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Energy landscape for directed polymers

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Abstract. We consider the directed polymer problem in two dimensions on a torus at zero temperature. For each site x we can compute the free energy $e(x)$ of the conformation of the polymer which goes by this site. We analyse the geometrical properties of this free energy landscape $e(x)$ which has the original property of being translationally invariant in terms of the one-point probability density of free energy. In particular, we study the statistical distribution of energies e as a function of the system size, and the spatial correlations parallel and perpendicular to the mean orientation of the polymer. The free energy field is shown to display an anisotropic self-affine structure. The scaling exponents obtained numerically are in good agreement with predicted values.

1. Introduction

The conformation of directed polymers (DP) at zero temperature in a random medium is a problem which has received a lot of attention recently. In particular, the exact solution of the scaling properties of the geometry of the optimal conformation, and of the free energy has been obtained in two dimensions by Kardar, Parisi and Zhang (KPZ) [1]. Since then many variants have been studied and the KPZ now constitutes the paradigm for many different statistical models developed in various contexts.

Among the main applications which have been considered beside polymers in a random medium, let us mention interfaces in random exchange Ising models [2], Ising spin-glasses in the high-temperature limit [3], and statistical growth models such as the Eden model [1, 4, 5]. In the context of transport phenomena, the DP problem is relevant for the non-Newtonian ('Bingham') fluid [6] and foam [7] flow in porous media, and perfect plasticity [8]. Derived from the latter example, extensions to earthquake models [9] and to fracture paths [10] have recently been proposed.

In most applications, only the optimal conformation of the polymers matters so that, for a given medium, a single directed path and a free energy are estimated. However, it is clear that, in a given medium, there is much more information than just the previously mentioned quantities. Zhang has considered the sensitivity to noise [11] of the conformation of the DP, which reveal interesting effects.

In [12], in the discussion of the relation between the DP model and the interfacial growth model described by KPZ, Cates and Ball have shown that the height of the interface at a position r and time t is the negative of the free energy of a polymer of length t with

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one end kept at a fixed position r . This mapping can be done in the continuum [12] using the Cole–Hopf transformation introduced in [1] by directly relating the Langevin equation for the growth to the Burgers' equation which governs the partition function of the polymer, or applied to a discrete model such as the Eden growth model which can be put in correspondence with the DP problem on the same lattice using the notion of waiting times [5].

Using this construction, the well studied geometric properties—and, in particular, the spatial correlations—of growth models governed by the KPZ equation can be used to analyse some spatial correlation in the free energy landscape of a polymer in a given medium.

However, using this mapping, one has to resort to particular boundary conditions, which introduce a bias. A full discussion of this is presented in [12]. We present here a peculiar type of geometry and boundary conditions such that all sites in the lattice are treated on the same footing. The construction we will use is very artificially related to a growth model. However, it is suited to the analysis of spatial correlations, in particular, in the direction along the polymer which cannot be obtained otherwise. For the application of the flow of Bingham fluids in a porous medium, the construction we will introduce is a natural way of determining the set of admissible paths for flow at a given pressure, by thresholding the 'energy' landscape at a value related to the pressure drop imposed.

A simple procedure can be implemented to study the free energy of the minimal directed path with the constraint that the path goes by a fixed point x and with toroidal boundary conditions imposed on the lattice. Using this construction, we derive the map of energies $e(x)$ for all sites x of a given medium. This free energy landscape with these kind of boundary conditions has never been considered before, and the purpose of this article is to report on some of its statistical properties.

2. Energy landscape

We consider a square lattice whose bonds are oriented at $\pm\pi/4$ with respect to the x -axis. Periodic boundary conditions are implemented in both directions along the x -axis and perpendicular to it, so that the topology is that of a torus. The lattice size is $L_x \times L_y$. Each bond i in the network is assigned a random weight w_i . An admissible polymer conformation \mathcal{P} is restricted to directed periodic paths, oriented along the x -axis. To each such path, we compute a free energy

$$E(\mathcal{P}) = \sum_{i \in \mathcal{P}} w_i. \quad (1)$$

The conformation a polymer will adopt at zero temperature is the path which has the lowest energy among all paths \mathcal{P} . Its free energy will be

$$E^* = \min_{\mathcal{P}} E(\mathcal{P}). \quad (2)$$

We will call \mathcal{P}^* the path for which the minimum is reached, $E^* = E(\mathcal{P}^*)$. We can also consider the set of paths \mathcal{P}_x which go through any prescribed site x . The minimum energy over this set is

$$E(x) = \min_{\mathcal{P}_x} E(\mathcal{P}_x). \quad (3)$$

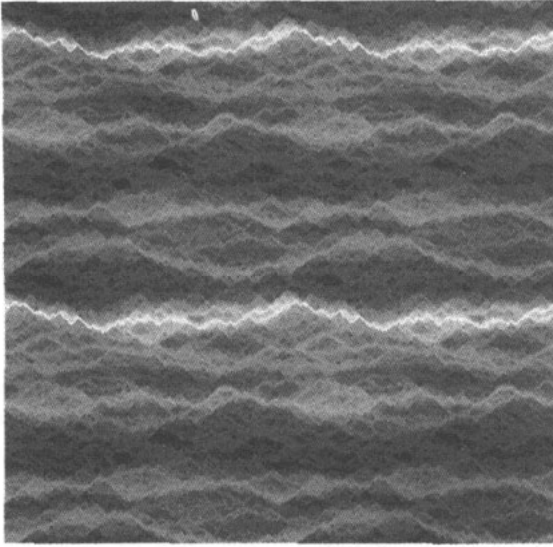


Figure 1. An example of a free energy landscape on a 100×100 lattice. The energy is coded in grey level from the lowest (white) to the highest (black). To illustrate the periodic boundary conditions, two periods are shown in each direction.

We furthermore introduce the energy cost per bond $e(x) = E(x)/L_x$. Since the dominant behaviour of $E(x)$ is a linear increase with L_x , e is expected to be directly comparable between different lattices. The field $e(x)$ is the energy landscape. Figure 1 gives one such example for $L_x = L_y = 100$ with a grey-scale coding for the e from white (lowest energy) to black (highest). Evidently, all sites which belong to \mathcal{P}^* will have an energy $E(x) = E^*$, and thus \mathcal{P}^* appears as a white line on the figure.

The computation of the energy field $e(x)$ does not involve any difficulties. A transfer-matrix approach [6] has been used to compute $E(x)$ starting from each individual site x , and taking account the periodic boundary conditions.

In order to further relate the field e to the KPZ growth model, we note that the value $e(x)$ at a given point corresponds to the height of the interface at the position x after a time L_x , with an initial seed at the point x . Thus to determine the landscape we have to consider $L_x \times L_y$ different seeds with the same noise. The latter problem is rather artificial for the growth problem, but it clearly reveals some additional information in connection with the directed polymer problem.

3. Distribution of energies

In order to characterize the field $e(x)$ we first analyse the one-point distribution function of e . We will study in the next section the pair distribution which will reveal the spatial correlations in the field.

Let us first recall a well known property [1] for the distribution of $e^* = E^*/L_x$. As the system size increases, the average minimal energy per bond will tend to a constant, with, however, non-analytic corrections:

$$e^*(L_x, L_y) = e_\infty^* + AL_x^{-1/\nu_1} + BL_y^{-1/\nu_1} + \text{higher-order terms} \quad (4)$$

where A and B are two constants. In two dimensions, the exponents $\nu_{\parallel} = \frac{3}{2}$ and $\nu_{\perp} = 1$. The asymptotic value e_{∞}^* has been estimated to the value 0.21 in [6]. The standard deviation, σ of e^* vanishes as the system size increases with a similar expression

$$\begin{aligned} \sigma &\propto L_x^{-1/\nu_{\parallel}} && \text{for } L_x \ll L_y^{\nu_{\parallel}/\nu_{\perp}} \\ \sigma &\propto L_y^{-1/\nu_{\perp}} && \text{for } L_x \gg L_y^{\nu_{\parallel}/\nu_{\perp}}. \end{aligned} \quad (5)$$

The difference of scaling in the x - and y -directions comes from the existence of two different correlation lengths, along and perpendicular to the mean orientation of the polymer, with different scaling behaviours.

The statistical distribution of energies for finite-size systems has been studied numerically in [13, 14] using point-like seeds and free end-points. The motivation of these two studies was to check numerically the theoretical predictions by Bouchand and Orland [15] concerning the value of the moments ratio, for the end-point distribution and for the free energy distribution. Although the boundary conditions are quite different from the one we have used, the results presented below are quite comparable.

Let us consider the distribution of energies e in the landscapes obtained for the entire lattice. It is observed that the histogram of e values becomes narrower as the system size increases. Therefore it is expected that most e values will concentrate around the asymptotic value e_{∞}^* when the system size diverges, since the absolute minimum is necessarily contained in the histogram. Due to the difference of scaling in the x - and the y -directions, it is expected that for square geometries, or even for rectangles having a moderate aspect ratio, the extension of the lattice along the x direction L_x will be the most stringent factor which limits the width of the distribution of the absolute minimum energy (the first case in (5)). Thus, extending the results (4) and (5) to the entire lattice, we are led to propose the following scaling form for the distribution $p(e)$ of e :

$$p(e) = L_x^{1/\nu_{\parallel}} \varphi[(e - e_0)L_x^{-1/\nu_{\parallel}}] \quad (6)$$

with $e_0 = e_{\infty}^*$. Moreover, we consider e_0 in the latter equations a free parameter to be fitted from the quality of the data collapse, obtained over various system sizes.

Figure 2 shows the data collapse obtained for $e_0 = 0.230$. We see on the figure that an excellent agreement is found for a set of 12 different system sizes. The estimate of e_0 is slightly larger than the previous estimate of e_{∞}^* . The function φ is shown with a semi-log scale and we see that the distribution can be nicely fitted by a Gaussian. In [13, 14], it was also found that a Gaussian provided a good fit to the distribution of free energy (obtained using different boundary conditions as mentioned above), however, a non-vanishing skewness was measured in qualitative but not quantitative agreement with [15].

In [16], a theoretical study of the statistical distribution of the minimal energy was presented for a simple geometry, namely that of a hierarchical lattice. It was shown, in particular, that the distribution is not Gaussian, and that the tails of the distribution behave as $\exp(-|e - e_{\infty}^*|^{\gamma_{\pm}})$ with two exponents γ_+ and γ_- for e , larger and smaller than e_{∞}^* , respectively. These exponents have been estimated to be $\gamma_+ = 3$ and $\gamma_- = \frac{3}{2}$.

The apparent discrepancy between the latter result and the numerical result reported in figure 2 is, however, to be considered very carefully. Indeed, the two exponents are only apparent for extremely low values of the probability. Dealing with a hierarchical lattice it is possible to have access to probability as small as 10^{-100} , compared with 10^{-4} at most for Monte Carlo simulations on a Euclidian lattice. If we restrict the range of analysis on the

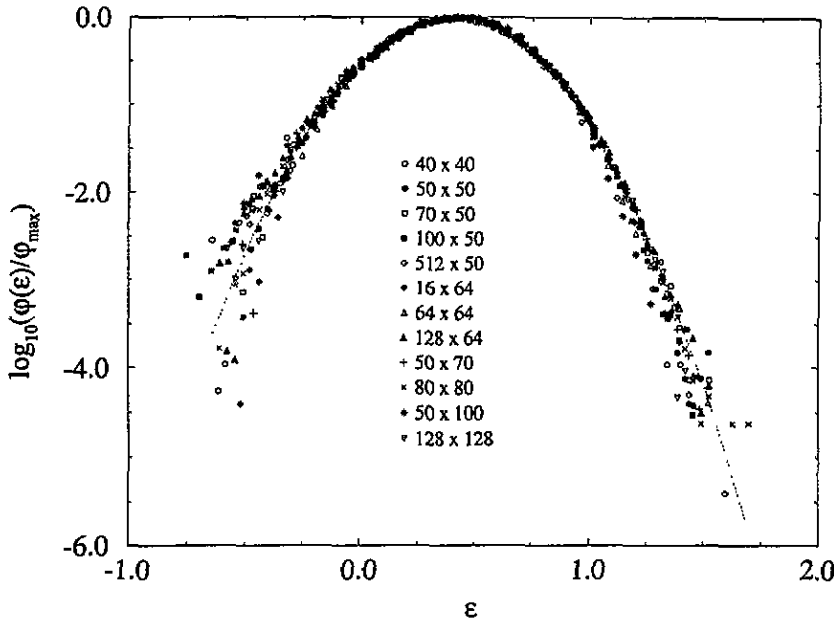


Figure 2. Distribution of energies for various system sizes (indicated in the insert) in rescaled units: $\log(\varphi(\varepsilon)/\varphi_{\max})$ versus $\varepsilon = (e - e_0)L_x^{-1/\nu_1}$ using $e_0 = 0.230$.

hierarchical lattice to a comparable level, then the probability distribution also appears to be well fitted by a Gaussian. Thus, the characterization of the probability distribution done on the hierarchical lattice, although more rigorous, appears to be rather academic, and it is hardly possible to be checked on Euclidian geometries.

4. Spatial correlations

Let us now turn to the study of spatial correlations in the energy landscape. We have seen above that the x - and y -directions have distinct scaling properties. Therefore, we analysed the correlations independently, in those two directions. We computed systematically, for all lines parallel to a given axis, the power spectra of the energy profiles and averaged the results over the different lines and realizations.

The power spectra obtained for various system sizes clearly revealed a power-law behaviour in an intermediate scale range. However, due to the finite size of the system, and the anisotropy of the correlations length, the small wavenumbers showed a saturation which rendered the determination of the scaling exponents unprecise.

In order to clarify this scaling property, we have performed an independent computation in a strip-like geometry, where the length L_x is much greater than the width L_y (the data shown below corresponds to $L_x > 250\,000$ and $L_y = 512$). In this case, we have not computed the full energy landscape, but rather we have obtained the minimal energy to connect any point to the first row. For each line (truncated in pieces of length L_y) and row, we have computed the power spectrum. Along the mean orientation of the polymers, the energy increases linearly with the distance. In order to avoid the effect of such a bias, an end-to-end linear drift is subtracted from each profile along x . (Such a drift would give rise in the power spectrum to a power-law k^{-2} which is trivially that of a periodic sawtooth

signal.) Moreover, transient effects (at small distance from the initial border) are eliminated by keeping the data generated in this early stage out of the averages so that the fluctuations are controlled by the width of the trip only. To this aim the initial part of the strip over a length of the order of 10% of L_x is not taken into account.

For this strip geometry, then the mapping between the DP problem and a KPZ growth model is fully valid including the boundary condition. The power spectrum of the free energy landscape along the y -direction can thus be compared directly to the Fourier transform of the height–height correlation function of the growth model considered in a similar geometry. Along the mean growth x -direction, after having removed the systematic bias due to the dominant linear increase of energy, correlations have not been considered before to our knowledge.

Figures 3(a) and 3(b) show the obtained spectra in log–log coordinates. The dotted lines are a linear regression through the data in the scaling regime (omitting the largest wavenumbers) with slopes equal to 1.9 ± 0.1 and 1.66 ± 0.1 , respectively. Let us introduce the following notations:

$$P(k_x) \propto k_x^{-1-2\zeta_{\parallel}} \quad P(k_y) \propto k_y^{-1-2\zeta_{\perp}} \quad (7)$$

with $\zeta_{\parallel} \approx 0.33$ and $\zeta_{\perp} \approx 0.45$. Thus the energy landscape can be seen as a self-affine surface with different roughness scaling exponents in the x - and y -directions.

We have introduced the roughness exponents so as to render more explicit their physical meaning. For points at a distance d_x along the x -axis the fluctuations of energy scale as $d_x^{\zeta_{\parallel}}$, whereas, if they are oriented along the y -axis, the fluctuations scale as $d_y^{\zeta_{\perp}}$.

We have also complemented this study by the direct analysis of the fluctuations in energy along intervals $y_0 \leq y < y_0 + \Delta$ at fixed x , averaging over y_0 , in the first toroidal geometry introduced in the second section. The fluctuations were analysed using two independent estimates. The first is the RMS fluctuation $\delta E(\Delta) = (\langle E(y)^2 \rangle - \langle E(y) \rangle^2)^{1/2}$, while the second is the difference between the maximum and the minimum value of E over the window. We have obtained a power-law increase $\delta E(\Delta) \propto \Delta^{\zeta_{\perp}}$ with $\zeta_{\perp} \approx 0.45$ and 0.51 for the RMS and the max–min estimates, respectively, as shown in figure 4. The latter computation performed on the toroidal geometry is consistent with the previous power spectrum analysis where the polymer extended only from an initial border to the current site.

We have also analysed the full statistical distribution of energy differences $n(\delta E, d_y)$ for pairs of sites at a varying distance d_y along the y -axis. We have found that the distribution can be considered as constant for small energy differences, with a sharp cut-off above a characteristic δE^* which itself is d_y -dependent. The self-affinity previously identified suggests analysing the distribution in terms of the reduced variable $u = \delta E/d_y^{\zeta_{\perp}}$, so that $n(\delta E, d_y)$ could be re-expressed as

$$n(\delta E, d_y) = d_y^{-\zeta_{\perp}} \psi(u). \quad (8)$$

Figure 5 shows the distribution $u\psi(u)$, i.e. the distribution of $\log(u)$. This plot has been obtained for a width $L_x = 128$, and various values of $d_y = 4, 8, 16, 32, 64$ and 128 . We see that the size effect is correctly accounted for with a choice of $\zeta_{\perp} = 0.45$.

Briefly, the different methods used provided consistent estimates of the two exponents $\zeta_{\perp} \approx 0.45 \pm 0.05$ and $\zeta_{\parallel} \approx 0.33 \pm 0.05$.

Let us now present an argument which allows us to estimate the exponents ζ . Let us consider two points M and M' with the same x -coordinate, and located at a distance d_y apart. The two minimal paths which go through M and M' , respectively, are expected to

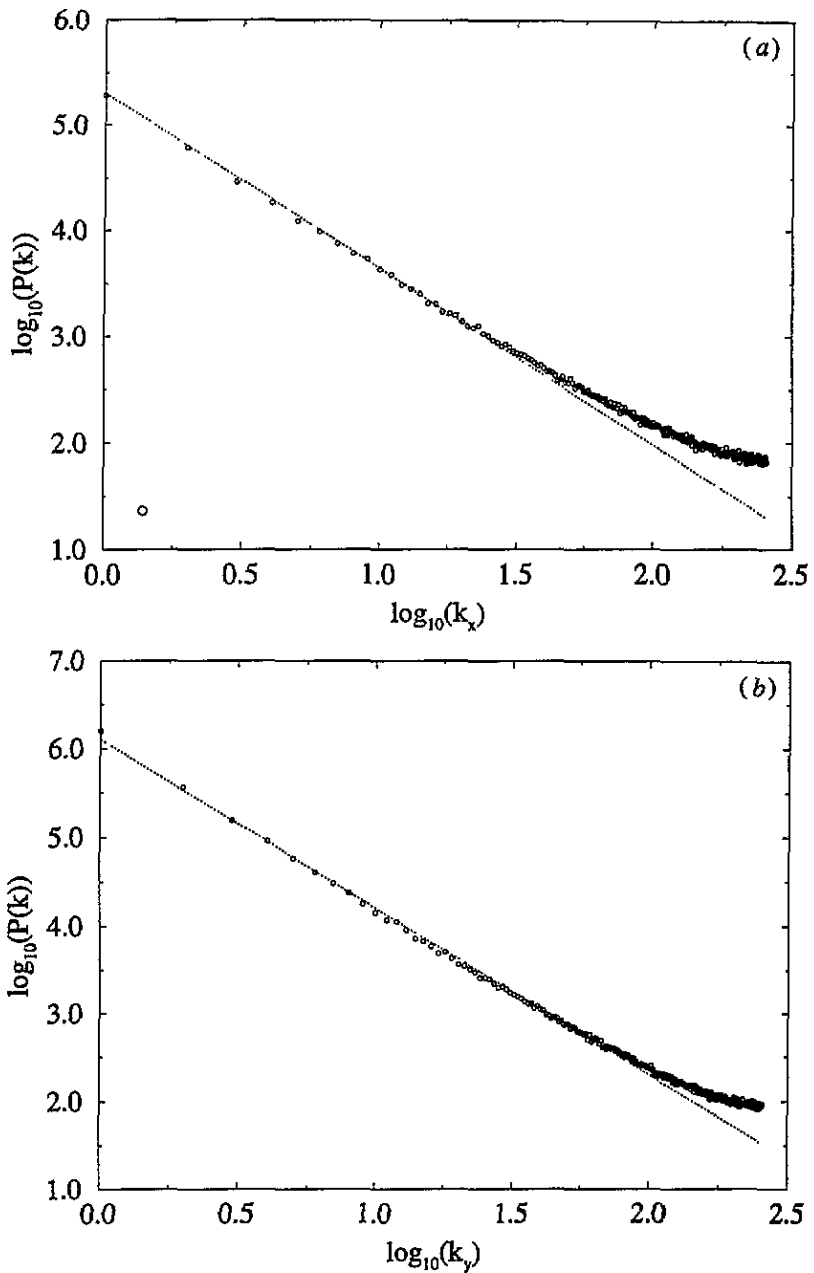


Figure 3. Average power spectrum of energy profiles (a) in the direction of the mean orientation of the polymers and (b) perpendicular to it. The straight lines shown on the graphs are linear regressions through the data with slopes 1.66 and 1.9, respectively. The lattice size is $250\,000 \times 512$.

merge after some distance d_x provided the length of the lattice L_x is large enough compared to d_y . The distance d_x should scale as $d_y^{v_{\parallel}/v_{\perp}}$. The difference in energy $E(M) - E(M')$ is only due to the fraction of the paths which are not in common, i.e. over a distance d_x .

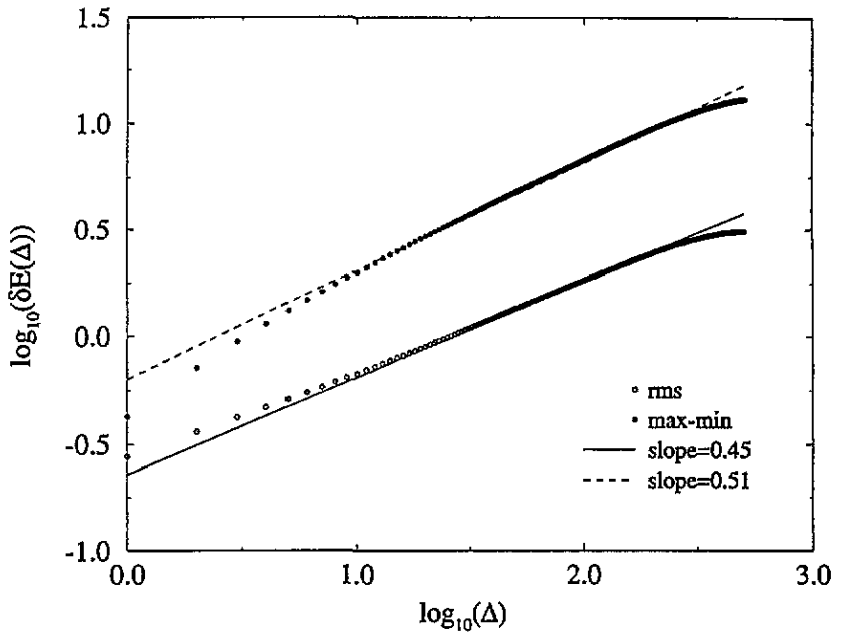


Figure 4. Fluctuation of energy δE along intervals of size Δ along the y -axis using two estimates, the RMS deviation of energy (symbol \circ) over the window, and the difference between the maximum and the minimum energy (symbol \bullet).

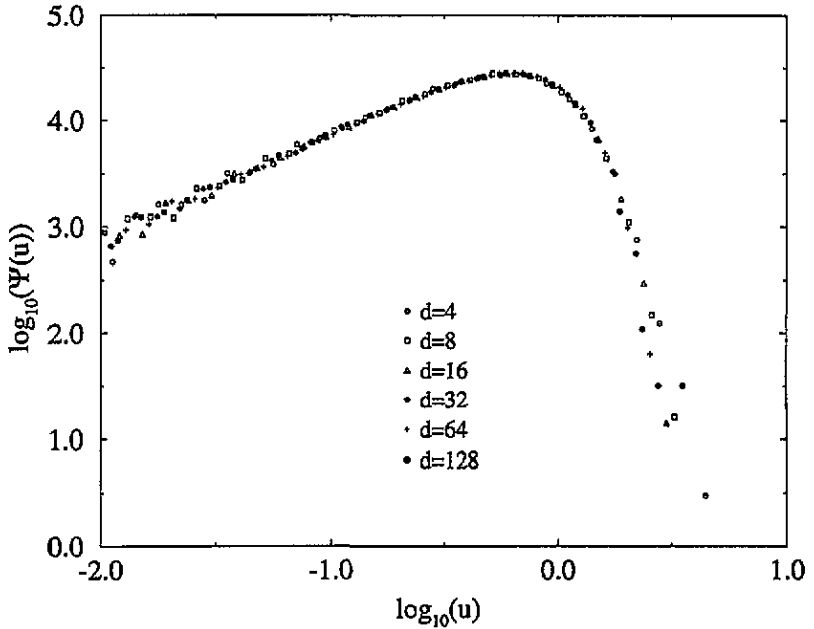


Figure 5. Rescaled distribution $\Psi(u)$ of the logarithm of energy difference δE between two points located at a distance d along the y -axis. The rescaled energy difference is $u = \delta E/d^{\zeta_{\perp}}$. The exponent ζ_{\perp} used in this graph is 0.45.

If we consider that when the paths are not joined they are statistically independent, we may use the above-stated result (5) which gives the scaling of the fluctuations in energy as $|E(M) - E(M')| \sim d_x^{1-1/\nu_{\parallel}}$. Inserting the expression of d_y in the latter expression gives a power-law increase of the fluctuations in energy with the distance d_y with an exponent

$$\zeta_{\perp} = \frac{\nu_{\parallel} - 1}{\nu_{\perp}}. \quad (9)$$

Numerically, in two dimensions, the latter expression amounts to $\zeta_{\perp} = \frac{1}{2}$.

Alternatively, one may have expected ζ_{\perp} to be given directly by the self-affine roughness exponent of the height profile in the KPZ growth model which is known [1] to be $\frac{1}{2}$. This exponent is the one which is measured in the strip-like geometry. In the toroidal geometry, it is not obvious that the same exponent holds. However, from the comparison between the two kinds of boundary conditions, it seems that these exponents are identical.

For the longitudinal correlation, it is not possible to resort to known results in the growth model. In order to estimate ζ_{\parallel} we use the self-affinity of the minimal paths in the x - y plane. Each such path is statistically invariant under the following transformation: $x \rightarrow \lambda^{\nu_{\parallel}}x$ and $y \rightarrow \lambda^{\nu_{\perp}}y$ for any λ . Therefore, we expect that the entire energy landscape obeys such an invariance. This implies that the energy fluctuation scaling exponents along both directions should be related through

$$\nu_{\parallel}\zeta_{\parallel} = \nu_{\perp}\zeta_{\perp}. \quad (10)$$

Combining this relation with (9), we obtain

$$\zeta_{\parallel} = \frac{\nu_{\parallel} - 1}{\nu_{\parallel}} \quad (11)$$

or in two dimensions, $\zeta_{\parallel} = \frac{1}{3}$. The latter value has not been considered previously to our knowledge. These two expressions (9) and (11) are in good agreement with the numerically determined values.

5. Conclusion

We have studied the free energy landscape of directed polymers in a random medium using a particular type of toroidal boundary conditions which gives a translational invariance for the average free energy. The one-point distribution of energy has been shown to be described by a scaling form which accounts for the size effects. The latter result is consistent with other numerical studies [13, 14] performed using standard boundary conditions. The two-point correlation functions parallel and perpendicular to the mean orientation of the polymers have been analysed numerically using different tools, and the resulting self-affine character of the energy distribution has been accounted for in a quantitative way by a simple scaling argument. The transverse correlations found in the free energy map are consistent with results known for the KPZ growth model which can be mapped onto the DP model with boundary conditions different from the one we introduced. The longitudinal correlations reported above have not been considered before to our knowledge.

Such a statistical description of the energy field may shed some light on problems related to the directed polymer model, in particular away from criticality, i.e. when a certain tolerance is allowed on the free energy of the polymer (i.e. not simply considering the lowest-energy configuration), or models such as the one introduced in [9], for non-zero values of the 'stress-drop' parameter which brings the system away from the zero-temperature directed-polymer problem.

Acknowledgments

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