close-packed lattices. The discontinuity in the vertical and horizontal scales should be noted.

3. ESTIMATION OF THE NATURE OF THE SPONTANEOUS MAGNETIZATION AT THE FERROMAGNETIC CRITICAL POINT

As is well known from the work of Yang,¹² Potts,¹³ and Naya,¹⁴ the spontaneous magnetization is proportional to $(T_c - T)^{1/8}$ for the two-dimensional Ising model lattices. If we assume that the spontaneous magnetization goes to zero at T_c like $(T_c - T)^n$, then, as in Sec. 2 for χ , the logarithmic derivative of the spontaneous magnetization has a simple pole at the critical point and we may study it by computing the $[N, N]$ Padé approximants to it. We remark that it is easy to see from the known exact values that this Padé approximant method will give the *exact* results for the two-dimensional cases by the computation of only a finite order approximant.

Using the results of Domb and Sykes¹ and the additional f functions

$$(sc) \quad f_9 = 24u^{14} + \dots,$$

$$(fcc) \quad f_6 = u^{24} + \dots,$$

we obtain for the logarithmic derivatives of the spontaneous magnetization, I_0/I_∞ ,

$$\begin{aligned} d \ln(I_0/I_\infty)_{fcc}/du &= -12u^5 - 264u^{10} + 288u^{11} - 720u^{14} - 4032u^{15} \\ &\quad + 11424u^{16} - 6996u^{17} - 3648u^{18} - 19680u^{19} \\ &\quad - 23184u^{20} + 266904u^{21} - 404064u^{22} + \dots, \end{aligned}$$

¹² C. N. Yang, Phys. Rev. **85**, 808 (1952).

¹³ R. B. Potts, Phys. Rev. **88**, 352 (1952).

¹⁴ S. Naya, Progr. Theoret. Phys. (Kyoto) **11**, 53 (1954).

TABLE IV. The $[N, N]$ Padé approximants to $[(1-u)(u_c-u)/u^2]d \ln(I_0/I_\infty)/du$ at u_c .

N	fcc	bcc	sc
1	...	0.54410588	0.30938496
2	...	0.32717390	0.28306575
3	0.43022570	0.32995454	0.30132063
4	0.31992175	0.19776749 ^a	0.30307992
5	0.32227436	0.32193537	0.30122094
6	0.32124883	0.30638038	
7	0.30826516		
8	0.30886220		
9	0.30741574		
10	0.30736227		

^a Pole at +0.577, zero at +0.557.

$$\begin{aligned} d \ln(I_0/I_\infty)_{bcc}/du &= -8u^3 - 112u^6 + 128u^7 - 1680u^9 + 3872u^{10} - 3368u^{11} \\ &\quad - 21216u^{12} + 81200u^{13} - 131280u^{14} + \dots, \end{aligned}$$

$$\begin{aligned} d \ln(I_0/I_\infty)_{sc}/du &= -6u^2 - 60u^4 + 72u^5 - 630u^6 + 1344u^7 - 6900u^8 \\ &\quad + 18960u^9 - 79332u^{10} + 246624u^{11} - 939900u^{12} + \dots, \end{aligned}$$

where

$$u = z^2, \quad z = \exp(-2J/kT) = (1-w)/(1+w).$$

Rather than proceeding as we did in Sec. 2, we may use our knowledge of the location of the critical point to proceed as we did in the construction of Table III; namely, we may remove the singularity by multiplying by $(u_c - u)$. As all the two-dimensional results had a singularity at $u = +1$ we will probably make our task simpler if we also remove it. Thus, we formed $[N, N]$ Padé approximants to

$$\frac{(1-u)(u_c-u) d \log(I_0/I_\infty)}{u^2 du},$$

where the u^2 in the denominator was included merely to keep the limit of the multiplying factor finite as $u \rightarrow \infty$. The reason for this requirement is that the logarithmic derivatives of the spontaneous magnetization in the two-dimensional cases tend to zero like

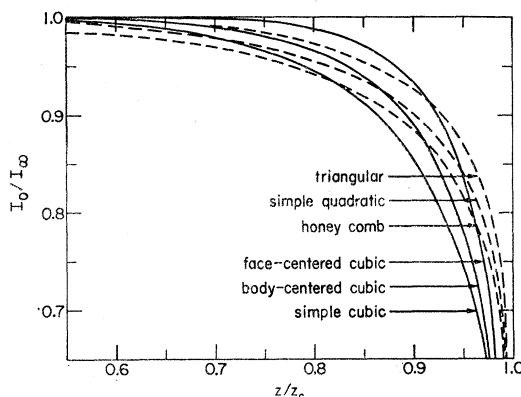


FIG. 3. Spontaneous magnetization vs z/z_c .

TABLE V. Results derived from $(I_0/I_\infty)^m$.

	fcc		bcc		sc	
	u_c	slope	u_c	slope	u_c	slope
3					0.45737318	-5.9809307
4			0.57254334	-6.0916502	0.41212918	-10.861860
5			0.41162508	-10.947899
6	0.70049101	-7.2065603	0.53413230	-10.224762	0.41164581	-10.944034
7	0.70049101 ^a	-7.2065603	0.53037024	-10.910849	0.41092472	-11.142299
8	0.53159797	-10.653271		
9	0.66360465	-12.661934				
10	0.66433442	-12.495958				
11	0.66399412	-12.577421				
12	0.66371331	-12.651636				
from χ	0.664658		0.5326607		0.411940	

^a The [6,6] and the [7,7] for the fcc are identical and the [8,8] does not exist. The [5,5] for the bcc does not exist.

u^{-1} (except for the honeycomb lattice where it is u^{-3}). We would expect the Padé approximants to do better further out if the functional behavior and the form of the approximant match at infinity. In Table IV we have listed the value of these Padé approximants at u_c . From these results we estimate that (I_0/I_∞) goes to zero like $(u_c - u)^{0.30}$ with an error of at most 10^{-2} in the power.

As a final check on the internal consistency of our results, if we form the $[N, N]$ Padé approximants to $(I_0/I_\infty)^{10/3}$ we should find a simple zero at the critical point. We see from Table V in which we list the location of the appropriate zero and the slope at that point that while the values for u_c obtained from the spontaneous magnetization are not as accurate as those from the magnetic susceptibility, they are however consistent with them within a few thousandths. The reason that these results are less accurate than those for the magnetic susceptibility is that the logarithm of spontaneous magnetization has roughly four complex

singular points which are as close or closer to the origin than the critical point. (There are not enough coefficients available for the simple cubic to identify more than one closer singularity.) In order to do a good job at the critical point, the Padé approximant must also take care of these other singularities.

In Fig. 3 we have plotted the spontaneous magnetization vs z/z_c over the whole ferromagnetic, ordered range. The difference between the appearance of Fig. 3 and Fig. 1 of Burley⁹ is more apparent than real and is the result of plotting vs z/z_c rather than T/T_c as he did. As the critical points for the three-dimensional lattices are generally at higher temperatures than for two-dimensional ones, this effect causes the difference in appearance.

ACKNOWLEDGMENTS

We wish to thank Mr. Herrick Lauson who coded the numerical calculations reported here for the IBM 704.

APPENDIX

We list here the Padé approximants from which the figures were prepared.

$$\begin{aligned} \chi_{\text{fcc}} &\approx [(1.0 - 6.4878493w + 29.266940w^2 - 11.816067w^3 - 7.4245573w^4) / \\ &\quad (1.0 - 16.087849w + 89.630294w^2 - 283.77802w^3 + 74.773566w^4)]^{5/4}, \\ \chi_{\text{bcc}} &\approx [(1.0 + 23.667027w + 134.51767w^2 + 176.26096w^3 - 92.930262w^4) / \\ &\quad (1.0 + 17.267027w - 15.671302w^2 - 666.90235w^3 - 1300.7945w^4)]^{5/4}, \\ \chi_{\text{sc}} &\approx [(1.0 + 6.1802658w + 6.3507605w^2 - 2.1384202w^3 + 25.127806w^4 + 4.8168171w^5) / \\ &\quad (1.0 + 1.3802658w - 21.394515w^2 - 26.707960w^3 + 24.087141w^4 - 122.05113w^5)]^{5/4}, \\ \chi_t &\approx [(1.0 + 0.87105230w + 3.0148162w^2 + 3.1175050w^3 + 3.0571423w^4 - 2.8165376w^5) / \\ &\quad (1.0 - 2.5575191w - 0.95124068w^2 - 8.4221376w^3 - 11.149369w^4 - 19.448134w^5)]^{7/4}, \\ \chi_{\text{sq}} &\approx [(1.0 + 4.4331741w + 6.6323991w^2 + 4.7961072w^3 + 1.7261877w^4 - 0.33157888w^5 \\ &\quad - 0.57263274w^6 - 4.3028266w^7) / (1.0 + 2.1474598w - 3.1740397w^2 - 11.015221w^3 - 13.264413w^4 \\ &\quad - 9.5895365w^5 - 6.7966830w^6 - 9.7192691w^7)]^{7/4}, \\ \chi_h &\approx [(1.0 + 1.7262288w + 3.2558681w^2 + 3.1997445w^3 - 6.1144361w^4 - 11.161589w^5 - 20.974653w^6 \\ &\quad - 14.779058w^7 + 4.1782428w^8 + 9.9072950w^9 + 17.623607w^{10} - 3.555816w^{11} + 2.8837465w^{12}) / \\ &\quad (1.0 + 0.011943082w + 0.90886364w^2 - 2.4094170w^3 - 11.214862w^4 - 2.9776.97w^5 - 7.1011106w^6 \\ &\quad + 19.066060w^7 + 27.538787w^8 + 15.376841w^9 + 8.8121770w^{10} - 23.012618w^{11} + 11.014469w^{12})]^{7/4}; \end{aligned}$$

$$\begin{aligned}
(I_0/I_\infty)_{\text{fcc}} &\approx [(1.0+3.8805092u+7.8281044u^2+13.419386u^3+14.181302u^4-1.7565205u^5-38.657407u^6 \\
&\quad -60.306173u^7-93.189067u^8-77.874280u^9-75.149353u^{10}+27.847042u^{11}-48.093601u^{12})/ \\
&\quad (1.0+3.8805092u+7.8281044u^2+13.419386u^3+14.181302u^4-1.7565205u^5-31.990740u^6 \\
&\quad -34.436111u^7-41.001704u^8+11.5882963u^9+19.392664u^{10}+96.136905u^{11}-53.146689u^{12})]^{3/10}, \\
(I_0/I_\infty)_{\text{bcc}} &\approx [(1.0+3.5481591u+7.8806661u^2-1.1714755u^3-19.310113u^4-46.487253u^5-37.851754u^6 \\
&\quad -26.364680u^7-39.358346u^8)/(1.0+3.5481591u+7.8806661u^2-1.1714755u^3-12.643446u^4 \\
&\quad -22.832859u^5+14.686020u^6+19.158817u^7-9.9683914u^8)]^{3/10}, \\
(I_0/I_\infty)_{\text{sc}} &\approx [(1.0+3.5495749u-5.7826623u^2-24.453557u^3-8.2315745u^4+15.570039u^5+49.840321u^6 \\
&\quad +13.621297u^7)/(1.0+3.5495749u-5.7826623u^2-17.786890u^3+15.432258u^4+17.018957u^5 \\
&\quad +11.021825u^6-35.665913u^7)]^{3/10}.
\end{aligned}$$

Measurement of the Refractive Index of Lucite by Recoilless Resonance Absorption*

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A method of frequency-modulating a monochromatic electromagnetic wave by varying the optical path length between the source and detector is described. The method has been applied to the measurement of the refractive index of Lucite for the 0.86 Å radiation emitted from Co^{57} ; the small frequency shift was detected by recoilless resonance absorption. The refractive index was found to be $1-n = (1.29 \pm 0.03) \times 10^{-6}$, in agreement with classical theory.

THIS paper describes a method of frequency-modulating a monochromatic electromagnetic wave by varying the optical path length between the source and detector. The method has been applied to, and is described in terms of, the measurement of the refractive index of Lucite for the 14.4-keV radiation emitted from Co^{57} . The measured refractive index agrees, within the 2% experimental uncertainty, with the simple theory applicable when the radiation energy is much greater than the binding energy of the electrons in the refractive medium, as in this case. The technique is in principle applicable to the nearly monochromatic radiation emitted from optical-frequency masers.

It is instructive to consider the method from two points of view, first in terms of frequency modulation and then in terms of a Doppler shift. Consider a source S and an observer (in our case a recoilless resonance absorber) A separated by a distance x [Fig. 1(a)]. A wave of angular frequency ω emitted by S will have the form $e^{i\omega(t-x/c)}$ at A . If a length L of material with refractive index n is placed in the optical path, the wave becomes $e^{i\omega(t-x/c)+i\phi}$, where the phase advance

$$\phi = (1-n)\omega L/c. \quad (1)$$

If ϕ changes with time, the instantaneous frequency seen by A will be $(\omega + d\phi/dt)$. This is done by moving a wedge-shaped piece of material to produce a frequency

shift

$$\frac{1}{2\pi} \frac{d\phi}{dt} = \Delta\nu = \nu \frac{(1-n) dL}{c dt}. \quad (2)$$

An equivalent point of view considers the radiation as being Doppler-shifted during the refraction by the moving wedge [Fig. 1(b)]. As it leaves the wedge the radiation is deflected (toward the normal, since $n < 1$) by an angle

$$\Delta\theta = (1-n) \tan\alpha.$$

The change in momentum of the photon is $\Delta p = p\Delta\theta$, and since the wedge is moving at a speed V it does work on the photon, increasing its energy by

$$\Delta E = V\Delta p = Vp(1-n) \tan\alpha = E[(1-n)/c]V \tan\alpha,$$

which is equivalent to Eq. (2) above.

For 14.4-keV radiation, the refractive index of Lucite is (see below)

$$(1-n) = 1.29 \times 10^{-6},$$

so that

$$(\Delta\nu/\nu)_{14 \text{ keV}} = 4 \times 10^{-17} dL/dt.$$

The frequency shift thus obtained for reasonable values of dL/dt can be detected by recoilless resonance scattering.¹

A schematic drawing of the experimental arrangement is shown in Fig. 2(a). The recoilless resonance

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¹ R. L. Mössbauer, *Z. Physik* **151**, 124 (1958); R. V. Pound and G. A. Rebka, Jr., *Phys. Rev. Letters* **4**, 337 (1960).