

Optimal path in two and three dimensions

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We apply the Dijkstra algorithm to generate optimal paths between two given sites on a lattice representing a disordered energy landscape. We study the geometrical and energetic scaling properties of the optimal path where the energies are taken from a uniform distribution. Our numerical results for both two and three dimensions suggest that the optimal path for random uniformly distributed energies is in the same universality class as the directed polymers. We present physical realizations of polymers in a disordered energy landscape for which this result is relevant. [S1063-651X(98)08212-9]

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Recently, there has been much interest in the problem of finding the optimal path in a disordered energy landscape. The optimal path can be defined as follows. Consider a d -dimensional lattice, where each bond is assigned with a random energy value taken from a given distribution. The optimal path between two sites is defined as the path on which the sum of the energies is minimal. This problem is of relevance to various fields, such as spin glasses [1], protein folding [2], paper rupture [3], and the traveling salesman problem [4]. Though much effort has been devoted to studying this problem, a general solution is still lacking. There exist two approaches developed recently to study this problem. Cieplak *et al.* [5] applied the max-flow algorithm for a two-dimensional energy landscape. Another approach is to restrict the path to be directed, that is, the path cannot turn backwards. This approach is the directed polymer problem which has been extensively studied in the past years; see, e.g., Refs. [6–8].

In this paper we adapt the *Dijkstra algorithm* from graph theory [9] for generating the optimal path on a lattice with randomly distributed positive energies assigned to the bonds. This algorithm enables us to generate the optimal path between any two sites on the lattice, not restricted to directed paths. We study the geometrical and energetic properties of the optimal paths in $d=2$ and 3 dimensions in a random uniform distribution of energies. We calculate the scaling exponents for the width and the energy fluctuations of the optimal path. We find that for both $d=2$ and 3 the exponents are very close to those of directed polymers, suggesting that the nondirected optimal path (NDOP) is in the same universality class as the directed polymer (DP). Our results are in agreement with those found by Cieplak *et al.* [5] for the two-dimensional case. This result indicates that, in the case of uniformly distributed energies, NDOP's are self-affine, and overhangs do not play an important role in the geometry of NDOP's.

Our results are relevant, for example, in the following polymer realizations: (i) Consider a d -dimensional energy landscape in which there is a spherical regime of randomly distributed high energies, while outside this sphere the energies are zero or have very low values. Consider as well a polymer of length N , one of whose ends is attached to the

center of the sphere while the other is free. The radius of the sphere is $r \ll N$ [see Fig. 1(a)]. The section of the polymer inside the sphere will reach the lowest energy path, which is the optimal path studied here, i.e., with a self-affine structure. (ii) Consider a polymer in a d -dimensional energy landscape which is divided into alternating strips of disordered low and high energies [see Fig 1(b)]. In the strips of high energies the polymer is expected to behave like the optimal path.

The Dijkstra algorithm enables one to find the optimal path from a given source site to each site on a d -dimensional lattice. During the execution of the algorithm, each site on the lattice belongs to one of three sets (see Fig. 2): (i) The first set includes sites for which their optimal path to the source site has already been found. (ii) The second set includes sites that are relaxed at least once, but their optimal path to the source has not yet been determined. This set is the perimeter of the first set. (iii) The third set includes all sites on the lattice which have not been visited yet.

The algorithm itself consists of two parts, initialization and the main loop. The main loop, in its turn, is composed of the search and the relaxation processes.

In the initialization part we prepare the lattice in the following way. Each bond is assigned with a random energy value taken from a given distribution. Each site is assigned an energy value of infinity. We pick up a certain source site

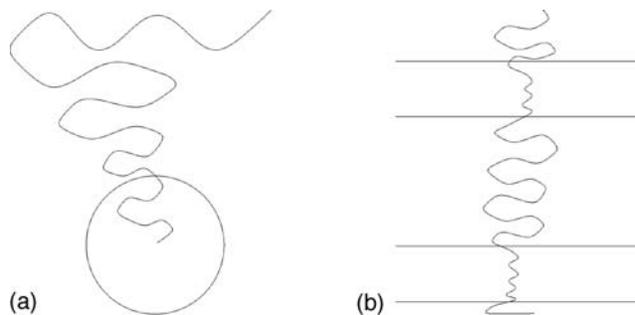


FIG. 1. Schematic illustrations of sections of a polymer having the structure of an optimal path. (a) Within the circle, energies are distributed. Outside the circle, zero or very low energies are distributed. (b) Alternating strips of high and low distributed energies.

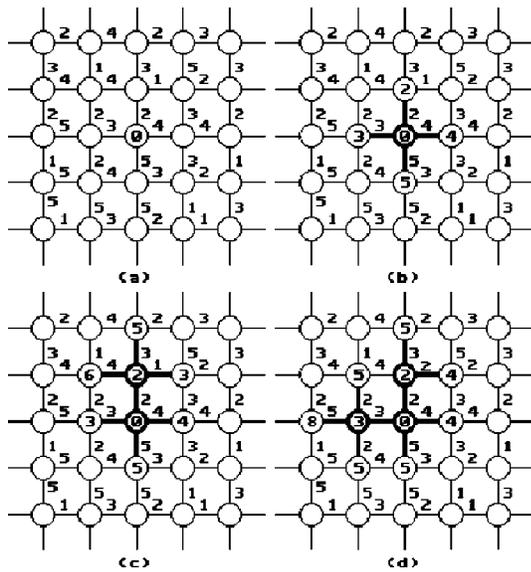


FIG. 2. Illustration of the first four steps of the Dijkstra algorithm applied to a square lattice. Numbers along the bonds represent the random energy assigned to them. Numbers inside circles represent the energies of sites, i.e., the total energy of the path connecting this site to the source. Empty sites possess infinite energy and belong to the third set, thick circles belong to the first set, and all other circles belong to the second set. Note, e.g., that the site marked 6 in (c) was relaxed one more time and became 5 in (d). During this second relaxation we broke its previous connection to the site with energy 2, and connected it to the site with energy 3. At each time step we identify the optimal path from each site in the first set to the source by going along the thick bonds.

and assign it an energy value of zero and insert it into the second set.

After that we enter the main loop. We perform the search among the sites from the second set, and find the one with the minimal energy value. Then we add it to the first set and proceed to the relaxation process. This site is called the *added* site. The relaxation process deals with sites neighboring the added site that do not belong to the first set.

In the relaxation process we compare two values: the energy value of the neighboring site and the sum of two values—the energy value of the added site and the energy value of the bond between these sites. If the value of the sum is smaller, then (a) we assign it to the neighboring site; (b) we connect the neighboring and the added site by a path (thick bond in Fig. 2); (c) if the neighboring site belongs to the second set, we break its previous connection to another site (thick bond); and (d) if the neighboring site does not belong to the second set, we insert it into the second set. The first four steps are demonstrated in Fig. 2. Normally, the main loop stops when the second set is empty; however, one might wish to break the loop earlier, e.g., at the moment when the first set reaches the edge of the lattice in order to avoid boundary effects.

Each site that belongs to the first set is connected to the source by a permanent path (thick bonds) that does not change during the execution of the algorithm; so, if we stop the algorithm at any given time, the first set will still be valid.

We simulate both DP's and NDOP's on a square lattice in

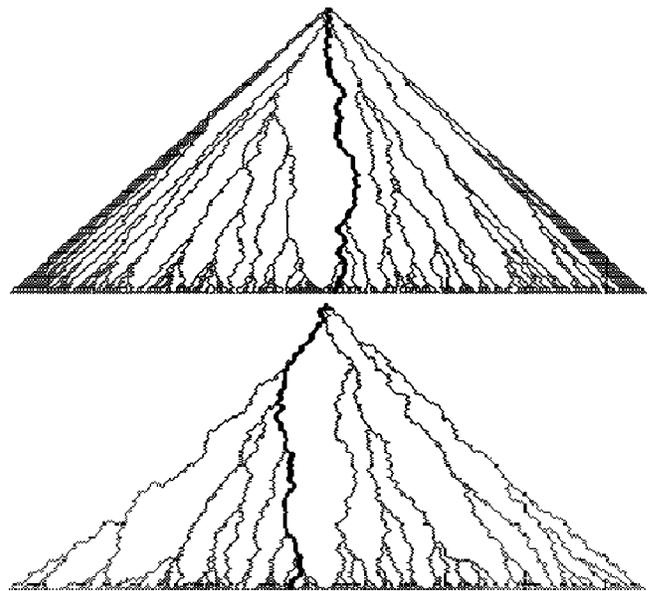


FIG. 3. The sets of all directed (the upper one) and nondirected (the lower one) optimal paths with $t=300$ obtained for the same realization of quenched randomness in the lattice. The global optimal path, which is the minimal energy path among all the paths with the same t , is shown by a thick line. In this particular case the directed and nondirected global optimal paths do not overlap. In other cases they might overlap significantly, though the rest of tree looks somewhat different.

the following way. Let x and y be the horizontal and vertical axes. We choose the origin to be the source site, and study the optimal paths connecting it with all the sites on the line between $[0,t]$ and $[t,0]$ for different values of t . The generalization to three dimensions is straightforward. The random energies assigned to bonds are taken from a uniform distribution. We find that our results are independent of the distribution interval.

In Fig. 3 we compare a configuration of DP and NDOP on the same disordered energy landscape. It is seen that in the NDOP only very few overhangs exist. To test the effect of the overhangs we calculate the mean end-to-end distance R of the global optimal path (thick line in Fig. 3) as a function of its length l . The global optimal path is the minimal energy path among all the paths with the same value of t . Our numerical results clearly indicate the asymptotic relation $l \sim R$, showing that the NDOP's are self-affine [7]. We should compare this result to the strong disorder limit, where

TABLE I. Width and energy fluctuation exponents of DP and NDOP in two and three dimensions. The exponents were derived from the slopes of the corresponding data points shown in Fig. 4. The error bar was estimated from taking ten ensembles of 10^4 configurations each for $d=3$, and 500 configurations each for $d=2$.

	$d=2$		$d=3$	
	DP	NDOP	DP	NDOP
ξ	0.66 ± 0.02	0.67 ± 0.02	0.60 ± 0.05	0.63 ± 0.05
ζ	0.32 ± 0.02	0.32 ± 0.02	0.19 ± 0.07	0.18 ± 0.07

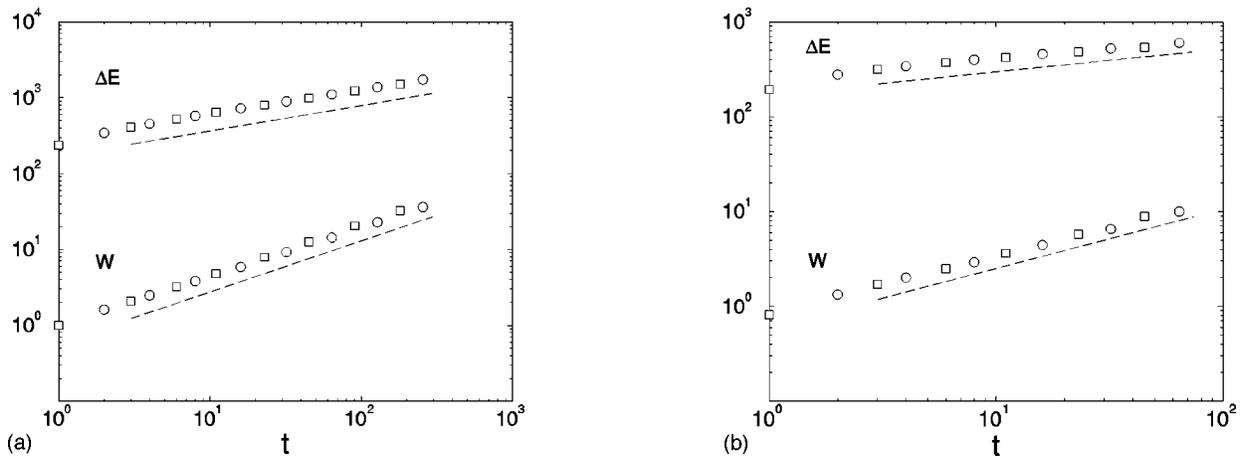


FIG. 4. The width and energy fluctuation as a function of t on a double logarithmic plot in (a) two and (b) three dimensions. Circles are used for directed polymers, and squares for nondirected optimal paths. For (a) 10^5 systems of linear size up to $t=300$ are used, and for (b) 5000 systems of linear size up to $t=75$. The dashed lines are given as a guide to the eye, and have slopes equal to the exponents known for DP: $\xi = \frac{2}{3}$ and $\zeta = \frac{1}{3}$ for $d=2$ and $\xi \approx 0.62$ and $\zeta \approx 0.24$ for $d=3$ [6]. For all cases we used a uniform distribution of energies between $E_1 = 1$ and $E_2 = 1000$. We also tested other energy intervals and found the same results.

the paths can be regarded as self-similar fractals, with $\mathcal{L} \sim R^{d_{\text{opt}}}$, where $d_{\text{opt}} \approx 1.22$ in $d=2$ and $d_{\text{opt}} \approx 1.42$ in $d=3$ [10,11].

In order to compare NDOP to DP we study several properties, such as the roughness exponent ξ , the energy fluctuation exponent ζ for two and three dimensions of DP and NDOP. The above exponents are defined by the relations $W \equiv \langle h^2 \rangle^{1/2} \sim t^\xi$ and $\Delta E \equiv \langle (E - \langle E \rangle)^2 \rangle^{1/2} \sim t^\zeta$. Here h is the transverse fluctuation of the global optimal path, which is the distance between its end point and the line $x=y$; E is the energy of the global optimal path which is the sum of all bond energies along the path. The average is taken over different realizations of randomness. Figure 4 shows the dependence of the width W and energy fluctuation ΔE of the DP and NDOP on t in two and three dimensions. The points are the data for both DP and NDOP, and the dashed lines repre-

sent the exponents of the DP. Our results indicate that the exponents for the NDOP are very close to those of DP (see also Table I).

Our results may be related to recent findings [12] that the roughness exponent of the minimal energy of the domain wall in the random Ising model and fracture interface are the same [3] in $d=2$. In these cases, similar to our case, although overhangs may occur, they do not play an important role.

In summary, our results suggest that the optimal path in the case of uniformly distributed energies, for any energy interval, is in a different universality class from the strong disorder limit, but in the same universality class as directed polymers. This result is relevant to several questions regarding the equilibrium state of polymers in different realizations of a disordered energy landscape.

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