Scaling behavior of linear polymers in disordered media

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It has long been known that the universal scaling properties of linear polymers in disordered media are well described by the statistics of self-avoiding walks (SAWs) on percolation clusters and their critical exponent ν_{SAW} , with the SAW implicitly referring to the average SAW. Hitherto, static averaging has been commonly used, e.g., in numerical simulations, to determine what the average SAW is. We assert that only kinetic, rather than static, averaging can lead to asymptotic scaling behavior and corroborate our assertion by heuristic arguments and a renormalizable field theory. Moreover, we calculate to two-loop order ν_{SAW} , the exponent ν_{max} for the longest SAW, and a family of multifractal exponents $\nu^{(\alpha)}$.

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In the past twenty years, the critical behavior of polymers in disordered media has generated a great deal of interest (for a recent review, see [1]). The problem is relevant in a vast range of different fields. To name a prominent example, the transport properties of polymeric chains in porous media might be exploitable commercially to enhance oil recovery. It has long been known that polymers in disordered media are well modeled by self-avoiding walks (SAWs) on percolation clusters. The term SAW usually refers implicitly to the average SAW. Despite the many ideas put forward and extensive numerical efforts, the critical behavior of polymers in disordered media is still far from being completely understood. The most unsettling problems are, perhaps, on the analytical side, that the only existing field theoretic model for studying average SAWs, the Meir-Harris (MH) model 2, has trouble with renormalizability 3,4 and, on the numerical side, that simulations lead to widespread results for the scaling exponent ν_{SAW} describing the mean length of average SAWs (see [1]).

A conceptual subtlety that apparently has not been appreciated much hitherto is the precise meaning of the average SAW. That is, there are, essentially, two qualitatively different ways of averaging over all SAWs between two connected sites for a given random configuration of a diluted lattice, one being static and the other being kinetic. In this Rapid Communication, we conjecture that the statistics of linear polymers in disordered media has no asymptotic scaling limit, when static averaging is used. Since it is static averaging that has been commonly employed in numerical work, many simulations might have suffered from this nonscaling behavior, which could explain the discrepancies between the numerical results for ν_{SAW} . In the following, we first corroborate our conjecture by heuristic arguments. Then, we resort to renormalized field theory. It turns out that, for achieving renormalizability, one has to use kinetic averaging; static averaging leads to nonrenormalizability. We then employ our field theory to calculate $\nu_{\rm SAW}$, the corresponding scaling exponents for the shortest and longest SAWs, and an entire family of multifractal exponents to two-loop order. Finally, we discuss the connection of kinetic averaging and the MH model.

First, let us define what we mean by static and kinetic averaging. In the framework of field theory, it is most convenient to model linear polymers in disordered media as SAWs between two connected sites x and y of a diluted lattice, where bonds are occupied with a probability p, and to focus on the length L(x,y) of a SAW (a random number proportional to the number of monomers of the corresponding polymer) rather than the Euclidian distance $|\mathbf{x}-\mathbf{y}|$ of its end points [2]. First, let us consider one given random configuration \mathfrak{C} of the diluted lattice. Averaging over all the SAWs belonging to the bundle $\mathcal{B}(x,y;\mathfrak{C})$ of SAWs directed from y to x yields the mean length

$$\langle L(x,y) \rangle_{\mathfrak{C}} = K \frac{\partial}{\partial K} \ln \left(\sum_{\gamma \in \mathcal{B}(x,y;\mathfrak{C})} p(\gamma) K^{L(\gamma)} \right),$$
 (1)

where $L(\gamma)$ is the length of γ , $p(\gamma)$, with $\sum_{\gamma} p(\gamma) = 1$, is a weight factor that depends on the averaging procedure, and K is the fugacity. Static averaging means that one simply uses $p(\gamma) \propto 1$. Kinetic averaging, on the other hand, means that a SAW γ earns a factor 1/z contributing to $p(\gamma)$ at each ramification where z-1 other SAWs from the bundle $\mathcal{B}(x,y;\mathfrak{C})$ split off. The experimentally relevant quantity, however, is not $\langle L(x,y) \rangle_{\mathfrak{C}}$, but rather its average $[\cdots]_p$ over all configurations \mathfrak{C} at fixed p subject to the constraint that xand y are connected. This average is expected to exhibit scaling behavior

$$M(x,y) = [\langle L(x,y) \rangle_{\mathfrak{C}}]_{p} \sim |\mathbf{x} - \mathbf{y}|^{1/\nu_{\text{SAW}}}$$
(2)

at a critical value K_c of the fugacity.

As we will demonstrate, SAWs on a percolation cluster are not merely standard fractals. Rather, they are multifractals. In order to capture this multifractality, we define the bond weights $m_b = \sum_{\gamma \in \mathcal{B}(x,y;\mathcal{C})} \chi_b(\gamma) p(\gamma) \leq 1$, where $\chi_b(\gamma)$ is 1 if the bond *b* belongs to the SAW γ and zero otherwise, and we introduce the multifractal moments HANS-KARL JANSSEN AND OLAF STENULL

FIG. 1. Percolation cluster in the node-link-blob picture.

$$L^{(\alpha)}(x,y) = \sum_{b} s_{b} m_{b}^{\alpha}$$
(3)

with s_b being the length of bond b. We will show that the scaling behavior of their quenched averages,

$$M^{(\alpha)}(x,y) = \left[L^{(\alpha)}(x,y)\right]_p \sim |\mathbf{x} - \mathbf{y}|^{1/\nu^{(\alpha)}},\tag{4}$$

is characterized by multifractal exponents $\nu^{(\alpha)}$ satisfying $\nu^{(0)} = 1/D_{bb}$, $\nu^{(1)} = \nu_{\text{SAW}}$, and $\nu^{(\infty)} = \nu$, where D_{bb} is the fractal dimension of the backbone and ν is the percolation correlation length exponent.

It is well known [5] that in a nonrandom medium (p=1)the exponent ν_{SAW} is the same for static and kinetic averaging. This may not be the case in a random medium, at least at the percolation point, and static averaging does not lead to a scaling law like Eq. (2). Heuristically, this can be understood by employing the node-link-blob picture of percolation clusters in which a percolation cluster connecting two terminal points, which is generically very inhomogeneous and asymmetric, can be envisaged as two nodes linked by tortuous ribbons that may contain blobs consisting of many short links in their interior. We will now use this picture to demonstrate that static averaging is unstable against coarse graining and that it therefore cannot be expected to produce the correct asymptotic scaling behavior. Let us for simplicity consider the cluster sketched in Fig. 1, which features two links, one with and the other without a blob. With static averaging the (upper) link with the blob acquires a much larger weight then the other (lower) one even if it is much shorter than the link with the blob. Then the statistics of the mean length is dominated by the short upper link with its many different SAWs induced by the blob. However, the weights change drastically upon coarse graining. Suppose we have some coarse graining procedure that culminates in condensing the blob into a single bond. After that, both links have the same weight. However, the lower one, since it is longer, now dominates the statistics. This demonstrates the instability of the weights of static averaging under real space renormalization as the group generated by repeated coarse graining. In contrast, kinetic averaging does assign the same weight to both links independent of the blob. Thus, kinetic averaging is stable under coarse graining even in a strongly inhomogeneous disordered medium.

To fortify our arguments, we now turn to renormalized field theory. We will propose a theory for calculating ν_{SAW} , as well as the entire family $\nu^{(\alpha)}$, that is renormalizable, provided that kinetic averaging is used. This theory is based on

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the nonlinear random resistor network (NRRN), where any bond on a *d*-dimensional lattice is occupied with a resistor with probability p or, respectively, empty with probability 1-p. Our theory, is motivated by the well known fact that the shortest and the longest SAWs (the former is also known as the chemical path) can be extracted from the NRRN [6] and its field theoretic formulation, the Harris model [7], by considering specific limits of the nonlinearity r of the generalized Ohm's law governing the bond resistors,

$$V_i - V_i = \rho_{(ij)} |I_{i,j}|^r \operatorname{sgn} I_{i,j},$$
 (5)

where V_i is the voltage at lattice site *i*, $\rho_{(ij)}$ is the resistance of bond (ij), and $I_{i,i}$ is the current flowing through that bond. As shown rigorously by Blumenfeld *et al.* [8], the shortest and the longest SAWs correspond to $r \rightarrow +0$ and $r \rightarrow -0$, respectively. Evidently, M(x, y) must lie between the average lengths of the shortest and the longest SAWs, which are, of course, very different. Since M(x, y) sits somewhere in this discontinuity at r=0, it is not known how to extract it from the NRRN by limit taking. Therefore, we propose here to study the average SAW by using our real world interpretation [9–12], in which the Feynman diagrams for the NRRN are viewed as being resistor networks themselves. The idea is to put SAWs on these diagrams. That this idea is fruitful can be checked explicitly with the instance of the chemical path. Our approach reproduces to two-loop order the corresponding exponent v_{\min} well established from dynamical percolation theory [13].

Our field theory is based on the Harris model as described by the Hamiltonian

$$\mathcal{H} = \int d^d x \sum_{\vec{\theta}} \left\{ \frac{\tau}{2} \varphi^2 + \frac{1}{2} (\nabla \varphi)^2 + \frac{w}{2} \varphi (-\vec{\partial}_{\theta})^{r+1} \varphi + \frac{g}{6} \varphi^3 \right\},\tag{6}$$

where $\vec{\theta}$ is a replicated discretized voltage taking on $(2N)^D$ values on a *D*-dimensional torus: $\vec{\theta} = (\pi/N)(n_1, \dots, n_D)$ with $n_i = -N+1, -N+2, \dots, N-1, N. \varphi = \varphi(\mathbf{x}, \vec{\theta})$ is the order parameter field, a continuum analog of a Potts spin. It transforms according to the one irreducible representation of the symmetric (permutation) group $S_{(2N)D}$ and thus, the model features only a single coupling constant g. τ and w are strongly relevant critical control parameters. The scaling behavior of SAWs is associated with the renormalization of w in the replica limit $D \rightarrow 0$. For details on the Harris model, we refer to [2,9,10]. The diagrammatic perturbation theory of the Harris model can be formulated in such a way that the Feynman diagrams resemble real RRNs. In this approach, which we refer to as the real world interpretation, the diagrams feature conducting propagators corresponding to occupied, conducting bonds and insulating propagators corresponding to open bonds. The conducting bonds carry replica currents conjugate to the replica voltages θ . The resistance of a conducting bond is given by its Schwinger parameter [14]. In the following, we will refer only to these very basic aspects of the real world interpretation which will be sufficient to follow the main line of argument. For further details on



FIG. 2. (Color online) Static and kinetic rule for averaging SAWs.

the real world interpretation, see Refs. [9–12].

Now we employ the real world interpretation to study the average SAW. As an example, let us consider a two-loop diagram that resembles the node-link-blob cluster in Fig. 1 and where all internal propagators are conducting. For determining the contribution of this diagram to M(x, y), the essential step in our approach is to find out the length L of an average SAW on that diagram. We can apply either the static or the kinetic rule to calculate L according to Eq. (3) with $\alpha = 1$, where now bond b is replaced by conducting propagator *i* and the Schwinger parameter $[14] s_i$ is interpreted as the corresponding length. As visualized in Fig. 2, static and kinetic averaging yield different results. The static rule gives $L^{(st)} = (s_1 + s_4 + s_5)/3 + 2(s_2 + s_3)/3$, whereas the kinetic rule produces $L^{(kin)} = (s_1 + s_2 + s_3)/2 + (s_4 + s_5)/4$. The remaining steps in calculating the diagram are essentially textbook matter [14]. It turns out that the static rule does not lead to a renormalizable theory. The reason is easily shown. In the two-loop calculation of our example diagram, the nonprimitive divergencies arising from the subintegrations of the oneloop self-energy insertion must be canceled through the counterterms introduced by the renormalization of this oneloop insertion. However, the weights of $L^{(st)}$ are not in conformity with the weights arising in the corresponding oneloop diagram with the counterterm insertion: crunching the insertion to a point (corresponding to $s_4+s_5 \rightarrow 0$) leads to $L^{(st)} = s_1/3 + 2(s_2 + s_3)/3$ in contrast to $L^{(kin)} = s_1/2 + (s_2)/3$ $(+s_3)/2$, which is equal to L of the one-loop self-energy diagram with a point insertion. Hence, only the weighting according to the kinetic rule works correctly in that it leads to a cancellation of nonprimitive divergencies by one-loop counterterms. Thus, the static rule has to be rejected on grounds of renormalizability.

Besides revealing the imperative of kinetic averaging, this theory yields two-loop results for the SAW exponents ν_{SAW} and ν_{max} , which previously have been calculated (correctly) only to one-loop order [2,7], and the family $\nu^{(\alpha)}$,

$$\nu_{\max} = \frac{1}{2} + \frac{\varepsilon}{168} + \left[\frac{5365}{16464} + \frac{15}{28}\left(\ln 2 - \frac{69}{70}\ln 3\right)\right] \left(\frac{\varepsilon}{6}\right)^2 + O(\varepsilon^3),$$
(7)



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FIG. 3. (Color online) The ε expansions of the exponents ν_{\min} (blue top curve), ν_{SAW} (red middle curve), and ν_{\max} (green bottom curve). Possible extrapolations at low dimensions *d* are shown by dashed lines. The squares with error bars symbolize numerical results for ν_{SAW} as compiled in [1].

$$\nu^{(\alpha)} = \frac{1}{2} + \left(\frac{5}{2} - \frac{3}{2^{\alpha}}\right) \frac{\varepsilon}{42} + \left(\frac{589}{21} - \frac{397}{14 \times 2^{\alpha}} + \frac{9}{4^{\alpha}}\right) \left(\frac{\varepsilon}{42}\right)^2 + O(\varepsilon^3),$$
(8)

where $\varepsilon = 6 - d$. ν_{SAW} is given by $\nu_{SAW} = \nu^{(1)}$. Our result for ν_{SAW} is compared to the available numerical estimates, to our result for the longest SAW, and to the well known exponent ν_{min} for the shortest SAW [9,10,13] in Fig. 3. The following points are worth noting. (i) $\nu^{(\alpha)}$ does not depend on α in a linear or affine fashion which implies that SAWs on percolation clusters are multifractal. (ii) $\nu^{(\alpha)}$ is in absolute agreement with the well known results for D_{bb} and ν in the cases $\alpha = 0$ and ∞ , respectively. (iii) ν_{min} and ν_{max} are not related to the family $\nu^{(\alpha)}$. (iv) The theory is renormalizable for arbitrary α if and only if kinetic averaging is used.

As mentioned above, the usual framework to study average SAWs on percolation clusters is the MH model as described by the Hamiltonian

$$\mathcal{H} = \int d^d x \Biggl\{ \sum_k \Psi_k (r_k - \nabla^2) \Psi_k + \frac{g}{6} \Psi^3 \Biggr\}.$$
(9)

Here, $\Psi_k = \{ \Psi_{k;\alpha_1,\dots,\alpha_k}^{i_1,\dots,i_k}(\mathbf{x}) \}, \ 1 \le k \le n$, is an order parameter field conjugate to an *n*-fold replicated *m*-component Heisenberg spin with vector indices i_l running from 1 to m and replica indices $\alpha_l \in \{1, ..., n\}$ ordered so that $\alpha_1 < \cdots < \alpha_k$. The *n* replicas transform according to *n* different irreducible representations of the direct product of the symmetric group S_n and the orthogonal (rotation) group SO(m). $r_k = \sum_l w_l k^l$, and Ψ^3 is a symbolic notation for the sum of the products of three Ψ_k fields. Only those cubic terms are allowed for which all pairs (i, α) appear exactly twice. In this model, one can extract ν_{SAW} from the renormalization of the relevant control parameter w_1 upon taking the replica limit $n \rightarrow 0$. The MH Hamiltonian (9) is nonrenormalizable as it stands. One difficulty that was pointed out by Le Doussal and Machta [3] several years ago is that the critical values $\{r_k^c\}$ of the control parameters are different for different k, i.e., the model is highly multicritical. A second problem, which to our knowledge has not been discussed hitherto, is that the order parameter fields Ψ_k for different k belong to different irreducible tensor representations of underlying symmetry group $S_n \times SO(m)$ (see above). Hence, strictly speaking, one needs independent coupling constants $g_{k,k',k''}$ for each product $\Psi_k \Psi_{k'} \Psi_{k''}$ [note that this is (i) not implemented in the original MH Hamiltonian (9) and (ii) different in the Harris model], and the fields Ψ_k need k-dependent renormalization factors [15]. Recently, these difficulties caused the failure of a two-loop calculation of ν_{SAW} by von Ferber *et al.* [4].

As far as its application to the average SAW is concerned, the renormalizability of the MH model can be rescued by a specific interpretation of the replica limit which has close ties to kinetic averaging. Our analysis of the MH model (details will be given elsewhere [17]) led to the following key findings. If the replica limit is taken after all summations over all possible arrangements of internal replica indices of a diagram, then the MH model reproduces static averaging and, as demonstrated above, is not renormalizable. If, however, the replica limit is taken, in the spirit of Ref. [16], as early as possible, i.e., loop after loop, or at least for each renormalization part, then the MH model reproduces kinetic averaging. This is the only interpretation of the replica limit of the MH model that leads to a renormalizable theory of SAWs in disordered media. With this interpretation, the MH model, in particular, produces the same result for ν_{SAW} as our real world interpretation and thereby provides an important consistency check for the validity of the application of the latter to SAWs.

Closing, we would like to emphasize that our renormalization group arguments are, although certainly well founded, not rigorous in the sense of a mathematical proof since they rely on our real world interpretation of Feynman diagrams. This interpretation thrives on analogy and there exist to date no rigorous mathematical arguments on how far its validity extends. However, given all its successes in the past, we would be surprised if it failed in describing SAWs on percolation clusters. The well known MH model, when interpreted carefully, corroborates the imperative of kinetic averaging and confirms our two-loop result for ν_{SAW} .

- [1] *Statistics of Linear Polymers in Disordered Media*, edited by B. K. Chakrabarti (Elsevier, Amsterdam, 2005).
- [2] Y. Meir and A. B. Harris, Phys. Rev. Lett. 63, 2819 (1989).
- [3] P. Le Doussal and J. Machta, J. Stat. Phys. 64, 541 (1991).
- [4] C. von Ferber, V. Blavats'ka, R. Folk, and Yu. Holovatch, Phys. Rev. E 70, 035104(R) (2004), and in [1].
- [5] L. Peliti, J. Phys. (Paris), Lett. 45, L925 (1984); K. Kremer and J. W. Lyklema, Phys. Rev. Lett. 55, 2091 (1985); L. Pietronero, *ibid.* 55, 2025 (1985).
- [6] S. W. Kenkel and J. P. Straley, Phys. Rev. Lett. 49, 767 (1982); J. P. Straley and S. W. Kenkel, Phys. Rev. B 29, 6299 (1984).
- [7] A. B. Harris, Phys. Rev. B 35, 5056 (1987).
- [8] R. Blumenfeld and A. Aharony, J. Phys. A 18, L443 (1985);
 R. Blumenfeld, Y. Meir, A. B. Harris, and A. Aharony, *ibid*. 19, L791 (1986).
- [9] O. Stenull, H. K. Janssen, and K. Oerding, Phys. Rev. E 59, 4919 (1999); H. K. Janssen, O. Stenull, and K. Oerding, *ibid.* 59, R6239 (1999).
- [10] H. K. Janssen and O. Stenull, Phys. Rev. E 61, 4821 (2000).
- [11] O. Stenull, Ph.D. thesis, Universität Düsseldorf (Shaker, Aachen, 2000).

- [12] O. Stenull and H. K. Janssen, Europhys. Lett. 51, 539 (2000);
 Phys. Rev. E 63, 036103 (2001).
- [13] H. K. Janssen, Z. Phys. B: Condens. Matter 58, 311 (1985); H.
 K. Janssen and U. C. Täuber, Ann. Phys. (N.Y.) 315, 147 (2005).
- [14] See, e.g., D. J. Amit, *Field Theory, the Renormalization Group, and Critical Phenomena* (World Scientific, Singapore, 1984); J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon, Oxford, 1996).
- [15] It is not possible to construct from the *n*-fold replicated *m*-vector model a simpler model where the order parameter fields Ψ_k for all *k* belong to one and the same irreducible representation of some higher-symmetry group. This is in contrast to the *n*-fold replicated *m*-state Potts model that combines to the *mⁿ*-state Potts model, where all fields belong to the same irreducible representation of S_{m^n} . Therefore, in the *n*-fold replicated *m*-state Potts model, one gets away with only one coupling parameter *g* and a unique (but *mⁿ*-dependent) renormalization factor for all fields.
- [16] A. B. Harris, Phys. Rev. B 28, 2614 (1983).
- [17] H. K. Janssen and O. Stenull (unpublished).