Crossover scaling function for exchange anisotropy: Heisenberg to XY-like crossover

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(Received 3 February 1975)

The crossover behavior of the susceptibility χ^{xx} of the classical Heisenberg model with XY-like anisotropic exchange coupling is studied following the methods of Pfeuty, Jasnow, and Fisher. The universal scaling function is obtained and, from it, the crossover of the effective susceptibility exponent $\gamma_{\rm eff}$ is found.

Recently, Pfeuty, Jasnow, and Fisher[1] reported the calculation of various susceptibility scaling functions for the crossover from Heisenberg to Ising-like behavior in the classical anisotropic Heisenberg model. Subsequently, Singh and Jasnow[2] reported a similar analysis for the XY and planar models. In this paper, the above program is carried out for the Heisenberg model, for the crossover from Heisenberg ($n=3$) to XY-like ($n=2$) behavior. We have employed essentially the same techniques as used in Refs. 1 and 2 for calculations. Hence we shall discuss the scaling theory very briefly and present the results; the reader is referred to Refs. 1, 2, and 4 for further details.

We shall deal with three-component classical spins on the fcc and sc lattice interacting with a nearest-neighbor ferromagnetic exchange in the absence of magnetic field. Let $\vec{\sigma}(\vec{R})$ be such a spin at lattice site $\vec{R}$. The isotropic Hamiltonian is given by

$$\mathcal{H}_0 = -\tfrac{1}{2}J \sum_{\vec{R}} \sum_{\vec{\delta}} \vec{\sigma}(\vec{R}) \cdot \vec{\sigma}(\vec{R}+\vec{\delta}) , \tag{1}$$

where $\{\vec{\delta}\}$ are the nearest-neighbor lattice vectors and J is a positive exchange constant. The anisotropy is introduced through[1,3,4] $\mathcal{H}=\mathcal{H}_0+g\mathcal{H}_1$, where

$$\mathcal{H}_1 = -\tfrac{1}{4}J \sum_{\vec{R},\vec{\delta}} [\sigma_x(\vec{R})\sigma_x(\vec{R}+\vec{\delta}) + \sigma_y(\vec{R})\sigma_y(\vec{R}+\vec{\delta}) - 2\sigma_z(\vec{R})\sigma_z(\vec{R}+\vec{\delta})] , \tag{2}$$

where g is the anisotropy parameter. (This corresponds to the case of axial anisotropy Q_2 with $g_1=0$, $g_2=-g<0$ in Ref. 1.) In the isotropic case, $g=0$, χ^{xx} $(=\chi^{yy}=\chi^{zz})$ diverges at a critical temperature T_{c0} with a critical exponent γ. For fixed small $g>0$, χ^{xx} $(=\chi^{yy})$ diverges at a new critical point $T_c(g)$ with a new exponent $\dot{\gamma}$. On going farther from the critical temperature however, the susceptibility appears to diverge with an isotropic exponent γ. This crossover behavior can be described by the extended scaling hypothesis[1,4]

$$\chi^{xx}(T,g) \approx At^{-\gamma}X(Bg/t^{\phi}) , \tag{3}$$

where we have defined

$$t=(T-T_{c0})/T_{c0} . \tag{4}$$

The parameters A and B are nonuniversal as is T_{c0}, but the crossover exponent ϕ is universal and, like γ, is characteristic of the isotropic system. The scaling function $X(x)$ is also expected to be universal. We shall use the normalization

$$X(0)=1, \quad \frac{dX}{dx}(0)=\frac{1}{2}. \tag{5}$$

(This choice of normalization leads to the identification of A and B with the corresponding parameters in the case of Heisenberg model with Q_1 or Q_2 anisotropy, used in Ref. 1.)

As stated previously, the susceptibility has the following behavior in the two limits of interest:

$$\chi^{xx}(T,0) \approx At^{-\gamma}, \quad g=0, \quad t\to 0 \tag{6}$$

$$\chi^{xx}(T,g) \approx \dot{A}(g)\dot{t}^{-\dot{\gamma}}, \quad g>0, \quad t\to \dot{t} \tag{7}$$

where we have introduced

$$\dot{t}=[T-T_c(g)]/T_{c0} . \tag{8}$$

Equation (6) follows from (3) and the normalization (5). To reproduce (7), the scaling function $X(x)$ should satisfy[1,2,4]

$$X(x) \approx \dot{X}(1-x/\dot{x})^{-\dot{\gamma}} \text{ as } x\to\dot{x} , \tag{9}$$

where we have written

$$\dot{x}=Bg/[t_c(g)]^{\phi} , \tag{10}$$

with,

$$t_c(g)=t-\dot{t}=[T_c(g)-T_{c0}]/T_{c0} . \tag{11}$$

The scaling hypothesis (3) guarantees the equality of ϕ with the shift exponent ψ, which is defined in

$$t_c(g) \approx \dot{w}g^{1/\psi} . \tag{12}$$

Further, it can be shown that[1,4] in the scaling rep-

TABLE I. Reduced susceptibility coefficients for χ^{xx} for the Heisenberg model on the fcc lattice [see Eqs. (15) and (16)].[a]

$a_0(g)=\frac{1}{3}, a_1(g)=\frac{4}{3}+\frac{2}{3}g,$

$a_2(g)=4.888\,888\,889+5.155\,555\,556g+1.155\,555\,556g^2,$

$a_3(g)=17.244\,444\,44+28.497\,777\,78g+13.191\,111\,11g^2+2.026\,666\,667g^3,$

$a_4(g)=59.486\,419\,75+136.003\,950\,6g+96.433\,439\,15g^2+30.981\,305\,11g^3+3.272\,028\,219g^4,$

$a_5(g)=202.248\,465\,6+596.817\,326\,3g+574.190\,686\,8g^2+284.385\,142\,9g^3+62.228\,200\,55g^4$
$+5.754\,831\,948g^5,$

$a_6(g)=680.700\,137\,2+2479.624\,503g+3029.558\,989g^2+2042.118\,645g^3+684.653\,717\,0g^4$
$+131.667\,947\,9g^5+8.648\,713\,642g^6,$

$a_7(g)=2273.984\,280+9912.374\,753g+14\,748.311\,27g^2+12\,637.841\,80g^3+5738.745\,767g^4$
$+1698.611\,340g^5+229.712\,947\,3g^6+16.468\,190\,16g^7,$

$a_8(g)=7553.120\,310+38\,502.819\,96g+67\,767.868\,97g^2+70\,707.465\,82g^3+40\,655.173\,80g^4$
$+16\,355.718\,10g^5+3381.665\,689g^6+500.879\,486\,3g^7+20.532\,640\,95g^8,$

$a_9(g)=24\,973.767\,74+146\,265.4618g+298\,108.2774g^2+367\,634.7066g^3+256\,519.5038g^4$
$+131\,007.4948g^5+36\,625.028\,06g^6+8336.114\,752g^7+699.398\,100\,8g^8+51.579\,518\,83g^9,$

$a_{10}(g)=82\,267.515\,40+545\,853.1327g+1\,267\,350.529g^2+1\,807\,558.464g^3+1\,486\,396.765g^4$
$+922\,929.8468g^5+326\,142.8975g^6+100\,878.9320g^7+12\,893.593\,39g^8+1954.333\,428g^9$
$+30.974\,595\,40g^{10}.$

[a] Forms for $a_9(g)$ and $a_{10}(g)$ have been kindly provided by W. J. Camp and J. P. Van Dyke (Ref. 5).

resentation

$$\dot{A}(g)\approx A_\infty g^{-(\gamma-\dot{\gamma})/\phi}, \tag{13}$$

$$\dot{A}_\infty = A\dot{X}\dot{w}^{\dot{\gamma}-\gamma}\phi^{-\dot{\gamma}} = AB^{(\dot{\gamma}-\gamma)/\phi}\dot{X}\dot{x}^{(\gamma-\dot{\gamma})/\phi}\phi^{-\dot{\gamma}}. \tag{14}$$

The parameters $\dot{w}$ and A_∞ are nonuniversal, whereas $\dot{x}$ and $\dot{X}$ are expected to be universal.

In order to calculate the nonuniversal and universal parameters and determine the scaling function, we have used the high-temperature series expansion[1] of the form

$$\chi^{xx}(T,g)=\sum_{k=0} a_k(g)K^k, \quad K=J/k_BT \tag{15}$$

with

$$a_k(g)=\sum_{l=0}^{k} b_{kl}g^l, \tag{16}$$

for the Hamiltonian $\mathcal{H}_0+g\mathcal{H}_1$. The coefficients $a_k(g)$ are available[1,5] to $k=10$ for the three cubic lattices. (We have, however, restricted our analysis to the fcc and the sc lattices only.) The coefficients $a_k(g)$ for the fcc case are given in Table I. We have used the following previously determined[1] parameters in our analysis:

$$\gamma=1.38, \quad \phi=1.25, \quad \dot{\gamma}=1.315 \text{ (fcc and sc)};$$
$$K_{c0}(\equiv J/k_BT_{c0})=0.3147 \text{ (fcc)}, \quad 0.6916 \text{ (sc)}. \tag{17}$$

[Note that the exponent ϕ is independent[1] of the type of anisotropy (Ising like or XY like).] Omitting the details of calculation,[1,2] the results are as follows. The nonuniversal parameters A and B are found to be

$$A=0.2799\pm0.0004, \quad B=1.143\pm0.007 \text{ (fcc)},$$
$$A=0.3182\pm0.0004, \quad B=1.328\pm0.002 \text{ (sc)}. \tag{18}$$

The uncertainties are for extrapolation only and do not include uncertainties in the isotropic parameters γ and ϕ. The universal amplitudes[1,2] R_l in the expansion[1]

$$X(x)=1+\frac{1}{2}x+\frac{R_1}{2!}\left(\frac{x}{2}\right)^2+\frac{R_1^2R_2}{3!}\left(\frac{x}{2}\right)^3+\cdots \tag{19}$$

are listed in Table II. The estimates for A, B, and the R_l agree well with the ones presented in Ref. 1. The estimates for R_l also agree closely with Pfeuty's preliminary renormalization group calculations also presented in Ref. 1. The expan-

TABLE II. Universal susceptibility ratio estimates.

Ratio	fcc	sc	Universal
R_1	1.521	1.504	1.512
R_2	1.581	1.586	1.584
R_3	1.169	1.172	1.170
R_4	1.425	1.421	1.423
R_5	0.954	$\cdots$	0.954

sion (19) now becomes

$$X(x)=1+\tfrac{1}{2}x+0.1890\,x^2+0.0754\,x^3+0.0264\,x^4+0.0105\,x^5+0.00334\,x^6\,, \tag{20}$$

with uncertainties of at most 0.3%, 1.3%, 3%, 8%, and 13% in the coefficients of $x^2 \to x^6$, respectively. The form (20) agrees with Eq. (5.15) of Ref. 1 under the transformation $g \to -g$ (or $x \to -x$). A preliminary analysis[1,2] of the series (20) gives

$$\dot{x}=2.901,\quad \dot{X}=1.075\,. \tag{21}$$

We turn now to the analysis for small finite g. The critical temperatures and the corresponding $\dot{w}_{\rm eff}(g)$, defined through[1,2]

$$\dot{w}_{\rm eff}(g)=g^{-1/\phi}(1-K_c(g)/K_{c0})\,, \tag{22}$$

are listed in Table III. Extrapolation[1,2] of $\dot{w}_{\rm eff}(g)$ to $g \to 0$ yields

$$\begin{aligned}\dot{w}&=0.436\pm0.025\ \text{(fcc)},\\ \dot{w}&=0.492\pm0.030\ \text{(sc)}.\end{aligned} \tag{23}$$

This allows us to determine $\dot{x}$. The results are,

$$\begin{aligned}\dot{x}&=3.23\pm0.23\ \text{(fcc)},\\ \dot{x}&=3.22\pm0.25\ \text{(sc)}.\end{aligned} \tag{24}$$

Universality is satisfied to the indicated uncertainties. For further analysis, we choose the value

$$\dot{x}=3.255\,. \tag{25}$$

We note that the ratio of $\dot{x}$ in the present case to the value calculated in Ref. 7 for the Heisenberg-Ising crossover (Q_2 anisotropy) is $\dot{x}(n=3 \text{ to } n=2)/\dot{x}(n=3 \text{ to } n=1)\simeq 2.51$. This is consistent with an estimate due to Fisher,[6] arising from the study of bicritical phase diagrams in spin-flop transitions. From the critical temperatures for finite g, we can get an estimate[1,2] for the shift exponent ψ. Our analysis is consistent with $\phi=\psi\simeq 1.25$; a direct analysis of ψ yields at best $\psi=1.21\pm0.07$.

The results of the finite g amplitude analysis[1,2] are now tabulated. Table IV lists $\dot{A}(g)$ and $\dot{A}_{\rm eff}(g)$ [defined from (13) in analogy with (22)]. Again, extrapolation to $g=0$ gives

$$\begin{aligned}A_\infty&=0.255\pm0.010\ \text{(fcc)},\\ A_\infty&=0.288\pm0.015\ \text{(sc)}.\end{aligned} \tag{26}$$

Using (14), (18), and (23) we can determine $\dot{X}$. The results from two separate calculations are

$$\begin{aligned}\dot{X}&=1.157\pm0.050\ \text{(fcc)},\\ \dot{X}&=1.159\pm0.065\ \text{(sc)}.\end{aligned} \tag{27}$$

Again, universality is verified to the indicated uncertainties. We adopt, for further analysis,

$$\dot{X}=1.158\,. \tag{28}$$

As a check on extrapolation consistency, we have repeated the above amplitude analysis for the functions[1,2] $\partial\chi/\partial g$ and $(\partial\chi/\partial g)/\chi$. In addition, we have estimated the universal parameters $\dot{x}$, $\dot{X}$ by making the assumption that the coefficients $a_k(g)$ [see Eq. (16)] themselves have a scaling form.[1] The results are consistent with the estimates presented above.

Now we have all the necessary information to construct the full scaling function. To do this, we first determine the amplitude function $P(z)$, defined by

$$P(z)=(1-z)^{\dot{\gamma}}X(x),\quad z=x/\dot{x} \tag{29}$$

as a polynomial in z to z^6. Next, we construct[1,2] Padé approximants to $P(z)$, subject to the constraint $P(1)=\dot{X}$. This gives us a representation of $P(z)$, and hence, of $X(x)$, valid in the region $0\le z\le 1$. As in earlier work,[1,2] we have examined two sets of Padé approximants (i) using values of $\dot{x}$ and $\dot{X}$ obtained directly from $X(x)$ [see Eq. (21)], (ii) using the parameters determined from a finite-

TABLE III. Critical point shifts and $\dot{w}_{\rm eff}(g)$. The critical points have uncertainties of about 0.1%. The uncertainties shown for $\dot{w}_{\rm eff}(g)$ are in the last decimal place quoted.

	fcc		sc	
g	$K_c(g)$	$\dot{w}_{\rm eff}(g)$	$K_c(g)$	$\dot{w}_{\rm eff}(g)$
0.02	0.308 59	0.444(22)	0.676 59	0.496(30)
0.03	0.306 18	0.447(16)	0.670 69	0.500(22)
0.04	0.303 91	0.450(12)	0.665 56	0.494(17)
0.05	0.301 75	0.452(10)	0.660 28	0.497(14)
0.06	0.299 63	0.455(9)	0.655 09	0.501(12)
0.07	0.297 61	0.456(8)	0.650 41	0.500(11)
0.08	0.295 64	0.457(7)	0.645 58	0.502(10)

TABLE IV. Anisotropic susceptibility amplitude estimates using $\dot{\gamma}=1.315$.

	fcc		sc	
g	$\dot{A}(g)$	$\dot{A}_{\rm eff}(g)$	$\dot{A}(g)$	$\dot{A}_{\rm eff}(g)$
0.02	0.313	0.255	0.352	0.287
0.03	0.3065	0.255	0.343	0.286
0.04	0.301	0.255	0.3405	0.288
0.05	0.2975	0.255	0.335	0.287
0.06	0.2935	0.254	0.3295	0.285
0.07	0.290	0.253	0.327	0.285
0.08	0.286	0.251	0.322	0.282

g analysis [see Eqs. (25) and (28)]. The results are very similar to those in Refs. 1 and 2. In the former case (i), most Padé approximants are defect free.[7] In addition, all of them agree with one another to within 0.1% for $0 \leq z \leq 1$. So we adopt, quite arbitrarily, the approximant,

$$P(z) = \frac{1 + 7.9645z + 39.521z^2 + 31.078z^3}{1 + 7.8292z + 38.571z^2 + 26.619z^3}, \tag{30a}$$

with

$$\text{(i)}\ \dot{\gamma} = 1.315, \quad \dot{x} = 2.901, \quad \dot{X} = 1.075. \tag{30b}$$

In the second case, about half of the entries in the Padé table are defect free. Most of them show a maximum near $z \approx 0.8 - 0.85$. In the [4, 3] Padé approximant, the maximum is near $z \approx 0.65$. The approximant [3, 4] forms a special case. It first grows to a maximum near $z \approx 0.5$, then drops to a *minimum* near $z \approx 0.8$ before rising to the required value at $z = 1$. (A single maximum in similar cases has been reported previously.[1,2]) We adopt the following approximant,

$$P(z) = \frac{1 - 0.80358z - 2.4239z^2 + 2.7187z^3 + 0.48114z^4}{1 - 1.1011z - 2.1488z^2 + 3.0894z^3}, \tag{31a}$$

with

$$\text{(ii)}\ \dot{\gamma} = 1.315, \quad \dot{x} = 3.225, \quad \dot{X} = 1.158. \tag{31b}$$

The approximants given in (30) and (31) and the linear approximant,

$$\text{(iii)}\ P(z) = 1 + (\dot{X} - 1)z, \tag{32}$$

using the value of $\dot{X} = 1.158$ from parameter set given in (31b), differ from one another by at most (in the vicinity of the peaks) 18% in the range $0 \leq z \leq 1$. The effective exponent[8,9]

$$\gamma_{\text{eff}} = -(T - T_c)\frac{\partial \ln\chi}{\partial T}, \tag{33}$$

rather than changing smoothly from $\dot{\gamma} \simeq 1.315$ to the isotropic $\gamma \simeq 1.38$, shows considerable structure when calculated from any of the three approximants. The structure is probably spurious and traceable to the lack of detailed knowledge of the shape of the scaling function near $x = \dot{x}$. On the other hand, sufficient details are known near $x = 0$ to guarantee a smooth fall from $\gamma = 1.38$ as z increases.

In Fig. 1 we have plotted γ_{eff} vs $\log_{10} \dot{t}$ for various values of g, using the approximant (30). Results based on (32) are similar; in both cases the minimum is probably spurious. It should be recalled that the scaling function is valid only for $\dot{t} \ll 1$, $g \ll 1$ for arbitrary values of the ratio $g/\dot{t}^{\phi}$. By the time $\dot{t}$ reaches, say, 0.1, we are receding from the critical (scaling) region, and for $\dot{t} \gtrsim 0.1$ alternative (conventional) analysis is possible for the behavior of the anisotropic susceptibility.[10] We have also plotted in Fig. 1 the *isotropic* γ_{eff} vs $\log t$. For small g, the isotropic and anisotropic curves should merge when $\dot{t} \simeq t$ is of order unity. Hence it can be seen that the full crossover from $\dot{\gamma} = 1.315$ to $\gamma = 1.38$ is not completed within the scaling regime unless $g \lesssim 10^{-6}$. This indicates that for physical anisotropy of a few percent, experiments in the range $10^{-5} \lesssim \dot{t} \lesssim 10^{-2}$ may yield an intermediate value of the susceptibility exponent.

Finally, it should be noted that the crossover region (defined in a reasonable manner) in the present case is narrower than in the $n = 2$ models presented previously.[2] This is consistent with the scaling theory, as the width of the crossover region is proportional to $g^{1/\phi}$ with $1.175 \simeq \phi(n=2) < \phi(n=3) \simeq 1.25$.

In concluding, we note that we have presented a calculation of the universal scaling function for the susceptibility $\chi^{xx}(T, g)$ of the Heisenberg $n = 3$ model with XY-like (Q_2) anisotropy. This, along with the work of Ref. 1, completes the study of the two *independent* crossovers in the $n = 3$ Heisenberg model, that is Heisenberg to Ising ($n = 3$ to $n = 1$) and Heisenberg to XY ($n = 3$ to $n = 2$).

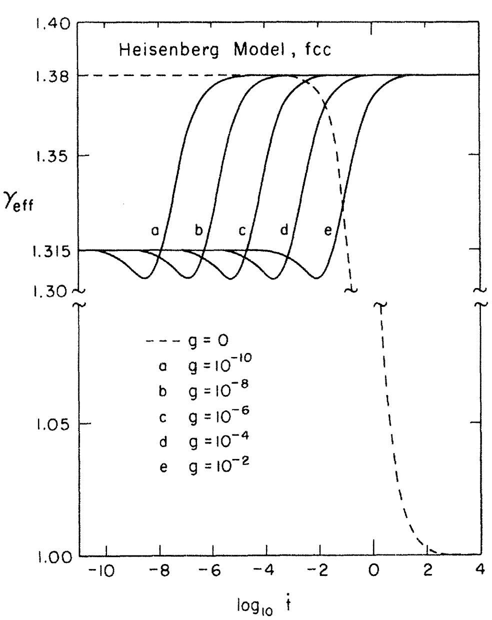

FIG. 1. Plot of γ_{eff} vs $\log_{10}\dot{t}$ for various values of g. Also included is γ_{eff} vs $\log_{10} t$ for $g = 0$. (Note $\dot{t} = t$ when $g = 0$).

ACKNOWLEDGMENTS

We thank Dr. W. J. Camp and Dr. J. P. Van Dyke for allowing us to use their series coefficients to carry out the analysis through tenth order. We wish to thank Professor M. E. Fisher for his interest and comments. The support of the National Science Foundation is gratefully acknowledged.

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[1]P. Pfeuty, D. Jasnow, and M. E. Fisher, Phys. Rev. B 10, 2088 (1974). References to original works on crossover phenomena and complete details of the calculations are provided in this paper. Note, however, the following additions, which apply to the above. (i) On comparison with the later work of Camp and Van Dyke (Ref. 5), it appears that the eighth-order *fcc Heisenberg* inversion coefficients, such as those given in Table I, are probably good to six figures. The accuracy of the $g \neq 0$ analysis is not affected, and the $g=0$ amplitudes are quoted to lower precision. The present work and that of Ref. 2 were based on more accurately known coefficients. (ii) It now appears that the tentative ϵ-expansion results quoted in (5.7) and (5.8) are correct to $O(\epsilon)$ but slightly inaccurate in order ϵ^2. [A. D. Bruce (private communication)].

[2]S. Singh and D. Jasnow, Phys. Rev. B 11, 3445 (1975).

[3]M. E. Fisher and P. Pfeuty, Phys. Rev. B 6, 1889 (1972).

[4]M. E. Fisher and D. Jasnow, in *Theory of Correlations in the Critical Region,* edited by C. Domb and M. S. Green (Academic, New York, to be published).

[5]In Ref. 1 the coefficients were determined to $k=8$ on the fcc lattice and to $k=9$ on the sc and bcc lattices. Subsequently, Van Dyke and Camp [J. P. Van Dyke and W. J. Camp, AIP Conf. Proc. 18, 878 (1973); W. J. Camp and J. P. Van Dyke (unpublished)] obtained the coefficients to tenth order. We are grateful to them for allowing us to use their coefficients to carry out the analysis through tenth order.

[6]M. E. Fisher, Conference on Magnetism and Magnetic Materials, 1974 (unpublished). Fisher demonstrates that the ratio is $2+O(\epsilon)$. Recent ϵ expansions by D. R. Nelson and A. D. Bruce indicate the ratio to be $2^{\phi}+O(\epsilon^3) \simeq 2.38$ in the present case. The value 2^{ϕ} is verified exactly in mean-field theory and for the spherical model.

[7]Some entries in the Padé table show a zero-pole pair in the range $z \leq 0 \leq 1$. Since we have, presumably, removed the singularities in $\chi(g,T)$, $P(z)$ should be relatively smooth.

[8]In calculating γ_{eff}, we use the complete susceptibility which is $\chi=\chi_{\text{ideal}}\chi_{\text{reduced}}$ where $\chi_{\text{ideal}} \propto T^{-1}$ and χ_{reduced} is given by (15) with coefficients $a_k(g)$ listed in Table I for the fcc case.

[9]See also the work of E. K. Riedel and F. J. Wegner [Phys. Rev. B 9, 294 (1974)] on the behavior of effective critical exponents.

[10]When one is outside the critical region, γ_{eff}, according to the definition (33), smoothly goes over to the mean-field value. An analogous "crossover" to Gaussian behavior can be understood in the framework of the renormalization-group recursion relations [D. R. Nelson (private communication)].