Scaling of Directed Polymers in Random Media

Mehran Kardar
Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

and

Yi-Cheng Zhang
Istituto Nazionale di Fisica Nucleare, I-00185 Rome, Italy, and Physics Department, University of Rome, I-00185 Rome, Italy

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Directed polymers subject to quenched external impurities (as in a polyelectrolyte in a gel matrix) are examined analytically, and numerically. Transverse fluctuations $|\mathbf{x}|$ scale with the length t of the polymer as $|\mathbf{x}| \sim t^\nu$. In all dimensions, for sufficiently strong disorder, ν can be different from the random-walk value of $\frac{1}{2}$. Extensive numerical simulations in two, three, and four dimensions in fact suggest a superuniversal exponent of $\nu = \frac{2}{3}$. The importance of the tree structure of the polymer ensemble is emphasized.

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To what extent are the scaling properties of polymers modified by impurities in the surrounding media? For self-avoiding polymers this interesting question has been debated for some time, and the resolution is not yet clear.[1-3] Here we address the simpler question of the behavior of a *directed* polymer in a random matrix.[3] A directed polymer (e.g., a polyelectrolyte), by the construction of being stretched in the longitudinal direction has no self-intersections, but can fluctuate in the transverse direction. The scaling of these fluctuations in the presence of quenched randomness is directly relevant to the conformations of a polyelectrolyte in a frozen gel matrix, but is also indirectly related to problems in optimization (best energy paths), growth (dynamic scaling of a growing interface), and fluid flow (the Burgers equation).

Without impurities, and due to entropy alone, typical transverse fluctuations $|\mathbf{x}|$ scale with the length t of the directed polymer as $|\mathbf{x}| \sim t^\nu$ with $\nu = \frac{1}{2}$ (i.e., as a typical random walk). In two dimensions, *with impurities,* the polymer behaves as the interface of an Ising model subject to disorder, where various results[4-7] indicate $\nu = \frac{2}{3}$ exactly. In higher dimensions, a mapping onto the randomly stirred Burgers equation,[8] again suggests the possibility of a new scaling regime with $\nu \neq \frac{1}{2}$, for strong disorder. We have investigated this regime in dimensions $d=3$ and 4 with extensive numerical simulations. Our results support nontrivial scaling (i.e., $\nu \neq \frac{1}{2}$) in these dimensions, and suggest that the exponent $\nu \sim \frac{2}{3}$ may be valid in *all dimensions.*

Because of the anisotropy of directed polymers, transverse and longitudinal directions are treated differently. The $d-1$ transverse directions are labeled by a vector $\mathbf{x}$, while the longitudinal direction is labeled t. Thus a configuration $\{\mathbf{x}(t)\}$ of the directed polymer can also be regarded as the world line of a $(d-1)$-dimensional particle. The path integral

$$W(\mathbf{x},t) = \int_{(\mathbf{0},0)}^{(\mathbf{x},t)} D\mathbf{x}'(t') \exp\left\{ -\int_0^t dt' \left[\frac{\gamma}{2} \left(\frac{d\mathbf{x}'}{dt'} \right)^2 + \mu(\mathbf{x}',t') \right] \right\} \tag{1}$$

represents the overall Boltzmann weight $W(\mathbf{x},t)$ of all directed polymers joining the points $(\mathbf{0},0)$ and $(\mathbf{x},t)$. The contributions to energy arise from a bare line tension γ, and an impurity term $\mu(\mathbf{x},t)$ which fluctuates in space. [We assume $\langle \mu(\mathbf{x},t)\mu(\mathbf{x}',t')\rangle = \sigma^2 \delta(t-t')\delta^{d-1}(\mathbf{x}-\mathbf{x}')$.] Equation (1) implies

$$\partial W/\partial t = [\gamma \nabla^2 + \mu(\mathbf{x},t)] W. \tag{2}$$

Without randomness, $W(\mathbf{x},t)$ behaves asymptotically as $\exp[-ft - x^2/2\gamma t]$, where f is the free energy, or line tension of the polymer, and $\langle x^2 \rangle = \gamma t$ is the expected diffusive behavior in the transverse direction. Similarly, with a quenched distribution of impurities, $W(\mathbf{x},t) \sim \exp[-\langle f \rangle t - g(x/t^\nu)]$, where $\langle f \rangle$ is a quench-averaged line tension, and ν describes the scaling of transverse fluctuations. Note that the important quantities appear in the exponent, and hence the logarithm of W (rather than W itself) has to be averaged. This subtlety is responsible for some of the confusion regarding scaling of polymers with randomness.[1-3]

Equation (2) appears in different disguises in a number of important physical situations. For example, the nonlinear transformation $W(\mathbf{x},t) = \exp[\lambda h(\mathbf{x},t)/2\gamma]$ converts Eq. (2) into

$$\frac{\partial h}{\partial t} = \gamma \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \frac{2\gamma}{\lambda} \mu(\mathbf{x},t), \tag{3}$$

which describes fluctuations of a growing interface, as in ballistic deposition processes.[9] Similarly $\mathbf{v} = \lambda \nabla h$ satisfies

$$\partial \mathbf{v}/\partial t + (\mathbf{v}\cdot\nabla)\mathbf{v} = \gamma \nabla^2 \mathbf{v} - 2\gamma\mu(\mathbf{x},t), \tag{4}$$

which is the Burgers equation for a randomly stirred, vorticity-free ($\nabla \times \mathbf{v} = \mathbf{0}$), fluid.[8] The connection between Eqs. (1) and (4) was first pointed out by Huse, Henley, and Fisher in the context of a 2D random-bond interface.[7] Equation (4) has been analyzed by Foster, Nelson, and Stephen (FNS)[8] using dynamical renormalization-group methods. They find that at the one-loop level the effective coupling constant $g = \sigma^2/\gamma$ ($\sigma^2 = \langle \mu(\mathbf{x},t)^2 \rangle$) obeys the rescaling equation

$$\frac{dg}{dl} = (3-d)g + \frac{K_{d-1}(2d-5)}{d-1} g^2, \tag{5}$$

where $K_d = S_d/(2\pi)^d$.

Equation (5) indicates a critical dimension of $d_c = 3$ in the sense that *weak* disorder is irrelevant for $d > 3$, but relevant for $d < 3$ leading to nontrivial scaling. In $d = 2$, the FNS calculation[8] gives an exponent of $\nu = \frac{2}{3}$. This one-loop result is in fact exact, and has been confirmed by numerical simulations,[4,6,10] and by replica analysis.[5] In the replica[5,10] method n copies of the polymer are generated, which can then be regarded as world lines of n particles in $d-1$ dimensions. The averaging over randomness produces a short-range attractive interaction $V(\mathbf{x}-\mathbf{y}) = \langle \mu(\mathbf{x},t)\mu(\mathbf{y},t)\rangle$ between these particles.

The FNS results[8] can easily be understood from this replica picture. In dimensions $d < 3$ (corresponding to world lines of particles in less than two spatial dimensions), the ground state dominating the large-t behavior is an n-body bound state. In the marginal dimension $d_c = 3$, there is still a bound state for any attractive potential, explaining the marginal *relevance* of g in Eq. (5), and indicating a nontrival scaling exponent ν. However, the bound-state energy in $d_c = 3$ has an essential singularity in g, and cannot be obtained by simple perturbation theory. (This accounts for the observation of $|\mathbf{x}| \sim t^{1/2}$ in a recent perturbation analysis by Bovier, Fröhlich, and Glaus.[10]) In dimensions $d > 3$, although small disorder is irrelevant, Eq. (5) indicates an unstable fixed point at $g^* = (d-3)(d-1)/K_{d-1}(2d-5)$, and a phase transition to new behavior for $g > g^*$. Similarly in the replica picture, although there is no bound state for weak potentials in $d > 3$, a bound state can be formed upon raising the strength of the potential [a finite range is then necessary for the potential $V(\mathbf{x})$]. Having thus established the existence of a new strong-coupling regime (corresponding to replica bound states) in *all dimensions,* we would like to investigate its scaling properties. This is unfortunately beyond perturbative schemes, and other techniques have to be employed.

Here we report *numerical studies* of directed polymers subject to strong disorder. To ensure that simulations are performed in the strong-coupling limit ($g \to \infty$) we consider the polymer problem at zero temperature. This is actually a considerable simplification, since rather than summing over contributions of all polymer configurations to the weight, as in Eq. (1), at zero temperature it is sufficient to examine only one path with lowest energy. We simulate directed polymers on a discrete hypercubic lattice, with random energies $\mu(\mathbf{x},t)$ assigned only to bonds parallel to the t direction. The polymer starts from $\mathbf{x} = \mathbf{0}$ at $t = 0$, and at each successive step moves up by one bond along the t direction. The polymer goes up either directly, or via a transverse jump to one of the neighboring bonds. To simulate the effects of the bare line tension in Eq. (1),[6] transverse jumps are at an energy cost of γ. Of course, the polymer takes advantage of such jumps to optimize its energy gain from the random bonds (taken from a uniform distribution of width w). The total energy after t steps is the sum of the random energies along the polymer length, plus the total cost of transverse jumps. Of the $(2d-1)^t$ possible polymers after t steps, the one with the lowest energy is selected.

This optimization problem can, in fact, be solved in polynomial time in t with use of a transfer-matrix method. The procedure has been described before,[4,6] and will only be outlined here. After t steps the polymer end point is in one of $(2t+1)^{d-1}$ positions. For a given realization of randomness, the energy of the optimal polymer configuration connecting the origin to *all* possible end points is calculated. The optimal paths to the $(2t+3)^{d-1}$ end points at $t+1$ are then calculated recursively by comparing possible evolutions of *all* optimal configurations after t steps. The transfer-matrix method is thus used to evolve the optimal energy landscape exactly, and the configuration of best energy at each t step is easily picked up. Note that this procedure circumvents the problems of metastability usually encountered in Monte Carlo simulations of disordered systems. As a measure of transverse fluctuations, the position of the optimal polymer $x^2(t)$ is recorded after each step. Similarly, to obtain typical energy fluctuations, the energy difference $\Delta E(t)$ between the optimal path and one constrained to terminate at $\mathbf{x} = \mathbf{0}$ is recorded for all t (note that $\Delta E \geq 0$ by construction). To get a meaningful description of the scaling of these fluctuations, we then perform averages over many realizations of randomness.

Such simulations were carried out for polymers in dimensions $d = 2$, 3, and 4 on a Cray XMP computer. For $d = 2$ the numerical results confirm the expected[4-7] scalings $|\mathbf{x}| \sim t^{2/3}$ and $\Delta E(t) \sim t^{1/3}$. The new results, for $d = 3$ and 4 are shown in Fig. 1. A bare "line tension" $\gamma = 0.1$ and random bonds of width $w = 5$ were chosen for these simulations. The results for $d = 3$ are obtained by averaging 400 realizations of polymers of length 1024, while the $d = 4$ results represent averages over 100 realizations of polymers of 512 steps.[11] These results are fitted to scaling forms $\langle |\mathbf{x}| \rangle \sim t^{\nu}$ and $\langle \Delta E \rangle \sim t^{\omega}$. For

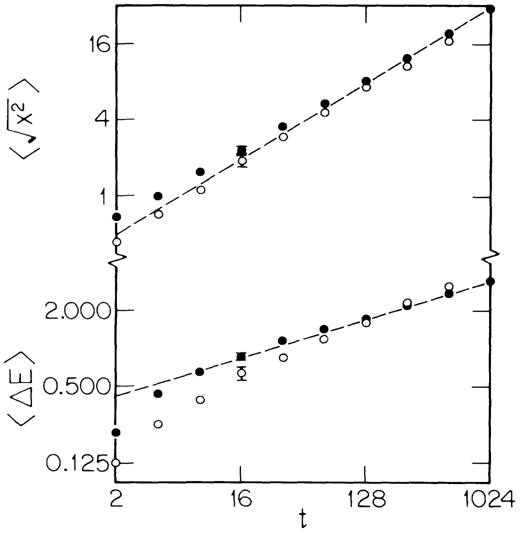

FIG. 1. Averaged energy fluctuations (lower part), and transverse positional fluctuations (upper part), for directed polymers in dimensions $d=3$ (solid circles), and 4 (open circles). Dashed lines of slopes $\frac{1}{3}$ and $\frac{2}{3}$ are drawn as guides to the eye. Representative error bars are depicted at $t=16$.

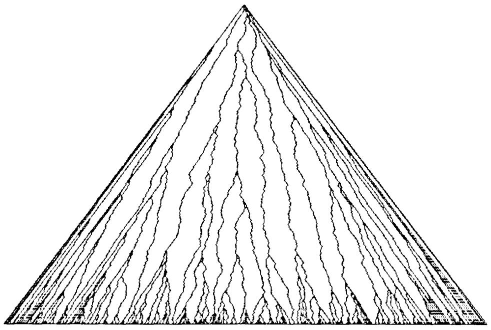

FIG. 2. A collection of polymers of lowest energy directed along the diagonals of a square lattice with random bonds. Each polymer (crossing 500 bonds) has one end fixed to the apex of the triangle, the other to various points on its base, and finds the optimal path in between.

$d=3$ we estimate $\nu=0.62\pm0.04$ and $\omega=0.33\pm0.02$, while for $d=4$, $\nu=0.64\pm0.07$ and $\omega=0.41\pm0.04$. The error bars represent a subjective assessment of the systematic errors, and we in fact believe that in both cases $\nu=\frac{2}{3}$ and $\omega=\frac{1}{3}$ are consistent with the data, and suggest that these exponents may be valid in all dimensions (i.e., superuniversal).

This conjecture is now examined by heuristic arguments. The starting point is a naive generalization of the usual approach to roughening of domain walls in random-field systems,[12-14] and is based on two assumptions: The first is that the polymer free energy can be described by continuum elastic theory.[4] This is fairly sensible at finite temperatures, and implies that the free-energy difference between two polymers whose end points are separated by $|\mathbf{x}|$ scales as x^2/t. Since $\Delta f\sim t^{\omega}$ and $|\mathbf{x}|\sim t^{\nu}$, this assumption leads to the exponent identity $\omega=2\nu-1$. The second assumption argues that since each polymer encounters t different random bonds along its path, typical energy fluctuations between paths scales as $t^{1/2}$ (i.e., $\omega=\frac{1}{2}$).[13] Together, these assumptions lead to $\nu=\frac{3}{4}$ and $\omega=\frac{1}{2}$, which although independent of dimension, are certainly incorrect! Since the continuum elastic identity $\omega=2\nu-1$ is valid in $d=2$,[4] and consistent with the numerical results in higher dimensions, it is the second assumption[13] for $\omega=\frac{1}{2}$ that requires scrutiny.[14]

Indeed, Fig. 2, depicting a collection of optimal paths of 500 steps, suggests the error in this argument. (These paths are actually directed along diagonals of a square, rather than the previously discussed model.) It can be seen that optimal configurations whose end points are separated by a small distance x *do not* cross t distinct bonds, but rather, on average, have a large number of bonds in common. Let z denote the distance along which the two paths are distinct. Figure 2 suggests that for small x, on average, z depends only on x and not on t. Since $z\ll t$, the previous exponent $\omega=\frac{1}{2}$ should be regarded only an an upper bound. The hierarchical (treelike) structure of optimal paths is thus important and needs to be discussed. One possibility is that paths converge as soon as possible, i.e., $\langle z\rangle\sim x$ (z is clearly bounded by x from below by light cone constraints). In this case if we modify the previous argument to $\Delta E\sim z^{1/2}\sim x^{1/2}$, implying $\omega=\nu/2$, then together with $\omega=2\nu-1$ we are led to $\nu=\frac{2}{3}$, and $\omega=\frac{1}{3}$. (This is again independent of dimension, and may justify the superuniversality gleaned from numerical data.) However, the argument is by no means exact, as it relies on the assumption $\Delta E\sim x^{1/2}$ based on $\langle z\rangle\sim x$. An equally valid alternative (suggested by Imbrie[15]) is that the global behavior continues at all scales, namely $z\sim x^{1/\nu}$ and $\Delta E\sim z^{\omega}\sim x^{\omega/\nu}$. This of course provides no explanation for the actual values of ω and ν, but the assumption that optimal paths constrained not to intersect behave as unconstrained paths is the simplest possible one (though not necessarily correct). Unfortunately, the allowed range of x in Fig. 2 is too small for a convincing analysis of the scaling of $\langle z\rangle$, although to the eye the second alternative is suggested. In any case, understanding this tree structure is likely to provide an avenue for a proof (or rebuttal) of the superuniversality conjecture.

In conclusion, we have considered conformations of directed polymers of length t subject to quenched random impurities. Extensive numerical simulations for $d=2$, 3, and 4 suggest that typical transverse fluctuations scale as $t^{2/3}$. Our results, via Eq. (3), also imply a new universality of fluctuations for growing interfaces.[9] Indeed, numerical simulations of growth in 3D observe a crossover towards a nontrivial fixed point, which has so far eluded convincing analysis.[16]

There are still a number of additional interesting unresolved questions: Our simulations were carried out at zero temperature, and although Eq. (5) suggests a finite range of validity for the strong-coupling fixed point, it would be reassuring to obtain similar results numerically at finite temperatures. This is a more formidable numerical task, and our early simulations in three dimensions are inconclusive, and indicate a wide crossover regime. More importantly, as in the replica analysis the shape of the potential for $d > 3$ is important in the formation of bound states, one could worry about universality at the strong-disorder fixed point. It would therefore be useful to do further simulations in $d > 3$ with different types of randomness, and polymer models.

The ensemble of optimal paths in Fig. 2 is highly reminiscent of patterns observed in river basins,[17] highway networks ($d=2$), or blood vessels, and neural connections ($d=3$). The ultrametric tree structure, which is characteristic of many optimization problems,[18] here appears quite naturally (using z as a distance). We thus believe that a complete understanding of this simple model can provide important insight into more complex optimization problems, and also random systems.

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