

## Higher-order corrections for the quadratic Ising lattice susceptibility

Solomon Gartenhaus and W. Scott McCullough

Department of Physics, Purdue University, West Lafayette, Indiana 47907

(Received 29 April 1988)

Four terms in the expansion for the zero-field susceptibility of the quadratic Ising lattice at criticality are known exactly. We have computed three additional terms in this expansion by analyzing Nickel's high-temperature series for this lattice with second-order homogeneous differential approximants and Padé techniques. These three terms are found to vary as  $|t|^{1/4}$ ,  $t$ , and  $|t|^{5/4}$  with  $t = 1 - T_c/T$ , and their respective coefficients are obtained to within 0.01% accuracy. It is shown that, if terms of the form  $|t|^{1/4} \ln|t|$  and  $|t|^{5/4} \ln|t|$  were present, their amplitudes would be less than  $10^{-5}$  of the amplitudes of the  $|t|^{1/4}$  and  $|t|^{5/4}$  terms, respectively. The results are in accord with the predictions of the renormalization group if irrelevant variables are neglected and indicate that, if singularities due to irrelevant variables are present, their associated exponents must exceed 2. The results are also used to predict the coefficients of the low-temperature series for this system. Agreement to as much as one part in  $10^5$  with the known first eleven coefficients of this series is obtained.

### I. INTRODUCTION

Consider the two-dimensional Ising model on a quadratic lattice with ferromagnetic nearest-neighbor interactions. Thanks to the work of Onsager<sup>1</sup> and Yang<sup>2</sup>, and subsequently of other workers,<sup>3</sup> we have available today explicit formulas for the zero-field free energy and the spontaneous magnetization for this and various other two-dimensional Ising lattices. Unfortunately, there are no corresponding formulas for the zero-field susceptibility  $\chi_0$ —nor of any higher field derivatives of the free energy—for any of these lattices.

More recently, Wu *et al.*<sup>4</sup> have developed an exact expression for the spin-spin correlation functions for the quadratic lattice in zero-field. Combining this with the fluctuation-dissipation theorem one can derive an exact—albeit somewhat formidable—formula for the zero-field susceptibility. Various authors<sup>4-6</sup> have analyzed this result to obtain an expansion for  $\chi_0$  about the critical point. Their results to date may be expressed by the formula

$$T\chi_0 = C_{0\pm} |t|^{-7/4} + C_{1\pm} |t|^{-3/4} + D_{0\pm} + \dots + E_{0\pm} t \ln|t| + \dots \quad (1)$$

where  $t = 1 - T_c/T$  with  $T$  the absolute temperature and  $T_c$  the critical temperature and the  $+$  ( $-$ ) sign refers to the region  $T > T_c$  ( $T < T_c$ ). The dots between the third and fourth terms serve to indicate that terms of the form  $|t|^{1/4}$  and  $|t|^{1/4} \ln|t|$  may also be present, but their coefficients have as yet not been computed from the correlation functions.

To 10 decimal places, the two constants  $C_{0\pm}$  have the values<sup>4,5</sup>

$$C_{0+} = 0.9625817322 \dots$$

$$C_{0-} = 0.0255369719 \dots \quad (2)$$

For  $C_{1\pm}$ , Barouch *et al.*<sup>5</sup> obtain the surprisingly simple formula

$$C_{1\pm} / C_{0\pm} = \pm \sqrt{2} K_c / 8 \quad (3)$$

with  $K_c = (1/2) \ln(1 + \sqrt{2}) \approx 0.441$ . The constants  $D_{0\pm}$  in Eq. (1) were first estimated by use of Padé methods by Guttman<sup>7</sup> who concluded the equality  $D_{0+} = D_{0-} \equiv D_0$ . More recently, this constant  $D_0$  has been evaluated exactly<sup>6</sup> and found to be

$$D_0 = -0.10413324511 \dots \quad (4)$$

With regard to the constants  $E_{0\pm}$ , they have also been found<sup>8</sup> to satisfy the relation  $E_{0+} = E_{0-} \equiv E_0$  with  $E_0$  calculated to have the value

$$E_0 = 0.0403255003 \dots \quad (5)$$

A previous evaluation of the constant  $E_0$  by Padé techniques<sup>9</sup> led to  $E_0 = 0.0402 \pm 0.0004$  in complete agreement with Eq. (5).

Besides the four terms displayed in Eq. (1), the nature of the higher order terms has not been clearly ascertained. Studies based on the spin-spin correlation functions indicate<sup>4</sup> that terms proportional to  $|t|^{1/4}$ ,  $|t|^{1/4} \ln|t|$  and  $t$  may also be present. However, the coefficients of such terms have, as yet, not been determined.

The purpose of this work is to describe an analysis of Nickel's high-temperature series<sup>10</sup>—which has been recently extended to 55 terms<sup>11</sup>—with Padé<sup>12</sup> and second order homogeneous differential approximant techniques.<sup>13</sup> In outline, the method used to obtain, say, the leading correction term to Eq. (1), involves first reexpressing the four known terms there in terms of the appropriate high-temperature variable  $v$  [ $\equiv \tanh(J/T)$ ] and subtracting the result from Nickel's corresponding series for  $T\chi_0$ . The results, as then analyzed by means of

second order differential approximant techniques, yield the leading correction to Eq. (1). With five terms in the expansion for  $T\chi_0$  thus available, the process is repeated to obtain the sixth and so on. It is in this way that three additional terms for  $T\chi_0$  in Eq. (1) have been obtained.

As discussed in a preliminary report<sup>9</sup> in general terms our results indicate that, at least to the order considered here, the formula for the susceptibility of the quadratic Ising lattice is precisely that predicted by the renormalization group<sup>14,15</sup> (RG) if irrelevant variables are neglected.<sup>16</sup> This theory, consistent with our results, predicts that the leading missing term in Eq. (1) varies as  $|t|^{1/4}$  and gives correctly its coefficient. It also predicts that there is no term varying as  $|t|^{1/4} \ln |t|$ . Analogous results are found for the terms  $|t|^{5/4}$  and  $|t|^{5/4} \ln |t|$ . Indeed, we find that our computed formula for  $T\chi_0$  is fully in accord with that given by the RG in the absence of irrelevant variables through terms of order  $t^2 \ln |t|$  and  $t^2$ .

In Section II we summarize the predictions of the RG when irrelevant variables are neglected for  $T\chi_0$ . Also included in this section is a brief description of second order differential approximants and how they can be used to test for the existence of logarithmic and other singularities. Some mathematical details of the latter are relegated to Appendix A. Section III is then devoted to details of the calculations carried out and a presentation of our main results. In Section IV we consider some limitations of the present work due to systematic errors. In turn, these considerations suggest that we reverse the process and use our expansion for  $T\chi_0$  to compute values for the coefficients of the high-temperature series. The results are compared with Nickel's coefficients of  $v^n$  for  $n$  values in the full range  $1 \leq n \leq 54$ . As a further test of our underlying hypothesis, we use our results to compute a low-temperature series for  $T\chi_0$  and compare these predictions with the known first eleven terms of this series. Section V contains a summary and some concluding remarks.

## II. PRELIMINARIES

In this section we present (1) a summary of the results of the RG when irrelevant variables are neglected, and (2) a brief description of second order partial differential approximants and how they can be used to analyze the high-temperature series for the susceptibility of the quadratic, ferromagnetic Ising lattice.

### A. Summary of the RG without irrelevant variables

Consider a ferromagnetic system from the point of view of the renormalization group<sup>14,15</sup> (RG). According to RG studies, if we neglect the effects of irrelevant variables, then near the critical point the free energy  $F$  may be expressed in the form

$$F(t, h) = |g_t|^{2-\alpha} Y_{\pm}(g_h / |g_t|^{\Delta}) + A(t, h) \quad (6)$$

where  $\alpha$  and  $\Delta$  are the usual critical exponents<sup>17</sup> and  $h = H/T$  with  $H$  the magnetic field. The  $Y_{\pm}$  are two

universal functions of the indicated variable, and  $A(t, h)$  is an analytic "background" term. The quantities  $g_t$  and  $g_h$  are nonlinear scaling fields, which in the absence of irrelevant variables are presumed to be<sup>14,16</sup> analytic functions of  $t$  and  $h$ . In the asymptotic region about the critical point  $g_t$  and  $g_h$  vary as

$$\left. \begin{aligned} g_t &\simeq t \\ g_h &\simeq h \end{aligned} \right\} t, h \rightarrow 0. \quad (7)$$

and magnetic symmetry requires that they be even and odd in  $h$  respectively. Note that Eq. (6) reduces to the asymptotic scaling formula<sup>17</sup> in this limit in Eq. (7).

A direct consequence of the presumed analyticity of the nonlinear scaling fields and the structure of  $F(t, h)$  in Eq. (6) is the imposition of certain constraints on the analytic structure of various thermodynamic functions. For the zero-field free energy  $F_0$ , the spontaneous magnetization  $M_0$ , and  $\chi_0$  one finds<sup>16</sup>

$$\begin{aligned} \frac{F_0}{T} &= A_{F\pm} |t|^{2-\alpha} f_0(t) + A_0(t), \\ M_0 &= B_0 |t|^{\beta} m_0(t), \\ T\chi_0 &= C_{0\pm} |t|^{-\gamma} p_0(t) + E_0 |t|^{1-\alpha} e_0(t) + D_0 d_0(t), \end{aligned} \quad (8)$$

where  $\beta$  and  $\gamma$  are critical exponents,<sup>17</sup>  $A_{F\pm}$ ,  $B_0$ ,  $C_{0\pm}$ ,  $D_0$ , and  $E_0$  are constants,  $A_0(t)$  is an analytic background term, and  $f_0(t)$ ,  $m_0(t)$ ,  $p_0(t)$ ,  $e_0(t)$ , and  $d_0(t)$  are analytic functions each normalized to unity at  $t=0$ . For the case  $\alpha=0$ , corresponding to the logarithmic specific heat singularity of two-dimensional Ising systems, the terms  $|t|^{-\alpha}$  in the first and third of Eqs. (8) are to be replaced by<sup>16</sup>  $\ln |t|$ .

Besides its prediction of the structure of  $F_0$ ,  $M_0$ , and  $\chi_0$  in Eqs.(8), the relation in Eq. (6) also predicts that the three analytic functions  $f_0(t)$ ,  $m_0(t)$ , and  $p_0(t)$  there are not independent, but are related by the important relation<sup>18</sup>

$$p_0(t) = \frac{m_0^2(t)}{f_0(t)}. \quad (9)$$

Thus for systems, such as two-dimensional Ising models, for which  $f_0(t)$  and  $m_0(t)$  are both known, the analytic corrections to scaling given by  $p_0(t)$  are fully determined. If we define a set of constants  $a_F$ ,  $b_F$ ,  $c_F$ ,  $a_M$ ,  $\dots$ ,  $a_{\chi}$ ,  $\dots$  by the formulas

$$\begin{aligned} f_0(t) &= 1 + a_F t + b_F t^2 + c_F t^3 + \dots, \\ m_0(t) &= 1 + a_M t + b_M t^2 + c_M t^3 + \dots, \\ p_0(t) &= 1 + a_{\chi} t + b_{\chi} t^2 + c_{\chi} t^3 + \dots, \end{aligned} \quad (10)$$

then Eq. (9) gives the relations

$$\begin{aligned} a_{\chi} &= 2a_M - a_F, \\ b_{\chi} &= 2b_M - b_F + (a_F - a_M)^2, \\ c_{\chi} &= 2c_M - c_F + 2a_M b_M - b_F a_{\chi} b_{\chi} a_F. \end{aligned} \quad (11)$$

The first two of these were first obtained by Aharony and

Fisher.<sup>16</sup> For systems for which we may neglect irrelevant variables, the analytic corrections to scaling for the leading singular behavior of the susceptibility are thereby fixed by those for the free energy and the spontaneous magnetization.

Let us now specialize to the case of the two-dimensional Ising model, for which  $\alpha=0$  (logarithmic),  $\beta=1/8$ , and  $\gamma=7/4$ . The fact that the analytic structure of the first two of Eqs. (8) (with  $|t|^{-\alpha}$  replaced by  $\ln|t|$ ) are precisely correct for this model is well known from the exact Onsager and Yang solutions for the quadratic lattice. Furthermore, the first of Eqs. (11) has been shown<sup>16</sup> to give correctly the known first-order correction,  $C_{1+}/C_{0+}$  to  $p_0(t)$  as given by Eq. (3). Making use of the exact solutions<sup>1,2</sup> for  $F_0$  and  $M_0$ , we find from Eqs. (9)–(11) the results

$$\begin{aligned} a_\chi &= \frac{\sqrt{2}K_c}{8}, \\ b_\chi &= \frac{151K_c^2}{192}, \\ c_\chi &= \frac{615\sqrt{2}K_c^3}{512}, \end{aligned} \tag{12}$$

with  $K_c=(1/2)\ln(1+\sqrt{2})$ .

**B. Second order differential approximants and logarithmic singularities**

As for related extrapolation schemes, the method of second order homogeneous differential approximants<sup>13</sup> makes it possible to study the singular behavior of a function  $F(v)$  which can be expressed in the form

$$F(v) = \sum_{n=0}^{\infty} a_n v^n \tag{13}$$

at a point  $v=v_c$  given a knowledge of the first  $N+1$  terms of its power series about the point  $v=0$ . [For the high-temperature series of the quadratic Ising lattice susceptibility,  $v=\tanh(J/T)$ ,  $v_c=\sqrt{2}-1$ .] That is, given the  $N+1$  numbers  $a_0, a_1, \dots, a_N$ , and thereby the polynomial approximation  $f_N(v)$  to  $F(v)$

$$f_N(v) = \sum_{n=0}^N a_n v^n, \tag{14}$$

this method enables us to study the singular behavior of  $F(v)$  at a point  $v=v_c$ . Of particular interest is the case where  $F(v) \sim |v-v_c|^\rho \ln|v-v_c|$  and  $|v-v_c|^\rho$  for values of  $v$  near  $v_c$ .

The basic tool of the method is the second order, homogeneous differential equation

$$R_K(v) \frac{d^2 f_N}{dv^2} + P_L(v) \frac{df_N}{dv} + Q_M(v) f_N = 0 \tag{15}$$

with  $f_N(v)$  the *known* partial series in Eq. (14). The three quantities  $R_K, P_L$ , and  $Q_M$ , which are to be determined, are polynomials in  $v$  of order  $K, L$ , and  $M$ , respectively, with the relation  $K+L+M+3 \leq N$  a necessary condition for fixing the coefficients of these polynomials. The

approximants  $f_{KLM}(v)$  for the function  $F(v)$  are then defined as appropriate solutions of this equation valid in a neighborhood about  $v_c$  with  $R_K, P_L$ , and  $Q_M$  now given. The zeros of  $R_K(v)$  are the singular points of the equation and hence of  $F(v)$ . Generally, we impose the constraints that near  $v=v_c$ ,  $R_K(v) \sim (v-v_c)^2$ , and  $P_L(v) \sim (v-v_c)$ , or equivalently that  $R_K(v_c)=R'_K(v_c)=P_L(v_c)=0$  while  $R''_K(v_c) \neq 0$ , where the primes denote the derivative. As described in Appendix A, under these circumstances the point  $v=v_c$  is a “regular singular point” of Eq. (15) and explicit solutions for the equation about this point are known. Specifically, the exponents characterizing the singular behavior of  $F(v)$  are given by the two roots of the indicial equation<sup>19,20</sup>

$$\rho^2 + (p_0 - 1)\rho + q_0 = 0 \tag{16}$$

where

$$\begin{aligned} p_0 &= 2P'_L(v_c)/R''_K(v_c), \\ q_0 &= 2Q_M(v_c)/R''_K(v_c), \end{aligned} \tag{17}$$

and where the *constant*  $p_0$  here is not to be confused with the function  $p_0(t)$  in Eqs.(8)–(10). Similarly, we can extrapolate values for the ratios of the correction terms to the leading singular term of  $f_{KLM}(v)$  by use of the polynomials  $R_K(v), P_L(v)$  and  $Q_M(v)$ . Complete details can be found in the literature.<sup>13</sup>

Of particular interest is the possibility of detecting confluent logarithmic singularities, such as the terms varying as  $|t|^{1/4}$  and  $|t|^{1/4} \ln|t|$  that correlation function studies indicate might appear in the formula for  $\chi_0$  in Eq. (1). The signature for a singularity of this type is that the roots of the indicial equation differ by an integer.<sup>19,20</sup> For the pair of singularities  $|t|^{1/4}$  and  $|t|^{1/4} \ln|t|$  for example, each root would have the value  $1/4$  and the difference of the roots would be zero.

As noted above, in this work we invariably “bias” the approximants by forcing the point  $v=v_c$  to be a regular singular point of Eq. (15). This reduces by three the number of terms of  $f_N(v)$  required to determine the  $K+L+M+2$  unknown coefficients of the polynomials  $R_K, P_L$ , and  $Q_M$  for a given choice of  $[K, L, M]$ . In practice then, in place of Eq. (15) we really use the equation

$$\begin{aligned} (v-v_c)^2 R_{K-2}(v) \frac{d^2 f_N}{dv^2} \\ + (v-v_c) P_{L-1}(v) \frac{df_N}{dv} + Q_M(v) f_N = 0 \end{aligned} \tag{18}$$

where usually  $R_{K-2}(v), P_{L-1}(v)$ , and  $Q_M(v)$  do not vanish at  $v_c$ . At times we bias the approximants further by requiring that one root of the indicial Eq. (16) assume a particular value. This reduces further the number of terms in  $f_N(v)$  required.

Finally, we note that as is usual in this kind of analysis,<sup>12,13,21</sup> not all approximants obtained in this way are reliable. Some may be “defective”, in the sense that a root of  $R_K(v)$  falls between  $v=0$  and  $v=v_c$  on the real axis. Others should be discounted because a root of

$R_K(v)$  is close to  $v_c$ , say within 7% of  $v_c$ , even though  $v > v_c$ . Approximants with these properties are duly noted and are not included in the final analysis.

### III. RESULTS

The basic result of this work can be summarized by the following statement: the zero-field susceptibility  $\chi_0$  of the ferromagnetic, quadratic Ising lattice can, near criticality and for  $T > T_c$ , be expressed in the form

$$T\chi_0 = C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4} + D_0 + C_{2+} |t|^{1/4} + E_0 t \ln |t| + D_1 t + C_{3+} |t|^{5/4} + O(t^2 \ln |t|, t^2). \quad (19)$$

Here  $C_{0+}$ ,  $C_{1+}$ ,  $D_0$ , and  $E_0$  are exactly known constants given respectively to ten decimal places by Eqs. (2), (3), (4) and (5), and the constants  $C_{2+}$  and  $C_{3+}$  are found numerically to be equal—to one part in  $10^4$ —to formulas analogous to that for  $C_{1+}$  in Eq. (3):

$$C_{2+}/C_{0+} = b_\chi = \frac{151}{192} K_c^2, \quad (20)$$

$$C_{3+}/C_{0+} = c_\chi = \frac{615\sqrt{2}}{512} K_c^3.$$

That is,  $C_{2+}$  and  $C_{3+}$  are indistinguishable from the values predicted by the RG in the absence of irrelevant variables as given in Eq. (12). Finally, the constant  $D_1$  is found to have the value

$$D_1 = -0.14869 \pm 0.00001. \quad (21)$$

To order  $(t^2 \ln |t|, t^2)$  then, the result in Eq. (19) is in accord in all respects with the predictions of the RG when irrelevant variables are neglected. In particular, there are no terms of the form  $|t|^{1/4} \ln |t|$  nor  $|t|^{5/4} \ln |t|$  as had been suggested earlier.<sup>6</sup> An analysis to detect the presence of any such terms was specifically carried out and led to the conclusion that if they did exist, their coefficients would be less than  $10^{-5}$  that of  $C_{2+}$  and  $C_{3+}$  in these two cases, respectively.

Let us consider in some detail the arguments that have led to these conclusions.

#### A. The $|t|^{1/4}$ term

Consider the function  $T\chi_A$  defined as the difference between  $T\chi_0$  and its four exactly known terms in Eq. (1):

$$T\chi_A \equiv T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 - E_0 t \ln |t|. \quad (22)$$

Making use of Nickel's high temperature series<sup>10,11</sup> for  $T\chi_0$  we express  $T\chi_A$  as a series in the high-temperature variable  $v = \tanh(J/T)$  (see Appendix B for details). Substituting this series for the function  $f_N$  in Eq. (15) and using  $v_c = \sqrt{2} - 1 = 0.41421$ . . . , we make use of second order differential approximants as described above, to determine the analyticity behavior of  $T\chi_A$ . The results for the two exponents<sup>22</sup>  $\rho_1$  and  $\rho_2$ —the roots of Eq. (16)—are displayed in Table I for 18 choices of  $(K, L, M)$

TABLE I. Exponents  $\rho_1$  and  $\rho_2$  ( $\rho_2 \leq \rho_1$ ) obtained from unbiased and biased second order homogeneous differential approximants to the series represented by the quantity  $T\chi_A$  defined in Eq. (22). An asterisk (\*) denotes an approximant with an intervening spurious singularity and a dagger (†) an approximant for which the polynomials  $R_K$ ,  $P_L$ , and  $Q_M$  possess an intervening common root.

$[K, L, M]$	Unbiased exponents		Biased exponents	
	$\rho_2$	$\rho_1$	$\rho_2$ ( $\rho_1 \equiv 1$ )	$\rho_1$ ( $\rho_2 \equiv 0.25$ )
[10,9,11]	0.2509	0.9547	0.2487	0.9719
[10,10,10]	0.2471	1.1488	0.2374*	1.2052*
[10,11,9]	0.2488	1.0505	0.2410*	1.0589*
[10,10,11]	0.2494	1.0218	0.2498	0.9921
[10,11,10]	0.2493	1.0275	0.2498	0.9922
[11,10,10]	0.2475	1.1247	0.2494	0.9697
[10,11,11]	0.2498	0.9993	0.2498	0.9916
[11,10,11]	0.2476	1.1158	0.2498	0.9930
[11,11,10]	0.2476	1.1179	0.2498	0.9933
[11,10,12]	0.2496	1.0121	0.2498	0.9923
[11,11,11]	0.2504	0.9751	0.2498	0.9919
[11,12,10]	0.2479*	1.1026*	0.2500†	1.0015†
[11,11,12]	0.2495	1.0133	0.2498	0.9921
[11,12,11]	0.2495	1.0167	0.2498	0.9921
[12,11,11]	0.2496	1.0112	0.2498	0.9919
[11,12,12]	0.2498	0.9997	0.2498	0.9919
[12,11,12]	0.2494	1.0188	0.2498	0.9876
[12,12,11]	0.2485	1.0717	0.2498	0.9902

with  $K + L + M$  in the range 30–35. The second and third columns are the results for the unbiased calculations in which  $\rho_1$  and  $\rho_2$  are unconstrained [although we still force  $v_c$  to be a regular singular point of Eq. (15)]. The fourth column gives the results obtained if one exponent is forced to be 1 and the fifth if one exponent is forced to be 1/4. An asterisk (\*) denotes that the approximant displays a spurious singularity and a dagger (†) that  $R_K(v)$ ,  $P_L(v)$ , and  $Q_M(v)$  have a common root  $v_r$  with  $0 < v_r < v_c$ . For reasons to be discussed in the next section, we retain no more than five places of decimals in all values for the exponents.

Reference to the table shows that with very few exceptions the exponents  $\rho_1$  and  $\rho_2$  are very close to 1.0 and 0.25, respectively. This is particularly so for the biased exponents in the last two columns where in almost all cases the deviations from these values are significantly less than 1%. Averaging over all the nonasterisked entries, but including the daggered values in these four columns, we obtain for approximants with free exponents the values

$$\langle \rho_1 \rangle = 1.04 \pm 0.06, \quad (23)$$

$$\langle \rho_2 \rangle = 0.249 \pm 0.001,$$

while for the biased ones

$$\langle \rho_1 \rangle = 0.990 \pm 0.008 \quad (\rho_2 \equiv 0.25), \quad (24)$$

$$\langle \rho_2 \rangle = 0.2497 \pm 0.0003 \quad (\rho_1 \equiv 1).$$

The conclusion that the leading behavior of  $T\chi_A$  is  $|t|^{1/4}$  and  $t$  is inescapable. Note especially that  $\rho_1$  is significantly different from  $\rho_2=1/4$ ; had this not been the case, it might have indicated the existence of a confluent logarithmic singularity of the form  $|t|^{1/4}\ln|t|$ . It is, of course, possible that  $T\chi_A$  has additional singular behavior characterized by an exponent less than unity; if so, we conclude that its coefficient must be very small.

Having thus made the case that the leading term in  $T\chi_A$  is  $|t|^{1/4}$  let us consider the problem of obtaining its coefficient. To this end consider the difference  $T\chi'_A$  defined by

$$T\chi'_A = T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 - (C_{2+} - \Delta C_2) |t|^{1/4} - C_{3+} |t|^{5/4} \quad (25)$$

where  $C_{2+}$  and  $C_{3+}$  are defined in Eq. (20) and  $\Delta C_2$  is a parameter which will be allowed to vary.<sup>23</sup> Note that this time we have *not* subtracted the  $t \ln |t|$  term.

First with  $\Delta C_2=0$ , we carry out an analysis, as above, to determine the leading singular behavior of  $T\chi'_A$ . The resulting exponents are now given in Table II. As above, the second and third columns display the exponents obtained from unbiased approximants and the fourth column shows the exponents obtained with one exponent forced to be unity. Note that now the results for the unbiased calculations are not as consistent as in Table I, but strongly suggest that both exponents are unity. This is clearly manifest in the results for the biased calculation as given in the fourth column where all values are unity to within 0.1%. The fact that some of the exponents in the second and third columns have small imaginary parts is no problem; indeed it is surprising that complex exponents do not appear more frequently in this case where  $\rho_1 \approx \rho_2$ . The average value of  $\rho$  from the fourth column is found to be

$$\langle \rho \rangle = 1.0013 \pm 0.0003. \quad (26)$$

As discussed in the preceding section and in Appendix A, this degeneracy with both roots unity implies that with  $\Delta C_2 \equiv 0$  the leading terms in  $T\chi'_A$  vary as  $t$  and  $t \ln |t|$ . But more importantly from the viewpoint of Eq.(19) it also implies that the coefficient  $C_{2+}$  of the  $|t|^{1/4}$  term there must be close to, if not equal to the value in Eq. (20). And finally, this also confirms that no term with an exponent less than 1 is present in  $T\chi'_A$ .

To obtain a measure of the accuracy with which we can confirm this value for  $C_{2+}$ , let us reanalyze the series for  $T\chi'_A$  in Eq. (25) but now for a range of values of  $\Delta C_2$  about  $\Delta C_2=0$ . For each value for  $\Delta C_2$ , we force one of the roots of Eq. (16) to be unity and compute a value for the second one. The calculations were carried out for all approximants with orders  $K=L=M$  and  $L=K\pm 1$ ,  $M=K\pm 1$  which require for their determination 30–35 terms in the series. This is the same as for the values in Tables I and II. Disregarding the approximants with spurious singularities the resulting values for  $\rho$  associated with the given  $\Delta C_2$  were used to obtain an average value  $\langle \rho \rangle$  and an associated standard deviation. The results are plotted in Fig. 1 which shows a graph of

TABLE II. Exponents obtained by use of second order homogeneous differential approximants for the quantity  $T\chi'_A$  defined in Eq. (25) with  $\Delta C_2 \equiv 0$ . The exponents listed in the last column under  $\rho$  are obtained from approximants for which one exponent is forced to be 1 exactly. An asterisk (\*) denotes an approximant with an intervening spurious singularity.

[K,L,M]	Unbiased exponents		Biased exponent $\rho$
[10,9,11]	0.9449±0.0982i		1.0011
[10,10,10]	1.2449	0.9227	1.0013
[10,11,9]	1.1239	0.9413	1.0013
[10,10,11]	1.0687	0.9579	1.0012
[10,11,10]	1.0932	0.9495	1.0013
[11,10,10]	1.0919	0.9497	1.0009
[10,11,11]	0.9979±0.0246i		1.0011
[11,10,11]	1.0494	0.9665	1.0016
[11,11,10]	1.0953	0.9491	0.9838*
[11,10,12]	0.9999±0.0120i		1.0010
[11,11,11]	1.0279	0.9786	1.0012
[11,12,10]	1.0523	0.9655	1.0020
[11,11,12]	0.9935±0.0386i		1.0010
[11,12,11]	1.3534	0.9180	1.0009
[12,11,11]	0.9814±0.0621i		1.0011
[11,12,12]	1.1147	0.9452	1.0012
[12,11,12]	0.9880±0.0510i		1.0008*
[12,12,11]	0.8736±0.1068i*		1.0019

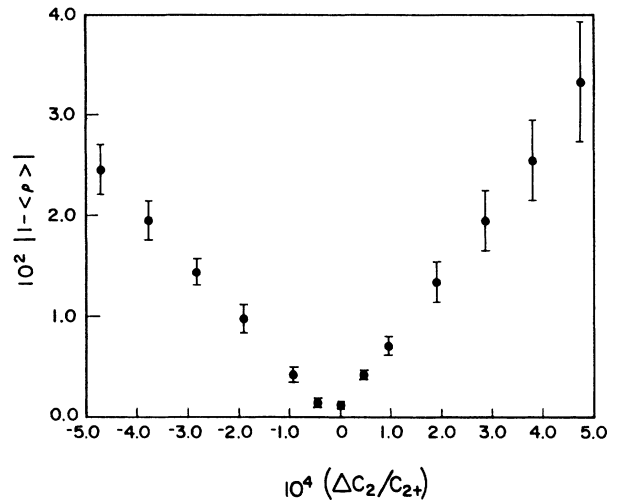


FIG. 1. Plot of  $10^2 |1 - \langle \rho \rangle|$  as a function of  $10^4 (\Delta C_2 / C_{2+})$ . Each value for  $\langle \rho \rangle$  was calculated by averaging the exponents obtained from a biased second order homogeneous differential approximant analysis of Eq. (25) with one exponent forced to be unity for various choices of the parameter  $\Delta C_2$  with  $C_{2+}$  as given in Eq. (20). The vertical bars indicate the standard deviation associated with the spread in the calculated values of  $\langle \rho \rangle$  for each value of  $\Delta C_2$ .

$|1 - \langle \rho \rangle| \times 10^2$  as a function of  $(\Delta C_2 / C_{2+}) \times 10^4$ . Each division along the vertical scale corresponds to a deviation of 1% in the value of the exponent from unity and each horizontal division a deviation of one part in  $10^4$  of  $C_{2+}$ . There is an unambiguous minimum near  $\Delta C_2 = 0$ , corresponding to the value for  $C_{2+}$  in Eq. (20) as the coefficient of the  $|t|^{1/4}$  term. As shown by the vertical bars, which represent one standard deviation, the fluctuations in the value for  $\langle \rho \rangle$  increase as  $\Delta C_2$  deviates more from zero. Since the minimum in the curve occurs for a value of  $\Delta C_2 / C_{2+}$  within  $10^{-4}$  of zero, we take this to be the uncertainty inherent in this method for determining the coefficient of  $|t|^{1/4}$ . That this is a reliable measure of the uncertainty has been confirmed by carrying out a similar analysis for the exactly known constant  $D_0$ .

### B. The $|t|^{5/4}$ term

With the  $C_{2+}|t|^{1/4}$  term established let us now consider the  $|t|^{5/4}$  term. To this end, we modify the difference in Eq. (22) by also subtracting out the  $|t|^{1/4}$  term and define a quantity  $T\chi_B$  by the formula

$$\begin{aligned} T\chi_B &= T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} \\ &\quad - D_0 - C_{2+} |t|^{1/4} - E_0 t \ln |t| \\ &\equiv T\chi_A - C_{2+} |t|^{1/4}. \end{aligned} \quad (27)$$

Repeating the same procedure as used above to deduce the  $|t|^{1/4}$  behavior of  $T\chi_A$ , we compute by use of second order differential approximants the values for the exponents characterizing the leading behavior of  $T\chi_B$ . The results for the same choices of  $(K, L, M)$  as above are shown in Table III. The second and third columns display the exponents obtained from unbiased approximants, the fourth column exponents obtained from approximants with  $\rho_1 = 1.25$  fixed, and the fifth column exponents with  $\rho_2 = 1$  fixed. Although the consistency of the values here is not nearly as good as those in Tables I and II—possibly due to the fact that  $\rho_1$  and  $\rho_2$  here are so close to each other—the conclusion that the leading terms of  $T\chi_B$  are associated with exponent values 1 and 1.25 seems plausible. Evidentially we cannot, on this basis alone, rule out additional singularities with exponents within a few percent of 1 or  $5/4$ , particularly if such terms have small coefficients. Averaging over the 18 nonasterisked values for  $\rho_1$  and  $\rho_2$  we obtain from the values listed in the unbiased columns the averages

$$\begin{aligned} \langle \rho_1 \rangle &= 1.20 \pm 0.03, \\ \langle \rho_2 \rangle &= 1.012 \pm 0.009. \end{aligned} \quad (28)$$

Thus, consistent with the earlier calculations  $\langle \rho_2 \rangle = 1$  but within 2% here. On the other hand the  $\langle \rho_1 \rangle$  value is somewhat smaller than 1.25 by  $\sim 4\%$ . However, on computing biased approximants with  $\rho_1 \equiv 1.25$  and with  $\rho_2 \equiv 1$ , we obtain from the values in the biased columns the averages (disregarding defective approximants)

$$\begin{aligned} \langle \rho_1 \rangle &= 1.240 \pm 0.003 \quad (\rho_2 \equiv 1.0), \\ \langle \rho_2 \rangle &= 0.997 \pm 0.001 \quad (\rho_1 \equiv 1.25). \end{aligned} \quad (29)$$

TABLE III. Exponents  $\rho_1$  and  $\rho_2$  ( $\rho_2 \leq \rho_1$ ) obtained from unbiased and biased second order homogeneous differential approximants to the quantity  $T\chi_B$  defined in Eq. (27). An asterisk (\*) denotes an approximant with an intervening spurious singularity and a dagger (†) an approximant for which the polynomials  $R_K, P_L$ , and  $Q_M$  possess an intervening common root.

[K,L,M]	Unbiased exponents		Biased exponents	
	$\rho_2$	$\rho_1$	$\rho_2$ ( $\rho_1 \equiv 1.25$ )	$\rho_1$ ( $\rho_2 \equiv 1$ )
[10,9,11]	1.0053	1.2199	0.9974	1.2396
[10,10,10]	0.9951	1.2595	0.9973	1.2390
[10,11,9]	0.9992	1.2423	0.9973	1.2392
[10,10,11]	1.0144	1.1918	0.9973	1.2393
[10,11,10]	1.0071	1.2140	0.9973	1.2393
[11,10,10]	1.0061	1.2163	0.9973	1.2388
[10,11,11]	1.0146	1.1911	0.9973	1.2391
[11,10,11]	1.0145	1.1915	0.9967	1.2373
[11,11,10]	1.0078	1.2123	0.9933	1.2316
[11,10,12]	1.0174	1.1833	0.9978*	1.2408*
[11,11,11]	1.0168	1.1849	0.9978*	1.2408*
[11,12,10]	1.0167	1.1855	0.9977*	1.2404*
[11,11,12]	1.0062†	1.2174†	0.9977†	1.2405†
[11,12,11]	1.0164	1.1868	1.0050*	1.2910*
[12,11,11]	1.0302	1.1518	0.9985	1.2434
[11,12,12]	1.0152	1.1901	0.9975†	1.2398†
[12,11,12]	1.0246	1.1644	0.9979†	1.2411†
[12,12,11]	1.0049	1.2255	0.9991	1.2458

These strongly suggest the exponents 1 and 1.25 although it should be noted that an exponent close to, but not exactly  $5/4$  is not clearly ruled out by these calculations. The argument below relating to the coefficient of the  $|t|^{5/4}$  term, however, strengthens the conclusion that  $\rho_1$  is indeed  $5/4$ .

The determination of the coefficient of the  $|t|^{5/4}$  term proceeds in a spirit similar to that used to determine the coefficient  $C_{2+}$ , but with some differences. We now analyze the quantity

$$\begin{aligned} T\chi_C &= T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 \\ &\quad - C_{2+} |t|^{1/4} - E_0 t \ln |t| - C_{3+} |t|^{5/4} \end{aligned} \quad (30)$$

with  $C_{2+}$  and  $C_{3+}$  given in Eq. (20). Computing values for the exponents by use of second order homogeneous differential approximants we find that the leading singular behavior of  $T\chi_C$  has the structure<sup>24</sup>  $t^2 \ln |t|$  and  $t$ . This is shown in Table IV. The unbiased columns give the exponents  $\rho_1$  and  $\rho_2$  obtained from unbiased approximants, and the biased columns the values obtained from approximants biased to force  $\rho_1 \equiv 2$  and  $\rho_2 \equiv 1$ . The values obtained clearly suggest that  $\rho_2 = 1$  and  $\rho_1 = 2$ , although the latter is confirmed only to within 2%. Averaging over the nondefective approximants in each column, we obtain from the unbiased values the averages

$$\begin{aligned} \langle \rho_1 \rangle &= 2.04 \pm 0.05, \\ \langle \rho_2 \rangle &= 1.0001 \pm 0.0002, \end{aligned} \quad (31)$$

TABLE IV. Exponents  $\rho_1$  and  $\rho_2$  ( $\rho_2 \leq \rho_1$ ) obtained from unbiased and biased second order homogeneous differential approximants to the quantity  $T\chi_C$  defined in Eq. (30). An asterisk (\*) denotes an approximant with an intervening spurious singularity and a dagger (†) an approximant for which the polynomials  $R_K, P_L$  and  $Q_M$  possess an intervening common root.

[K,L,M]	Unbiased exponents		Biased exponents	
	$\rho_2$	$\rho_1$	$\rho_2$ ( $\rho_1 \equiv 2$ )	$\rho_1$ ( $\rho_2 \equiv 1$ )
[10,9,11]	0.9997	1.9969	0.9997*	1.8044*
[10,10,10]	0.9999	2.0153	0.9996*	2.0194
[10,11,9]	1.0000	2.0238	0.9996*	2.0245
[10,10,11]	1.0000	2.0247	0.9997	2.0227
[10,11,10]	1.0000	2.0280	0.9998	2.0253
[11,10,10]	1.0000	2.0124	1.0002	2.0098
[10,11,11]	1.0000	1.9858	1.0000	2.2177*
[11,10,11]	1.0001	2.0368	0.9999	2.0202
[11,11,10]	1.0001	2.0463	0.9999	2.0224
[11,10,12]	1.0000	1.9979	1.0000	2.0032
[11,11,11]	1.0001	2.0263	1.0000	1.9616*
[11,12,10]	1.0002	2.0572	0.9997†	2.0332
[11,11,12]	0.9688*	1.0953*	1.0000	2.0023
[11,12,11]	1.0004	2.1400	1.0000	2.0043
[12,11,11]	1.0004*	2.1536*	1.0000	1.9994
[11,12,12]	1.0003	2.1045	1.0000	1.9934
[12,11,12]	1.0005*	2.2019*	1.0000*	2.0143*
[12,12,11]	1.0004	2.1461	1.0008*	2.3337*

TABLE V. Exponents obtained from second order homogeneous differential approximants for the quantity  $T\chi_D$  as defined in Eq. (33) with  $\Delta C_3 \equiv 0$ . The exponents  $\rho$  are obtained from approximants for which one exponent is forced to be 2 exactly. An asterisk (\*) denotes an approximant with an intervening spurious singularity.

[K,L,M]	Unbiased exponents		Bias exponent
	$\rho_2$	$\rho_1$	$\rho$
[10,9,11]	1.8646*	3.0399*	1.9985
[10,10,10]	1.9219	2.1547	1.9975
[10,11,9]	1.9161	2.1797	1.9983
[10,10,11]	1.9080	2.2224	1.9989
[10,11,10]	1.9064	2.2328	1.9989
[11,10,10]	1.8873	2.4069	1.9988
[10,11,11]	1.8742*	2.6653*	1.9982
[11,10,11]	1.9168	2.1764	1.9986
[11,11,10]	1.9138	2.1911	1.9987
[11,10,12]	1.9127*	2.1942*	2.0057*
[11,11,11]	1.9982±0.01700i		1.9983
[11,12,10]	1.9783±0.07757i		1.9985
[11,11,12]	1.9028*	2.2527*	1.9983
[11,12,11]	1.8578*	3.6504*	1.9983
[12,11,11]	1.8847*	2.4496*	1.9983
[11,12,12]	1.5852*	1.7532*	1.9974*
[12,11,12]	1.7622±0.1234i*		1.9946*
[12,12,11]	1.4552*	1.7813*	2.0014*

and for the biased values the averages

$$\begin{aligned} \langle \rho_1 \rangle &= 2.01 \pm 0.01 \quad (\rho_2 \equiv 1.0), \\ \langle \rho_2 \rangle &= 0.9999 \pm 0.0001 \quad (\rho_1 \equiv 2.0). \end{aligned} \tag{32}$$

Thus we conclude that<sup>24</sup> the leading “singular” behavior of  $T\chi_C$  is  $t^2 \ln |t|$  and  $t$ . As anticipated above, this also implies that the coefficient of  $C_{3+}$  of the  $|t|^{5/4}$  term in  $T\chi_0$  is close to, if not equal to the value given in Eq. (20). No further singularity characterized by an exponent close to 5/4 shows up in this analysis.

With the value for  $C_{3+}$  tentatively established, let us now obtain a measure for its accuracy by analyzing the quantity

$$\begin{aligned} T\chi_D &= T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 \\ &\quad - C_{2+} |t|^{1/4} - E_0 t \ln |t| - D_1 t \\ &\quad - (C_{3+} - \Delta C_3) |t|^{5/4} \end{aligned} \tag{33}$$

where  $\Delta C_3$  is a variable parameter and with  $C_{3+}$  as given by Eq. (20). Note the appearance of the  $D_1 t$  term with  $D_1$ , as determined in the next section, to have the value  $D_1 = -0.14869 \pm 0.00001$ .

Let us first analyze  $T\chi_D$  with  $\Delta C_3 = 0$ . Table V shows the exponents obtained by use of a second order differential approximant analysis of this quantity. The unbiased values in the second and third columns show considerable scatter about the value 2.0. However, averaging over the biased (one exponent forced to be 2) values of  $\rho$  in the last column we find

$$\langle \rho \rangle = 1.9984 \pm 0.0004 \tag{34}$$

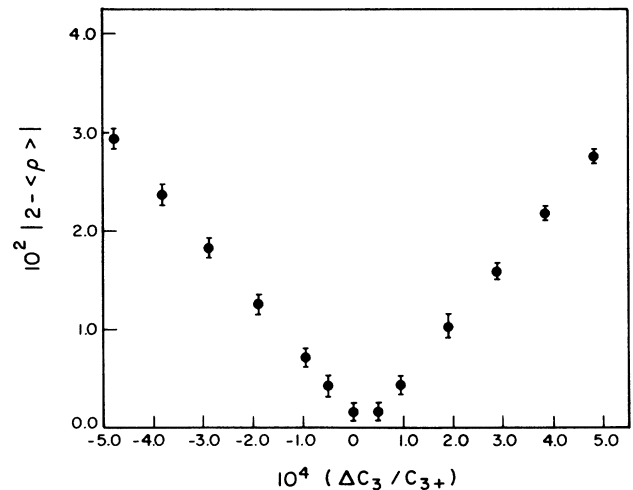


FIG. 2. Plot of  $10^2 |2 - \langle \rho \rangle|$  as a function of  $10^4 (\Delta C_3 / C_{3+})$ . Each value for  $\langle \rho \rangle$  was calculated by averaging the exponents obtained from a biased second order homogeneous differential approximant analysis of Eq. (33) with one exponent forced to be 2 for various choices of the parameter  $\Delta C_3$  with  $C_{3+}$  as given in Eq. (20). The vertical bars indicate the standard deviation associated with the spread in the calculated values of  $\langle \rho \rangle$  for each value of  $\Delta C_3$ .

thus indicating that the leading terms for  $T\chi_D$  are  $t^2 \ln |t|$  and  $t^2$ . This incidentally also confirms that the coefficient  $C_{3+}$  of the  $|t|^{5/4}$  term in  $T\chi_0$  is given correctly by Eq. (20).

We now set a numerical bound on possible deviations of  $C_{3+}$  from the value in Eq. (20) by analyzing  $T\chi_D$  for various choices of  $\Delta C_3$  near  $\Delta C_3=0$ . For each value of  $\Delta C_3$  we bias the approximants so that one of the roots of Eq. (16) is 2 exactly and obtain in this way a value for the second root. For the same choices of  $K$ ,  $L$  and  $M$  used previously we obtain an average value  $\langle \rho \rangle$  and a standard deviation as a function of  $\Delta C_3$ . The results are shown in Fig. 2 where we plot  $|2 - \langle \rho \rangle| \times 10^2$  versus  $\Delta C_3 / C_{3+} \times 10^4$ . As for Fig. 1, the result here leads to the conclusion that the coefficient of the  $|t|^{5/4}$  term is given to within one part in  $10^4$  by the value called for by the RG in the absence of irrelevant variables; that is, by the value in Eq. (20). As noted above, this was the value of  $C_{3+}$  used<sup>23</sup> in obtaining the coefficient  $C_{2+}$  of the  $|t|^{1/4}$  term from  $T\chi'_A$  in Eq. (25).

### C. The $t$ term

Besides their usage in obtaining the  $|t|^{1/4}$  and the  $|t|^{5/4}$  terms, the arguments above, and particularly the values for  $\rho_1$  and  $\rho_2$  listed in Tables I–IV, make it evident that the linear  $t$ -term from the analytic background term  $A(t, h)$  in Eq. (6) is present in the susceptibility. Indeed, we have been using the existence of the  $t$  and  $t \ln |t|$  terms as a probe for some of the other terms. Let us now consider the problem of obtaining the value for its coefficient  $D_1$  in Eq. (19).

Unlike the  $|t|^{1/4}$  and the  $|t|^{5/4}$  terms, whose respective coefficients  $C_{2+}$  and  $C_{3+}$  can be “guessed” from the predictions of the RG in the absence of irrelevant variables, there is no corresponding guidance regarding the analytic background term  $D_0 d_0(t)$  in the third of Eqs. (8). Thus we cannot use the same procedure as above of “guessing”  $D_1$  as in Eq. (20) and considering small variations about these values.

To determine  $D_1$  [ $\equiv D_0 d'_0(0)$ ] let us consider the quantity

$$T\chi_E = T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 - C_{2+} |t|^{1/4} - C_{3+} |t|^{5/4} - E_0 t \ln |t| \quad (35)$$

and carry out a Padé analysis<sup>12</sup> of the quantity  $T\chi_E/t$  evaluated at  $t=0$ . Using up to 48 terms in Nickel’s high-temperature series for  $T\chi_0$ , the exactly known values  $C_{0+}$ ,  $C_{1+}$ ,  $D_0$ , and  $E_0$ , and the values given in Eq.(20) for  $C_{2+}$  and  $C_{3+}$ , we find on expanding  $T\chi_E/t$  in terms of the high-temperature variable  $v$ , the results given in Table VI. The notation  $[N, M]$  for the Padé approximants is the usual one<sup>12</sup> with  $N$  ( $M$ ) the order of the numerator (denominator) polynomial of the approximant. Averaging over all values listed in the table (except the defective ones that are indicated by an asterisk) we conclude for  $D_1$  a value  $D'_1$  given by

$$D'_1 = -0.1490 \pm 0.0001 \quad (\text{Padé}). \quad (36)$$

Unfortunately, although this value follows unambiguously

TABLE VI. Values of the coefficient  $D_1$  of  $t$  obtained by the Padé technique. An asterisk (\*) denotes a defective approximant. The notation  $[N, M]$  for the Padé approximants denotes the order of the numerator and denominator polynomials, respectively.

$N$	$[N-1, N]$	$[N, N]$	$[N, N-1]$
15	-0.14935*	-0.14918	-0.14921
16	-0.14915	-0.14965*	-0.14911
17	-0.14902	-0.14910	-0.14895
18	-0.14906	-0.14904	-0.14904
19	-0.14908*	-0.14898	-0.14904
20	-0.14898	-0.14898	-0.14898
21	-0.14893	-0.14895	-0.14889
22	-0.14894	-0.14890	-0.14893
23	-0.14887	-0.14888	-0.14886
24	-0.14888	-0.14810*	-0.14887

ly from the Padé analysis and appears to be fairly accurate, it fails the more sensitive test of our differential approximant analysis in a sense described immediately below.

To see this and to obtain an improved value for  $D_1$  consider the quantity

$$T\chi_F = T\chi_E - \bar{D}_1 t \quad (37)$$

with  $\bar{D}_1$  a variable parameter which has the approximate value  $D'_1$  above. [This is essentially the same as the quan-

TABLE VII. Exponents obtained from second order homogeneous differential approximants, biased to force one exponent to be 2, for the quantity  $T\chi_F$  defined in Eq. (37). Each column represents a different choice for the parameter  $\bar{D}_1$  given in the top row. An asterisk (\*) denotes an approximant with an intervening spurious singularity and a dagger (†) an approximant for which the polynomials  $R_K$ ,  $P_L$  and  $Q_M$  possess an intervening common root.

$[K, L, M]$	-0.1490	-0.14870	-0.14869	-0.14868
[10,9,11]	2.7742*	2.0191	2.0026	1.9849
[10,10,10]	2.6263*	2.0191	2.0018	1.9833*
[10,11,9]	2.6783*	2.0197	2.0025	1.9846
[10,10,11]	2.7376*	2.0193	2.0031	1.9853
[10,11,10]	2.6802*	2.0197	2.0030	1.9852
[11,10,10]	2.8271*	2.0197	2.0029	1.9852
[10,11,11]	1.9438†	2.0196	2.0025	1.9834
[11,10,11]	3.2513*	2.0197	2.0028	1.9850
[11,11,10]	4.0165*	2.0130	2.0028	1.9852*
[11,10,12]	1.1534*	2.0197*	2.0084*	1.9920*
[11,11,11]	1.9055†	2.0196*	2.0026	1.9837
[11,12,10]	1.8062†	2.0166*	2.0028	1.9838
[11,11,12]	1.4772†	2.0195*	2.0022	1.9843
[11,12,11]	1.6048†	2.0180*	2.0024	1.9840
[12,11,11]	1.7094†	2.0165*	2.0027	1.9833
[11,12,12]	1.5849†	2.0195*	2.0014*	1.9834
[12,11,12]	1.9594†	2.0161*	1.9990*	1.9799*
[12,12,11]	1.6322†	2.0220*	2.0057	1.9865



tity  $TX_D$  defined in Eq. (33), but with  $\Delta C_3=0$  and  $D_1$  replaced by the variable  $\tilde{D}_1$ .] Table VII shows, for various choices of  $\tilde{D}_1$ , the exponents obtained from approximants to  $TX_F$  which are biased to force one exponent to be 2. Note that almost half of the exponents obtained with the Padé value  $\tilde{D}_1 = -0.1490$  in the first column are associated with defective approximants and are inconsistent, ranging from a high of 4.0 to a low of 1.2; clearly a very unsatisfactory situation. The remaining columns for various choices of the parameter  $\tilde{D}_1$  near the Padé value  $D'_1$  serve to clarify this situation. From the last three columns in Table VII we see that the “best” value for  $D_1$ —in the sense of giving consistent values for the exponents and with a small number of defects and with a minimum value for the quantity  $|2 - \langle \rho \rangle|$ —corresponds to the value  $\tilde{D}_1 = -0.14869$ .

The last three columns in Table VII suggest that we estimate the accuracy of the value for  $D_1$  quoted in Eq. (21) by carrying our computations for choices of  $\tilde{D}_1$  in the range  $-0.14870 \leq \tilde{D}_1 \leq -0.14868$ . Unexpectedly, we find the results of such an analysis to be extremely sensitive to the sixth decimal place of  $\tilde{D}_1$ . For reasons to be discussed in Section IV, accuracy to better than 5 decimal places is unwarranted here. Thus  $D_1$  in Eq. (21) is given to five decimal places and making use of the entries in the last three columns in Table VII we estimate the uncertainty in  $D_1$  to be 1 part in  $10^4$ , or 0.01%.

**D.  $|t|^{1/4} \ln |t|$  and  $|t|^{5/4} \ln |t|$  terms**

Finally, let us test for the possibility that  $TX_0$  also has terms of the form  $|t|^{1/4} \ln |t|$  and/or  $|t|^{5/4} \ln |t|$ . To this end consider the quantity

$$TX_G = TX_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 - C_{2+} |t|^{1/4} + \lambda C_{2+} |t|^{1/4} \ln |t| - C_{3+} |t|^{5/4} \tag{38}$$

with  $\lambda$  a variable parameter and where the  $t$  and  $t \ln |t|$  terms have *not* been subtracted. Carrying out a biased second order differential approximant analysis of  $TX_G$  for various choices of  $\lambda$  and with one exponent forced to be unity, we obtain Fig. 3 with  $\lambda$  along the abscissa. Reference to the graph shows that the minimum occurs for values of the parameter  $|\lambda| \lesssim 10^{-5}$ . This means that if a term  $|t|^{1/4} \ln |t|$  were present its coefficient could be at most  $10^{-5}$  that of the value  $C_{2+}$ .

Similarly to test for the possibility of a  $|t|^{5/4} \ln |t|$  term we consider the quantity  $TX'_G$  given by

$$TX'_G = TX_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4} - D_0 - C_{2+} |t|^{1/4} - E_0 t \ln |t| - D_1 t - C_{3+} |t|^{5/4} + \mu C_{3+} |t|^{5/4} \ln |t|, \tag{39}$$

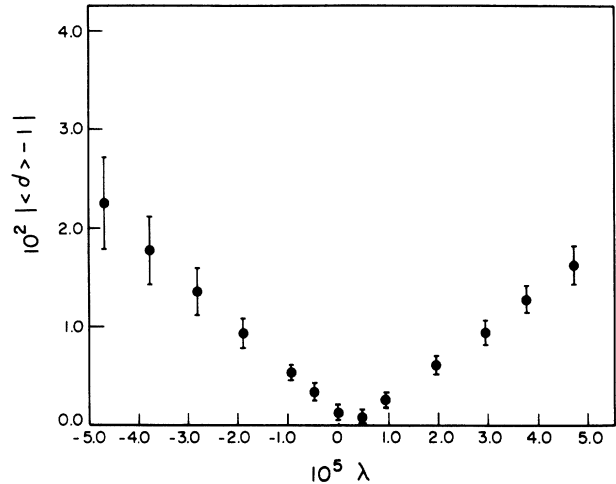


FIG. 3. Plot of  $10^2 |1 - \langle \rho \rangle|$  as a function of  $10^5 \lambda$  showing that the coefficient of a hypothesized  $|t|^{1/4} \ln |t|$  term in  $TX_0$  must be very small or zero. Each value for  $\langle \rho \rangle$  was calculated by averaging the exponents obtained from a biased second order homogeneous differential approximant analysis of Eq. (38) with one exponent forced to be 2 for various choices of the parameter  $\lambda$ . The vertical bars indicate the standard deviation associated with the spread in the calculated values of  $\langle \rho \rangle$  for each value of  $\lambda$ .

with the terms  $t$  and  $t \ln |t|$  now included in the subtraction. Carrying out a biased second order differential approximant analysis of  $TX'_G$  for various choices of  $\mu$  and with one exponent now forced to be 2, we conclude (see Fig. 4) that if the term  $|t|^{5/4} \ln |t|$  were present, its coefficient would be less than  $10^{-5}$  that of  $C_{3+}$ .

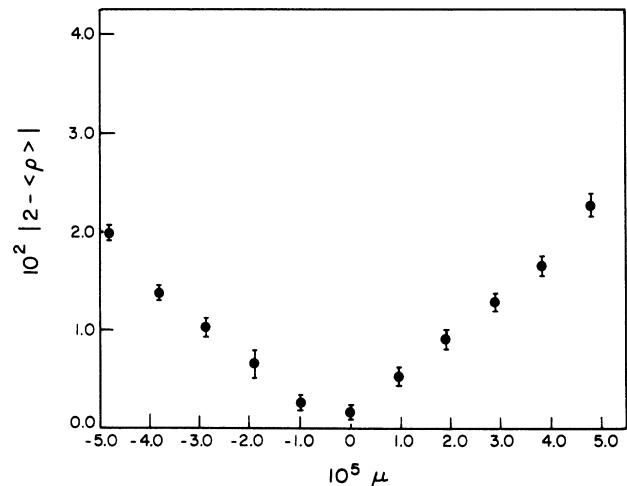


FIG. 4. Plot of  $10^2 |2 - \langle \rho \rangle|$  as a function of  $10^5 \mu$  showing that the coefficient of a hypothesized  $|t|^{5/4} \ln |t|$  term in  $TX_0$  must be very small or zero. Each value for  $\langle \rho \rangle$  was calculated by averaging the exponents obtained from a biased second order homogeneous differential approximant analysis of Eq. (39) with one exponent forced to be 2 for various choices of the parameter  $\mu$ . The vertical bars indicate the standard deviation associated with the spread in the calculated values of  $\langle \rho \rangle$  for each value of  $\mu$ .

## IV. FURTHER CONSIDERATIONS

In this section we turn to the question of the accuracy of our calculations. As will be discussed below, the principle limitation to the accuracy attainable in the present work is that the constant  $C_{0+}$  (and to a lesser extent  $D_0$  and  $E_0$ ) is known at the present time to "only" 10 decimal places. Although there is an exact expression<sup>4</sup> for  $C_{0+}$ , its evaluation to more than 10 places remains a formidable task and has not yet been carried out. This limited precision for  $C_{0+}$  leads to a systematic degradation in the accuracy of the series coefficients when the subtractions in Eqs. (22), (27), ... for  $T\chi_A$ ,  $T\chi_B$ , ... are carried out. This is particularly important for us since throughout this work we have had to subtract numerical coefficients, some of which have limited precision, and frequently, common digits. It must be kept in mind that ten digit agreement between two such coefficients would leave a residue devoid of any numerical significance. In addition, as we shall see, this naturally leads us to considerations which reinforce the validity of our underlying hypothesis that irrelevant variables can be neglected for two-dimensional Ising systems.

To introduce the idea let us see to what accuracy the coefficients of  $v^n$  in the high-temperature expansion of the quantity  $T\chi_0 - C_{0+} |t|^{-7/4}$  can be determined. The coefficients of the  $T\chi_0$  expansion are integers, and as such may be regarded as "infinitely" precise real numbers. On the other hand, the coefficients of the high-temperature expansion of the term  $C_{0+} |t|^{-7/4}$  are limited to 10 place significance by the value of  $C_{0+}$  as given in Eq. (2). Thus the coefficients of the series for  $T\chi_0 - C_{0+} |t|^{-7/4}$  can be at most accurate to 10 decimal places. On comparing Nickel's exact series for  $T\chi_0$  with the series for  $C_{0+} |t|^{-7/4}$ , we find that the respective coefficients of the two series are of the same order of magnitude and for the higher orders agree with each other up to two decimal places. For example, the coefficients of  $v^{25}$  for  $T\chi_0$  and  $C_{0+} |t|^{-7/4}$  are 36212402548 and  $3.574241397 \times 10^{10}$ , respectively, and these agree to two places. Thus the coefficient of  $v^{25}$  for the expansion of  $T\chi_0 - C_{0+} |t|^{-7/4}$  is accurate only to eight decimal places rather than ten. Similarly the corresponding coefficients of  $v^{53}$  are 3254615979848876064244 and  $3.234271265 \times 10^{12}$ , respectively; on subtraction these yield a number accurate again only to eight places. A comparison for all the coefficients in the expansion of  $T\chi_0 - C_{0+} |t|^{-7/4}$  shows that the degradation in accuracy is worst for the higher orders, with no case more severe than the examples just given.

This loss of accuracy is more serious for the series representing the difference  $T\chi_0 - C_{0+} |t|^{-7/4} - C_{1+} |t|^{-3/4}$ . This time, if we construct the high-temperature expansion for the sum  $C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4}$ , we find that the resulting coefficients agree much more closely with the exact coefficients of the series for  $T\chi_0$ . For the same orders 25 and 53 as above we now find for the coefficients of  $v^{25}$  and  $v^{53}$  the respective values  $3.621174159 \times 10^{10}$  and  $3.254616722 \times 10^{21}$ . Comparing these with the exact coefficients for the  $T\chi_0$

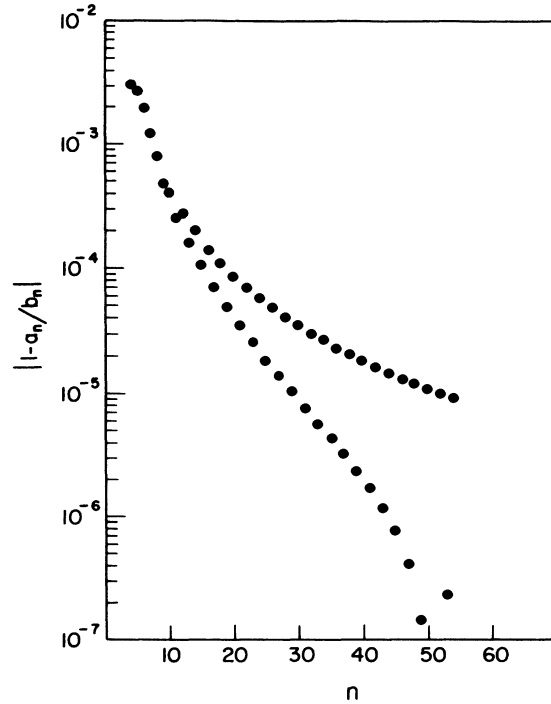


FIG. 5. Plot of the quantity  $|1 - a_n/b_n|$  as a function of the order  $n$ , with  $a_n$  the coefficient of  $v^n$  in the high-temperature expansion of the quantity  $C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4}$  and  $b_n$  Nickel's exact coefficient of  $v^n$  in the high-temperature expansion for  $T\chi_0$ . For an explanation of the anomalous point on the lower curve, corresponding to  $n = 53$  see Ref. 25.

expansion given above, we see that the agreement is now to five and six places, respectively. Hence the differences now yield values accurate at best to only five or four places.

Figure 5 shows as a function of  $n$  the quantity  $|1 - a_n/b_n|$ , where  $a_n$  is the coefficient of  $v^n$  for the high-temperature expansion of  $C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4}$  and  $b_n$  is the exact coefficient of  $v^n$  for Nickel's high-temperature series of  $T\chi_0$ . There are two "curves," the upper one corresponding to even values of  $n$  and the lower one to odd values. For small values of  $n$  the quantity  $|1 - a_n/b_n|$  is relatively large so that the low-order coefficients for the expansion of  $C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4}$  are not too close to the exact coefficients of  $T\chi_0$ . However, as  $n$  increases, the quantity  $|1 - a_n/b_n|$  becomes steadily smaller. With increasing order the coefficients ( $b_n - a_n$ ) of the series for  $T\chi_0 - (C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4})$  become much less accurate and for the highest orders are reliable at best to four decimal places. Therefore, quite apart from any uncertainties inherent in the method used to analyze the series itself, results obtained by the use of all 54 terms in such series cannot be treated as being more reliable than four decimal places.

With the difference  $T\chi_0 - (C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4})$  reducing us from 10 to 5 or 4 significant figures, it is crucial to see what is the effect of subtracting additional terms such as  $C_{2+} |t|^{1/4}$ ,  $C_{3+} |t|^{5/4}$ , and

$E_0 t \ln |t|$  from  $T\chi_0$ . Fortunately, we find that these additional terms modify the difference ( $a_n - b_n$ ) only slightly.<sup>26</sup> Table VIII shows the results of these computations for  $1 \leq n \leq 54$ . The exact values of the coefficients of  $v^n$  for the expansion of  $T\chi^0$  as communicated to us by Nickel<sup>11</sup> are given in the column labeled "exact." The neighboring columns labeled "partial" list the coefficients of  $v^n$  obtained by expanding the right-hand side of Eq.(19) in a high-temperature series. Reference to the table shows that except for the very lowest values of  $n$  the computed values in the "partial" column are in substantial agreement with the exact coefficients. The differences between the coefficients in the two columns are given as a percent in the third column labeled "%." These percent differences alternate in sign—being positive for odd  $n$  and negative for even  $n$ —and are generally very small, corresponding to 0.01% for  $n=17$ , 0.001% for  $n=39$ , and going down to 0.00044% for  $n=54$ . This means that for all terms with  $n > 17$ , the computed coefficients agree with the exact ones to from 4 to as many as 6 decimal places. In turn, this implies that the difference in the coefficients of the high-temperature expansion for  $T\chi_0$  and the seven terms on the right-hand side of Eq. (19) can be determined only to  $\sim 4$ -5 places.

This remarkable agreement between these latter two sets of coefficients can also be viewed from an alternate perspective. In obtaining the three new terms on the right-hand side of Eq.(19) we made use only of the first 35 of Nickel's high-temperature coefficients. In effect therefore, we "predicted," to 5-6 place accuracy, the last 19 terms  $b_n$  for  $36 \leq n \leq 54$ , of Nickel's high-temperature series. It is reasonable to suppose that corresponding predictions for the higher order coefficients would agree as well. In any event, this agreement reinforces the credibility of the underlying hypothesis that for two-dimensional Ising systems, irrelevant variables can be neglected to the order considered here.

Before turning to another implication of this rather surprising agreement between the two sets of coefficients in Table VIII, let us consider why it is that we have calculated approximants using only the first 35 terms in Nickel's series rather than the full 55 terms that are available. Generally, we would expect for approximation schemes of the kind used here that the approximants would converge better with increasing order.<sup>12,21</sup> In fact we found that the quality of the approximants—in the sense of consistency among the calculated exponent values and the encountering of fewer defective approximants—improves, as expected, with increasing order, but only up to a point; thereafter the quality diminishes for higher orders. We believe that this is due to the limited accuracy to which  $C_{0+}$  is known. In carrying out computations of the type described in the preceding section we have found that results from approximants constructed with 30 to 35 term series are the most consistent. Values obtained from approximants that make use of fewer than 30 coefficients are overall less consistent in the sense that they do not appear to converge as well. Similarly, approximants that require more than 35 coefficients generally yield more defective approximants, especially when  $\rho_1 = \rho_2$ . It appears that the expected in-

crease in accuracy with increased order is offset by the decreasing accuracy of the series coefficients in the expansions of the differences  $T\chi_A$ ,  $T\chi_B$ , etc., used in the analysis.

Let us finally consider an implication of the above unexpected agreement displayed in Table VIII between the high-temperature series coefficients obtained from the right hand side of Eq. (19) and the exact Nickel coefficients but now for the low-temperature range  $T < T_c$ . Reference to Eqs. (19) and (20)—the direct consequences of the hypothesis that irrelevant variables may be neglected—shows that since the quantities  $f_0(t)$ ,  $A_0(t)$ ,  $m_0(t)$ ,  $p_0(t)$ ,  $e_0(t)$ , and  $d_0(t)$  are analytic functions of  $t$ , if we know these functions for  $T > T_c$  we also know them for  $T < T_c$ . We can thus write for  $T < T_c$

$$\begin{aligned} T\chi_0 = & C_{0-} |t|^{-7/4} + C_{1-} |t|^{-3/4} + D_0 \\ & + C_{2-} |t|^{1/4} + E_0 t \ln |t| + D_1 t \\ & + C_{3-} |t|^{5/4} + O(t^2 \ln |t|, t^2), \quad T < T_c \end{aligned} \quad (40)$$

where<sup>5</sup>

$$\begin{aligned} C_{0-} &= 0.0255369719 \dots, \\ C_{1-}/C_{0-} &= -a_\chi \equiv -\frac{\sqrt{2}}{8} K_c, \\ C_{2-}/C_{0-} &= b_\chi \equiv \frac{151}{192} K_c^2, \\ C_{3-}/C_{0-} &= -c_\chi \equiv -\frac{615\sqrt{2}}{512} K_c^3, \end{aligned} \quad (41)$$

and where we have used the fact that  $E_0$ ,  $D_0$ , and  $D_1$  are the same on the high- and low-temperature sides. It is to be emphasized that Eqs. (40) and (41) are valid for  $T < T_c$  only if the underlying assumption that irrelevant variables can be neglected is correct.

Let us now take this formula for  $T\chi_0$  in Eq. (40) and expand the right hand side in a power series in the low-temperature variable<sup>3</sup>  $u = e^{-4J/T}$ . With all coefficients in Eq. (40) known we can compute for  $T < T_c$  the coefficients of the power series for  $T\chi_0$  in  $u$  analogous to those in the "partial" column in Table VIII for  $T > T_c$  (Appendix B). The resulting low-temperature coefficients are shown in Table IX in the column labeled "partial." Also displayed are the 11 exactly known low-temperature series coefficients for this system<sup>27</sup> in the column labeled "exact." As in Table VIII we have computed coefficients through  $n=54$  even though the "exact" column now has only 11 values, as does the "%" column. Again, there is significant agreement between the "predicted" and the 11 known exact values. The coefficients listed in the partial column are here consistently above the exact values, with the difference, as one might expect, decreasing rapidly with increasing values of  $n$ . For the highest-order exactly known coefficient,  $n=11$ , the difference is  $-4.8 \times 10^{-4}\%$  whereas the corresponding difference at  $n=11$  for  $T > T_c$  was larger by a factor of nearly 100 at  $2.9 \times 10^{-2}\%$ . The predicted values for the coefficients for  $T < T_c$  increase much more rapidly with order  $n$  than do the high-temperature coefficients. Thus for  $n=54$ , the low-

TABLE VIII. Exact and partial high-temperature series coefficients for the zero-field quadratic Ising lattice susceptibility. The partial series coefficients were calculated from the expression  $C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4} + C_{2+} |t|^{1/4} + C_{3+} |t|^{5/4} + E_0 |t| \ln |t|$  and the exact coefficients were calculated by B.G. Nickel (Ref. 11). The column labeled “%” indicates the percent difference between the values in the “exact” and “partial” columns. The decimal points for the listings in the partial column were chosen to emphasize the digits that agree with those in the exact column.

n	Exact	Partial	%	n	Exact	Partial	%
1	4	3.263250589	18.	28	552460084428	$5524.745775 \times 10^8$	-0.0026
2	12	12.39122620	-3.3	29	1367784095156	$13677.52555 \times 10^8$	0.0023
3	36	35.74572098	0.71	30	3383289570292	$3383.363211 \times 10^9$	-0.0022
4	100	100.4333361	-0.43	31	8363078796612	$8362.917432 \times 10^9$	0.0019
5	276	$27.54035271 \times 10^1$	0.22	32	20656054608404	$20656.43203 \times 10^9$	-0.0018
6	740	$74.16216307 \times 10^1$	-0.22	33	50987841944612	$50987.00988 \times 10^9$	0.0016
7	1972	$196.9809553 \times 10^1$	0.11	34	125771030685740	$12577.29801 \times 10^{10}$	-0.0015
8	5172	$517.6200472 \times 10^1$	-0.081	35	310070329656964	$31006.60086 \times 10^{10}$	0.0014
9	13492	$1348.573999 \times 10^1$	0.046	36	763956047852548	$7639.661867 \times 10^{11}$	-0.0013
10	34876	$348.8957050 \times 10^2$	-0.039	37	1881332450300692	$18813.09868 \times 10^{11}$	0.0012
11	89764	$897.3962385 \times 10^2$	0.027	38	4630413888204372	$46304.66945 \times 10^{12}$	-0.0011
12	229628	$2296.853259 \times 10^2$	-0.025	39	1139155886485432	$11391.44018 \times 10^{12}$	0.0010
13	585508	$585.3973997 \times 10^3$	0.019	40	28010951274197380	$28011.23045 \times 10^{12}$	-0.0010
14	1486308	$1486.562144 \times 10^3$	-0.017	41	68849212197171604	$68848.58533 \times 10^{12}$	0.00091
15	3763460	$3762.962294 \times 10^3$	0.013	42	16915009736533708	$16915.15736 \times 10^{13}$	-0.00087
16	9497380	$949.8510050 \times 10^4$	-0.012	43	415419639494357940	$41541.63129 \times 10^{13}$	0.00080
17	23918708	$2391.644779 \times 10^4$	0.0094	44	1019816266252636316	$101982.4108 \times 10^{13}$	-0.00077
18	60080156	$6008.533033 \times 10^4$	-0.0086	45	2502715799503410388	$25026.98072 \times 10^{14}$	0.00071
19	150660388	$1506.497699 \times 10^5$	0.0070	46	6139555263040186116	$61395.97092 \times 10^{14}$	-0.00068
20	377009364	$3770.338578 \times 10^5$	-0.0065	47	15056658258453004340	$150565.6343 \times 10^{14}$	0.00063
21	942106116	$9420.549456 \times 10^5$	0.0054	48	36912183772984767964	$36912.40773 \times 10^{15}$	-0.00061
22	2350157268	$2350.275621 \times 10^6$	-0.0050	49	90466431959611708308	$90465.92290 \times 10^{15}$	0.00056
23	5855734740	$5855.484462 \times 10^6$	0.0043	50	221649470925554607500	$22165.06741 \times 10^{16}$	-0.00054
24	14569318492	$14569.89853 \times 10^6$	-0.0040	51	542914755497182676020	$54291.20138 \times 10^{16}$	0.00050
25	36212402548	$3621.116268 \times 10^7$	0.0034	52	1329440077424712435476	$132944.6562 \times 10^{16}$	-0.00049
26	89896870204	$8989.975176 \times 10^7$	-0.0032	53	3254615979848876064244	$32546.01170 \times 10^{17}$	0.00046
27	222972071236	$22296.58514 \times 10^7$	0.0028	54	7965488065940462105380	$79655.23121 \times 10^{17}$	-0.00044

TABLE IX. Exact and partial low-temperature series coefficients for the quadratic Ising lattice susceptibility. The partial series coefficients are calculated from Eq. (41). The column labeled “%” indicates the percent difference between the values in the “exact” and “partial” columns.

n	Exact	Partial	%	n	Partial
1	0	0.3296233		28	$2.482731 \times 10^{21}$
2	4	3.800798	+ 5.0	29	$1.485698 \times 10^{22}$
3	32	32.63967	-2.0	30	$8.882647 \times 10^{22}$
4	240	240.1660	$-6.9 \times 10^{-2}$	31	$5.306289 \times 10^{23}$
5	1664	$166.5551 \times 10^1$	$-9.3 \times 10^{-2}$	32	$3.167373 \times 10^{24}$
6	11164	$1116.561 \times 10^1$	$-1.4 \times 10^{-2}$	33	$1.889245 \times 10^{25}$
7	73184	$7318.944 \times 10^1$	$-7.4 \times 10^{-3}$	34	$1.126100 \times 10^{26}$
8	472064	$4720.767 \times 10^2$	$-2.7 \times 10^{-3}$	35	$6.707850 \times 10^{26}$
9	3008032	$30080.75 \times 10^2$	$-1.4 \times 10^{-3}$	36	$3.993215 \times 10^{27}$
10	18985364	$18985.51 \times 10^3$	$-7.8 \times 10^{-4}$	37	$2.375801 \times 10^{28}$
11	118909888	$1189.105 \times 10^5$	$-4.8 \times 10^{-4}$	38	$1.412728 \times 10^{29}$
12		$7.400687 \times 10^8$		39	$8.396168 \times 10^{29}$
13		$4.581670 \times 10^9$		40	$4.987568 \times 10^{30}$
14		$2.823711 \times 10^{10}$		41	$2.961368 \times 10^{31}$
15		$1.733538 \times 10^{11}$		42	$1.757525 \times 10^{32}$
16		$1.060676 \times 10^{12}$		43	$1.042619 \times 10^{33}$
17		$6.470628 \times 10^{12}$		44	$6.182629 \times 10^{33}$
18		$3.937068 \times 10^{13}$		45	$3.664815 \times 10^{34}$
19		$2.389932 \times 10^{14}$		46	$2.171549 \times 10^{35}$
20		$1.447735 \times 10^{15}$		47	$1.286273 \times 10^{36}$
21		$8.753313 \times 10^{15}$		48	$7.616380 \times 10^{36}$
22		$5.283387 \times 10^{16}$		49	$4.508401 \times 10^{37}$
23		$3.184015 \times 10^{17}$		50	$2.667844 \times 10^{38}$
24		$1.916102 \times 10^{18}$		51	$1.578221 \times 10^{39}$
25		$1.151579 \times 10^{19}$		52	$9.333610 \times 10^{39}$
26		$6.912652 \times 10^{19}$		53	$5.518370 \times 10^{40}$
27		$4.144877 \times 10^{20}$		54	$3.261789 \times 10^{41}$

temperature coefficient is predicted to be  $\approx 3 \times 10^{41}$  while the corresponding high-temperature one is 20 orders of magnitude smaller than this at  $\approx 8 \times 10^{21}$ . This may be the reason why it is so much more difficult to compute exact values for the low-temperature series coefficients than for the high-temperature ones. We stress that the values listed in Table IX are a projection based on Eqs. (40) and (41) and should be interpreted in that light. It would be of considerable interest to have available additional exact values with which to compare our  $T < T_c$  predictions.

## V. SUMMARY AND CONCLUSIONS

The main result of this paper for the zero-field quadratic Ising lattice susceptibility can be summarized by the statement that through terms of order  $t^2$  and  $t^2 \ln |t|$ , we have confirmed the predictions of the renormalization group when irrelevant variables are neglected. Specifically, we have shown the existence of the  $|t|^{1/4}$  and  $|t|^{5/4}$  terms for  $T\chi_0$  and that the respective coefficients  $C_{2+}$  and  $C_{3+}$  are very close to and possibly equal to the values given by Eqs.(20). Also, we have established that the coefficients of terms varying as  $|t|^{1/4} \ln |t|$  and  $|t|^{5/4} \ln |t|$  are very small and possibly zero by showing that if the latter terms are present, their coefficients would be less than  $10^{-5}$  of the values of

$C_{2+}$  and  $C_{3+}$  respectively. By making use of Kong’s recently calculated value<sup>8</sup> of the coefficient  $E_0$  of the  $t \ln |t|$  term, we were able to obtain an improved value for the coefficient  $D_1$  of the  $t$  term and were able to conclude that if there is a confluent singularity in the two-dimensional Ising susceptibility due to an irrelevant variable, it must have an associated exponent greater than 2.

A second important conclusion derives from the high-temperature series expansion of Eq. (19) in terms of the variable  $v$  and its low temperature analogue in Eq. (40) in terms of the variable  $u$ . These derived coefficients are in remarkable agreement with the exact series coefficients (Tables VIII and IX, respectively) and thereby lend additional confirmation to the underlying hypothesis that irrelevant variables can be neglected for two-dimensional Ising systems. Besides its intrinsic interest, this comparison of the exact and partial series coefficients also indicates that the numerical precision to which  $C_{0+}$  is known is the principle limitation to the accuracy which can be achieved by analyzing series which are obtained by subtracting from  $T\chi_0$  expansions of various singularities in Eq.(19).

Finally, we have introduced a new method for verifying and analyzing logarithmic singularities by means of second-order homogeneous differential approximants. The method relies on the signature of an integer difference in the roots of the indicial equation for logarithmic solutions of homogeneous, second order, ordi-

TABLE X. Comparison of additional exact low-temperature series coefficients [R.J. Baxter and I.G. Enting, J. Stat. Phys. **21**, 103 (1979)] for the quadratic Ising lattice susceptibility with their partial counterparts from Table IX. The column labeled “%” indicates the percent difference between the values in the “exact” and “partial” columns.

n	exact	partial	%
12	740066448	$74006.87372 \times 10^4$	$-3.1 \times 10^{-4}$
13	4581660832	$45816.70416 \times 10^5$	$-2.1 \times 10^{-4}$
14	28237063308	$28237.10454 \times 10^6$	$-1.5 \times 10^{-4}$
15	173353630848	$173353.8119 \times 10^6$	$-1.0 \times 10^{-4}$
16	1060674765568	$106067.5572 \times 10^7$	$-7.6 \times 10^{-5}$
17	6470624695296	$647062.8323 \times 10^7$	$-5.6 \times 10^{-5}$
18	39370663086596	$393706.7948 \times 10^8$	$-4.2 \times 10^{-5}$
19	238993166711328	$238993.2408 \times 10^9$	$-3.1 \times 10^{-5}$
20	1447734754083760	$144773.5087 \times 10^{10}$	$-2.3 \times 10^{-5}$
21	8753312020985216	$875331.3496 \times 10^{10}$	$-1.7 \times 10^{-5}$
22	52833859249062184	$528338.6564 \times 10^{11}$	$-1.2 \times 10^{-5}$
23	318401517346021368	$3184015.440 \times 10^{11}$	$-8.4 \times 10^{-6}$

nary differential equations. This technique has hitherto been unexploited in this type of analysis.<sup>13,21</sup>

The results of this work raise several questions. Among these is whether the neglect of irrelevant variables is justified for other planar Ising lattices, for example the triangular and honeycomb lattices. If so, can the present method be extended to the zero-field susceptibilities of these lattices? This problem is currently under investigation for the triangular and hexagonal lattices. Also, the analysis of the quadratic Ising lattice susceptibility by means of the pair correlation function<sup>4</sup> is an active area of interest<sup>6,8</sup> and our results, while posing perplexing mathematical questions, may help point the way to further exact results. Finally, in a more speculative vein, we note that the above results for the ferromagnetic susceptibility may apply to the quadratic Ising *antiferromagnetic* susceptibility,<sup>28</sup> with  $p_0(t)$  in Eqs. (8) and (9) now predicted to be zero.

*Note added.* After submitting this paper, I.G. Enting brought to our attention a calculation of the low-temperature series for the quadratic Ising lattice susceptibility through terms of order  $u^{23}$  [R.J. Baxter and I.G. Enting, J. Stat. Phys. **21**, 103 (1979)]. On comparing the “partial” coefficients in Table IX with these additional exact coefficients, we find that they agree to as many as 7 decimal places. These new coefficients and their “partial” counterparts from Table IX are shown in Table X.

#### ACKNOWLEDGMENTS

The authors wish to thank Professor B. G. Nickel for sending us his extended high-temperature series for the Ising susceptibility and for permission to list the new coefficients in Table VIII. We also wish to thank Professor J.H.H. Perk for calling our attention to the evaluation of  $E_0$  in the unpublished thesis of Dr. X.P. Kong, and Professor C.A. Tracy and Professor H. Nakanishi for helpful comments.

#### APPENDIX A

The purpose of this appendix is to provide some mathematical details concerning the solutions of second-order homogeneous ordinary differential equations relevant to the use of homogeneous differential approximations to determine confluent logarithmic and other singularities.

Consider the second order equation

$$(z - z_0)^2 \frac{d^2 y}{dz^2} + (z - z_0)P(z) \frac{dy}{dz} + Q(z)y = 0 \quad (\text{A1})$$

where  $P$  and  $Q$  are analytic about the point  $z = z_0$  and thus can be expressed

$$P(z) = p_0 + p_1(z - z_0) + p_2(z - z_0)^2 + \dots, \quad (\text{A2})$$

$$Q(z) = q_0 + q_1(z - z_0) + q_2(z - z_0)^2 + \dots. \quad (\text{A3})$$

with  $p_0 \neq 0$  and  $q_0 \neq 0$ . The assumption that a solution of (A1) has the form

$$y = (z - z_0)^\rho \left[ 1 + \sum_{n=1}^{\infty} a_n (z - z_0)^n \right] \quad (\text{A4})$$

yields,<sup>19,20</sup> when substituted into (A1), relations for the unknowns  $\rho, a_1, a_2, a_3, \dots$  as follows:

$$\rho^2 + (p_0 - 1)\rho + q_0 = 0 \quad (\text{A5})$$

and

$$a_n = -\frac{1}{F(\rho + n)} \left[ \sum_{m=1}^{n-1} a_{n-m} [(\rho + n - m)p_m + q_m] + \rho p_n + q_n \right] \quad (\text{A6})$$

where  $a_n = 0$  for  $n \leq 0$  and the quantity  $F$  is defined by

$$F(x) = x^2 + x(p_0 - 1) + q_0. \quad (\text{A7})$$

The relation in (A5), which can also be written as

$F(\rho)=0$ , is known as the *indicial equation* and determines two values for  $\rho$ ; call them  $\rho_1$  and  $\rho_2$ . For cases of interest to us, these will in general be real, and we will take  $\rho_1$  to be the larger of the two. Provided that  $\rho_1-\rho_2$  is not a positive integer or zero the denominator  $F(\rho+n)$  in (A6) does not vanish and (A4)–(A6) yield two linearly independent solutions<sup>19,20</sup> to (A1).

The case when this latter condition is violated is of particular interest to us since for this case a confluent logarithmic singularity can arise. To see this, suppose

$$\rho_1-\rho_2=n_0 \tag{A8}$$

with  $n_0$  a non-negative integer. Then (A4)–(A6) will still yield one solution of (A1) associated with the larger root,  $\rho_1$ , of the indicial equation. But now, since  $F(\rho_2+n_0)=F(\rho_1)=0$ , (A4)–(A6) do not yield a second solution. However, it can be shown for this case, that if  $y_1=y_1(z)$  is the solution of (A1) for  $\rho=\rho_1$ , then a second solution  $y_2$  of (A1), when  $n_0 \neq 0$ , has the form

$$y_2(z) = Ay_1 + B \left\{ \mu y_1(z) \ln(z-z_0) + (z-z_0)^{\rho_2} \left[ \frac{-1}{n_0} + \sum_{n=1}^{\infty} h_n(z-z_0)^n \right] \right\} \tag{A9}$$

where  $A$  and  $B$  are constants of integration and  $\mu, h_1, h_2, \dots$  are fixed constants. For the case  $n_0=0$ , corresponding to  $\rho_1=\rho_2$ , the structure of  $y_2$  is

$$y_2(z) = Ay_1 + B \left\{ y_1(z) \ln(z-z_0) + (z-z_0)^{\rho_2} \sum_{n=1}^{\infty} h_n(z-z_0)^n \right\}. \tag{A10}$$

In general, unless the constant  $\mu$  happens to vanish, the second solution of (A1) involves a logarithmic singularity of the form  $(z-z_0)^{\rho_1} \ln(z-z_0)$ . It is precisely this feature of (A1) that makes it so useful for our purposes.

APPENDIX B

The purpose of this appendix is to provide some of the details involved in obtaining the high- and low-temperature expansions for the terms  $C_{0\pm} |t|^{-7/4}$ ,  $C_{1\pm} |t|^{-3/4}$ ,  $C_{2\pm} |t|^{1/4}$ ,  $C_{3\pm} |t|^{5/4}$ , and  $E_0 |t| \ln |t|$  which are used to obtain the series represented by the various quantities  $T\chi_A, T\chi_B, \dots$  in Eqs. (22), (27),  $\dots$ .

Consider first the high-temperature case. The variable for the high-temperature series of  $T\chi_0$  for the quadratic Ising lattice is  $v = \tanh(J/T)$  rather than the variable  $t = 1 - T_c/T$ . In order to carry out a term by term subtraction of series for the singular terms  $C_{0+} |t|^{-7/4}$ ,  $C_{1+} |t|^{-3/4}$ , etc., from the series for  $T\chi_0$ , we must express the quantity

$$C_{0+} |t|^{-7/4} + C_{1+} |t|^{-3/4} + D_0 + C_{2+} |t|^{1/4} + E_0 t \ln |t| + D_1 t + C_{3+} |t|^{5/4} \tag{B1}$$

in terms of the variable  $(v_c - v)$ . The result can be expressed as

$$C'_{0+} (v_c - v)^{-7/4} + C'_{1+} (v_c - v)^{-3/4} + D'_{0+} + C'_{2+} (v_c - v)^{1/4} + E'_{0+} (v_c - v) \ln(1 - v/v_c) + D'_{1+} (v_c - v) + C'_{3+} (v_c - v)^{5/4} \tag{B2}$$

where  $v_c = \sqrt{2} - 1$  and with  $C'_{0+}, C'_{1+}$ , etc., as appropriate coefficients. Since  $v < v_c$  for  $T > T_c$  we drop the absolute value signs in (B2). It is the formula in (B2) which is expanded about  $v=0$  and then subtracted term-by-term from the series for  $T\chi_0$  to obtain series for the various quantities  $T\chi_A, T\chi_B$ , in Eqs. (22), (27),  $\dots$ .

Let us now determine the constants  $C'_{0+}, C'_{1+}, D'_{0+}, C'_{2+}, E'_{0+}, D'_{1+}$  and  $C'_{3+}$  in (B2) in terms of the values of  $C_{0+}, C_{1+}, D_0$  and  $E_0$  given in Eqs. (2)–(5), the values of  $C_{2+}$  and  $C_{3+}$  given in Eqs. (20), and the value of  $D_1$  given in Eq. (21). We expand  $t$  in powers of  $(v_c - v)$  through terms of order  $(v_c - v)^4$  to obtain

$$t = \frac{1}{2v_c K_c} \left[ (v_c - v) - \frac{1}{2}(v_c - v)^2 + \frac{(3 + \sqrt{2})}{6}(v_c - v)^3 - \frac{(2 + \sqrt{2})}{4}(v_c - v)^4 + \dots \right] \tag{B3}$$

and substitute this expansion into (B1). Keeping only terms through order  $(v_c - v)^{5/4}$  and  $(v_c - v) \ln(1 - v/v_c)$ , we obtain with  $K_c = (1/2) \ln(1 + \sqrt{2})$ ,

$$\begin{aligned} C'_{0+} &= C_{0+} (2v_c K_c)^{7/4} = 0.1650479829 \dots, \\ C'_{1+} / C'_{0+} &= \frac{16 + \sqrt{2}}{16} \approx 1.088388348 \dots, \\ D'_{0+} &= D_0 = -0.10413324511 \dots, \\ C'_{2+} / C'_{0+} &= \frac{93 + 32\sqrt{2}}{256} \approx 0.5400579453 \dots, \\ E'_{0+} &= \frac{E_0}{2v_c K_c} = 0.110457553 \dots, \\ D'_{1+} &= \frac{D_1 - E_0 \ln(2K_c)}{2v_c K_c} = -0.39333 \pm 0.00003 \dots, \\ C'_{3+} / C'_{0+} &= \frac{5872 + 4135\sqrt{2}}{4096} \approx 2.861272725 \dots \end{aligned} \tag{B4}$$

It is by use of these formulas that the various series represented by the quantities  $T\chi_A, T\chi_B$ , etc., were obtained.

The situation for the low-temperature series coefficients in Table IX is similar with the low-temperature variable  $u = e^{-4J/T}$ . We expand  $t$  in powers of  $(u_c - u)$  to obtain

$$t = -\frac{1}{4K_c u_c} \left[ (u_c - u) + \frac{1}{2u_c} (u_c - u)^2 + \frac{1}{3u_c^2} (u_c - u)^3 + \frac{1}{4u_c^3} (u_c - u)^4 + \dots \right] \quad (\text{B5})$$

with  $u_c = 3 - 2\sqrt{2}$ . Substituting into Eq. (40) we obtain

$$\begin{aligned} C'_{0-} (u_c - u)^{-7/4} + C'_{1-} (u_c - u)^{-3/4} + D'_{0-} \\ + C'_{2-} (u_c - u)^{1/4} + E'_{0-} (u_c - u) \ln(1 - u/u_c) \\ + D'_{1-} (u_c - u) + C'_{3-} (u_c - u)^{5/4} \end{aligned} \quad (\text{B6})$$

where now

$$\begin{aligned} C'_{0-} &= C_{0-} (4u_c K_c)^{7/4} = 0.00314982951 \dots, \\ C'_{1-} / C'_{0-} &= \frac{-(88 + 59\sqrt{2})}{32} \approx -5.357456256 \dots, \\ D'_{0-} &= D_0 = -0.10413324511 \dots, \\ C'_{2-} / C'_{0-} &= \frac{1461 + 1032\sqrt{2}}{1024} \approx 2.852019918 \dots, \\ E'_{0-} &= \frac{E_0}{4u_c K_c} = -0.133334061 \dots, \\ D'_{1-} &= \frac{-(D_1 - E_0 \ln(4K_c))}{4K_c u_c} = 0.56722 \pm 0.00003 \dots, \\ C'_{3-} / C'_{0-} &= \frac{-(90808 + 64213\sqrt{2})}{32768} \approx -5.542568832 \dots \end{aligned} \quad (\text{B7})$$

<sup>1</sup>L. Onsager, Phys. Rev. **65**, 117 (1944).

<sup>2</sup>C.N. Yang, Phys. Rev. **85**, 808 (1952).

<sup>3</sup>C. Domb, Adv. Phys. **9**, 149 (1960).

<sup>4</sup>T.T. Wu, B.M. McCoy, C.A. Tracy and E. Barouch, Phys. Rev. **B 13**, 316 (1976).

<sup>5</sup>E. Barouch, B.M. McCoy, and T.T. Wu, Phys. Rev. Lett. **31**, 1409 (1973); C.A. Tracy and B.M. McCoy, *ibid.* **31**, 1500 (1973).

<sup>6</sup>X.P. Kong, H. Au-Yang, and J.H.H. Perk, Phys. Lett. **A 116**, 54 (1986).

<sup>7</sup>A.J. Guttmann, J. Phys. **A 8**, 1236 (1975).

<sup>8</sup>X.P. Kong, Ph.D. thesis, State University of New York at Stony Brook, 1987.

<sup>9</sup>S. Gartenhaus and W.S. McCullough, Phys. Lett. **A 127**, 315 (1988).

<sup>10</sup>B.G. Nickel, in *Phase Transitions: Cargèse 1980*, Vol. 72 of *NATO Advanced Study Institute, Series B*, edited by M. Lévy, J.-C. Le Guillou and J. Zinn-Justin (Plenum, New York, 1981), p. 291.

<sup>11</sup>B.G. Nickel (private communication). See the column labeled "exact" in Table VIII for these coefficients.

<sup>12</sup>D.S. Gaunt and A.J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic, New York, 1974), Vol. 3, p.181; D.L. Hunter and G.A. Baker, Jr., Phys. Rev. **B 7**, 3346 (1973).

<sup>13</sup>G.S. Joyce and A.J. Guttmann, J. Phys. **A 5**, L81 (1972); J.J. Rehr, G.S. Joyce, and A.J. Guttmann, *ibid.* **13**, 1587 (1980).

<sup>14</sup>F.J. Wegner, Phys. Rev. **B 5**, 4229 (1972); M.E. Fisher, Rev. Mod. Phys. **46**, 597 (1974).

<sup>15</sup>A. Aharony, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M.S. Green (Academic, New York, 1976), Vol. 6, p. 357; F.J. Wegner, *ibid.*, p. 7.

<sup>16</sup>A. Aharony and M.E. Fisher, Phys. Rev. Lett. **45**, 679 (1980); Phys. Rev. **B 27**, 4394 (1983).

<sup>17</sup>For the definitions of the critical exponents, see for example

H.E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford University Press, New York, 1971).

<sup>18</sup>S. Gartenhaus and W.S. McCullough, Phys. Rev. **B 35**, 3299 (1987).

<sup>19</sup>E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, London, 1962), Chap. X.

<sup>20</sup>E. L. Ince, *Ordinary Differential Equations* (Dover, New York, 1957), Chap. XVI.

<sup>21</sup>D.L. Hunter and G.A. Baker, Jr., Phys. Rev. **B 19**, 3808 (1979).

<sup>22</sup>We order the roots so that  $\rho_1 \geq \rho_2$ .

<sup>23</sup>Note the subtraction of the term  $C_{3+} |t|^{5/4}$  here. In anticipation of subsequent results, we have subtracted this term from  $T\chi_0$  in the expression for  $T\chi'_4$  since this enhanced the reliability and consistency of the calculated exponents considerably. We presume this enhancement is due to the fact that the exponent 5/4 is so close to unity.

<sup>24</sup>Recall from Appendix A that if the exponents differ by an integer, in general there is a logarithmic singularity associated with the larger exponent.

<sup>25</sup>Professor Nickel has informed us that the coefficients of  $v^{48}$  through  $v^{54}$  for the  $T\chi_0$  series may not be fully correct. This may explain why the last point on the lower curve in Fig. 5, related to the coefficient of  $v^{53}$ , does not seem to follow the pattern of the previous odd coefficients. Any such deviations in the last 7 exact coefficients for  $T\chi_0$  will not affect our results, which make use of only the first 35 coefficients.

<sup>26</sup>Note that subtracting high-temperature series expansions for the terms  $D_0$  and  $D_1 t$  affects only the coefficients of  $v^0$  and  $v^1$  and so are not considered here.

<sup>27</sup>M.F. Sykes, D.S. Gaunt, J.L. Martin, and S.R. Mattingly, J. Math. Phys. **11**, 1071 (1972).

<sup>28</sup>M. Kaufman, Phys. Rev. **B 36**, 3697 (1987).