# Sign of corrections to scaling amplitudes: Field-theoretic considerations and results for self-repelling walks

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I discuss the application of renormalized field theory to such critical systems where the renormalized coupling approaches the fixed point from the "wrong" (strong-coupling) side. In contrast to a belief sometimes expressed in the literature, I find that also this situation can be described within the standard formalism, only the interpretation of the strong-coupling branch relies on the existence of a finite cutoff. I illustrate these considerations with an analysis of Monte Carlo data for self-avoiding walks, finding that the data support the theory in all respects. However, it is stressed that the nonuniversal parameters of the renormalized theory in general have no simple relation to the parameters of the underlying bare model.

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## I. INTRODUCTION

Universal scaling behavior found at a critical point can be explained by the renormalization group [1], which exploits the scale covariance of a critical system. Consider, for instance, the local magnetization of a ferromagnet, modeled in terms of an interacting vector field $\phi(\mathbf{r}_j)$ defined on a $d$-dimensional hypercubic lattice $\{\mathbf{r}_j\}$ of spacing $l_0$. The lattice version of the standard Landau-Ginzburg Hamiltonian reads

$$\frac{\mathcal{H}}{k_B T}=l_0^d \sum_i \left\{ \frac{1}{2} \sum_{j=1}^{d} \left[ \frac{\phi(\mathbf{r}_i+\mathbf{l}_j)-\phi(\mathbf{r}_i)}{l_0} \right]^2 + \frac{m_0^2}{2}\phi^2(\mathbf{r}_i) + \frac{u_0}{8}[\phi^2(\mathbf{r}_i)]^2 - h_0\phi(\mathbf{r}_i) \right\}, \quad (1)$$

where the $\mathbf{l}_j$ are the primitive lattice vectors. The "mass" $m_0$ incorporates the temperature dependence: $m_0 = m_0(T)$, and $h_0$ represents a magnetic field. $u_0$ is known as the interaction constant. Renormalization maps this "bare" model onto a renormalized model of characteristic length scale $l_R$, the mapping preserving the macroscopic properties of the system. The renormalization group (RG) studies the dependence of the renormalized model on the scale $l_R$, showing that this dependence embodies the qualitative form of the observed scaling laws. Furthermore, the renormalized theory allows for quantitative calculations, the results generally comparing well to experiment. This holds true in particular for properties right at the critical point, to be described by a renormalized theory where the dimensionless renormalized coupling constant $u$ takes a special value $u^*$. This value is a fixed point under the RG, which means that it is invariant under a change of $l_R$. Universality of critical properties is established, since in the infrared limit $l_R \rightarrow \infty$ the renormalized coupling $u(l_R)$ tends to $u^*$, irrespective of its starting value $u(l_R \sim l_0) > 0$. This starting value is nonuniversal, i.e., specific to the bare model under consideration. In physical applications $l_R$ must be taken to be of the order of the correlation length in the system, and therefore it is the infrared limit which describes a critical system with its infinite range correlations.

Concerning the approach of $u(l_R)$ towards $u^*$ it is found that in a field-theoretic realization of the renormalization scenario, working with the renormalized counterpart of a continuum version of the Hamiltonian (1), $u(l_R)$ has to reach $u^*$ from below, values $u > u^*$ being unphysical. (See, for instance, [2], Sec. 9.5 or [3], Secs. 23.1 and 32.1.) This is at variance with some results of computer simulations. In particular, for the three-dimensional Ising model [4] or for self-avoiding walks (SAW) on cubic lattices [5], the approach to criticality ($T \rightarrow T_c$ in the Ising model, step number $n \rightarrow \infty$ for the SAW) is such that it would need values $u > u^*$. This has been taken as an indication that the powerful methods of renormalized field theory cannot be applied to these systems in standard form. We here are confronted with some puzzle, since the renormalized expressions intrinsically do not seem to rely on the constraint $u \leq u^*$. Using a so-called "massless" renormalization scheme I find expressions which seem to be well defined also in some range $u > u^*$. Indeed the restriction $u \leq u^*$ reflects the way the renormalized theory is derived by starting from a continuum version of the bare model, i.e., taking as a first step the limit of vanishing lattice spacing in the Hamiltonian (1) or the limit of vanishing step size of the SAW, respectively. This raises the question of whether we are entitled to use the thus derived results also in the range $u > u^*$.

A detailed analysis of the problem has been presented by Bagnuls and Bervillier [6], who carefully discuss the different limiting procedures involved. They furthermore analyze other implementations of the renormalization scenario which clearly allow for values $u > u^*$. Here it must be recalled that in general the RG works in a space of infinitely many parameters specifying the microscopic Hamiltonian. The field-theoretic approach by construction concentrates on the flow of a few most relevant "scaling fields" in the sense of Ref. [7], suppressing all "nonuniversal corrections" due to "irrelevant perturba-

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tions." In the context of an analysis of nonuniversal corrections in polymer physics, i.e., the SAW problem, Krüger and present author [8] recently have argued that the results of standard field theory can be used also for $u > u^*$. In the present paper I rephrase the argument in terms of general critical phenomena (Sec. II), and then I illustrate the power of the approach with an analysis data on self-avoiding walks (Sec. III). Both lattice walks and walks in continuous three-dimensional space will be considered. In Sec. IV I summarize the results.

It is of interest to note that a footnote of [6] mentions field-theoretic calculations done in the range $u > u^*$. Results and further discussions are presented in copies of recent unpublished work [24], which I received after submission of the present paper. Furthermore, in [9] the relation of the field-theoretic formulation of the SAW problem to the general Wilson-type RG framework is reexamined.

## II. GENERAL DISCUSSION OF THE PROBLEM $u > u^*$

As indicated in the Introduction, the field-theoretic approach to critical phenomena consists of two steps: (i) Mapping of the bare model onto a renormalized model of arbitrary scale $l_R$: (ii) studying the change of the renormalized model under a change of $l_R$. I first consider step (ii).

The RG mapping is constructed in the form of flow equations giving the change of the renormalized parameters under an infinitesimal change of $l_R$. (I should note that often $l_R$ is replaced by a momentum-type variable $\mu = 1/l_R$.) The flow equation for the renormalized coupling can be cast in the form

$$-l_R \frac{du(l_R)}{dl_R} = \beta(u(l_R),\epsilon) , \tag{2}$$

$$\beta(u,\epsilon) = -\epsilon u + u^2 \hat{\beta}(u) , \tag{3}$$

where

$$\epsilon = 4-d . \tag{4}$$

Other parameters, such as the renormalized number of steps of a SAW or the renormalized mass or magnetic field of the Landau-Ginzburg model obey equations of the general structure

$$-l_R \frac{d}{dl_R} \ln Q = \eta_Q(u(l_R)) , \tag{5}$$

where $Q$ stands for the quantity considered. $\hat{\beta}(u)$ or $\eta_Q(u)$ are smooth functions depending only on the renormalized coupling. Within the special scheme of "minimal subtraction" they even are independent of spatial dimensionality.

Of special importance is the flow of $u$ [Eq. (2)]. Fixed points are zeros of $\beta(u,\epsilon)$. There always is the trivial fixed point $u=0$. For the theories of interest there also is a nontrivial fixed point $u^* = O(\epsilon)$, $u^* > 0$ for $\epsilon > 0$. I introduce the slope of $\beta(u,\epsilon)$ at $u^*$:

$$\omega = \left. \frac{\partial \beta(u,\epsilon)}{\partial u} \right|_{u^*} > 0, \ \epsilon > 0 . \tag{6}$$

Assuming that in the range of interest there is no other zero of $\beta(u,\epsilon)$ I write

$$\frac{1}{\beta(u,\epsilon)} = -\frac{1}{\epsilon u} + \frac{1}{\omega(u-u^*)} + p_u(u) , \tag{7}$$

where $p_u(u)$ is some regular function. Using this ansatz in the integration of Eq. (2) I find

$$\frac{l_R}{l_{R,0}} = \left[ \frac{u(l_R)}{u(l_{R,0})} \right]^{1/\epsilon} \left[ \frac{u(l_{R,0}) - u^*}{u(l_R) - u^*} \right]^{1/\omega} \times \exp[P_u(u(l_{R,0})) - P_u(u(l_R))] , \tag{8}$$

where $P_u(u)$ again is some regular function. Using Eq. (2) to eliminate $l_R$ from Eq. (5) and integrating the resulting equation using the form (7) I furthermore find

$$Q(l_R) = \left[ \frac{u(l_{R,0})}{u(l_R)} \right]^{\eta_Q^{(0)}/\epsilon} \left[ \frac{u(l_R) - u^*}{u(l_{R,0}) - u^*} \right]^{\eta_Q^*/\omega} \times \exp[P_Q(u(l_R)) - P_Q(u(l_{R,0}))] Q(l_{R,0}) , \tag{9}$$

where

$$\eta_Q^{(0)} = \eta_Q(0) , \quad \eta_Q^* = \eta_Q(u^*) , \tag{10}$$

and $P_Q(u)$ again is some regular function. Equations (8) and (9) are standard results representing the general field-theoretic RG mapping in global form. They relate renormalized parameters on scale $l_R$ to those on scale $l_{R,0}$.

Inspecting these results I find that they allow for three different branches, sketched in Fig. 1.

*(i) Weak-coupling branch.* Starting from a value $u(l_{R,0}) < u^*$ I find $u(l_R) < u^*$, reaching $u^*$ for $l_R \to \infty$ from below. This branch continuously is connected to $u=0$.

*(ii) Strong-coupling branch.* Starting from $u(l_{R,0}) > u^*$ I find $u(l_R) > u^*$, reaching $u^*$ for $l_R \to \infty$ from above. This branch is not connected to $u=0$ but runs off towards $u \gg u^*$, eventually leaving the region $u \lesssim 1$ where a perturbation expansion in powers of $u$ can be considered a

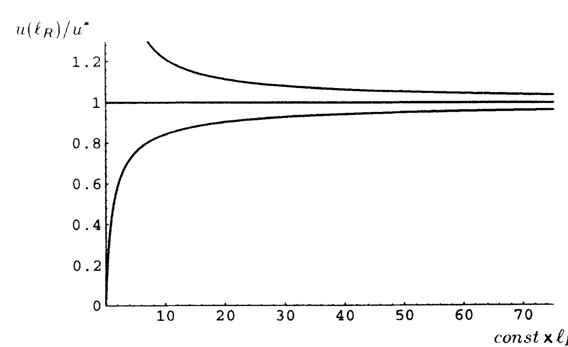


FIG. 1. Running coupling constant $u(l_R)/u^*$ as a function of $l_R$. Schematic plot showing the three branches. The scale of $l_R$ is in arbitrary units.

useful tool.

*(iii) Fixed point branch.* Branches (i) and (ii) are separated by a separatrix

$$u(l_{R,0}) \equiv u^* \equiv u(l_R) ,$$

where Eq. (5) yields pure power law behavior:

$$Q(l_R) = \left[ \frac{l_{R,0}}{l_R} \right]^{\eta_Q^*} Q(l_{R,0}) . \tag{11}$$

These three branches are the analog in the present scheme of the RG trajectories discussed in the context of Fig. 1 in Ref. [6].

These results are based on the assumption that the functions $\hat{\beta}(u), \eta_Q(u)$ show no singularity at $u = u^*$, an assumption clearly underlying all field-theoretic renormalization group work. In the present context it is hard to see how this could go wrong. As mentioned above, the functions $\hat{\beta}(u), \eta_Q(u)$ can be constructed to be independent of $\epsilon$, whereas $u^* \sim \epsilon$ vanishes for $\epsilon \to 0$. Singular behavior at the continuously varying value $u^*(\epsilon)$ thus would imply that the functions $\hat{\beta}(u), \eta_Q(u)$ do not exist at all. (It should be noted that this argument explicitly refers to the minimal subtraction scheme or to formulations derived from it by an analytic reparametrization of the coupling constant flow. For other formulations, for instance, those defining the renormalized parameters in terms of vertex functions, the situation may be less clear.)

As derived above, the field-theoretic RG mapping by itself does not indicate that the strong-coupling branch (ii) or the fixed point branch (iii) must be rejected. To understand the argument leading to the belief that only the weak-coupling branch is relevant physically I must consider more closely the mapping from bare to renormalized theory [step (i)]. I first recall the structure of bare perturbation theory, based on a model with finite cutoff $\Lambda \sim l_0^{-1}$ like the Hamiltonian (1) or the SAW of finite step length. In the following I use wording adequate for the magnetic model.

Being interested in a neighborhood of the critical point $T = T_c$ I first must carry through a mass subtraction, introducing the deviation of $m_0^2$ from the critical mass $m_{0c}^2 = m_0^2(T_c)$. To avoid delicate problems connected to that step (see, for instance, Ref. [10]), which are not relevant to the present discussion, I imagine having eliminated $m_0^2$ in favor of a correlation length $\xi^2$. Now considering some dimensionless observable I note that it can depend only on the dimensionless parameters $u_0 l_0^\epsilon$, $h_0 l_0^{1+d/2}$, $l_0^2/\xi^2$, besides the possible occurrence of momentum variables $pl_0$. Bare perturbation theory is found to proceed in powers of

$$u_0 l_0^\epsilon \left[ \frac{\xi^2}{l_0^2} \right]^{\epsilon/2} = u_0 \xi^\epsilon ,$$

with leading corrections of order $(l_0/\xi)^{k\epsilon}$, $k \geq 1$. These corrections are taken care of by multiplicative renormalization. I write

$$u_0 = u l_R^{-\epsilon} Z_u(u, l_0/l_R) , \tag{12}$$

with similar equations for the other parameters, and I determine the coefficients in the perturbation expansion of the renormalization factors $Z$ so as to absorb all the leading corrections. [Subleading corrections of canonical order $(l_0/\xi)^2$ *a priori* survive. They are related to the nonuniversal corrections mentioned in the Introduction.] The renormalization factors must be chosen such that the renormalized theory exists for $d \leq 4$.

The analysis is greatly simplified by first taking the continuum limit $l_0 \to 0$ for $d < 4$, keeping $u_0$, $\xi^2$, etc. fixed. This suppresses all $l_0$ dependence at the price of introducing singularities for $d \to 4$. The $Z$ factors then have to be chosen to absorb these singularities, the special scheme of "minimal subtraction" of dimensional poles leading to functions $\hat{\beta}(u)$, $\eta_Q(u)$ independent of $\epsilon$.

How is the starting value $u(l_{R,0} = l_0)$ of the renormalized coupling constant related to the coupling $u_0$ of the original model (1)? Clearly $u(l_0)$ is not identical to the dimensionless coupling $u_0 l_0^\epsilon$ of the bare theory, but being defined on the microscopic scale $l_0$ it is reasonable to assume that $u(l_0)$ is an analytic function of $u_0 l_0^\epsilon$,

$$u(l_0) = c u_0 l_0^\epsilon [1 + O(u_0 l^\epsilon)] . \tag{13}$$

Thus $u(l_0) \to 0$ in the continuum limit, and we necessarily find ourselves on the weak-coupling branch. This result can be sharpened by noting that in the continuum limit Eq. (8) reduces to

$$c u_0 l_R^\epsilon = u(l_R) \left[ 1 - \frac{u(l_R)}{u^*} \right]^{-\epsilon/\omega} \exp[-\epsilon P_n(u(l_R))] . \tag{14}$$

For $l_R$ fixed, all the range $0 \leq u_0 < \infty$ is mapped on the range $0 \leq u(l_R) < u^*$, leaving no room for the strong-coupling branch. It, however, should be clear that the argument is specific to the continuum limit. A contradictory statement may be found in [1], Sec. 9.5. A closer inspection, however, shows that it uses a form of the coupling constant flow equivalent to Eq. (14), derived with explicit use of the continuum limit [Ref. [1], Eqs. (8.18)–(8.21)].

There exists a second line of argument [11] leading to the constraint $u < u^*$. Using a massive renormalization scheme one finds that the renormalized correlation functions show a cut starting at the fixed point coupling. In that scheme the renormalized functions depend on a coupling $u_m$ and the mass $m = \xi^{-1}$, besides momentum variables $\{q\}$. They obey inhomogeneous Callan-Symanzik equations which do not allow for solutions regular at $u_m = u_m^*$ for fixed $m$, $\{q\}$. Rather the critical power-type singularities induce a cut for $u_m > u_m^*$. In contrast, in the present paper I have in mind a massless renormalization scheme, the correlation functions depending on the coupling $u$, temperature $t$, and a scale $l_R^{-1} = \mu$, besides $\{q\}$. These functions obey homogeneous renormalization group equations, which are consistent with analyticity at $u = u^*$ for $t, \mu, \{q\}$ fixed. In fact this analyticity underlies the standard discussion of corrections to scaling. The apparent contradiction is resolved by noting that the mass $m = m(t, u, \mu)$ itself is singular at $u = u^*$. Being the inverse correlation length it indeed lives on one of the three branches $u<u^*$, $u=u^*$, $u>u^*$ which are not analytically connected at $u=u^*$. The cut therefore reflects the choice of variables in the massive scheme.

There remains the question whether a renormalized theory, constructed by starting from the continuum limit, can be used to describe the strong-coupling or fixed point branches, even though those branches, properly speaking, are unphysical in the continuum limit. The answer is positive, since the same RG flow equations can be derived from both the continuum limit or cutoff theories. To formulate it in somewhat more detail, in the cutoff theory the leading microstructure dependence comes in the form of powers of $\Lambda^{-\epsilon}=l_0^{\epsilon}$, as has been mentioned above. Such terms have to be absorbed into renormalization factors [see Eq. (12)], taking the general form

$$Z_x\left[u,\frac{l_0}{l_R}\right]=1+\sum_{j=1}^{\infty}u^jP_j\left[\frac{l_0}{l_R}\right], \tag{15}$$

where $P_j$ is a finite polynomial in $(l_0/l_R)^{\epsilon}$. Choosing the zero-order term of that polynomial to coincide with the equivalent term in the minimal subtraction scheme we are guaranteed to find renormalization group equations identical to those of the minimal subtraction scheme, even without taking the continuum limit $l_0\to 0$. With this latter derivation there is no reason to discard the fixed point or strong-coupling branches.

The renormalized correlation functions, calculated by renormalizing the cutoff model as outlined above, differ from the correlation functions calculated in the continuum limit only by terms of canonical order $l_0^2/\xi^2$. Corrections of the same order of magnitude would be created by irrelevant perturbations not included in the original model. Close to the fixed point $u^*$ these terms are dominated by the so-called corrections to scaling proportional to $u-u^*$. An extensive discussion of that "preasymptotic" regime may be found in [12]. Going further away from the fixed point the irrelevant terms numerically may become important, however. It is here that an important difference among the strong- or weak-coupling branches emerges. For some systems we may have a handle on the starting value $u(l_0)$, allowing us to reduce it to zero continuously. A noteworthy example is the physics of polymer solutions, where the role of temperature in critical phenomena is played by the inverse of the chain length (i.e., step number of the SAW), the physical temperature influencing $u(l_0)$. A so-called $\Theta$ temperature might be reached, where $u(l_0)$ vanishes. We then may work with very long chains: $l_0/\xi\ll 1$ (the role of $\xi$ is played by the radius of the polymer coil in solutions), staying so close to the $\Theta$ temperature that still $u(l_R\sim\xi)$ is much smaller than $u^*$. Then clearly corrections $\sim(l/\xi)^2$ are negligible and we in principle can map out all of the weak-coupling branch. For the strong-coupling branch no such tool is available. It would amount to making $u(l_0)$ very large, so that the perturbative construction of the RG mapping breaks down. For the strong-coupling branch only results in some region close to $u^*$ should be trusted.

In summary I have found (see also [24]) that the results of standard renormalized field theory can be used also in some range above $u^*$. The interpretation of the strong-coupling or fixed point branches implicitly makes use of the existence of a finite cutoff. In the next section I apply these results to an example taken from the topic of self-avoiding walks.

## III. THE END-TO-END DISTANCE OF A SELF-AVOIDING WALK

I here discuss Monte Carlo results on three-dimensional self-avoiding walks both on a lattice and in continuous space. Computer experiments have the advantage of a well defined step number, whereas physical experiments on long macromolecules necessarily deal with samples showing some distribution of chain lengths. This gives rise to additional complications of data analysis, and a discussion of physical data will be published elsewhere. The most extensive set of numerical data is available for the mean squared end-to-end distance $R_E^2$, and I therefore restrict my discussion to this quantity.

For the SAW the important parameters are the renormalized coupling $u$ and the renormalized chain length $n_R$. In three dimensions the RG mapping, written in the form of Eqs. (8) and (9), is found as

$$\frac{l_R}{l}=\frac{f}{f_0}\left[\frac{1-f}{1-f_0}\right]^{-1/\omega}\left[\frac{1+0.824f}{1+0.824f_0}\right]^{0.25}, \tag{16}$$

$$n_R=\left[\frac{f}{f_0}\right]^{-2}\left[\frac{1-f}{1-f_0}\right]^{1/\nu\omega}\left[\frac{1+0.824f}{1+0.824f_0}\right]^{-0.50}\times Z_n^{-1}(f_0,1)n\;, \tag{17}$$

$$\omega=0.80\;,\quad \nu=0.59\;. \tag{18}$$

Here

$$f=\frac{u(l_R)}{u^*}\;,\quad f_0=\frac{u(l_0)}{u^*}\;, \tag{19}$$

and $n$ denotes the unrenormalized chain length. This form of the mapping is based on a most precise calculation of Schloms and Dohm [10], using the minimal subtraction scheme of field theory. It is an analytical fit reproducing the results numerically within 1% deviation.

For a discussion of the weak- or strong-coupling branches a more lucid form of the mapping introduces two parameters $\tilde z$, $\tilde R_0^2$.

$$\tilde z=\tilde v n^{1/2}\;, \tag{20}$$

$$\tilde v=f_0|1-f_0|^{-1/2\nu\omega}(1+0.824f_0)^{0.25}Z_n^{-1/2}(f_0,1)\;, \tag{21}$$

$$\tilde R_0^2=\tilde l^{\,2}n\;, \tag{22}$$

$$\tilde l=|1-f_0|^{(1/\omega)(1-1/2\nu)}Z_n^{-1/2}(f_0,1)l_0\;. \tag{23}$$

Then fixing the renormalized length scale $l_R$ by the condition $n_R=1$, which amounts to $l_R^2\sim R_E^2/6$, I find Eqs. (4.26) and (4.27) of [8]:

$$f|1-f|^{-1/2\nu\omega}(1+0.824f)^{0.25}=\tilde{z} , \quad (24)$$

$$l_R^2=|1-f|^{(1/\omega)(1/\nu-2)}\tilde{R}_0^2 . \quad (25)$$

Thus the mapping from bare to renormalized theory in general involves two nonuniversal microscopic parameters $\tilde{v}$, $\tilde{l}$, such theories in polymer physics traditionally being addressed as "two-parameter theories." The theory makes no precise quantitative prediction on the size of these parameters.

To reach the fixed point branch I take the limit $f\to 1$, $f_0\to 1$ in Eqs. (23) and (24) to find

$$l_R^2=B^2n^{2\nu} , \quad (26)$$

$$B=1.824^{0.25(1-2\nu)}\tilde{l}\tilde{v}^{2\nu-1}|_{f_0\to 1}$$
$$=Z_n^{-\nu}(1,1)l_0 . \quad (27)$$

The two parameters have merged into a single one.

The mean squared end-to-end distance of a SAW in [8] has been calculated to first nontrivial order of renormalized perturbation theory, evaluated directly in three dimensions. Ignoring the irrelevant perturbations I find from [8], Eq. (4.29),

$$\tfrac{1}{6}R_E^2=l_R^2(1-0.192f) . \quad (28)$$

Evaluated for the fixed point branch this yields

$$\tfrac{1}{6}R_E^2=0.808B^2n^{2\nu} . \quad (29)$$

For the weak- or strong-coupling branches I can define a generalized "swelling factor," which is a function of $\tilde{z}$ only:

$$\tilde{\alpha}_E^2=\frac{R_E^2}{6\tilde{R}_0^2}=|1-f|^{-0.381}(1-0.192f) . \quad (30)$$

$f=f(\tilde{z})$ has to be taken from Eq. (24). In Fig. 2 I have plotted the two branches of $\tilde{\alpha}_E^2(\tilde{z})$ together with their common asymptote.

$$\tilde{\alpha}_{\rm as}^2(\tilde{z})=0.765\tilde{z}^{0.360}, \quad \tilde{z}\to\infty \quad (31)$$

which in such a plot replaces the fixed point branch.

For a comparison to data it is useful to construct a more explicit form of $\tilde{\alpha}_E^2(\tilde{z})$. The surprisingly simple expressions

$$\tilde{\alpha}_{E,w}^2(\tilde{z})=(1+1.066\tilde{z}+0.226\tilde{z}^2)^{0.18}$$
(weak coupling) (32a)

or

$$\tilde{\alpha}_{E,s}^2(\tilde{z})=(1.704-1.096\tilde{z}+0.226\tilde{z}^2)^{0.18}$$
(strong coupling) (32b)

numerically reproduce my results to an accuracy better than 0.5%.

Using Borel resummation methods based on sixth-order bare perturbation theory for a three-dimensional continuous chain model, Muthukumar and Nickel [13] have constructed a very accurate expression for the weak-coupling branch. Their result is parametrized as

$$\tilde{\alpha}_{E,\rm MN}^2=(1+7.524z+11.06z^2)^{0.1772} , \quad (33)$$

employing a value $\nu=0.5886$ instead of my value $\nu=0.59$. In the experimentally relevant range $\tilde{z}\lesssim 100$ the rescaling $z=0.150\tilde{z}$ yields agreement among Eqs. (32a) and (33) up to deviations less than 0.5%. This shows that my result for the weak-coupling branch is quite accurate.

Turning now to the Monte Carlo data I note that for SAW's on the three cubic lattices the corrections to the asymptotic power law behavior are known to be negative. According to Fig. 2 I clearly am on the strong-coupling branch. I have analyzed the recent accurate data collected by Barrett, Mansfield, and Benesch [14], covering chain lengths $26\le n\le 3328$. The values of $\tilde{v}$ [Eq. (20)] or $6\tilde{l}^2$ [Eq. (22)] used in the fit are collected in Table I. (In my notation the step size of a random walk of fixed length steps is $\sqrt{6}\tilde{l}$.) All lengths are measured in units of the lattice spacing: $l_0=1$. Figure 3 shows the data for

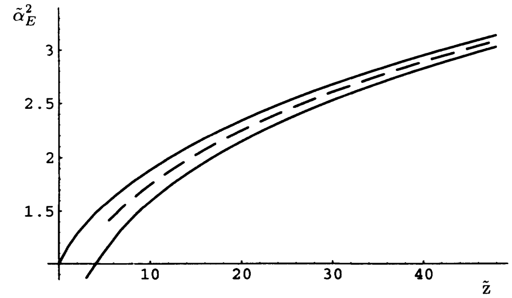


FIG. 2. Swelling factor $\tilde{\alpha}_E^2$ [Eq. (30)] as a function of $\tilde{z}$. The broken line represents the asymptotic power law (31). The upper branch is the weak-coupling branch.

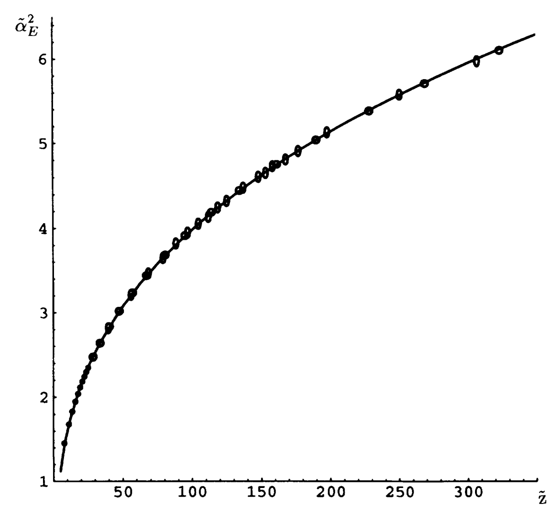


FIG. 3. $\tilde{\alpha}_E^2$ as a function of $\tilde{z}$. Strong-coupling branch. Data for SAW's on the simple cubic lattice, as collected in [14]. Circles: data of Nickel; ellipsoids: data of Barrett *et al.*; points: exact enumeration data.

TABLE I. Parameter values for SAW's on cubic lattices [14]. Also included is the four-way SAW on the simple cubic lattice [23].

| Lattice | sc | bcc | fcc | sc four way |
|---|---|---|---|---|
| $6\tilde{l}^2$ | 0.825 | 0.636 | 0.645 | 1.190 |
| $\tilde{v}$ | 5.611 | 8.462 | 7.341 | 1.464 |
| $6\tilde{l}^2\tilde{v}^{0.360}$ | 1.535 | 1.372 | 1.322 | 1.365 |

SAW's on the simple cubic (SC) lattice as compared to my calculation of the strong-coupling branch. I included also exact enumeration data [14], starting at $n=2$. Clearly the fit is excellent over all the range of $\tilde{z}$. In particular, no sign of irrelevant perturbations can be detected. In view of the short chains included this is quite a surprising feature. (I should note that the exact enumeration data cover even values of $n$ only, so that odd-even effects are not seen.) A fit of the same quality is found for all the other lattice or off-lattice data analyzed here, supporting the view that my calculation indeed yields an excellent representation also of the strong-coupling branch.

In Fig. 4 I show the Monte Carlo data for the three cubic lattices, where I divided out the leading asymptotic variation $\sim\tilde{\alpha}^2_{\text{as}}$. This plot magnifies the scatter of the data, but allows for a clear distinction among the three branches. Clearly theory and data agree within at most 0.5% deviation. It should be noted that in all this and the subsequent analysis I encountered values $f(l_R)\lesssim 1.15$ only, so that I stay well within the domain of renormalized perturbation theory.

Yuan and Masters [15] recently published very accurate data on SAW's on a diamond lattice, $42\leq n\leq 210$. They included and varied an attractive nearest neighbor interaction $\epsilon_{\text{YM}}$. Analyzing these data I find the results of Fig. 5. The parameter values are collected in Table II. For pure self-avoiding walks ($\epsilon_{\text{YM}}=0$), I again am on the strong-coupling branch. For $\epsilon=-0.1$ within the accuracy of the data I seem to have hit the fixed point branch. Only the combination $5\tilde{l}^2\tilde{v}^{0.360}\sim B^2$ can be determined, but for including the data into the figure I arbitrarily assigned a value $\tilde{v}=3$. For $\epsilon_{\text{YM}}\leq -0.2$ I am on the weak-coupling branch. According to Yuan and Masters the Gaussian coil behavior (corresponding to the $\Theta$ temperature) is reached for $\epsilon_{\text{YM}}=-0.51$, and in Fig. 4 I omitted the data for $\epsilon_{\text{YM}}=-0.5$ reaching values $\tilde{z}\leq 0.2$ only, where that plot is not adequate. Clearly theory and data match very well.

I finally consider data on off-lattice chains, constructed from segments of length $l_0$ connecting the centers of hard beads of diameter $a_0$. In that model the parameter

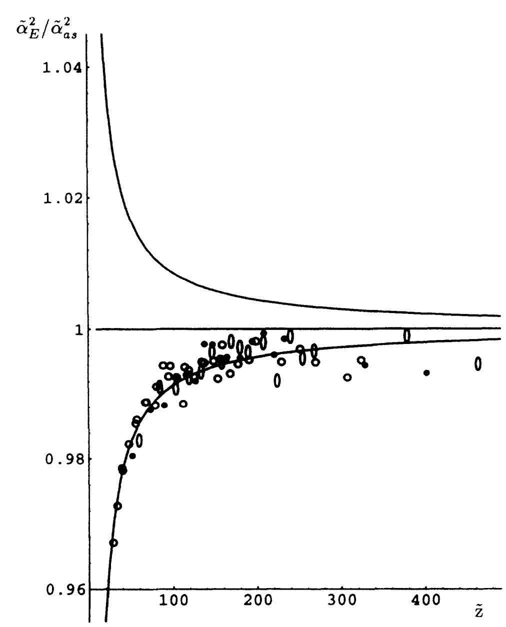


FIG. 4. $\tilde{\alpha}_E/\tilde{\alpha}^2_{\text{as}}$ as a function of $\tilde{z}$. Data [14] for cubic lattices. Circles: sc; ellipsoids: bcc; points: fcc.

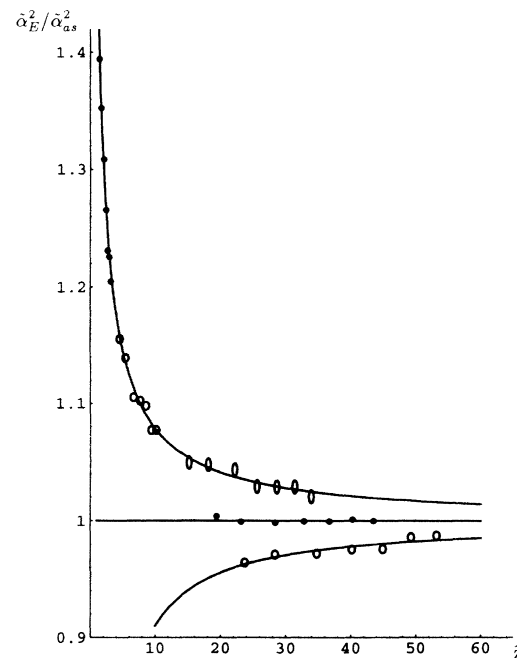


FIG. 5. $\tilde{\alpha}_E/\tilde{\alpha}^2_{\text{as}}$ as a function of $\tilde{z}$. Data [15] for interacting SAW's on the diamond lattice. Lower branch (strong coupling) $\epsilon_{\text{YM}}=0$. Horizontal branch (fixed point) $\epsilon_{\text{YM}}=-0.1$. The horizontal position of the points has been fixed arbitrarily by taking $\tilde{z}=3n^{1/2}$. Upper branch (weak coupling), ellipsoids: $\epsilon_{\text{YM}}=-0.2$; circles: $\epsilon_{\text{YM}}=-0.3$; points: $\epsilon_{\text{YM}}=-0.4$.

TABLE II. Parameter values for interacting SAW's on the diamond lattice [15]. Nearest neighbor interaction $\epsilon_{YM}$.

| $\epsilon_{YM}$ | 0 | −0.1 | −0.2 | −0.3 | −0.4 | −0.5 |
|---|---|---|---|---|---|---|
| $6\tilde{l}^2$ | 1.170 | | 1.149 | 1.523 | 1.804 | 1.988 |
| $\tilde{v}$ | 3.668 | | 2.342 | 0.701 | 0.211 | 0.011 |
| $6\tilde{l}^2\tilde{v}^{0.360}$ | 1.868 | 1.727 | 1.561 | 1.340 | 1.030 | 0.388 |

$$\delta=\frac{a_0}{l_0} \tag{34}$$

can be varied, $0\le\delta\le 1$, thus changing the excluded volume. Using an ingenious combination of Monte Carlo results and RG ideas Baumgärtner and co-workers [16] concluded that the fixed point branch is found for $\delta^*=0.52\pm0.02$. Figure 6 shows the results of my analysis of the accurate data of Barrett, Mansfield, and Benesch [14], covering chain lengths $50\le n\le 1000$. Again the data nicely confirm the theory. The parameter values are collected in Table III, where I included parameters extracted from the (few and not very precise) data of Refs. [16,17].

There remains the question of to what extent we can understand the variation of the parameters $\tilde{l},\tilde{v}$ as exhibited, for instance, in Table III. This question directly relates to the traditional analysis of such data, where $6\tilde{R}_0^2$ typically is identified [18] with the mean squared end-to-end distance of a random walk chain, i.e., $\sqrt{6}\tilde{l}$ is identified with the elementary step length $l_0$, modified by including the bond angle constraints imposed. $\tilde{v}$ is determined by estimating the elementary excluded volume, the precise expression being a matter of some debate. (For a discussion of this approach I refer to [19], and references given therein.) Now the results of Tables II and III show a strong variation of the parameters $\tilde{l},\tilde{v}$, not compatible with the philosophy outlined above. Outside a $\Theta$ region of very small excluded volume the parameters of two-parameter theory cannot naively be identified with parameters of the bare model. This also is obvious from Eqs. (21) and (23), showing that $\tilde{l},\tilde{v}$ nontrivially depend on the starting value of the renormalized coupling, which in turn is an unknown function of the bare parameters. Also $l_0$ is an unknown function of the bare parameters, implicitly being fixed by taking $n$ as the physical chain length. Furthermore, the function $Z_n(f_0,1)$ is microstructure dependent and cannot be calculated reliably. Still, Eqs. (21) and (23) involve some useful information, showing that $\tilde{l}$ vanishes for $f_0\to 1$, whereas $\tilde{v}$ diverges in that limit. The combination $\tilde{v}^{4\nu-2}6\tilde{l}^2/l_0^2$ shows no singularity, however. This qualitatively explains the variation of the parameters. In Fig. 7 I have plotted the numerical values of Table III together with the functions

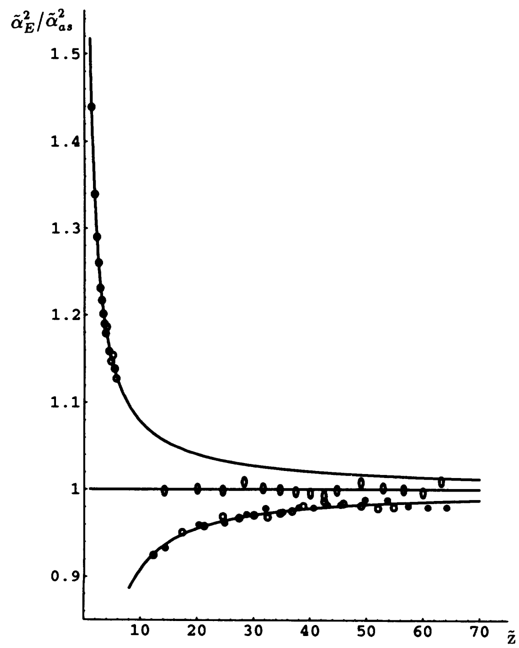


FIG. 6. Same as Fig. 5, but for continuum chains. Data from [14]. Strong-coupling branch, circles: $\delta=0.99$; points: $\delta=0.75$. Fixed point branch: $\delta=0.5$. I arbitrarily took $\tilde{z}=2n^{1/2}$. Weak-coupling branch: $\delta=0.25$.

TABLE III. Parameter values for three-dimensional continuum walks. $\delta=a_0/l_0$: ratio of bead diameter to segment length.

| $\delta$ | $6\tilde{l}^2$ | $\tilde{v}$ | $6\tilde{l}^2\tilde{v}^{0.360}$ |
|---|---|---|---|
| 1[a] | 1.8 | 1.8 | 2.2 |
| 0.99[b] | 1.804 | 1.733 | 2.199 |
| 0.93[a] | 1.6 | 1.9 | 2.0 |
| 0.79[a] | 1.3 | 2.1 | 1.8 |
| 0.75[b] | 1.330 | 2.029 | 1.716 |
| 0.71[a] | 1.4 | 1.8 | 1.7 |
| 0.63[a] | 1.0 | 3.1 | 1.5 |
| 0.60[c] | 0.80 | 4.38 | 1.37 |
| 0.55[c] | 0.70 | 5.25 | 1.27 |
| 0.55[a] | 0.7 | 6.3 | 1.3 |
| 0.50[b] | | | 1.143 |
| 0.45[c] | 0.64 | 3.38 | 1.00 |
| 0.45[a] | 0.7 | 2.3 | 1.0 |
| 0.40[c] | 0.70 | 1.97 | 0.98 |
| 0.30[a] | 0.9 | 0.4 | 0.6 |
| 0.25[b] | 0.956 | 0.178 | 0.514 |
| 0.10[b] | 0.999 | 0.010 | 0.190 |

[a]Reference [17].
[b]Reference [14].
[c]Reference [16].

$$\tilde{v}=1.45 f_0|1-f_0|^{-1/2\nu\omega}\,, \tag{35}$$

$$\frac{6\tilde{l}^2}{l_0^2}=|1-f_0|^{(2/\omega)(1-1/2\nu)}\,, \tag{36}$$

$$\left[\frac{6\tilde{l}^2}{l_0^2}\right]^{1/(4\nu-2)}\tilde{v}=1.45 f_0\,, \tag{37}$$

using the simple ansatz

$$f_0=\left[\frac{\delta}{\delta^*}\right]^3\,, \tag{38}$$

$\delta^*=0.52$. The factor 1.45 has been chosen such that Eq. (37) fits the data for small values of $\delta$. It clearly is illustrated that the main trend of the parameters just maps out the singularity structure of Eqs. (21) and (23). It also is clear that neither $\tilde{v}$ nor $\tilde{l}$ naively can be identified with parameters of the bare model.

In closing this section I want to comment on some previous theoretical analysis of such data. Notably over the years Domb and co-workers have published a series of papers (see [19] for details and further references), aiming at a construction of two-parameter results such as the equation for $\tilde{\alpha}_E^2(\tilde{z})$. Typically they combine results of bare perturbation theory valid for small excluded volume ($\tilde{z}<1$) in the continuous chain model with numerical results on lattice SAW's, thus constructing semiempirical formulas. According to the present analysis I feel this attempt is likely to fail, trying to interpolate smoothly among the weak- and strong-coupling branches. Still the method has met with considerable success (see [20], for instance), as can be understood from Fig. 2. Clearly for larger $\tilde{z}$ the shapes of the strong- or weak-coupling branches are not too different, and in some restricted range of $\tilde{z}$ a rescaling of that parameter might bring the two branches in close agreement. It is only with the recent very accurate data, covering a large range of chain lengths, that I clearly can resolve the difference.

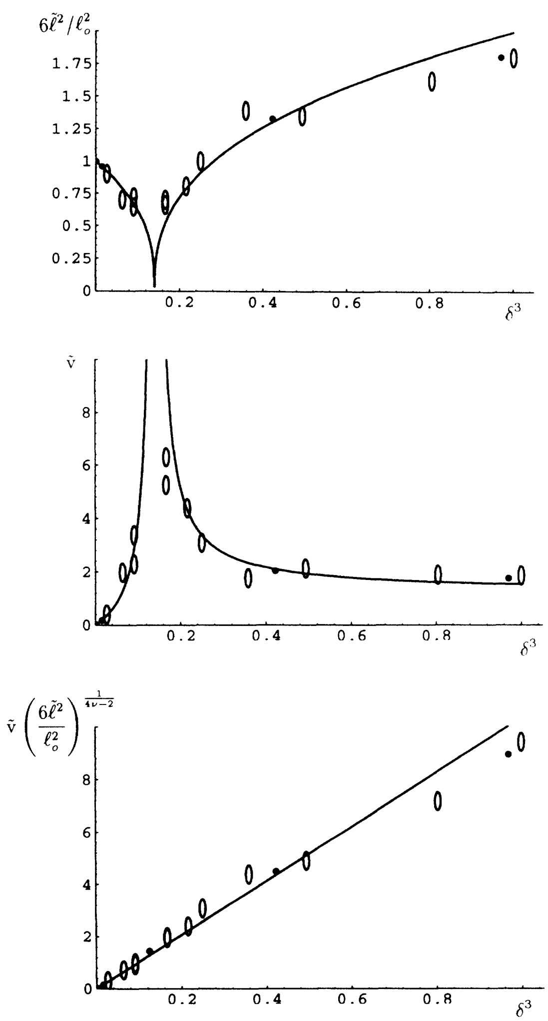


FIG. 7. Parameter values for continuum walks, plotted as a function of $\delta^3$. Points: Ref. [14]. Ellipsoids: less precise data of Refs. [16,17]. (a) $6\tilde{l}^2/l_0^2$; curve given by Eq. (36). (b) $\tilde{v}$; curve given by Eq. (35). (c) $(6\tilde{l}^2/l_0^2)^{1/(4\nu-2)}\tilde{v}$; curve given by Eq. (37).

The existence within the two-parameter model of a weak- and a strong-coupling branch recently has been clearly noted and stressed by Nickel [5]. He uses results of bare perturbation theory for the continuous chain model to construct recursion relations corresponding to successive decimations of the chain length by a factor of 2. He furthermore reformulates these relations in the style of a "direct renormalization" scheme, which in field-theoretic terms amounts to using a not minimally subtracted renormalization scheme, identifying the coupling $u(l_R)$ with some observable quantity. From both versions of his flow equations he derives the different branches. The present analysis is in complete accord with his findings.

Finally, Chen and Noolandi [21] presented an approach similar to the present one in that it is based on renormalized field theory. They use a form of $u(l_R)$ which essentially is based on a two loop calculation of the RG flow, and which first has been presented in [22]. They combine this with a kind of improved zero loop approximation for the scaling functions, fitting some numerical constants to asymptotic results of higher-order bare perturbation theory. In this way they reach a fit of similar quality to that shown here, except that they do not observe the structure of three universal branches but besides a quantity $\bar{u}$ corresponding to $f(l_R)$ keep an additional variable $z$ corresponding to the interaction parameter introduced in traditional unrenormalized theories.

## IV. CONCLUSIONS

I have argued that the standard methods of renormalized field theory can be applied also in some region where the renormalized coupling is larger than the nontrivial fixed point value. Basically I exploit the fact that the renormalized theory is independent of the details of the underlying bare theory. Arguments in favor of $u<u^*$ based on the infinite cutoff limit are relevant in quantum field theory, but do not apply to statistical mechanics with its finite cutoff. Also arguments based on massive renormalization do not apply to the present scheme. In agreement with the general RG framework I find three

universal branches $u < u^*, u = u^*, u > u^*$, all described by the same RG flow equations. There is no need to invoke irrelevant perturbations to give a meaning to the strong-coupling branch $u > u^*$. However, such perturbations inevitably influence the observables in the strong-coupling regime, if I am driven away from $u^*$ too far, going outside the preasymptotic regime [12]. Still it must be noted that in my analysis of results on self-avoiding walks I have found no sign of such corrections.

I have illustrated the usefulness of the approach with an analysis of Monte Carlo data on self-avoiding walks. The data nicely conform to the theory. I, however, should note that for each set of data I have two nonuniversal parameters available, so that the quantitative success should not be overestimated. In fact, it is well known that a one loop calculation of scaling functions, as exploited here, in general is accurate only up to a few percent. For instance, the ratio of the radius of gyration to the end-to-end distance differs from the results of Monte Carlo experiments or of a two loop calculation by about 3%. More important than the quantitative success is the basic qualitative agreement, convincingly exhibited in Figs. 5 and 6.

The analysis has stressed that the nonuniversal parameters of renormalized theory should not be mixed up with parameters of the bare model. In general there is no simple matching point, where these parameters could be identified naively. This point of view also has been stressed in Ref. [12]. Indeed, I work entirely in the renormalized framework, not invoking matching to bare theory. The resulting effective parameters show a behavior quite different from the parameters of the bare model. In particular, the parameter $\tilde{u}$ which relates the scaling variable $\tilde{z}$ to the chain length and which traditionally is considered to be a measure of the bare interaction strength, in the strong-coupling regime even decreases with increasing excluded volume. Renormalization thus induces some type of screening of strong interactions. In the strong-coupling regime the decrease of $\tilde{u}$ is accompanied by an increase of the effective segment size $\tilde{l}$, which may indicate that the interaction induces a local stretching of the chain.

All the qualitative results found here should hold generally for critical systems. Clearly a similar analysis of numerical data for three-dimensional Ising models should be feasible and seems highly appropriate.


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