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ABSTRACT

In the past decade a number of authors have reported the measurement of a non-zero value for the critical exponent η. We analyze the method of data analysis in these critical scattering experiments and conclude that no experiment to date unambiguously and directly establishes that η is greater than zero. We then discuss what we feel would be an unambiguous determination of η. These conclusions are a result of our computation of the k-dependent susceptibility $\chi(\vec{k},T)$ for the two-dimensional Ising model in zero magnetic field. In the scaling limit $k\to 0$, $\xi\to\infty$ such that $y=k\xi$ is fixed, $\chi(\vec{k},T)=\xi^{\gamma/\nu}X_{\pm}(y)+o(\xi^{\gamma/\nu})$ (ξ is the correlation length). We compare these exact results with the various phenomenological scattering approximates (Ornstein-Zernike, Fisher-Burford, etc.) This comparison provides insight into those regions of $y=k\xi$ where these approximates are applicable. Such insight is important since the region of experimentally accessible y is rather limited.

INTRODUCTION

In the past decade a great amount of work has gone into the study of critical magnetic scattering. If the inelasticity effects are negligible and multiple scattering may be neglected, then the neutron scattering cross section is proportional to the $\vec{k}$-dependent susceptibility $\chi(\vec{k},T)$, where $\vec{k}$ is the momentum transfer. This is the so-called quasielastic approximation.[1] For a simple spin system the $\vec{k}$-dependent susceptibility $\chi(\vec{k},T)$ is related to the static spin-spin correlation function $\langle\sigma_0\sigma_{\vec{R}}\rangle$ by

$$\chi(\vec{k},T) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}[\langle\sigma_0\sigma_{\vec{R}}\rangle - M_s^2] \quad (1)$$

where M_s is the spontaneous magnetization. For $\vec{k}=0$ $\chi(\vec{k},T)$ reduces to the thermodynamic susceptibility $\chi(T) \equiv \chi(0,T)$.

As T approaches the critical temperature T_C, the correlation length $\xi(T)$ and the thermodynamic susceptibility $\chi(T)$ diverge and are usually parametrized by[2]

$$\xi \sim \xi_0^{\pm}|1-T/T_C|^{-\nu} \qquad (T\to T_C^{\pm}) \quad (2)$$

and

$$\chi(T) \sim C_{0\pm}|1-T/T_c|^{-\gamma} \qquad (T\to T_C^{\pm}). \quad (3)$$

The critical exponent η is defined[3] by

$$\chi(\vec{k},T_C) \sim \bar{C}_1 k^{-2+\eta} \qquad (T=T_C, k\to 0). \quad (4)$$

One notes that the exponent η is defined by a property of the system for T exactly equal to T_C, whereas γ and ν are defined by an approach to T_C. In Table I se summarize the experimental results for η (for magnetic systems).

The scaling region is defined by the limit

$$T\to T_C,\ k\to 0 \quad (5a)$$

such that the scaled variable

$$y=k\xi \quad \text{is fixed.} \quad (5b)$$

In this scaling limit Kadanoff[4] and Fisher[2,3] assume that $\chi(\vec{k},T)$ which is a function of two variables $\vec{k}$ and T reduces to essentially a function of one variable

$$\chi(\vec{k},T) = \xi^{\gamma/\nu}X_{\pm}(y) + o(\xi^{\gamma/\nu}). \quad (6)$$

The functions $X_{\pm}(y)$ are referred to as scaling functions.

As $y\to\infty$ the large-y behavior of $X_{\pm}(y)$ defines an exponent $\hat{\eta}$

$$X_{\pm}(y) \sim C_1 y^{-2+\hat{\eta}} \qquad (y\to\infty). \quad (7)$$

The one-length scaling hypothesis states that η defined by (4) and $\hat{\eta}$ defined by (7) are the same. Furthermore it is implicity assumed that C_1 is non-zero and it reproduces the constant $\bar{C}_1$ in (4). Thus the one-length scaling hypothesis states that

$$\hat{\eta} = \eta \qquad \text{and } C_1 \neq 0. \quad (8)$$

Table I. Experimental results for the critical exponent η determined by direct measurements of the neutron scattering cross section. The last column gives the reference to this work.

System	η	Ref.
DAG[2]	0.12±0.1	5
MnF_2	0.05±0.02	6
$RbMnF_3$	0.055±0.01	7
K_2NiF_4	***[b]	8
K_2CoF_4	0.2±0.1	9
$MnTiO_3$	0.2±0.15	10

[a] Dysprosium Aluminum garnet

[b] Recent re-analysis of the data now gives the scattering cross section consistent with the Ornstein-Zernike pole approximation in the range $y\lesssim 10$.

If there were more than one length scale present in the problem, then we would find (8) being violated. From here on we assume $\hat{\eta}=\eta$ and no longer distinguish between η and $\hat{\eta}$.

Once one has (8) and demands that the scaling functions connect onto (3) in the $y\to 0$ limit and onto (4) in the $y\to\infty$ limit, then one obtains the relationship[2,3,4]

$$(2-\eta)\nu=\gamma. \quad (9)$$

PHENOMENOLOGICAL SCALING FUNCTIONS

We now discuss the problem of the measurement of η. First of all, the mere definition (4) of η makes it impossible to directly measure for the simple reason that no experiment is performed exactly at $T=T_c$. From an experimental point of view, the definition (7) is more appropriate. Thus a direct measurement of η involves measuring cross sections for large y. If one assumes the one-length scaling hypothesis, then small-y measurements allow one to determine γ and ν and by (9) to deduce η. Unfortunately the mathematical limit $y\to\infty$ in (7) cannot be performed in the laboratory. Experimental values[5-10] of y range up to 65 but perhaps 20 to 30 is more typical. Thus one has the problem of extrapolating the data into the regime where (7) is a valid approximation to the scaling functions $X_{\pm}(y)$. This extrapolation involves assuming a phenomenological formula for $X_{\pm}(y)$ and using this in a least squares fitting program. Thus to discuss further the measurement of η we must discuss various phenomenological approximates for $X_{\pm}(y)$.

In general $X_{\pm}(y)$ are functions which depend on the system under consideration. However, for physically realistic systems no exact calculation of $X_{\pm}(y)$ has ever been carried out. Therefore the phenomenological formulas for $X_{\pm}(y)$ have been of an approximate nature, and over the years a large number of approximates[3,11-18] have been proposed. The most famous of these phenomenological approximates is that of Ornstein and Zernike[11]

$$X_{OZ}(y) = x_0(1+y^2)^{-1} \quad (10)$$

while some of the more recent approximates are those of Fisher,[3]

$$X_F(y) = A(1+y^2)^{-1+\eta/2}, \quad (11)$$

and those of Fisher and Burford,[12]

$$X_{FB}(y) = A\,\frac{(1+\phi_c^2y^2)^{\eta/2}}{1+y^2}. \quad (12)$$

One notes that for $y\to\infty$ both (11) and (12) incorporate the expected large-y behavior (7) of $X_{\pm}(y)$. Because of this the "η" emerging from the least-squares fitting of these formulas to the data is interpreted as a determination of η. We discuss the validity of this procedure below.

Recently Wu, McCoy, Tracy, and Barouch[19-23] have computed exactly in the scaling limit the spin-spin correlation function $\langle\sigma_{0,0}\sigma_{M,N}\rangle$ for the two-dimensional Ising model in zero magnetic field. It is possible therefore to compare the above phenomenological approximates with the exact scaling functions $X_{\pm}(y)$ for the two-dimensional Ising model. This has been done by Tracy and McCoy[21], and in Table II we present some of their results.

DETERMINING η

Furthermore one can ask how well do the commonly used phenomenological approximates extract η ($\eta=\frac{1}{4}$ for the two-dimesional Ising model) from the exact $X_{\pm}(y)$. That is to sa we can use the exact values of $X_{\pm}(y)$ as "data" over various ranges of y and try by using various phenomenological formu to extract the exponent η. From Table II we can see that the Ornstein-Zernike pole dominates $X_{+}(y)$ in the region $y<10$. Thus since the Ornstein-Zernike pole term has zero η one should not use data from this region in attempting

Table II. This table compares the exact scaling function $X_+(y)$ for the two-dimensional Ising model with various approximate scaling functions. The approximates $X_{OZ}(y)$, $X_F(y)$, and $X_{FB}(y)$ are all normalized to unity at y=0, and hence, are compared with the scaling function $X_+(y)/X_+(0)$. The quantity $X_{FL}(y)=C_1y^{-7/4}[1+C_2 \times \ell ny+C_3)y^{-1}]$ is the Fisher-Langer approximate. The error in percent is defined as the exact value minus the approximate value, divided by the exact value. The upper row gives the error. Thus, for instance, the Ornstein-Zernike pole approximate $X_{OZ}(y)$ agrees with the exact $X_+(y)/X_+(0)$ to within 5% over the range $0 \le y \le 11.2$.

Approx.	1%	5%	10%
$X_{OZ}(y)$	$0 \le y \le 4.0$	$0 \le y \le 11.2$	$0 < y \le 21$
$X_F(y)$	$1170<y<\infty$	$163<y<\infty$	$64<y<\infty$
$X_{FB}(y)$	$0 \le y<4.2$	$0 \le y<15$	$0 \le y<\infty$
	$1145<y<\infty$	$138<y<\infty$	
$C_1y^{-7/4}$	$1170<y<\infty$	$163<y<\infty$	$64<y<\infty$
$X_{FL}(y)$	$5.4<y<\infty$	$2.5<y<\infty$	$1.7<y<\infty$
$X_{FB}(y)$ with LSV[a]	$8.8<y<103$	$0 \le y<310$	$0 \le y<800$

[a]Least-squares value.

Table III. This table gives the predicted critical exponent η from a least-squares fit to a phenomenological formula. The formulas are given in the left-hand column. The upper row gives the interval over which the formula was fitted. The number of data points, which are equally spaced and equally weighted, is also given. All data is for $T>T_c$. Recall $\eta=\frac{1}{4}$ is the exact result.

Approx.	(10,30) 50 pts.	(20,40) 50 pts.	(20,60) 100 pts.
$X_F(y)$	0.086	0.123	0.131
$X_{FB}(y)$	0.143	0.168	0.176
$C_1y^{-2+\eta}$	0.095	0.125	0.133
Fisher-Langer $C_1y^{-2+\eta}+C_2(\ell ny)y^{-3+\eta}$	0.299	0.264	0.260
Fisher-Langer $C_1y^{-2+\eta}+[C_2\ell ny+C_3]y^{-3+\eta}$	0.256	0.2510	0.2507
$C_1y^{-2+\eta}+By^{-3+\eta}\frac{y^{\lambda-1}}{\lambda}$	0.248	0.247	0.247

proximate $X_F(y)$ [see (11)] to fit the data in the range $0 \le y \le 10$, then a least-squares fitting program gives $\eta \approx 0.02$. The results are presented in Table III. One notes there is no real difference between the Fisher approximate and the $y^{-2+\eta}$ approximate. The Fisher-Burford approximate fits the data quite well in the sense that the computed values from the fitted $X_{FB}(y)$ reproduce the exact input values of $X_+(y)$ to three significant figures. In Table II, the last row, the Fisher-Burford approximate $X_{FB}(y)$ with values $\eta=0.1756$, $\phi_c=0.0571$ and A=2.6687 [those parameters were determined from a least-squares fit of $X_{FB}(y)$ to 100 values of $X_+(y)$ equally spaced and equally weighted over the interval $20<y<60$] is compared with the exact $X_+(y)$. The fit is excellent over experimentally accessible y, but the predicted η is in approximately 30% error.

The reason for these large errors is that $X_F(y)$ and $X_{FB}(y)$ are not really valid in the range of experimentally accessible y. The "η" appearing in these formulas is the true η from a least-squares-fitting point of view only when $y^{-2+\eta}$ is a good approximation. But as can be seen from Table II this is not the case in the region $y<1000$.

When $y^{-2+\eta}$ is not a good approximation to $X_\pm(y)$ one must consider the correction terms to (7). Fisher[24] and Fisher and Langer[25] have argued that for $y\to\infty$

$$X_\pm(y) \sim C_1y^{-2+\eta}[1 \pm C_2y^{-(1-\alpha)/\nu}+C_3^\pm y^{-1/\nu}], \quad (13)$$

with α the critical exponent describing the divergence of the specific heat. For the two-dimensional Ising model ν=1 and $y^{\alpha/\nu}$ is replaced by ℓny (see Ref. 21 for the constants C_1, C_2, and C_3). The form (13), which we call the Fisher-Langer approximate, has more recently been discussed by Stell,[26] Tracy and McCoy,[20,21] Stell and Hochen,[27] Fisher and Aharony,[14] and Brézin,et.al.[28]

We now use the same "data" as above but this time we use the Fisher-Langer approximate as the fitting function. As one sees from Table III the results are remarkably improved. The experimental results listed in Table I used either the Fisher or the Fisher-Burford of the $y^{-2+\eta}$ approximates in analyzing the data. From our least-square experiment we have shown that these three approximates are not trustworthy in the present experimental range of y values. Furthermore, our "data" suffer no problems of resolution[29] or inelasticity corrections,[30] and still these approximates are unable to extract the exponent η. Also the value $\eta=\frac{1}{4}$ is a large number for η, and thus the two-dimensional Ising model should provide the easiest test for these phenomenological formulas. Thus we must conclude that any analysis of critical scattering data that makes use of the Fisher, Fisher-Burford, or $y^{-2+\eta}$ approximates must be seriously questioned when it comes to extracting the exponent η from the scattering data. Recently Birgeneau[31] has reanalyzed his neutron scattering data for Ki_2NiF_4 and has concluded that his data is consistent with the Ornstein-Zernike pole approximate (1) in the range $y \le 10$. Basically the pole dominates the cross-section to such an extent in th range of experimental y that it is impossible to disting uish between the simple Ornstein-Zernike pole approximat and the more mathematically complicated forms that one expects on theoretical grounds.[14,20-23,28]

We would like to give a series of steps that we feel will lead to an unambiguous measurement of η (this assum of course, that the resolution and inelasticity correcti are also make). We consider the case $T>T_c$, and only at the end remark about the case $T<T_c$.

(i) Data must exist in both the large- and small- k regions (a priori one doesn't know large kξ from small kξ, but in practice, some estimate for ξ is usually avai able). The data in the small-kξ region in conjunction with the Ornstein-Zernike pole approximation allows one to determine ξ, and hence the scaled variable y=kξ.

(ii) Test the data to determine if it scales.

(iii) Determine the value of y at which deviations from the Ornstein-Zernike pole first become significant (we denote this value by y_{OZ}).

(iv) For data which satisfy $y>y_{OZ}$ (and y>>1) use th Fisher-Langer approximate (13) as a fitting function. ' not have too many fitting parameters one might first tr setting $C_3^+=0$. As a check on the Fisher-Langer approxim the value of the exponent α obtained from the least-squares fit should be compared with independent measurements of α.

(v) If the data are good enough to have seen the e ponent α, then fixing α to the best known value is perh wise. A final fit with the Fisher-Langer approximate w this fixed α then gives an improved estimate for η. Fu thermore if the data warrant it, one can include the C_3^+

term to get a better fit. This term may prove important for small α.

(vi) The value of η obtained should be independent of the cutoff y_{0Z}.

(vii) If data exist below T_C, then this can provide additional checks on the Fisher-Langer approximate. For instance, the only difference in the second term in (13) above and below T_C is the sign.[25] Furthermore, Hocken and Stell[27] and Brézin, et.al[28] have shown that the ratio C_3^+/C_3^- is the negative of the ratio of the specific-heat amplitudes above and below T_C.

SCALING FUNCTIONS for the TWO-DIMENSIONAL ISING MODEL

In conclusion we give the analytical results of Wu, McCoy, Tracy, and Barouch[20-23] for the scaling functions for the two-dimensional Ising model in zero magnetic field. For a derivation of these results along with a discussion of their analytic properties, the interested reader is referred to Ref. 20-23.

$$X_+(y)=2^{9/4}\pi(\sinh\beta_c E_1+\sinh 2\beta_c E_2)^{1/8}\int_0^\infty d\theta\ \theta[1-\eta(\theta)]\exp\left(\int_\theta^\infty dx\ x\ \ln x[1-\eta^2(x)]-h(\theta)\right)J_0(2\theta y), \quad (14)$$

$$X_-(y)=2^{9/4}\pi(\sinh 2\beta_c E_1+\sinh 2\beta_c E_2)^{1/8}\int_0^\infty d\theta\left[[1+\eta(\theta)]\exp\left(\int_\theta^\infty dx\ \ x\ln x[1-\eta^2(x)]-h(\theta)\right)-2\right]J_0(2\theta y), \quad (15)$$

$$h(\theta)=\left(\frac{\theta\eta'(\theta)}{2\eta(\theta)}+\frac{\theta^2}{4\eta^2(\theta)}\ [(1-\eta^2(\theta))^2-(\eta'(\theta))^2]\right)\ln\theta, (16)$$

$\eta(\theta)$ is a Painlevé funciton of the third kind[32] and satisfies the differential equation

$$\frac{d^2\eta}{d\theta^2}=\frac{1}{\eta}\left(\frac{d\eta}{d\theta}\right)^2-\frac{1}{\eta}+\eta^3-\frac{1}{\theta}\ \frac{d\eta}{d\theta} \quad (17)$$

with the boundary conditions

$$\eta(\theta)=-\theta[\ln(\theta/4)+\gamma_E]+O(\theta^5\ln^3\theta) \quad (18)$$

as $\theta\to 0$, $\gamma_E=0.577215\cdots$ is Euler's constant, and

$$\eta(\theta)\ =\ 1-2\pi^{-1}K_0(2\theta)+O(e^{-4\theta}) \quad (19)$$

as $\theta\to\infty$ where $K_0(x)$ and $J_0(x)$ are Bessel functions. Furthermore it is known[22,23] that $\eta(\theta)$ can be written for sufficiently large θ as ($\theta=\frac{1}{2}t$)

$$\frac{1-\eta(t/2)}{1+\eta(t/2)}=\sum_{k=0}^{\infty}g^{(2k+1)}(t), \quad (20)$$

$$g^{(2k+1)}(t)=(-1)^k\pi^{-(2k+1)}\int_1^\infty dy_1\cdots\int_1^\infty dy_{2k+1}\prod_{j=1}^{2k+1}\frac{e^{-ty_j}}{(y_j^2-1)^{\frac{1}{2}}}\prod_{j=1}^{2k}(y_j+y_{j+1})^{-1}\prod_{j=1}^{k}(y_{2j}^2-1) \quad (21)$$

(for k=0 the last two products are replaced by unity). The analytic structure of $X_\pm(y)$ is shown in Fig. 1.

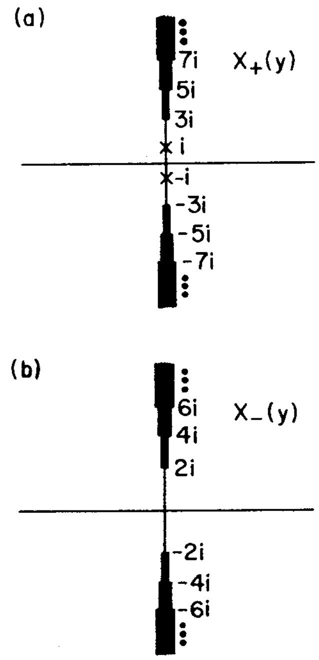

Fig. 1.a)Analytic structure of $X_+(y)$ in the complex y plane. The branch points at $\pm(2n+1)i$, n=1,2,3,..., are square-root-type singularities, and the symbol × denotes a simple pole. The poles are the Ornstein-Zernike poles. b) Analytic structure $X_-(y)$ in the complex y plane. $X_-(y)$ has only branch points which are located at $\pm 2ni$, n=1,2, 3,... .

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