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Visibility of Critical-Exponent Renormalization

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The extent to which the renormalization of critical-point behavior should be visible experimentally is investigated on the basis of detailed numerical calculations for a three-dimensional soluble model (a mobile-electron Ising ferromagnet). If a dilution parameter x is defined such that the change in critical temperature from the "pure" or unrenormalized system is $|T_c(x) - T_c^0| = xT_c/f$, where $f = 0.6-0.9$, then we conclude that the effective exponents $\beta_{\text{fit}}(x)$ and $\gamma_{\text{fit}}(x)$ which will be observed experimentally, vary *roughly* as $\beta_{\text{fit}} \approx \beta + x\Delta\beta_X$ and $\gamma_{\text{fit}} \simeq \gamma + \frac{1}{5}x \times (1+2x^2)\Delta\gamma_X$. Here β and γ are the ideal exponents for the order parameter and total fluctuation or susceptibility of the pure system, while $\Delta\beta_X = \beta_X - \beta$ and $\Delta\gamma_X = \gamma_X - \gamma$, in which $\beta_X = \beta/(1-\alpha')$ and $\gamma_X = \gamma/(1-\alpha)$ are the fully renormalized exponents, while α and α' (assumed positive) describe the divergence of the specific heats of the pure system. [Theoretically the true limiting asymptotic behavior at the transition is described by $\beta(x) = \beta_X$ and $\gamma(x) = \gamma_X$ for all $x > 0$.] The renormalized specific heats are found to be sensitive to x but their true renormalized behavior is not evident until $x \gtrsim 0.3$. Various techniques of data analysis such as logarithmic, semilogarithmic, Heller-Benedek, and Kouvel-Fisher plots have been tested.

I. INTRODUCTION AND SUMMARY

Under a fairly wide range of circumstances the critical exponents occurring in a natural or a model system are expected to become "renormalized".[1] As shown by Fisher[1] (see also Buckingham and Lipa[2]) renormalization occurs when an "ideal" or "pure" system possessing a critical point is perturbed homogeneously by some influence which, in turn, is subject to a "constraint". Various different physical examples of this general situation were discussed in Ref. 1. A typical one is a gasliquid transition in a pure single-component fluid which is perturbed (but not destroyed) by the presence of impurities. The constraint in this case would be the requirement of constant over-all impurity concentration (although as p and T varied the impurities would redistribute themselves and come to an internal equilibrium). On the other hand, impurities in a solid system with a critical point, such as a ferromagnet, are often "frozen" into an immobile random configuration. In such a case renormalization, as described below, is *not* expected; rather, the transition is likely to be rounded or smeared (probably in quite a subtle way[3]). Similarly, a gravitational field will "spread out" a fluid critical point (by inducing large scale inhomogeneities) and a magnetic field imposed on a ferromagnet destroys the transition: Specific heats, etc. will look different ("rounded") in these cases but these also are not renormalization effects. However, the case of an *anti*ferromagnet in a uniform applied field is one where simple renormalization is expected.[1] The critical (or Néel) temperature is changed (frequently reduced) but the transition is not destroyed. A constraint arises through the demagnetization phenomenon which implies that the (more fundamental) internal field varies through the transition when the applied field is held constant.[1] In certain circumstances the interaction with other degrees of freedom, such as the elastic modes of a crystal, may also be regarded as a renormalization effect.[1,4] Again, in the model described in Sec. 2 an ideal interacting spin system is renormalized by the constraint of over-all electroneutrality imposed on the mobile electrons which couple the ionic spins. (See also Ref. 1 where other, earlier models are reviewed.)

To describe the effects of critical exponent renormalization explicitly, suppose that the exponents of the ideal system are, in standard notation,[5] α, α' for the specific heat above and below T_c, β for the order parameter (spontaneous magnetization, density discontinuity, etc), γ, γ' for the total fluctuation (susceptibility or compressibility). Then the renormalized exponents governing the true asymptotic behavior of the "real" (or renormalized) system as $T \to T_c$ are

$$\alpha_X = -\alpha/(1-\alpha), \quad \alpha'_X = -\alpha'/(1-\alpha'), \tag{1.1}$$

$$\beta_X = \beta/(1-\alpha'), \tag{1.2}$$

$$\gamma_X = \gamma/(1-\alpha), \quad \gamma'_X = \gamma'/(1-\alpha'). \tag{1.3}$$

These relations presuppose that α and α' are positive so that the ideal specific heat diverges. The negative values of the renormalized specific-heat exponents indicate that the specific heats remain finite[1b] at the critical point but exhibit cusps there (with infinite slopes). When the ideal specific-heat singularities are logarithmic ($\alpha = \alpha' = 0$) renormalization with finite cusped specific heat again occurs but the renormalized temperature dependence is not given asymptotically by a pure power law. (See Ref. 1 for the details in this case.)

A crucial point concerning the renormalization results (1.1)–(1.3) is that the exponents α_X, β_X, γ_X, ..., while they are the true asymptotic values, will in general describe the behavior of the system closely only *inside* some transition region about the critical temperature T_c. Outside this transition region, the system may well appear to exhibit a temperature variation characteristic of the original ideal behavior. Furthermore, it was shown theoretically in Ref. 1 that the transition region may be rather small. This situation leads to the following questions, of importance in studying real physical systems: (a) Under what circumstances will critical-exponent renormalization be experimentally visible when expected on theoretical grounds? (b) If renormalization effects are visible, how close will the "observed" renormalized exponents correspond with the theoretically predicted values? (c) When renormalization effects are only partially observable how will the "observed" value of the critical temperature compare with the true value? (d) More generally what are the main factors influencing the size of the renormalization effects? By their nature these questions can be answered properly only by a detailed quantitative numerical analysis. This paper provides answers based on calculations for a theoretical model displaying renormalization which can, in effect, be solved exactly.[6] The model is, naturally, a somewhat special one (see below) but, on the grounds that many features of equilibrium critical behavior are known to be fairly insensitive to the system or the model,[4] it is believed that the results we have found will provide a realistic guide to the situation in more general and realistic cases. Our procedure has been to calculate from the model a set of (exact) "data points" such as might be obtained in an accurate experiment. In terms of the reduced temperature variable,

$$\begin{aligned} t &= (T/T_c) - 1, \quad T \ge T_c \\ t &= 1 - (T/T_c), \quad T \le T_c, \end{aligned} \tag{1.4}$$

we have obtained values of the specific heat, order parameter, total fluctuation, etc. for values of t spaced roughly equally on a logarithmic scale with about 10 points per decade over the range $1 \ge t \ge 10^{-8}$. The complete set of data for a given value of the dilution parameter x (or n, see below) have been examined and analyzed to determine apparent values of critical exponents and critical temperatures. In the analysis we have employed various standard techniques frequently used for handling real experimental data. The apparent or fitted values have then been compared with the exact values known from the theory of the model.

In order to summarize our conclusions we first define a properly normalized dilution parameter x. Suppose n is some parameter of the system or model which measures the density of impurities, the perturbing field, or other diluting influence. (In the model studied below it is actually a density of "electrons" through which spins are coupled.) Let n_0 be the value of n for the ideal or pure system with critical temperature T_c^0. We expect in most typical circumstances that the diluting influence will lower the critical temperature linearly with n for small $n-n_0$. In simple cases $T_c(n)$ will actually go to zero at a critical value of n, say n_c (e.g., a critical density of nonmagnetic impurities in a ferromagnet). When this happens, we define the dilution parameter simply by

$$x=(n-n_0)/(n_c-n_0), \tag{1.5}$$

so that $x=0$ corresponds to the ideal system, $0<x<1$ to the renormalized system, while for $x\geq 1$ there is no transition (of the same kind). This is the parameter we will use in our model. More generally, however, some other transition may intervene before $T_c(n)$ vanishes or, for experimental reasons, it may be impossible to follow T_c to large values of $n-n_0$. In these circumstances we may define x by

$$x=f\left|T_c^0-T_c\right|/T_c^0 \tag{1.6}$$

or, provided $T_c(n)$ varies linearly with n near $n=n_0$, by

$$x=f\left|n-n_0\right|\left|\left(\frac{\partial T_c}{\partial n}\right)^0\right|\Big/T_c^0, \tag{1.7}$$

where the superscript zero denotes the ideal limit $n=n_0$. These definitions imply

$$T_c(n)\approx T_c^0(1+f^{-1}x), \quad \text{as } x\to 0, \tag{1.8}$$

where f is a factor expected to be in the range, say 0.6–0.9, which allows for the differences from the definition (1.5). Note that these last two definitions can be used when no critical value of n exists or even when the "diluting influence" actually raises the transition temperature.

With these preliminaries, we may summarize our conclusions as follows. Firstly, essentially no renormalization effects are visible unless $x>0.01$. The specific heat changes quite sensitively with the dilution parameter but the nature of the asymptotic behavior does not change unambiguously until x is so large (≥ 0.3) that the finite height of the cusp can be seen experimentally. These effects *do* appear to have been seen unmistakably in recent experiments on the λ transition in liquid He^3-He^4 mixtures,[7] which should provide a good example of the general theory. The changes due to renormalization in the specific heat and in the other thermodynamic variables are much more pronounced *below* T_c than above T_c. Correspondingly, the changeover or transition temperature is much closer to T_c above the transition than below. These features are mainly due to the characteristic asymmetry in the ideal specific heats which, for equal values of t are typically 2 to 4 times larger below T_c than above.

A second principal conclusion is that even when renormalization effects are clearly occurring, it is nonetheless essentially *impossible* experimentally to measure the fully renormalized critical exponents. Instead, the fitted or observed exponents β, γ, γ',... increase smoothly with x, there being very little if any indication from the fits that the apparent exponent is not asymptotically exact. For the order-parameter exponent we find that the approximate formula

$$\beta_{\text{fit}}(x)\simeq\beta+x\Delta\beta_X, \quad (\Delta\beta_X=\beta_X-\beta) \tag{1.9}$$

gives a fair account of the situation. We expect γ'_{fit} to vary according to a similar formula although we have not examined this exponent in detail. Above T_c, on the other hand, the true renormalized exponent is even less accessible to experiment: We find roughly that

$$\gamma_{\text{fit}}(x)\simeq\gamma+\tfrac{1}{5}\,x\,(1+2x^2)\Delta\gamma_X, \; (\Delta\gamma_X=\gamma_X-\gamma) \tag{1.10}$$

describes the behavior if x is not too close to unity. Of course these last two formulas have no theoretical status. They merely summarize what will appear to be the case experimentally on the basis of measurements in which the temperature resolution is not better than 1 in 10^6 or 10^8. At present these represent realistic if not overoptimistic limits. An experimental test which bears out the insensitivity of the exponent γ to dilution has been performed recently by Bak and Goldburg[8] who studied the scattering of light near the consolute point of the binary fluid mixture phenol and water in the presence of hypophosphorous acid (H_3PO_2) as an impurity. A small consolation for the difficulty of measuring the true renormalized exponents is that use of the observed or fitted exponents leads to quite reliable estimates of the true critical temperatures when the data are accurate (i.e., bearing in mind the actual resolution in t available).

The explicit, albeit rough and ready, formulas (1.9) and (1.10) for the "effective" exponents have been found, as explained, only for a particular model. The question, naturally, arises as to how far they will remain quantitatively valid in other models and in real systems with, now, the more general definitions (1.6)–(1.8) of the dilution parameter x. By altering the parameters of the model (see Sec. II) this point may be checked to some extent: We have not made a full-scale study but examination of the thermodynamic functions of the model over a range of parameter values[9,10] indicates that the above results remain valid to within factors of 0.7–1.5 in the definition of x. More generally, consideration of the renormalization mechanism reveals that the magnitude of the specific-heat anomaly is the prime quantitative determinant. One knows from a variety of model studies (and to some extent also from experimental data) that the amplitude of the singularity changes quite strongly with x. In particular, when $T_c(x) \to 0$ the amplitude itself approaches zero. From this viewpoint the conclusions (1.9) and (1.10) together with the definitions (1.6)–(1.8) simply embody a law of corresponding states. Experience with other critical properties[3] suggests that such a law should be valid to within factors of 0.5–2 on the scaling variables, provided one considers systems with simple predominantly short-ranged interactions. As with the critical exponents themselves, significant long-range forces probably lead to appreciable quantitative differences. (Competing short-range forces could also give rise to quantitative changes.)

The detailed calculations and graphs leading to our main conclusions are presented in the remainder of the article. The model used is explained briefly in Sec. II while Secs. III–V are devoted, respectively, to the specific heats, order parameter, and total fluctuation or susceptibility above T_c.

II. MODEL

The model employed in this study is one of a class of decorated Ising models described by Fisher[1,11] which are completely soluble in terms of the underlying standard Ising lattice. The particular model, a "mobile-electron Ising ferromagnet," has been studied in detail by Scesney.[9,10] It consists generally of a lattice of spin-$\frac{1}{2}$ ions which interact with nearest neighbor ions, only via interactions with one or more "mobile electrons" which may have moved into association with the ion-ion bond. The energy associated with the bond and the strength of the induced spin-spin coupling of Ising character depends on the number of electrons present locally. Although the number of electrons on a bond may fluctuate, the total number is subject to the constraint of electroneutrality. As demonstrated in Ref. 10 the model displays several interesting different modes of behavior depending on n, the over-all mean number of electrons per bond, and on two energy parameters b and c, which arise naturally in the analysis. For the present purposes we have restricted attention to the cases for which $b=0$, $c=2$. This combination of parameter values leads to some mathematical simplifications but the general behavior is quite typical of other values and, as indicated in the Introduction, our results are not very sensitive to the particular choice (provided the over-all mode of behavior is not changed, e.g., *lower* critical points may arise in the model but are not considered here).

With the choice $b=0$, $c=2$, the model exhibits only three modes of behavior: At maximum electron concentration $n=n_0=2$ all ions are coupled in an identical fashion with no fluctuations. This is the ideal or pure state which is ferromagnetically ordered at low temperatures but disorders above a unique critical temperature T_c^0. The critical exponents in this case are identical with those of the standard Ising ferromagnet. (We have considered only an underlying simple cubic lattice although bcc and fcc lattices could have been analyzed with equal ease.) Of course, the exact critical point and exponents are not known for any three-dimensional Ising lattices. However, there is a wealth of numerical evidence[12] which supports the conclusions

$$\alpha=\alpha'\simeq 0.1250, \quad \beta\simeq 0.3125, \quad \gamma\simeq 1.250. \quad (2.1)$$

In the present analysis we will accept these values (and the corresponding numerical estimates of the critical temperature, the energy, specific heat, magnetization and susceptibility)[10] without further question. The essential point is that we are interested only in *relative* effects, namely, the changes brought about by renormalization. Any errors in the values of (2.1), etc. will only lead to changes of a percent or so in the data we calculate; they will not seriously change orders of magnitude, general trends, or important qualitative features. Thus doubts, for example, as to the equality of α and α', need not concern us here. (As a matter of fact, some calculations have been run with the assumption $\alpha'=0.0625$ and these confirm our assertions.)

When the electron concentration n is decreased below n_0 fluctuations of the effective spin-spin interactions are allowed (we may think of impurity "holes" being admitted to the lattice) and renormalization effects set in as predicted by the general theory.[1] With the values (2.1) the exact asymptotic renormalized critical exponents of the model are

$$\alpha_X=\alpha'_X\simeq -0.1429, \quad (2.2)$$

$$\beta_X\simeq 0.3571, \quad \gamma_X\simeq 1.4286. \quad (2.3)$$

It is from this range of the model that our conclusions have been drawn. As n decreases to the critical value $n_c\simeq 0.2642$ the critical temperature $T_c(n)$ falls to zero. For $n\geq n_c$ there is no transition

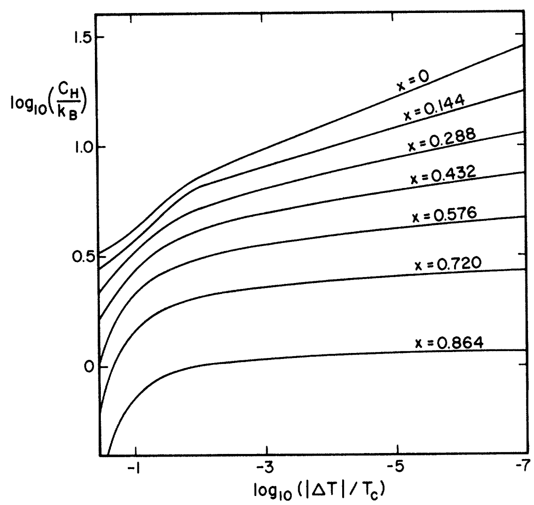

FIG. 1. Logarithmic plot of specific heat C_H below T_c versus the reduced temperature t for various values of the dilution parameter x.

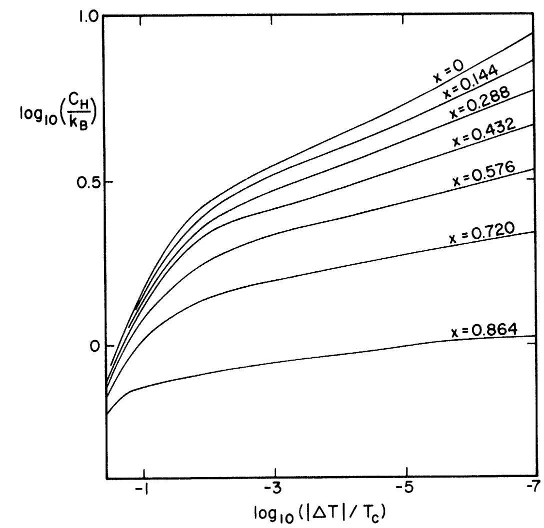

FIG. 2. Logarithmic plot of the specific heat above T_c versus t for the various values of x used in Fig. 1.

and the system always remains in the magnetically disordered (paramagnetic) state. (Physically the number of available electrons is too few to link together a macroscopic number of the ionic spins so as to form a single magnetized domain which can exhibit long-range order. In fact, n_c is fairly close to the percolation probability for random occupation of the bonds.[13])

Finally, we recall that the dilution parameter x is related to the concentration n of mobile electrons via (1.5).

III. SPECIFIC HEAT

While the specific heat of the pure or ideal system diverges at T_c with exponents α and α' (equal to $\frac{1}{8}$), the renormalized specific heat sufficiently close to the critical point varies as[1,4]

$$C_H/k_B \approx A + B_+ t^{\alpha/(1-\alpha)}\ , \quad \text{as } T \to T_{c+} \tag{3.1}$$

$$C_H/k_B \approx A + B_- t^{\alpha'/(1-\alpha')}\ , \quad \text{as } T \to T_{c-}\ . \tag{3.2}$$

The "constants" A, B_+, and B_- depend, of course, on the degree of dilution x. To see the extent to which the change from divergent to cusped behavior is visible in temperature ranges accessible to experiment we present, in Figs. 1 and 2, log-log plots of specific heat versus t above and below T_c for various values of x. The curves for $x = 0$ in both plots approach limiting straight lines of slopes corresponding to $\alpha = \alpha' = \frac{1}{8}$. For large values of x the cusped behavior [i.e., the finite maximum in $C_H(T)$] is clearly visible when $T < T_c$ although, for the same value of x it is less obvious above T_c.

For small degrees of dilution, however, the height of the cusp is so great that there are no signs of the plots bending over or levelling out, even for $t < 10^{-6}$ or 10^{-7}. Instead the plots appear to be quite closely linear on a scale of 2 to 3 decades (especially if allowance is made for "experimental uncertainties" in the values of C_H which, in practice, increase as T approaches T_c). The slopes of these pseudoasymptotic lines decrease smoothly with increasing x from the maximum value $\frac{1}{8}$ to close to zero. Although the full renormalization effects are not visible unless x is large, we note that the specific heat is quite sensitive to changes in x both above and below T_c.

In Figs. 3 and 4, the same specific-heat data

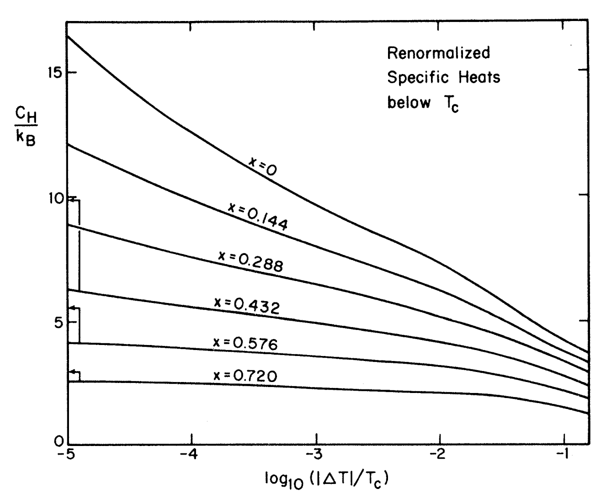

FIG. 3. Semilogarithmic plot of the specific heat below T_c for the same values of x used in Fig. 1.

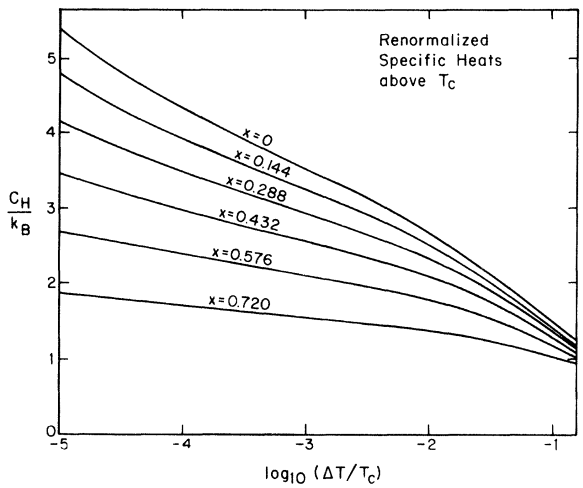

FIG. 4. Semilogarithmic plot of the specific heat above T_c for the same values of x used in the previous figures.

are plotted linearly versus $\log_{10} t$ as is very often done in practice. For small x, a clear upward curvature is visible for low t as is characteristic of some (low) power-law divergence. For $x > \frac{1}{2}$, the plots below T_c again show evidence of the finite cusp. (Note that the limiting maxima are indicated on the axis by arrows.) Above T_c, however, the maxima although finite, are so much greater than the values of the specific heat even at $t = 10^{-5}$, that there is essentially no visible evidence of their presence in the curves. On the contrary, for $x > 0.3$ the last $2-2\frac{1}{2}$ decades of the plots can be fitted quite accurately by straight lines as would be the case if the specific heats were diverging logarithmically. A similar linearity is seen below T_c for intermediate values of x from 0.2 to 0.6.

As indicated above, the general behavior can be understood by realizing how the height of the cusp depends on the degree of dilution. For the present simple cubic lattice model this is described fairly accurately by the formula

$$A(x) \simeq 7.50(1-x)/x. \tag{3.3}$$

Thus A is rather large even for $x \simeq \frac{1}{2}$. For the models based on other lattices, a similar form would hold but with a slightly different ($\pm 10\%$) numerical constant.

IV. ORDER PARAMETER

Asymptotically close to the critical point the order parameter or spontaneous magnetization $M_0(T)$ vanishes as

$$M_0(T) \approx D(x) t^{\beta(x)}, \quad \text{as } T \to T_c(x)-, \tag{4.1}$$

with exponent $\beta = 0.3125$ in the ideal limit $x = 0$. [The normalization chosen is such that $M_0(T) \to 1$ as $T \to 0$ when $x = 0$.] For $x > 0$, the renormalized value $\beta_X = 0.3571$ must be evident sufficiently close to T_c: We will show, however, that this may be very close indeed.

To study the effects of renormalization the (M_0, T) data were analyzed as if the values of $T_c(x)$, $\beta(x)$, and $D(x)$ were unknown. In the first instance the numerical data for a fixed value of x were separated into groups with different temperature ranges. Generally two consecutive decades of $\Delta T = T_c - T$ were selected since this sort of range is typical of real experiments. Each group of data was then fitted, using a standard least-squares procedure, to the logarithmic form

$$\ln M_0(T) = \beta \ln[1-(T/T_c)] + \ln D \tag{4.2}$$

in order to determine optimal values of T_c, β, and D for the given limited temperature ranges. The fitted critical temperatures $T_{c,\text{fit}}$ are found to be slightly lower than the exact critical temperature T_c, known by direct calculation, but the magnitude of the deviations are found to be quite negligible. Typically, $(T_c - T_{c,\text{fit}})$ was a factor of 10 to 100 smaller than the smallest values of $|\Delta T| = t T_c$ provided in the data. From an experimental viewpoint, this high accuracy is somewhat illusory since it is based on arbitrarily precise and accurate data with no "experimental" uncertainties in the values of M_0 or T. Not withstanding the high precision, the straight line fits on the log-log plots are found to be perfect to within graphical accuracy. [The maximum deviation of $\log_{10} M_0(T)$ from the fitted line is $\sim 10^{-3}$.] The most interesting results of the fitting process are displayed in Fig. 5, where $\beta_{\text{fit}}(x)$, the optimal fitted value of β in (4.2), is plotted versus the dilution parameter x for various different temperature ranges. [The curves labeled k to $(k+2)$ describe the results of fitting about 20 data points in the range of $t = |\Delta T| / T_c$ of 10^{-k} to 10^{-k-2}: The corresponding error in $T_{c,\text{fit}}$ is about 1 part in 10^{-k-4} as mentioned.] It is evident from Fig. 5 that β_{fit} is an approximately linear function of x for accessible temperature ranges. To a rough but useful approximation, the formula

$$\beta_{\text{fit}}(x) \simeq \beta + x\Delta\beta_X, \quad \Delta\beta_X = \beta_X - \beta \tag{4.3}$$

describes the data in the normally best accessible range $t = 10^{-3}-10^{-6}$. Quite clearly, β_{fit} only approximates the fully renormalized value β_X for x rather close to 1. In fact even at the limit $x = 1$ very small values of t are needed to obtain a good estimate of β_X.

Note, incidentally, that the curve for the range $10^{-2} > t > 10^{-4}$ underestimates β by about 1% at the ideal limit $x = 0$. Of course, this is just an indica-

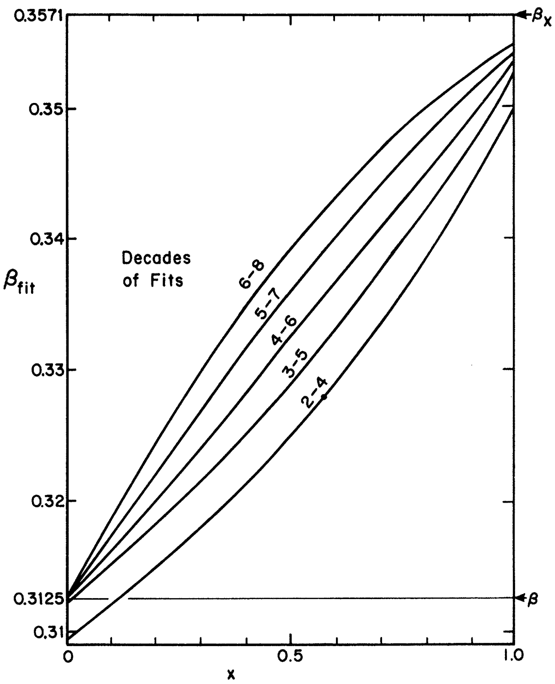

FIG. 5. Apparent value $\beta_{fit}(x)$ of the exponent β for the order parameter as a function of the dilution parameter x for fits over different temperature ranges (see text).

tion of the importance of the ever-present higher-order corrections to the leading asymptotic behavior. As is usually done, these have been neglected in (4.1) and (4.2). This observation should, however, serve as a warning against placing much confidence in the third decimal place of any real experimental estimate of β. Even in the ideal case, one cannot be sure the corrections are small and they usually cannot be estimated independently.

In Fig. 6 we show the variation of the apparent amplitude $D(x)$ as fitted on the log-log plots. The changes with x are fairly mild until one approaches close to the limit $x=1$ where the amplitude rapidly drops to zero. However, the magnitude of the amplitude is sensitive to the range of fit. It can be shown theoretically that as x changes from zero to nonzero the asymptotic values of both the exponent β and the amplitude D change discontinuously. The asymptotic value of D for $x>0$ is found to be proportional to $x^{-\beta_x}$ and hence, for small x, is greater than the finite asymptotic value of D for $x=0$.[14] The tendency for the curves describing the various ranges $10^{-k}>t>10^{-k-2}$ to bow upward as k increases merely reflects their approach to the asymptotic value.

In order to illustrate further how good the least-squares log-log fits actually are, a particular set of data similar to some of the best published data[15] have been singled out for further analysis. The data selected correspond to

$$x=0.576, \quad t>10^{-4}, \quad \beta_{fit}=0.3280;$$

they are denoted by a solid dot on the 2-4 curve in Fig. 5. As an alternative to the log-log fits the graphical technique of Heller and Benedek[13] was tried. Values of the spontaneous magnetization [reduced by some convenient value, such as $M_1=M_0(0)$] are raised to various powers which it is hoped will approximate $1/\beta$, and are plotted linearly versus T. If the "true" value of β is chosen the data are expected to lie asymptotically on a straight line which intersects the T axis at the critical point T_c (which is thereby located by the data). As can be seen from Fig. 7, the data do indeed lie on a good straight line if the previously fitted value $\beta=0.3280$ is adopted. On the other hand if either the ideal value $\beta=0.3125$, or the renormalized value $\beta_x=0.3571$ is employed to make the plot, the data deviate markedly from a straight line near T_c. (In the figure, T_1 is a convenient scaling temperature equal to J/k_B, where J is a spin-spin coupling parameter for the model.)

As a further test of the choice of β_{fit} and to study

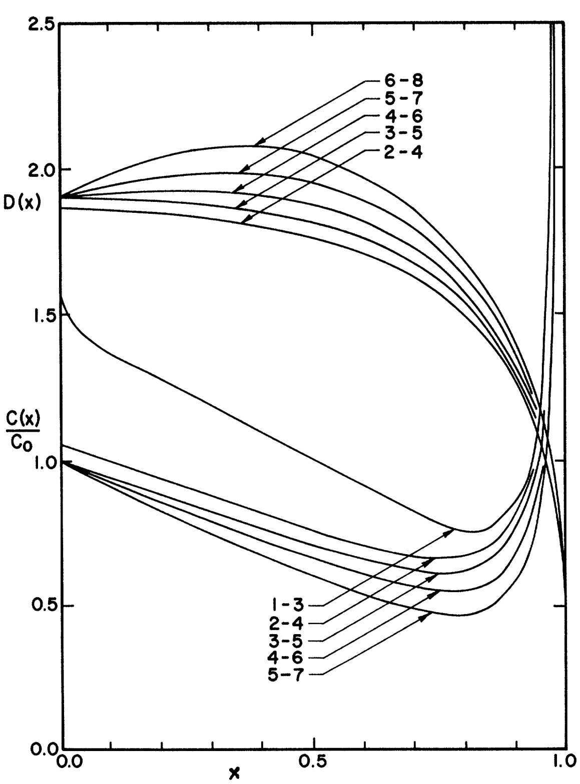

FIG. 6. Apparent values of the amplitudes $D(x)$ (upper set of curves) and $C(x)/C_0$ (lower set) as a function of x and for various temperature ranges (see text). C_0 is the asymptotic limiting value of $C(0)$.

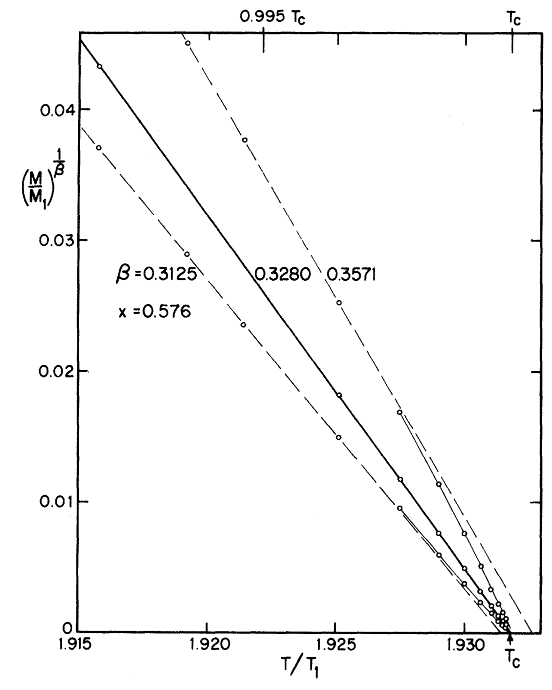

FIG. 7. Heller-Benedek plots of $M^{1/\beta}$ versus T (on conveniently reduced scales) for the case $x=0.576$ comparing the ideal, best fit, and fully renormalized exponent values.

the approach of the data to the chosen asymptotic form, a number of values of β bracketing β_{fit} were chosen. With these values assigned, two-parameter least-squares fits were made using the form (4.2) again. (The same data over the decades $t=10^{-2}-10^{-4}$ were employed as previously.) The values T_c and D so determined, together with the corresponding value of β, describe curves in the (M_0, T) plane. Following Heller[15] we test the goodness of fit by calculating the temperature deviation $T_{fit}(M_0)-T_{data}(M_0)$ of the fitted curve from the exact value $T_{data}(M_0)$ at the same fixed value M_0 of magnetization. These deviations are normalized by the corresponding $T_{c,fit}$ and plotted versus $T(M_0)/T_{c,fit}$ in Fig. 8 (see solid curves). Again, the entire analysis is carried out as though the exact value of T_c were unknown. This figure does indeed illustrate that a value of β within $\frac{1}{2}\%$ of 0.328 is the best choice for fitting the data near T_c. As T falls below $0.995\,T_c$ all the deviations increase (owing again to the neglected higher-order correction terms) but the fits are clearly worse for the other assigned values of β, including the ideal value $\beta=0.3125$ and the renormalized value $\beta_X=0.3571$. We may recall, nonetheless, that $\beta=\beta_X$ must be asymptotically exact.

Finally we remark that there is a certain arbitrariness in plots such as Fig. 8 unless one specifies an explicit method for estimating the amplitude D (as we did using the log-log fits). The criteria employed by Heller for the choice of D in his original applications of the method[15] were not clearly stated.[16] By suitably altering our own choice of D, however, we can mimic the deviation structure found by Heller; this is illustrated by the dashed lines for the extreme values of β in Fig. 8. These values of D reduce the deviations when t is in the range 0.970–0.995, at the cost of much larger relative deviations when t is in the region of 10^{-3} where our fitting was performed. The arbitrariness does not seem, however, to have a serious effect on the choice of the optimum value of β_{fit}.

In conclusion we reiterate that none of the methods examined (or others known to the authors) will give good fits to the data for intermediate values of x which isolate either the correct value of β or of β_X.

V. SUSCEPTIBILITY AND TOTAL FLUCTUATION

We now investigate the renormalization of the susceptibility or total squared fluctuation of the order parameter above the transition. The suscep-

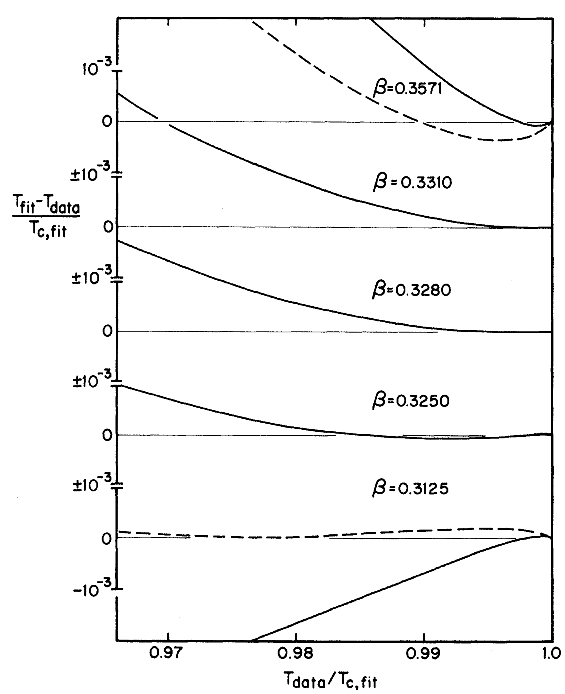

FIG. 8. Reduced temperature deviations versus temperature for the data with $x=0.576$ fitted by assuming various values of β.

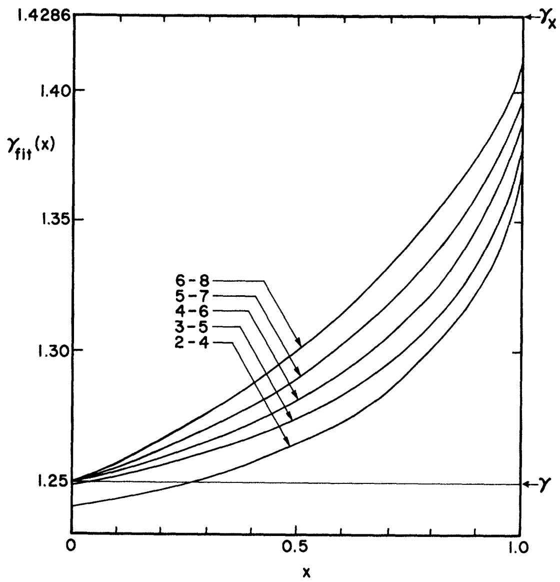

FIG. 9. Apparent values of $\gamma_{fit}(x)$ of the exponent γ for the susceptibility above T_c as a function of x for various temperature ranges. [The notation k to $(k+2)$ denotes a fit made over the two decades 10^{-k} to 10^{-k-2} of reduced temperature $t = |\Delta T|/T_c$.]

tibility χ varies asymptotically as

$$(k_B T_c/m^2)\chi = \hat{\chi} \sim C(x)\, t^{-\gamma(x)}, \quad (T \to T_c+) \qquad (5.1)$$

where in the ideal limit $x = 0$ we have $\gamma = 1.250$; but for $0 < x < 1$ the renormalized value $\gamma_X \simeq 1.429$ will apply sufficiently close to T_c. Note that the ideal free spin susceptibility per ion is $\chi = m^2/kT$ in this normalization. We will describe the results of two numerical techniques used to analyze the (χ, T) data. The first one is simple least-squares fitting to the logarithmic relation

$$\ln\hat{\chi} = -\gamma \ln[(T/T_c) - 1] + \ln C, \qquad (5.2)$$

as used for the spontaneous magnetization. The data were again grouped into sets of about 20 points, each set spanning two decades in t. The critical temperature $T_c(x)$, and $\gamma(x)$, and $C(x)$ were fitted independently. The errors in the estimation of T_c were quite negligible relative to the range of t studied just as found in the case of the magnetization. The actual fitted values $T_{c,fit}$ however, were slightly higher than the true values of T_c. Again the goodness of the fits over the chosen two decades of the log-log plots was perfect to within graphical accuracy.

The best values $\gamma_{fit}(x)$ of the exponent obtained by this procedure is plotted versus x in Fig. 9. The effects of the renormalization on χ are relatively much weaker and more subtle then they were on the magnetization. Whereas $\beta_{fit}(x)$ varied fairly linearly with x from β to β_x, the variation of $\gamma_{fit}(x)$ for comparable temperature ranges is linear only for small $x (\lesssim 0.3)$; as x increases even to 0.95 the apparent exponent remains below 1.37 (compared with $\gamma_X \simeq 1.43$). In the range $x < 0.8$, the approximate formula

$$\gamma_{fit}(x) \simeq \gamma + \tfrac{1}{5} x (1 + 2x^2) \Delta\gamma_X, \quad \Delta\gamma_X = \gamma_X - \gamma \qquad (5.3)$$

gives a rough description of the behavior when t is in the range 10^{-3}–10^{-6}. For larger values of t less renormalization is visible for small x and indeed when temperatures in the range $t \simeq 0.01$ are utilized the fits actually fall *below* γ even at the ideal limit. Just as for the spontaneous magnetization, this is merely an indication of the neglected higher-order corrections to (5.1).

The variation of the apparent amplitude $C(x)$ is shown in Fig. 6 where it is scaled by C_0, the asymptotic limiting value of $C(0)$, [14] and plotted as a function of x for various ranges of t. Note the divergence of $C(x)$ as x approaches the limit $x = 1$. As was also the case with the magnetization, the asymptotic value of the amplitude changes discontinuously when x becomes nonzero. The asymptotic value of $C(x)$ for $x > 0$ is proportional to x^{γ_X} and for small x, is less than the asymptotic value of $C(0)$.[14] This accounts for the initial downward trend of the fitted values of $C(x)$ for small x.

As a second method of analysis we try the method of Kouvel and Fisher[17] which is useful for extrapolation when observations very close to T_c are not available. A function $T^*(T)$ is defined from the data by

$$T^*(T) = \left(\frac{d}{dT} \ln\chi^{-1}\right)^{-1} = \left(\chi \frac{d\chi^{-1}}{dT}\right)^{-1}. \qquad (5.4)$$

If χ is described asymptotically by the power law (5.1) then as $T \to T_c+$ the function $T^*(T)$ varies asymptotically as $(T - T_c)/\gamma$, that is, linearly with T. A linear extrapolation of $T^*(T)$ to the T axis thus yields an estimate T_c' for the critical temperature. Figure 10 shows such a plot of $T^*(T)$ and χ^{-1} for the special case $x = 0.576$ studied in Sec. IV. Although the $T^*(T)$ plot appears highly linear over a wide range of temperatures, its actual slope is found to decrease slightly as T approaches T_c. This, of course, indicates the start of the change from $1/\gamma$ to the renormalized value $1/\gamma_X$. Most of this bending, however, occurs so close to T_c even for $x \simeq 0.6$, that, as before, the error in estimating T_c is quite negligible relative to the closest data points.

Once a reliable estimate of T_c is obtained, the Kouvel-Fisher method defines an effective exponent

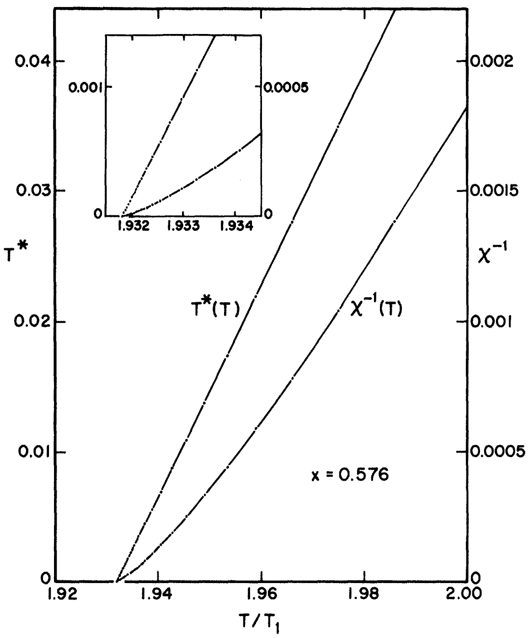

FIG. 10. The inverse susceptibility χ^{-1} and the Kouvel-Fisher function $T^*(T)$ versus T for $x = 0.576$.

$$\gamma^*(T) = (T - T_c')/T_c{}^*(T), \tag{5.5}$$

where T_c' denotes the estimated critical temperature. If T_c' is sufficiently accurate $\gamma^*(T)$ will eventually approach close to the fully renormalized asymptotic exponent γ_X. [Indeed when T_c' is exact, the limit of $\gamma^*(T)$ as $T \to T_c$ can be taken as a definition of the true exponent.] The behavior of $\gamma^*(T)$ as a function of T/T_c for various values of the dilution parameter x is shown in Fig. 11. The curve for $x = 0$ is readily extrapolated to yield the correct ideal exponent $\gamma = 1.250$. The curves for large x lie higher and are not so linear. They would probably be extrapolated roughly to values comparable to (or for the same range of t, somewhat higher than) the values obtained from the log-log fits (see Fig. 9). However, at the end of the range close to T_c the curves for all $x > 0$ exhibit rather clearly a sharp "upswing" which serves as a warning that the exponent is being underestimated. Nevertheless, even with a generous allowance for this upswing, it would be quite impossible to guess a reliable value for γ_X. Furthermore, in an experimental situation one must expect that the curvature might be hidden in the noise level provided by uncertainties in the value of $\gamma^*(T)$; these are necessarily fairly large because of the numerical differentiation involved in reducing the data to obtain $\gamma^*(T)$.[17]

We conclude then, that it is impossible in practice to measure the fully renormalized exponent γ_X. For sufficiently large values of the dilution parameter the apparent value of γ will increase but, as indicated by (5.3), only by a proportionately rather small fraction of the full difference $\gamma_X - \gamma$. The recent experimental test by Bak and Goldburg[8] which bears out the insensitivity of γ to dilution was mentioned already in the Introduction. Indeed, we expect our conclusions to remain valid both as regards other methods of analysis that might be tried and, as explained in the introduction, for more general models and for real physical systems.

ACKNOWLEDGMENTS

We are grateful for the support of the Advanced

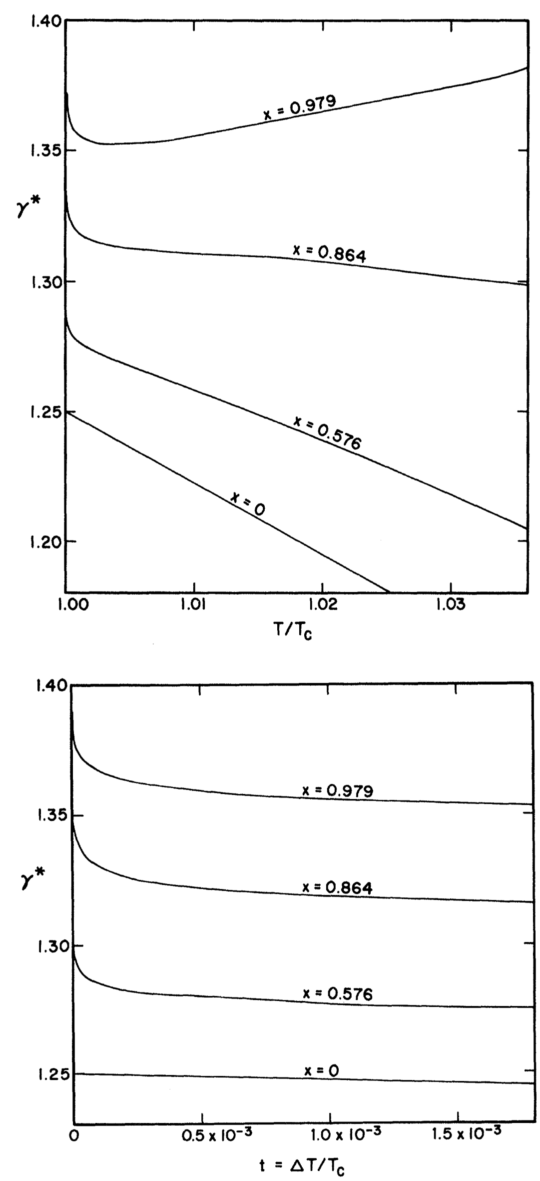

FIG. 11. Plots of the exponent function $\gamma^*(T)$ versus T/T_c for various values of the dilution parameter x.

Research Projects Agency through the Materials Science Center at Cornell University. Comments and correspondence from Professor B. Widom and Dr. George Neece are gratefully acknowledged.

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[1](a) M. E. Fisher, Phys. Rev. 176, 257 (1968). This paper contains references to most of the relevant earlier literature. (b) Attention should be drawn to a mistake in this article by Fisher, where, following Eq. (2.47), it was stated that the renormalized specific heat would in general be discontinuous at T_c with $B_X' \neq B_X$. In fact it is easily verified from the definitions in Ref. 1 that B_X, as defined by Eq. (2.45), depends only on the critical-point values of variables which are continuous at T_c. It follows that $B_X = B_X' = C(T_c)/k_B$ so that the renormalized specific heat is *continuous* through the critical point even though it is cusped there. [Fig. 1(b) of Ref. 1 is thus also misleading.] In fact, a discontinuous renormalized specific heat is only to be expected when either α or α' or both are already negative in the ideal system.

[2]B. J. Lipa and M. J. Buckingham, Phys. Letters 26A, 643 (1968).

[3]B. M. McCoy and T. T. Wu, Phys. Rev. 176, 631 (1968); 188, 982 (1969); B. M. McCoy, *ibid.* 188, 1014 (1969); B. M. McCoy, Phys. Rev. Letters 23, 383 (1969); R. B. Griffiths, *ibid.* 23, 17 (1969); P. G. Watson, J. Phys. C 2, 948 (1969).

[4]See G. A. Baker and J. W. Essam, Phys. Rev. Letters 24, 520 (1970).

[5]For reviews of critical-exponent notation, etc., see: (a) M. E. Fisher, J. Appl. Phys. 38, 981 (1967); (b) L. P. Kadanoff *et al.*, Rev. Mod. Phys. 39, 393 (1967); (c) M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967).

[6]Some similar calculations have been undertaken by Dr. George Neece who has employed a binary fluid model [G. A. Neece, J. Chem. Phys. 47, 4112 (1967); R. K. Clark and G. A. Neece, *ibid.* 48, 2575 (1968)] and mainly studied the two-dimensional case where the specific heat is logarithmic.

[7](a) T. Alvesado, P. Berglund, S. Islander, G. Pickett, and W. Zimmerman, Phys. Rev. Letters 22, 1281 (1969); (b) F. Gasperini and M. R. Moldover, *ibid.* 23, 749 (1969).

[8]C. S. Bak and W. I. Goldburg, Phys. Rev. Letters 23, 1218 (1969).

[9]M. E. Fisher and P. E. Scesney, J. Appl. Phys. 40, 1554 (1969).

[10]P. E. Scesney, Phys. Rev. B 1, 2274 (1970).

[11]M. E. Fisher, Phys. Ref. 5(c). 969 (1959).

[12]See the review Ref. 5(c).

[13]See, e.g., M. E. Fisher, *Proceedings I.B.M. Scientific Computing Symposium on Combinatorial Problems*, 16-18, *March* 1964, (I.B.M. Corporation, New York, 1966) Chap. 11; and J. W. Essam and H. Garelick, Proc. Phys. Soc. (London) 92, 136 (1967).

[14]The asymptotic behavior of $D(x)$ and $C(x)$, although not treated in Ref. 1 or Ref. 10, is easily derived from the information contained therein. Note that as a feature of the model we have $C(0) = 1.46$ which is some 40% higher than values of C typical of other systems.

[15]P. Heller, Rept. Progr. Phys. 30, 731 (1967).

[16]Heller's deviation plots and the dashed lines in Fig. 8 show the deviation of $M^{1/\beta}$ versus T plots from linearity. The choice of the straight line and hence "best" D when the plot is curved is not obvious.

[17]J. S. Kouvel and M. E. Fisher, Phys. Rev. 136, A1626 (1964).