Determination of Critical Behavior in Lattice Statistics from Series Expansions. I.*

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A method is developed for determining the critical point and the critical exponent from terms of a series expansion for a restricted class of functions. The advantage of the method is that under certain reasonable assumptions it provides estimates for errors which are narrower than those usually given. As examples, we consider the high-temperature susceptibility series for the Ising model and the analogous chain-generating function for the excluded volume problem.

1. INTRODUCTION

IN recent years there has been renewed interest, both theoretically and experimentally, in the behavior of fluids and magnets in the neighborhood of their critical points. The system most studied theoretically has been the Ising model. Exact analytical results are known for the two-dimensional model, but since no analytical results are known for the three-dimensional model, considerable effort, chiefly by Domb, Sykes, and coworkers,[1] has been devoted to obtaining series expansions for the quantities of interest, and to obtaining the maximum amount of analytic information from the available terms in the series. Mathematically, the simplest problem that occurs can be stated as follows:

A function $f(x)$ has a power-series expansion about the origin of the form

$$f(x)=\sum_{n=0}^{\infty} a_n x^n, \tag{1.1}$$

and the coefficients a_n are known exactly for $n=0$, $1, \cdots, k$. Given that $f(x)$ has at least one singularity on the positive real axis, and that the closest such singularity μ^{-1} is algebraic, find μ and the exponent γ under the assumption

$$f(x)=(1-\mu x)^{-\gamma}h(x), \tag{1.2}$$

where $h(x)$ is analytic in and on the circle $|\mu x|\leq 1$ in the complex x plane, except possibly at $\mu x=-1$.

As examples, we consider here the high-temperature susceptibility χ of the Ising model and the analogous chain-generating function C for the excluded volume problem. In asserting that χ and C have the form (1.2) we are assuming (i) the closest singularity to the origin is at $|\mu x|=1$ and (ii) the "ferromagnetic" singularity at $\mu x=+1$ ($\mu x=-1$ corresponds to the "antiferromagnetic" singularity)[2] factors. Both assumptions are commonly made in the literature.[1] We stress, however, that they are not generally valid for Ising-model and excluded volume functions. For example, the specific-heat ferromagnetic singularity almost surely does not factor, and for the low-temperature Ising-model series one in general has singularities inside the circle $|\mu x|\leq 1$. In fact, the only functions for the Ising and excluded volume problems that we believe have the form (1.2) are the high-temperature susceptibilities and the chain-generating functions.

Two methods that have been used extensively in the problem of determining μ and γ from terms of a series expansion are the ratio method[1] and the method of Padé approximants.[3] Both methods give sequences of values for μ and γ, which are assumed to be convergent, and the results for μ and γ represent extrapolated limit points of the sequences, with errors stated being confidence limits rather than true errors.

Our purpose here is to present a simple method, applicable to functions of the form (1.2), for determining μ and γ. The advantage of the method is that under certain reasonable assumptions, precise error estimates for μ and γ can be given. Moreover, if either one of μ or γ is known, the estimate of the other is extremely accurate. The results for the high-temperature susceptibilities and the chain-generating functions are summarized in Tables I and II, respectively, where for comparison we have included the values usually quoted from the ratio and Padé methods.

Although the method presented here applies only to a very restricted class of functions, we believe that it can be generalized to cover a wider class of functions, and we hope to report on this at a later date.

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[1] For reviews and detailed references, see C. Domb, Advan. Phys. **9**, 34 (1960); M. E. Fisher, J. Math. Phys. **4**, 278 (1963); M. E. Fisher, *Boulder Lectures, 1964* (University of Colorado Press, Boulder, Colo., 1965); and C. Domb, Natl. Bur. Std. Publ. **273** (1966).

[2] For the Ising model it is trivial to prove that the antiferromagnetic singularity (for loose-packed lattices) occurs at $\mu x=-1$ if the ferromagnetic singularity occurs at $\mu x=+1$. The analogous result for the excluded volume problem has not been proved, although from the known terms of the series expansions for $C(x)$ it seems very likely that the distribution of the singularities of $C(x)$ in the complex x plane for a given lattice is identical with that of $\chi(x)$ and depends only on the lattice in question.

[3] G. A. Baker, Jr., Advan. Theoret. Phys. **1**, 5 (1965).

2. METHOD AND AN EXAMPLE

Consider a function $f(x)$ of the form (1.2), and let us assume initially that

$$h(x) \sim A(1+\mu x)^{\alpha} \quad \text{as} \quad \mu x \to -1. \tag{2.1}$$

Our method rests on the simple observation that for functions of the form (1.2), with $h(x)$ satisfying (2.1), *the coefficients* a_m *of* $(\mu x)^m$ *in*

$$h_n(x) = (1+\mu x)^n (1-\mu x)^{\gamma} f(x) \tag{2.2}$$

alternate in sign and decrease in magnitude for $n+\alpha > -1$ *and for sufficiently large* m [i.e., for $m \geq M(n)$, where $M(n)$ will in general be an increasing function of n]. This is proved simply by using the asymptotic form of the coefficients for $(1+\mu x)^n h(x)$ [remembering (2.1)], viz.,

$$[(-1)^m A(m+n+\alpha-1)!/m!(n+\alpha-1)!]. \tag{2.3}$$

Combinations of algebraic and logarithmic singularities [rather than (2.1)] can of course be treated in the same way with the same result (2.2).

If the function $f(x)$ does not have a singularity at $\mu x = -1$, we consider instead of $f(x)$ in (2.2), $\tilde{f}(x)$ defined by $\tilde{f}(x) = f(x)\, f(-x)$, i.e.,

$$\tilde{f}(x) = (1-\mu x)^{-\gamma} (1+\mu x)^{-\gamma} h(x) h(-x). \tag{2.4}$$

To demonstrate how the result (2.2) can be applied

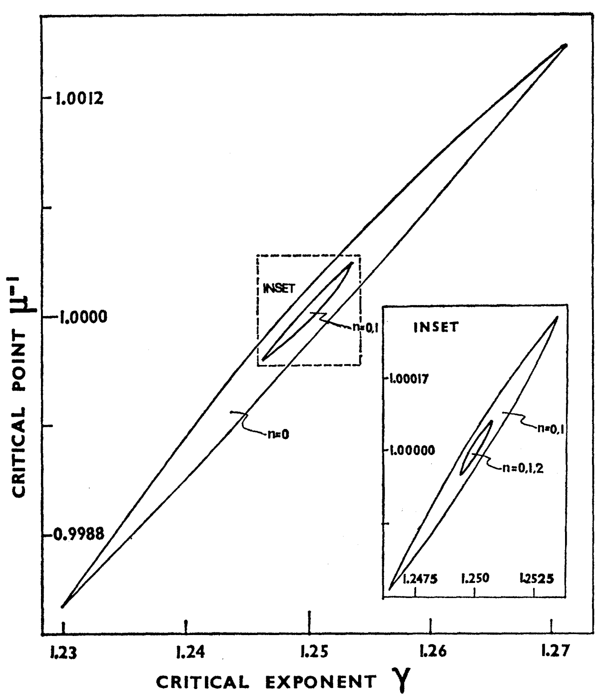

FIG. 1. Contour map of n values in the μ^{-1}-γ plane for the function (2.5).

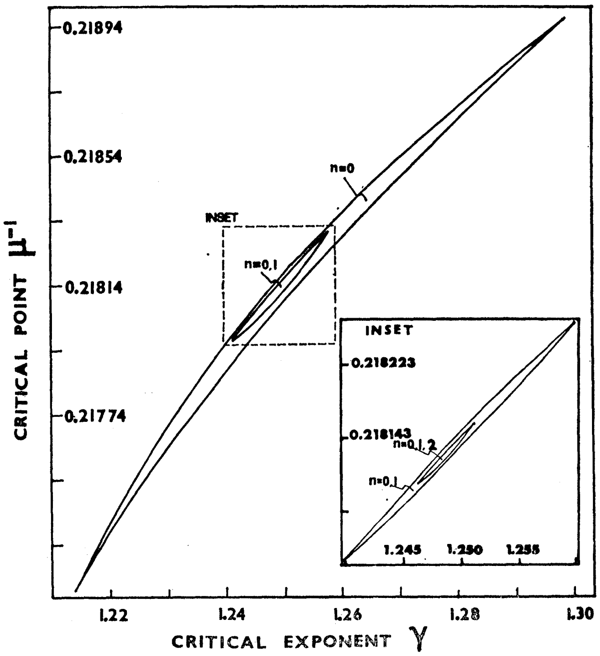

FIG. 2. Contour map of n values in the μ^{-1}-γ plane for the simple cubic high-temperature susceptibility.

to series analysis, let us examine the function

$$\begin{aligned} f(x) &= (1-x)^{-5/4}\{1.125 - 0.125(1+x^{-1}) \ln(1+x)\} \\ &= 1 + 1.1875x + 1.34896x^2 + 1.45117x^3 + 1.54596x^4 \\ &\quad + 1.61915x^5 + 1.68859x^6 + 1.7467x^7 + 1.8024x^8 \\ &\quad + 1.85109x^9 + \cdots, \end{aligned} \tag{2.5}$$

which may be considered as a prototype of the high-temperature susceptibilities for the loose-packed two-dimensional lattices,[4,5] and let us imagine that only the first 12 terms of the series are known, and initially, that μ is known to be unity. From (2.5) we have that

$$\begin{aligned} (1-x)^{5/4} f(x) &= 1 - 0.0623x + 0.02092x^2 - 0.01035x^3 \\ &\quad + 0.006296x^4 - 0.004128x^5 + 0.003007x^6 \\ &\quad - 0.002205x^7 + 0.001759x^8 - \cdots, \end{aligned} \tag{2.6}$$

which quickly settles down to the required alternating and decreasing behavior [note that the "antiferromagnetic" singularity is weaker than a simple pole so that (2.2) should and does hold for $n=0$]. We would say then that $\frac{5}{4}$ is a possible value for γ. Consider now

$$\begin{aligned} (1-x)^{1.248} f(x) &= 1 - 0.0605x + 0.02171x^2 - 0.009769x^3 \\ &\quad + 0.006710x^4 - 0.003780x^5 + 0.003287x^6 \\ &\quad - 0.001957x^7 + 0.001971x^8 \cdots. \end{aligned} \tag{2.7}$$

This series does not settle down to the required behavior

[4] M. F. Sykes and M. E. Fisher, Physica **28**, 919 (1962).
[5] M. E. Fisher and M. F. Sykes, Physica **28**, 939 (1962).

TABLE I. High-temperature susceptibility critical exponents and critical points.

		(1) Two-dimensional lattices.[a]					
	Method	Quadratic[b]	r	Honeycomb[b]	r	Triangular[b]	r
γ	Ratio and Padé	1.750 ± 0.003		1.750 ± 0.003		1.750 ± 0.003	
	Present $\bar{n}=0$	1.750 ± 0.005	13	1.77 ± 0.03	23	1.82 ± 0.15	13
	$\bar{n}=1$	1.7497 ± 0.0004	8	$\cdots$	$\cdots$	1.749 ± 0.005	12
	$\bar{n}=2$	1.7499 ± 0.0002	6	$\cdots$	$\cdots$		$\cdots$
μ	Exact	$1+\sqrt{2}$		$\sqrt{3}$		$2+\sqrt{3}$	

		(2) Three-dimensional lattices.					
	Method	sc[c]	r	bcc[c]	r	fcc[c]	r
γ	Ratio and Padé	1.250 ± 0.004		1.250 ± 0.004		1.250 ± 0.004	
	Present $\bar{n}=0$	1.26 ± 0.04	10	1.250 ± 0.060	8	1.30 ± 0.30	9
	$\bar{n}=1$	1.250 ± 0.008	8	1.247 ± 0.010	6	1.248 ± 0.046	8
	$\bar{n}=2$	1.249 ± 0.002	5	$\cdots$	$\cdots$	1.248 ± 0.011	7
μ^{-1}	Ratio and Padé	0.21815 ± 0.00030		0.15617 ± 0.00020		0.10175 ± 0.00001	
	Present $\bar{n}=0$	0.21809 ± 0.00090	10	0.15609 ± 0.00090	8	0.10179 ± 0.00280	9
	$\bar{n}=1$	0.21814 ± 0.00020	8	0.15612 ± 0.00020	6	0.10170 ± 0.00018	8
	$\bar{n}=2$	0.21812 ± 0.00004	5	$\cdots$	$\cdots$	0.10175 ± 0.00013	7
μ^{-1} assuming $\gamma=5/4$	Padé	0.218156 ± 0.000006		0.156179 ± 0.000009		0.101767 ± 0.000007	
	Present $\bar{n}=0$	0.218134 ± 0.000040	10	0.156152 ± 0.000051	8	0.101763 ± 0.000240	9
	$\bar{n}=1$	0.218144 ± 0.000009	8	0.156171 ± 0.000010	6	0.101759 ± 0.000032	8
	$\bar{n}=2$	0.2181437 ± 0.0000004	5	$\cdots$		0.101770 ± 0.000014	7

[a] The references given for each lattice indicate where the series may be found. For the quadratic lattice, the blank entry indicates that the zeros close up so far from $\gamma=7/4$ that no results are given. For the honeycomb lattice, the presence of further singularities on the circle of convergence requires a specialized analysis (see text) which leads to only one result. Other blank entries denote that there are insufficient terms in the series for results to be given in these cases.

[b] M. F. Sykes, J. Math. Phys. 2, 51 (1961).

[c] Reference 6.

and in fact is beginning to diverge. We conclude, therefore, that 1.248 is not a possible value for γ. With the aid of a computer it is possible to try a sequence of values for γ, and, using as a criterion for selecting possible values for γ that the last 12 terms of the series for $(1-x)^{\gamma}f(x)$ oscillate and decrease, we find that

$$\gamma=1.250\pm0.002, \qquad (n=0). \tag{2.8}$$

Our basic assumption [apart from (1.2)] is, of course, that if the correct value of γ is chosen, "regularities," once "established" in the known terms of the series for $h(x)$, will persist for all terms. Similar regularity assumptions are inherent in both ratio and Padé methods and in fact, in most, if not all, extrapolation techniques. In all cases, whether a trend is judged to be established or not is a matter of personal taste.

If one is willing to relax one's regularity requirements somewhat, the estimate (2.8) can be improved by investigating the $h_n(x)$ series [Eq. (2.2)] for $n=1, 2, \cdots$, and for a range of values of γ. For example, with $n=1$ we find that

$$(1+x)(1-x)^{5/4}f(x)=1+0.9375x-0.04167x^2 +0.01042x^3-0.004167x^4+0.00208x^5-0.001190x^6 +0.000744x^7-0.000496x^8+\cdots, \tag{2.9}$$

which converges much more rapidly than (2.6). If one then examines $h_1(x)$ for a range of values for γ and uses as a criterion that the last 10 terms of the series alternate and decrease, one has

$$\gamma=1.2500\pm0.0006, \qquad (n=1) \tag{2.10}$$

which is a considerable improvement on the $n=0$ estimate, Eq. (2.8).

Similarly, with $n=2$ and $n=3$, using as a criterion that the last nine and eight terms of $h_2(x)$ and $h_3(x)$, respectively, alternate and decrease, we find that

$$\gamma=1.2500\pm0.0002, \qquad (n=2)$$

and

$$\gamma=1.2500\pm0.0001, \qquad (n=3). \tag{2.11}$$

For $n>3$ the $h_n(x)$ series show no convincing regularity, so that one can conclude nothing with confidence. In general (although not with our present example), the irregularities in the coefficients for higher n values occur simply because multiplying by powers of $(1+\mu x)$, although diminishing the strength of the singularity at $\mu x=-1$, amplifies the effect of other singularities. (Eventually, of course, the coefficients must oscillate and decrease if we have chosen the correct exponent.) One must therefore exercise some caution when obtaining error estimates from large n values.

So far we have assumed that the exact value of μ is known. Let us now assume that μ is not known, which is in fact the case for the three-dimensional Ising model and the excluded volume problem in two and three dimensions. We proceed exactly as above except that now we examine the convergence of $h_n(x)$ for a range of

TABLE II. Chain-generating function critical exponents and critical points.

	Method	Quadratic[b,c]	r	Honeycomb[c,d]	r	Triangular[b,c]	r
		(a) Two-dimensional lattices.[a]					
γ	Ratio	1.333 ± 0.005		$\approx\frac{4}{3}$		1.333 ± 0.005	
	Present $\bar{n}=0$	···		···		1.43 ± 0.41	17
	$\bar{n}=1$	1.326 ± 0.014	4	···		···	
μ^{-1}	Present $\bar{n}=0$	···		···		0.2404 ± 0.0042	17
	$\bar{n}=1$	0.378867 ± 0.00026	4				
μ^{-1} assuming $\gamma=\frac{4}{3}$	Ratio	0.378932 ± 0.000071		0.5420 ± 0.0044		0.240862 ± 0.000063	
	Present $\bar{n}=0$	0.379008 ± 0.000088	13	···		0.24090 ± 0.00027	17
	$\bar{n}=1$	0.3790045 ± 0.0000038	4	0.5410904 ± 0.0000082	23	···	
		(2) Three-dimensional lattices.					
	Method	sc[b,e]	r	bcc[b,e]	r	fcc[b,e]	r
γ	Ratio	1.167 ± 0.010		1.167 ± 0.010		1.167 ± 0.010	
	Present $\bar{n}=0$	1.166 ± 0.039	14	1.187 ± 0.030	7	1.208 ± 0.202	13
	$\bar{n}=1$	1.1631 ± 0.0059	4	1.163 ± 0.009	6	1.165 ± 0.019	12
μ^{-1}	Present $\bar{n}=0$	0.213631 ± 0.00042	14	0.153099 ± 0.00089	7	0.09977 ± 0.0014	13
	$\bar{n}=1$	0.213512 ± 0.000078	4	0.153152 ± 0.00017	6	0.099636 ± 0.000150	12
μ^{-1} assuming $\gamma=7/4$	Ratio	0.213557 ± 0.000012		≈0.1529		0.0996528 ± 0.0000074	
	Present $\bar{n}=0$	0.213562 ± 0.000016	14	0.153185 ± 0.000053	7	0.099663 ± 0.000078	13
	$\bar{n}=1$	0.213561 ± 0.000001	4	0.153207 ± 0.0000010	6	0.0996529 ± 0.0000063	12

[a] The references given for each lattice indicate where the series may be found. For the quadratic lattice, the blank entry indicates that the zeros close up so far from $\gamma=4/3$ that no results are given. For the honeycomb lattice, the presence of further singularities on the circle of convergence requires a specialized analysis (see text) which leads to only one result. Other blank entries denote that there are insufficient terms in the series for results to be given in these cases.

[b] M. E. Fisher and B. J. Hiley, J. Chem. Phys. **34**, 1253 (1961).

[c] M. F. Sykes, J. Math. Phys. **2**, 51 (1961).

[d] M. E. Fisher and M. F. Sykes, Phys. Rev. **114**, 45 (1959).

[e] M. F. Sykes, J. Chem. Phys. **39**, 410 (1963).

values of μ as well as γ. Thus for a range of values of μ and γ we obtain the values of n for which at least the last r terms of $h_n(x)$ oscillate in sign and decrease in magnitude (the value of r depends on the number of available terms and how reasonable one is). The results for example (2.5) are shown in Fig. 1 as a contour map of n values in the μ^{-1}-γ plane for the case $r=8$. For $n\geq4$ the $h_n(x)$ series are not sufficiently regular for reasonable conclusions to be drawn. Also, if one demands more regularity, for example, by requiring that at least the last nine terms of $h_n(x)$ oscillate and decrease, one obtains no $n=3$ values and therefore a wider range of possible μ and γ values. Similarly, if one requires that the last 10 terms oscillate and decrease, one obtains no $n=2$ or $n=3$ values. The prescription one adopts then is that the maximum value of n, denoted by $\bar{n}(r)$, where r is the number of terms of the $h_n(x)$ series one requires to alternate and decrease, corresponds to the correct μ and γ. As can be seen from the figure, this condition is satisfied by a range of values lying in a thin closed region, the extremities of which give bounds for both μ and γ. For this example we have

$$\begin{aligned} &\mu^{-1}=0.9999\pm0.0017 && \gamma=1.2506\pm0.022 && r=12,\\ &\mu^{-1}=1.00005\pm0.00026 && \gamma=1.2505\pm0.003 && r=10,\\ &\mu^{-1}=1.00000\pm0.00005 && \gamma=1.2500\pm0.0006 && r=9,\\ &\mu^{-1}=1.000000\pm0.000016 && \gamma=1.2500\pm0.0002 && r=8. \end{aligned} \tag{2.12}$$

Note that the estimates for γ are not nearly so accurate as those given above assuming μ is known to be unity.

In addition to the above example, we have studied some more complicated functions and have concluded that if nine to fifteen terms of a series are known for functions of the type (1.2), requiring at least the last five or six terms of the series for $h_n(x)$ to alternate and decrease provides a reasonable criterion for determining μ and γ.

3. APPLICATIONS

A. Ising Model

Let us consider first the high-temperature susceptibility for the simple cubic lattice. Eleven terms of this series are known,[6] and the ratio and Padé estimates for μ and γ are usually quoted at about $\mu^{-1}=0.21815\pm0.00030$ and $\gamma=1.250\pm0.004$, respectively (with two extra terms Sykes[7] has recently estimated that $\mu^{-1}=0.21814$ with a possible error of a few parts in the last figure). We have scanned a range of values for μ and γ as indicated above and the resulting contour map is shown in Fig. 2, which is almost identical in form with that shown in Fig. 1. $\bar{n}=0$, 1, and 2 in this case are

[6] C. Domb and M. F. Sykes, J. Math. Phys. **2**, 63 (1961). The last two terms of the simple cubic series are in error, but are corrected in Ref. 5.

[7] M. F. Sykes (private communication).

appropriate if one requires that at least the last ten, eight, or five terms, respectively, of $h_n(x)$ oscillate and decrease. The results are tabulated in Table I. If one assumes that $\gamma=\frac{5}{4}$, which is the value commonly assumed to be correct, one finds that

$$\begin{aligned}\mu^{-1}&=0.2181338\pm0.0000375 \quad \text{for} \quad r=10 \quad (\bar{n}=0),\\ &=0.2181439\pm0.0000089 \quad \text{for} \quad r=\ 8 \quad (\bar{n}=1),\\ &=0.2181437\pm0.0000004 \quad \text{for} \quad r=\ 5 \quad (\bar{n}=2).\end{aligned} \tag{3.1}$$

These estimates differ somewhat from the Padé estimate[3] of $\mu^{-1}=0.218156\pm0.000006$ (also assuming $\gamma=\frac{5}{4}$) but are quite close to Sykes's recent estimate of 0.21814.

The same method can be applied directly to the high-temperature susceptibility for the quadratic, honeycomb, and body-centered cubic lattices (since these have antiferromagnetic singularities), and the results are also given in Table I.

For the quadratic lattice it is known that $\mu=1+\sqrt{2}$ so we have only tabulated the results for γ, which support very strongly the generally accepted result[1,6] of $\gamma=7/4$ exactly in two dimensions.

Similarly, for the honeycomb lattice it is known that $\mu=\sqrt{3}$ and that a pair of singularities occur at $x=\pm i\mu^{-1}$. The latter is reflected in the series for $h_1(x)$ which shows the characteristic $++--$ sign periodicity resulting from such a pair of singularities.[4]

For the triangular and face-centered cubic lattices, which have no antiferromagnetic singularities, we first form the series for $\chi(x)\ \chi(-x)$ [see Eq. (2.4)] and then apply the above method. These results are also given in Table I.

B. Excluded Volume Problem

The chain-generating function

$$C(x)=\sum_{n=0}^{\infty} c_n x^n, \tag{3.2}$$

where c_n is the number of n-step self-avoiding random walks on a lattice, is the analog of the high-temperature susceptibility χ for the Ising model (in fact, the series coefficients for χ are related to the c_n's). In this case, however, there is no physical analog to the antiferromagnetic singularity and in fact no proof exists that there is such a singularity. As mentioned, however,[2] the behavior of the series coefficients indicates the presence of such a singularity for the loose-packed lattices, and moreover it seems that the distribution of singularities for $C(x)$ in the complex x plane is identical with that for the Ising model for a given lattice. For example, if one investigates $h_1(x)$ for the honeycomb lattice, one encounters the same four-term sign periodicity for $C(x)$ as for χ. If one assumes that this periodicity persists for the correct μ and γ, one can eliminate those values for which $h_1(x)$ does not show the required periodicity. In this way one obtains the results given in Table II.

Assuming then that $C(x)$ is of the form (1.2), the method described in the previous section can be applied directly to $C(x)$ for the loose-packed lattices, and to $C(x)C(-x)$ for the close-packed lattices. The results are given in Table II.

In general, the $C(x)$ series is not so well behaved as the corresponding Ising-model series, and we do not feel confident in giving results beyond $\bar{n}=1$. The results, however, support the generally accepted values of $\gamma=\frac{4}{3}$ in two dimensions and $\frac{7}{6}$ in three dimensions. Assuming these values to be correct, we obtain the estimates for the attrition μ given in Table II, which are considerably more accurate than those previously published.

It is of interest to note that with these values for the triangular and honeycomb lattices μ_T and μ_H, respectively, we have

$$\mu_T+\mu_H=5.999\pm0.006$$

(or, using the result of Sykes *et al.*[8] for the triangular lattice, we obtain $\mu_T+\mu_H=5.9999\pm0.0015$), which supports very strongly Sykes's conjecture that the sum should be precisely six. (The analogous result for the Ising model is $\mu_T-\mu_H=2$, and a similar result holds for the percolation problem.)

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[8] J. L. Martin, M. F. Sykes, and F. T. Hioe, J. Chem. Phys. **46**, 3478 (1967).