Absence of self-averaging in global optimization problems

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We study the distribution of (1+1)-dimensional self-affine lines resulting from the zero-temperature directed polymer in a random medium or from critical directed percolation problems. The related amplitude ratios depend on whether the finite size scaling statistics is made over finite segments of the infinite objects or over the finite objects of diverging size. As a by-product we obtain the correction to scaling exponents for the finite size scaling of the distribution functions. [S1063-651X(96)50206-0]

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Self-affine objects are abundant in nature. In particular, they seem to be the typical case when interfaces are created by noisy processes [1-3]. To mention an everyday example, the fracture surface created when, say, a piece of pottery breaks, or a sheet of paper is torn, shows self-affinity typically over more than two orders of magnitude variation in the length scales [4-8]. Global optimization processes like the determination of the minimum energy conformation of directed polymers [9,10] in a random medium or critical directed percolation [11] backbones lead to self-affine lines and they are both good candidates for describing surface lines resulting from two-dimensional [(1+1)-dimensional] breaking processes [7,8]. Due to the fact that the roughness exponents for these two models are rather close to each other (2/3 and 0.633) there is a need to characterize them in more detail in order to help distinguish between them.

The moments of the distribution functions of height differences on self-affine lines have attracted interest in recent years for two reasons. First, there are cases where the different moments scale differently leading to multiaffinity [12,13]. Second, the non-Gaussian character of the distribution of directed polymer lines was investigated this way [14].

In this paper we investigate the moments of the height difference distributions in two self-affine objects in 1+1 dimensions: (1) The minimum-energy conformation of directed polymers in random media [9,10], and (2) critical "pinning lines" in directed percolation [15,16].

We have studied two cases: (i) The distribution of height differences between the end points of the self-affine lines where the sizes *L* were increasing and (ii) the distribution of height differences between points at distance *x* where $x \ll L \rightarrow \infty$ but $x \rightarrow \infty$. The striking result is that the two limits are not equivalent, i.e., from the point of view of the moments of the distributions the cases $x \rightarrow L$; $L \rightarrow \infty$ and $L \rightarrow \infty$; $x \rightarrow \infty$ are not interchangeable. The scaling of the moments is, however, always described by the corresponding unique universal exponent.

The statistical distribution of self-affine lines may be described by the function $p_{x_1,x_2}(y_1,y_2)$, giving the conditional probability density that the curve y(x) passes the point (x_2,y_2) provided it passes (x_1,y_1) . It can be assumed that the function only depends on the differences $\Delta x = x_2 - x_1$ and $\Delta y = y_2 - y_1$ and self-affinity imposes the invariance

$$p_{\Delta x}(\Delta y) = \frac{1}{\lambda^{\zeta}} p_{\Delta x/\lambda}(\Delta y/\lambda^{\zeta}) \tag{1}$$

on the distribution function where ζ is the roughness or Hurst exponent. We do not consider here multiaffine objects [12,13]. The distribution leads to the moments (or *k*th order correlation functions):

$$C_{k}(\Delta x) = \left[\int_{-\infty}^{\infty} d\Delta y |\Delta y|^{k} p_{\Delta x}(\Delta y) \right]^{1/k}.$$
 (2)

Due to the scaling assumption (1) we have $C_k(\Delta x) \propto |\Delta x|^{\zeta}$. The distribution is therefore best characterized by the amplitude ratios:

$$R_k(\Delta x) = C_k(\Delta x) / C_2(\Delta x).$$
(3)

The linear sizes of the objects are denoted by *L*. We concentrate on the question whether $\lim_{\Delta x\to\infty} \lim_{L\to\infty} R_k(\Delta x)$ is equivalent to $\lim_{L\to\infty} \lim_{\Delta x\to L} R_k(\Delta x) = \lim_{L\to\infty} R_k(L)$ and how these quantities are related to the ratios resulting from Gaussian distributions.

Both directed polymers and critical directed percolation paths are results of global optimization problems. In order to describe these two problems, we start with a square lattice at 45° with respect to the two directions x and y. We imagine that the size of the lattice is L in the x direction and W in the y direction. To each node (x, y) in the lattice, we assign a random number $e_{(x,y)}$ obtained from some probability distribution — for example, a uniform distribution between zero and one. The problem now consists of identifying the path y(x) between x=0 and x=L for which the sum of the random numbers is minimal,

$$E = \min_{y(x)} \left(\sum_{x} e_{(x,y(x))} \right). \tag{4}$$

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We may interpret the path as being a polymer without overhangs — hence *directed* — which is strongly interacting with a surrounding medium with quenched disorder. This interaction gives rise to a local interaction energy $e_{(x,y)}$, and the path determined through Eq. (4) is the ground state configuration of the polymer at zero temperature. It has been shown [9,10] that in (1+1) dimensions the ground state conformation of the directed polymer is self-affine with a roughness exponent $\zeta = 2/3$. This result is valid as long as the distribution of interaction energies falls off towards negative values at least as fast as a power law, $1/e^{1+\mu_c}$, where μ_c is a dimension-dependent critical value [17], which, e.g., for the hierarchical lattice [18] is $\mu_c = 6$, or if the distribution towards positive values is not so broad that a single energy $e_{(x,y)}$ dominates all others.

In the latter case we may substitute the sum in Eq. (4) by a maximum,

$$E = \min_{y(x)} \left(\max_{x} e_{(x,y(x))} \right).$$
 (5)

This is in fact a formulation of the directed percolation problem [19,20]. The max in (5) picks the bottlenecks for all possible lines and the min in the front assures that the optimal, i.e., the critical percolation line is chosen. For a system of size L this is not a unique definition since there could be several lines satisfying the condition (5) corresponding to the whole critical directed percolation backbone. However, there are ways to suppress this ambiguity. One is the following: The maximal value of $e_{(x,y)}$ on the backbone divides it into two pieces. Now one can look for the maximal values left and right from this point and so on until a unique line is determined. This global optimization model was recently formulated by Roux and Zhang [21]. Another possibility is that one chooses the lowermost line which corresponds to the pinning line in models of fluid displacement in a random environment [15,16]. We applied in our investigations the latter choice.

For the critical directed percolation line the roughness exponent is $\zeta = \nu_{\perp} / \nu_{\parallel} \approx 0.633$, where $\nu_{\perp} = 1.733 \pm 0.001$ is the correlation length exponent in the *y* direction and $\nu_{\parallel} = 1.097 \pm 0.001$ is the correlation length exponent in the *x* direction. The numerical values are based on series expansions [22,23].

In order to identify the minimum-energy path in the directed polymer problem, we use a transfer matrix tech-



FIG. 1. The moment ratios R_k for the directed polymer problem as calculated for the *L* limit. The extrapolated values marked for $L \rightarrow \infty$ agree well with those of Ref. [14] and are given in Table I. The lines connect the data points.

nique. We define the matrix element $E_{(x,y)}$ as the minimum energy of a directed polymer starting at x=0 and y=0 and ending at (x,y). The relation between the mininum energies at level x and x+1 is then simply $E_{(x+1,y)} = \min(E_{(x,y-1)})$ $+ e_{(x+1,y)}, E_{(x,y+1)} + e_{(x+1,y)})$. Likewise, in the directed percolation problem, we update a transfer matrix $E_{(x,y)}$ by the rule [20] $E_{(x+1,y)} = \min(\max(E_{(x,y-1)}, e_{(x+1,y)}), \max(E_{(x,y+1)}, e_{(x+1,y)}))$.

In the directed polymer problem, once a matrix element $E_{(x,y)}$ has been assigned to each node in the lattice, the minimum energy conformation y(x) is easily identifiable: We start by identifying the minimum $E_{(x=L,y)}$. Once this element has been identified, we have the end point of the minimum energy configuration. We then identify the minimum of the two neighboring elements $E_{(x=L-1,y+1)}$ and $E_{(x=L-1,y-1)}$. Once this element has been identified, we then move on to identifying the minimum matrix element among the two neighbors with x=L-2 of this element. Doing this "burning" backwards recursively, until x=0 has been reached, the entire minimum-energy configuration is finally mapped out.

A similar method is used to map out the directed percolation path. However, the ambiguity mentioned above shows up here in the following way: There is typically a large number of paths with the same "energy" $E_{(x,y(x))}$

TABLE I. Extrapolated amplitude ratios R_k for the directed polymer, the critical directed percolation lines, and random walks in the L and x limits. The last column contains the exact Gaussian values from (8).

k	Dir. pol. L limit	Dir. pol. <i>x</i> limit	Dir. perc. L limit	Dir. perc. <i>x</i> limit	Rand. walk L limit	Rand. walk x limit	Gauss.
1	0.807	0.800	0.675	0.793	0.797	0.796	0.7979
3	1.157	1.164	1.265	1.170	1.169	1.169	1.1686
4	1.291	1.306	1.475	1.317	1.318	1.317	1.3161
5	1.409	1.432	1.65	1.450	1.451	1.450	1.4488
6	1.515	1.547	1.79	1.571	1.574	1.573	1.5704
7	1.610	1.652	1.91	1.683	1.687	1.686	1.6833
8	1.698	1.750	2.01	1.775	1.793	1.792	1.7892



FIG. 2. The moment ratios R_k for the directed polymer problem, as calculated for the x limit. The extrapolation was carried out according to (9) with $\omega_{\text{polymer}}=0.67$ and it is indicated by the straight lines for $\Delta x \rightarrow \infty$. The extrapolated values are listed in Table I.

given by Eq. (4). This degeneracy results from situations where in Eq. (5) the two expressions $\max(E_{(x,y-1)}, e_{(x+1,y)})$ and $\max(E_{(x,y+1)}, e_{(x+1,y)})$ are equal. When this situation occurs, we choose the path passing through the point (x,y-1). The path we have thus identified corresponds to the shape of an interface in a medium with quenched disorder at the depinning transition [15,16]: We therefore refer to the path thus identified as a "pinning line."

Our statistics is based on N runs with W=2000, L=1000, and $N=10^5$ for the $\lim_{\Delta x\to L} \lim_{L\to\infty}$ cases (in the following to be referred to as the L limit) and W=400, L=2000, and $N=5\times10^4$ for the $\lim_{L\to\infty} \lim_{\Delta x\to\infty}$ cases (to be referred to as the x limit) where the largest Δx was L/2.

We first checked the scaling assumption in the *L* limit and concluded that the distributions can be characterized with the roughness exponents $\zeta = 0.662$ for the directed polymer and $\zeta = 0.638$ for directed percolation, in good agreement with the generally accepted values.

Halpin-Healy concluded [14] that the ratios $R_k(L)$ for directed polymers in (1+1) dimensions are not Gaussian. The Gaussian ratios can be calculated analytically from the assumption

$$p_{\Delta x}(\Delta y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-(\Delta y)^2/2\sigma^2]$$
(6)

with $\sigma \propto (\Delta x)^{\zeta}$ resulting in $R_k = \sqrt{2} [\Gamma((k+1)/2)/\sqrt{\pi}]^{1/k}$. Halpin-Healy studied the *L* limit and our calculations (Fig. 1, Table I) are in full agreement with his results. Figure 2 shows the calculations of the ratios $R_k(\Delta x)$ for the directed polymers in the *x* limit. In order to extrapolate the data for $\Delta x \rightarrow \infty$ we applied the concept of corrections to scaling:

$$R_k(\Delta x) = R_k(\Delta x \to \infty) + A_k / \Delta x^{\omega}, \qquad (7)$$

where the value of ω is determined by the possibly smoothest extrapolation. The curves in Fig. 2 were obtained with $\omega_{polymer}=0.67$ (perhaps 2/3?) and the straight parts of the



FIG. 3. The moment ratios R_k for the critical directed percolation lines as calculated for the *L* limit. The extrapolation was carried out according to (9) with $\omega_{\text{percolation}} = 0.4$. The values are indicated for $L \rightarrow \infty$ and are given in Table I. The lines connect the data points.

lines justify this choice. In fact, we observed that the straightness of the lines depends strongly on the value of $\omega_{polymer}$ but the extrapolated ratio values (Table I) do not. The lines for different *k* values bend for Δx approaching *L* showing finite size effects. Of course, for $\Delta x = L$ we should obtain the same limits as for Fig. 1. The interesting result comes from the comparison of the two limits. The precision of our data is certainly good enough to conclude that the two limiting ratios differ from each other significantly. Since the errors become larger for the higher values of *k* the Gaussian behavior cannot be ruled out (Table I) in the *x* limit.

We carried out a similar calculation for the critical directed percolation lines. The *L* limit (Fig. 3) shows in this case a stronger *L* dependence than in the case of directed polymers, so we had to apply an extrapolation procedure as given by (7). The fit is acceptably good with



FIG. 4. The moment ratios R_k for the critical directed percolation lines, as calculated for the x limit. The extrapolation was carried out according to (9) with $\omega_{\text{percolation}} = 0.35$ and it is indicated by the straight lines for $\Delta x \rightarrow \infty$. The extrapolated values are given in Table I.

 $\omega_{\text{percolation}} = 0.4 \pm 0.1$ and the limiting ratios are again non-Gaussian.

For the x limit (Fig. 4) we used $\omega_{\text{percolation}} = 0.35$. The finite size effects are somewhat more pronounced than for the directed polymer case. However, we see again that the L and x limits are not interchangeable. Moreover, the x limit leads to values which are very close to the Gaussian values strongly indicating that in this limit the distribution approaches a Gaussian. The results for the directed percolation are also summarized in Table I.

For comparison, we also generated a sample of similar size of random walks. The scaling exponent is in this case $\zeta = 1/2$. Carrying out the extrapolations with $\omega_{walk} = 1$, we get values which are in excellent agreement with the Gaussian ones for both *L* and *x* limits indicating that the effect we have found for the global optimization problems is real; see Table 1.

Our main result is therefore that although the scaling exponents are robust with respect to the L and x limits, the distributions do depend on them. The distributions are generally considered to be universal, e.g., the ratios R_k should be independent of the type of the lattice, extent of short-range interaction, etc. Our result indicates, however, that the limiting distribution is sensitive to the order of the limits.

This finding can be interpreted in the following way. In the L limit we take the objects of size L, carry out the statistics on them and let the system size L go to ∞ . Due to the fact that we consider global optimization problems as we go from one size to the other the objects under consideration change, i.e., the objects at size L_1 are *different* from the objects at L_2 . On the other hand, if we consider increasing parts of large samples (x limit) the objects on which the statistics is carried out do not change. The global restriction which is imposed onto the ensemble of the lines with the same scaling exponents results in the change of the distribution functions. We can therefore conclude that in the considered models self-averaging is valid for the scaling exponents but not for the distributions. This has a bearing on the comparison between experimental and numerical studies of rough surfaces: Experimental measurements are typically carried out over pieces of the rough surface in question which places them in the x limit, while numerical studies are more easily carried out in the L limit.

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