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Where two fractals meet: the scaling of a self-avoiding walk on a percolation cluster

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Зустріч двох фракталів: скейлінг випадкових блукань без самоперетинів на перколяційному кластері

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Анотація. У рамках теоретико-групового підходу проаналізовано скейлінгові властивості випадкових блукань без самоперетинів на d -вимірній розведеній перколяційній гранці. З цією метою розглядається модель, запропонована у роботі Мейра та Гаріса (Phys. Rev. Lett., **63**, 2819 (1989)). У той час як отриманий попередниками результат на базі першого порядку теорії збурень не узгоджувався із даними інших досліджень, ми отримали, що асимптотична поведінка випадкових блукань без самоперетинів на перколяційному кластері керується показником $\nu_p = 1/2 + \varepsilon/42 + 110\varepsilon^2/21^3$, $\varepsilon = 6 - d$. Цей аналітичний результат добре узгоджується із відомими даними досліджень Монте Карло та методів точного підрахунку у широкій ділянці значень вимірності $2 \leq d \leq 6$.

Where two fractals meet: the scaling of a self-avoiding walk on a percolation cluster

C. von Ferber, V. Blavats'ka, R. Folk, Yu. Holovatch

Abstract. The scaling properties of self-avoiding walks on a d -dimensional diluted lattice at the percolation threshold are analyzed by a field-theoretical renormalization group approach. To this end we reconsider the model of Y. Meir and A. B. Harris (Phys. Rev. Lett., **63**, 2819 (1989)). While the former first order perturbation did not agree with the results of other methods, we find that the asymptotic behavior of a self-avoiding walk on the percolation cluster is governed by the exponent $\nu_p = 1/2 + \varepsilon/42 + 110\varepsilon^2/21^3$, $\varepsilon = 6 - d$. This analytic result gives an accurate numeric description of the available MC and exact enumeration data in a wide range of dimensions $2 \leq d \leq 6$.

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Polymers and percolation clusters are among the most frequently encountered examples of fractals in condensed matter physics [1–3]. When a long polymer chain is immersed in a good solvent its mean-square end-to-end distance $\overline{R^2}$ scales with the monomer number N as:

$$\overline{R^2} \sim N^{2\nu_{\text{SAW}}}, \quad N \rightarrow \infty \quad (1)$$

with the exponent $\nu_{\text{SAW}}(d)$ which depends on the (Euclidean) space dimension d only. This scaling of polymers (1) is perfectly described by the self-avoiding walk (SAW) on a *regular* d -dimensional lattice [1] and the fractal dimension of a polymer chain readily follows: $d_{\text{SAW}} = 1/\nu_{\text{SAW}}$. For space dimensions d above the upper critical dimension $d_{\text{up}} = 4$ the scaling exponent becomes trivial: $\nu_{\text{SAW}}(d > 4) = 1/2$, whereas for $d < d_{\text{up}}$ the non-trivial dependence on d is described e.g. by the phenomenological Flory formula [1] $\nu_{\text{SAW}} = 3/(d + 2)$. This found its further support by the renormalization group (RG) $\tilde{\epsilon} = 4 - d$ -expansion known currently to the high orders [4]: $\nu_{\text{SAW}} = 1/2 + \tilde{\epsilon}/16 + 15\tilde{\epsilon}^2/512 + \dots$

When a SAW resides on a *disordered* (quenched diluted) lattice – such a situation might be experimentally realized studying a polymer solution in a porous medium, but is of its own interest as well – the asymptotic scaling behavior is a more subtle matter [5–7]. Numerous MC simulations [8–13] and exact enumeration studies [14–20], which last since early 80-ies [7], lead to the conclusion that there are the following regimes for the scaling of a SAW on a disordered lattice: (i) weak disorder, when the concentration p of bonds allowed for the random walker is higher than the percolation concentration p_{PC} and (ii) strong disorder, directly at $p = p_{\text{PC}}$. By further diluting the lattice to $p < p_{\text{PC}}$ no macroscopically connected cluster, “percolation cluster”, remains and the lattice becomes disconnected. In regime (i) the scaling law (1) is valid with the same exponent ν_{SAW} for the diluted lattice independent of p , whereas in case (ii) the scaling law (1) holds with a new exponent $\nu_p \neq \nu_{\text{SAW}}$. A hint to the physical understanding of these phenomena is given by the fact that weak disorder does not change the dimension of a lattice visited by a random walker, whereas the percolation cluster itself is a fractal with fractal dimension dependent on d : $d_{\text{PC}}(d) = d - \beta_{\text{PC}}/\nu_{\text{PC}}$, where β_{PC} and ν_{PC} are familiar percolation exponents [2]. In this way, $\nu_{\text{SAW}}(d)$ must change along with the dimension d_{PC} of the (fractal) lattice on which the walk resides. A modified Flory formula [8] for the exponent of a SAW on the percolation cluster $\nu_p = 3/(d_{\text{PC}} + 2)$ along with results of similar theoretical studies [21–28] gives numbers in an astonishing agreement with the data observed (see Table). Since $d_{\text{up}} = 6$ for percolation [2], the exponent $\nu_p(d \geq 6) = 1/2$ [32].

Although the Flory-like theories [21–28] offer good approximations for $\nu_p(d)$ in a wide range of d , even more astonishing is the fact that up to now there do not exist any satisfactory theoretical estimates for $\nu_p(d)$ based on a more refined theory, which takes into account non-Markovian properties of the SAW, a task which was completed for regular lattices already in mid-70-ies [1]. Existing real-space RG studies [14, 21, 29, 33] give satisfactory estimates for $d = 2$, whereas the field-theoretical approaches aimed to describe the situation at higher dimensions lead to contradictory conclusions. In particular, the field theory developed in Ref. [14] supported $d_{\text{up}} = 6$ and presented a calculation of ν_p in the first order of $\epsilon = 6 - d$. However the numerical estimates obtained from this result are in poor agreement with numbers observed by other means, leading in particular to the surprising estimate $\nu_p \simeq \nu_{\text{SAW}}$ in $d = 3$ (see Table). In turn, a subsequent study [34] even questioned the renormalizability of this field theory and suggested another theory with $d_{\text{up}} = 4$ which is obviously disproved by computer simulations and exact enumerations at dimensions $d = 4, 5$ [13, 14].

There is another important reason, why the scaling of a SAW on a percolation cluster calls for further theoretical study. As it became clear now, higher-order correlations of a fractal object at another fractal lead to multifractality [35]. Recently studied examples of multifractal phenomena are found in such different fields as diffusion in the vicinity of an absorbing polymer [36], random resistor networks [37], quantum gravity [38]. A SAW on a percolation cluster is a good candidate to possess multifractal behavior. Indeed such behavior is found in computer simulations [19], moreover it naturally emerges in the RG scheme, as we will explain below.

Let us consider a diluted lattice with sites \mathbf{x}_i in terms of variables $p_{ij} = 0, 1$ that indicate whether a given bond between the sites \mathbf{x}_i and \mathbf{x}_j is present or not. To describe the critical properties of SAWs on this lattice following the idea of de Gennes [1] we introduce m -component spin variables $S_\alpha(\mathbf{x}_i)$, $\alpha = 1, \dots, m$, and evaluate the theory for $m = 0$. To allow for the averaging over the *quenched* disorder the spins are n -fold replicated which gives for the Hamiltonian:

$$e^{-\mathcal{H}_s} = \langle \exp\left\{-\frac{K}{2} \sum_{i,j} p_{ij} \sum_{\alpha=1}^m \sum_{\beta=1}^n S_\alpha^\beta(\mathbf{x}_i) S_\alpha^\beta(\mathbf{x}_j)\right\} \rangle_p \quad (2)$$

where we denote by $\langle \dots \rangle_p$ the average over the random variables p_{ij} which take the value 1 and 0 with probabilities p and $(1 - p)$ respectively, and K is an interaction parameter. In the following we will work with a field theoretical representation of the effective Hamiltonian defined in

Table 1. The exponent ν_p for a SAW on a percolation cluster. FL: Flory-like theories, EE: exact enumerations, RS, RG: real-space and field-theoretic RG. The first line shows ν_{SAW} for SAW on the regular lattice ($d = 2$ [30], $d = 3$ [31]).

d	2	3	4	5	6
ν_{SAW}	3/4	0.5882(11)	1/2	1/2	1/2
FL, [21]	0.778	0.662	0.593	0.543	1/2
[22]	0.69(1)	0.57(2)	0.49(3)		1/2
[23]		0.70(3)	0.63	0.56	1/2
[24]	0.770	0.656	0.57	0.52	1/2
[25]	0.76	0.65	0.58		1/2
[26]	0.75-0.76	0.64-0.66	0.57-0.59	0.55-0.57	1/2
[27]	0.77	0.66	0.62	0.56	1/2
MC, [8]		$\simeq 2/3$			
[9]	$\simeq \nu_{\text{SAW}}$	0.612(10)			
[10]	$\simeq \nu_{\text{SAW}}$	0.605(10)			
[11]	0.77(1)				
[12]	0.783(3)				
[13]		0.62-0.63	0.56-0.57		
EE, [14]	0.76(8)	0.67(4)	0.63(2)	0.54(2)	
[15]	0.81(3)				
[15]	0.745(10)	0.635(10)			
[16]		0.65(1)			
[17]	0.745(20)	0.640(15)			
[18]	0.770(5)	0.660(5)			
[19]	0.778(15)	0.66(1)			
[19]	0.787(10)	0.662(6)			
RS, [29]	0.767				
[21]	0.778	0.724			
RG, [14]	0.595	0.571	0.548	0.524	1/2
(9)	0.785	0.678	0.595	0.536	1/2

(2). This is achieved [14] via a Stratonovich-Hubbard transformation to tensor fields $\psi_k(\mathbf{x})$ with components $\psi_{k;\beta_1,\dots,\beta_k}^{\alpha_1,\dots,\alpha_k}(\mathbf{x})$ conjugated to the product $\Pi_{j=1}^k S_{\alpha_j}^{\beta_j}(\mathbf{x})$ of k components of the replicated spin with $\beta_1 < \dots < \beta_k$. This results in the effective Hamiltonian up to order ψ^3 [14]:

$$\mathcal{H}_\psi = \frac{1}{2} \int d^d q \sum_k (r_k + q^2) \psi_k(\mathbf{q}) : \psi_k(-\mathbf{q}) +$$

$$\frac{w}{6} \int d^d x \psi^3(\mathbf{x}), \quad (3)$$

where $\psi_k(\mathbf{q})$ is the Fourier transform of $\psi_k(\mathbf{x})$, the inner product reads:

$$\psi_k(\mathbf{q}) : \psi_k(-\mathbf{q}) = \sum_{\{\alpha_i\}} \sum_{\{\beta_i\}} |\psi_{k;\beta_1,\dots,\beta_k}^{\alpha_1,\dots,\alpha_k}(\mathbf{q})|^2,$$

and $\psi^3(\mathbf{x})$ is a symbolic notation for a product of three ψ_k fields. Only those cubic terms ψ^3 are allowed for which all pairs (α_i, β_i) appear exactly twice. A second condition on the diagrammatic contributions to perturbation theory can be derived from the de Gennes limit $m = 0$, namely, if any index (α, β) appears only on the internal propagator of a diagram, then its contribution vanishes.

We note the unusual dependence of “masses” r_k on k . This is reminiscent of the fact that in the $m = 0$ limit the theory (2) becomes multicritical [14, 39]. This has impact on the renormalization of the theory (3) as we will show in the following.

We choose to calculate the critical properties of the theory by analyzing its vertex functions, in particular $\Gamma^{(2)}(q)$, $\Gamma^{(3)}(\{q\})$, and $\Gamma^{(2,1)}(\{q\})$ where the latter includes an insertion of the $\psi:\psi$ operator. Each of these Γ -functions will depend on the family of masses $\{r_k\}$. The Feynman graphs of the contributions to the two-point vertex function $\Gamma^{(2)}(q)$ in the two lowest orders are shown in Fig. .

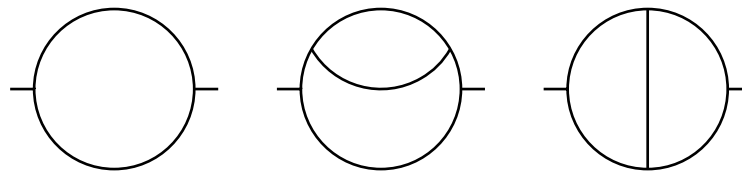


Figure 1. The Feynman graphs of the vertex function $\Gamma^{(2)}(q)$ in the two lowest orders.

The contributions to $\Gamma^{(2,1)}$ are found from this by placing an insertion on each of the inner propagator lines. These integrals are evaluated then in dimensional regularization in dimension $d = 6 - \varepsilon$ and minimal subtraction [40] using a Laurent-expansion in ε . Usually the renormalization of the vertex functions is defined in terms of Z -factors in such a way that the products $Z_\psi \Gamma^{(2)}$, $Z_w \Gamma^{(3)}$, $Z_{\psi^2} \Gamma^{(2,1)}$ are free of ε -poles. However, the insertion of the $\psi:\psi$ -operator together with the k -dependence of the

masses r_k leads to the following renormalization procedure. The vertex function $\Gamma^{(2,1)}$ even when evaluated at zero mass remains k -dependent:

$$\Gamma^{(2,1)} = \Gamma_0^{(2,1)} + k\Gamma_1^{(2,1)} + k^2\Gamma_2^{(2,1)} + \dots \quad (4)$$

and it can not be renormalized by one multiplicative Z -factor. The essential feature of this expansion is that each term shows a different scaling behavior. In this way the multicriticality recognized already by Derrida [39] and Meir and Harris [14] manifests itself in our present formalism and leads to a *spectrum of exponents*. Instead of a single Z -factor Z_{ψ^2} a whole family of factors $Z_{\psi:\psi}^{(i)}$ is necessary to renormalize each $\Gamma_i^{(2,1)}$ in (4). This allows to define RG-functions

$$\beta(w) = \frac{d}{d\kappa} \ln Z_w, \quad (5)$$

that describes the RG-flow of the coupling with respect to the rescaling parameter κ and

$$\eta(w) = \frac{d}{d\kappa} \ln Z_\psi, \quad \eta_{\psi:\psi}^{(i)}(w) = \frac{d}{d\kappa} \ln Z_{\psi:\psi}^{(i)} \quad (6)$$

which define the anomalous dimensions of the corresponding operators. At the stable fixed point w^* with $\beta(w^*) = 0$ the family of correlation exponents is given by

$$\nu^{(i)} = [2 - \eta(w^*) + \eta_{\psi:\psi}^{(i)}(w^*)]^{-1}. \quad (7)$$

We note that $\nu^{(0)} \equiv \nu_{\text{PC}}$ and $\nu^{(1)} \equiv \nu_{\text{p}}$ as introduced above, whereas the $\nu^{(i)}$ for $i \geq 2$ are connected with higher order correlations. The β -function (5) is the familiar RG function of the ψ^3 Potts model [41].

The explicit calculations proceed as follows: (i) One starts with the vertex function $\Gamma_{\psi_k}^{(2)}$ corresponding to the propagator of the field ψ_k . (ii) For the masses one inserts the expansion $r_k = \mu \sum_{j=0}^{\infty} u_j k^j$. (iii) The insertion of $\psi:\psi$ is defined by the derivative $\frac{\partial}{\partial \mu} \Gamma_{\psi_k}^{(2)}$ evaluated at zero mass for $\mu = 0$. (iv) Performing the summation over the replica indices the contributions to the different $\Gamma_i^{(2,1)}$ are generated by rearranging the expansion in k . One finds the multiplicative renormalization for $\Gamma_i^{(2,1)}$ for appropriate linear combinations of the different orders of k .

Following this procedure we obtain $\varepsilon = 6 - d$ expansions for $\eta_{\psi:\psi}^{(i)}$. Substituting them together with the known result [41] $\eta = -\varepsilon/21 -$

$206\varepsilon^2/21^3$ into (7) we arrive at the following spectrum of correlation exponents:

$$\nu^{(0)} = \nu_{\text{PC}} = 1/2 + 5\varepsilon/84 + 589\varepsilon^2/42^3, \quad (8)$$

$$\nu^{(1)} = \nu_{\text{p}} = 1/2 + \varepsilon/42 + 110\varepsilon^2/21^3, \quad (9)$$

$$\nu^{(2)} = 1/2 + \varepsilon/24 + 13907\varepsilon^2/1100736, \dots \quad (10)$$

By (8) we recover the familiar ε -expansion for the percolation exponent ν_{PC} [41] and in (9) we extend the first order result for ν_{p} [14]. The physical interpretation and properties of the remaining exponents $\nu^{(i)}$ of the family is the subject of a separate study [42]. Contrary to the family of ν -exponents defined in Ref. [19], the $\nu^{(i)}$ govern the non-trivial scaling of properly defined cumulants of the distribution of SAWs for given end-to-end distance [42]. Evaluating the result for ν_{p} (9) by direct substitution of $\varepsilon = 6 - d$ one finds nearly perfect correspondence with available MC and exact enumeration results over the range $d = 2, \dots, 5$, see Table . This presents a *qualitative* improvement over the linear result as seen in Fig. where we also show that the result is in between the limits given by the shortest and longest SAWs on percolation cluster [44].

A rather peculiar finding is that results of the phenomenological Flory-like formulae evaluated using the fractal characteristics of the percolation cluster are numerically very close to our result in the same region of dimensions. Note however the ambiguity [18] in defining a Flory-like scheme leading to the different results in Table .

The ψ^3 theory as applied to the present problem inevitably has the upper critical dimension $d_{\text{up}} = 6$. This in particular allows us to describe the discussed non-trivial scaling for dimensions $d = 4, 5$. This is out of reach following the approach of Ref. [34] which gives trivial scaling for $d \geq d_{\text{up}} = 4$ and relies on a ϕ^4 -theory with two couplings of different symmetry. Moreover, in the de Gennes limit $m = 0$ the symmetry of the two couplings coincides [6] leading back to a theory of SAWs on the pure lattice with a redefined coupling parameter, a fact neither exploited in Ref. [34] nor in the similar approaches [45, 46].

From the physical point of view, our result for the exponent ν_{p} together with the data of EE and Flory-like theories (see Table) predicts a swelling of a polymer coil on the percolation cluster with respect to the pure lattice: $\nu_{\text{p}} > \nu_{\text{SAW}}$ for $d = 2 - 5$. Up to now, this phenomenon has clearly been observed only in MC simulations for $d = 2$ [12]. Although simulations on $d = 3$ percolation clusters have been claimed to show this effect [8–10, 13], these studies were subsequently criticized for using inappropriate data analysis [9, 15, 20] and for lack of accuracy. At $d = 3$

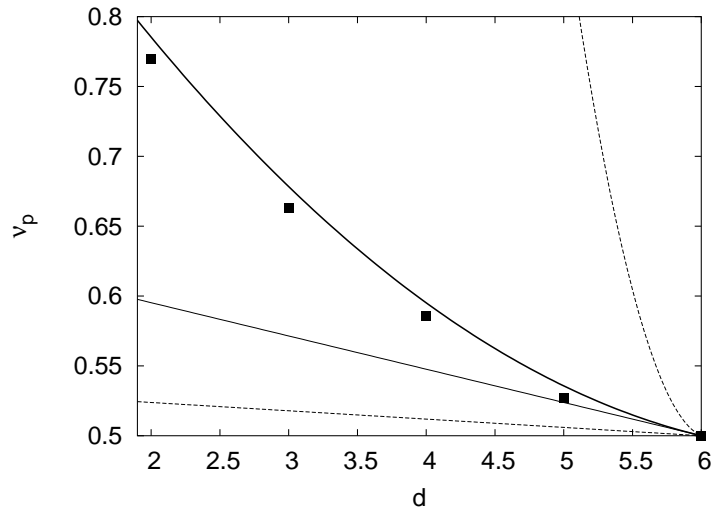


Figure 2. The correlation exponent ν_p . Bold line: (9), thin line: one-loop result [14], filled boxes: Flory result $\nu_p = 3/(d_{PC} + 2)$ with d_{PC} from [43]. Exponents for the shortest and longest SAW on percolation cluster [44] are shown by dotted lines.

our formula (10) predicts a 13% increase of ν_p with respect to ν_{SAW} which is larger than at $d = 2$ (5%) and should be more easily observed by current state-of-art simulations. Given that even at $d = 2$ we are in nice agreement with MC and EE data and the reliability of the perturbative RG results increases with d , this number calls for verification in MC experiments of similar accuracy.

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