

Stretching of a fractal polymer around a disc reveals KPZ-like statistics

Kirill E. Polovnikov¹, Sergei K. Nechaev^{2,3}, Alexander Y. Grosberg⁴

¹*Skolkovo Institute of Science and Technology, 121205 Moscow, Russia*

²*Interdisciplinary Scientific Center Poncelet (CNRS IRL 2615), 119002 Moscow, Russia*

³*P.N. Lebedev Physical Institute RAS, 119991 Moscow, Russia*

⁴*Department of Physics and Center for Soft Matter Research,
New York University, 726 Broadway, NY 10003, New York, USA*

While stretching of a polymer along a flat surface is hardly different from the classical Pincus problem of pulling chain ends in free space, the role of curved geometry in conformational statistics of the stretched chain is an exciting open question. Here by means of the scaling analyses and computer simulations we examine stretching of a fractal polymer chain around a disc in 2D (or a cylinder in 3D) of radius R . Surprisingly, we reveal that the typical excursions of the polymer away from the surface scale as $\Delta \sim R^\beta$, with the Kardar-Parisi-Zhang (KPZ) growth exponent $\beta = 1/3$, for *any* fractal dimension of the chain. Moreover, we find that the curvature-induced correlation length of a fractal chain behaves as $S^* \sim R^{1/z}$ with the KPZ dynamic exponent $z = 3/2$, suggesting that the crossover from flat to curved geometry of a stretched polymer corresponds to the crossover from large to short time scales in the KPZ stochastic growth. Thus, we argue that curvature of an underlying boundary furnishes universal KPZ-like statistics to the stretched fractal paths, which further suggests numerous connections with several branches of mathematical physics.

I. INTRODUCTION

The phenomenon of stretching a polymer chain by pulling on its ends is a standard subject in polymer physics, with important applications in cell biology; as a recent example see, e.g., [1] about chromatin stretching by optical tweezers. By analogy with macroscopic examples (e.g., mooring line around a bollard), here we examine another efficient way to stretch a polymer, when it is tight around a curved obstacle. As a model, it is prototypical for several biological contexts. As just one example, we mention the recently documented (via imaging [2, 3] and Hi-C experiments [4]) chromosomes morphology in a certain algae (dinoflagellates) that form cylindrical rods with helically twisted bundles of wrapped DNA. In addition, the model turns out to have surprisingly rich connections with several other fields of theoretical physics, first and foremost with KPZ statistics.

Winding of a Gaussian polymer around a topological point-like obstacle in 2D is also a classical problem in polymer physics, pioneered by S.F. Edwards [5], Prager and Frisch [6] and Saito and Chen [7]. For a finite size obstacle in 2D (or a cylinder in 3D), Green's function of a Gaussian polymer was considered by Comtet et al in [8] and later formally expressed in terms of an infinite series of linear combinations of Bessel functions [9]. Although the latter result is exact, addressing the limit of strongly stretched chain based on this expression remains a steep challenge. A significant progress in this direction was recently achieved by B.Meerson and N.Smith [10, 11], some related problems were also examined by some of us [12–14].

The model that we address in this paper is depicted in Fig. 1, with panels (a,b) and (c) showing polymer chain stretched along a flat and curved boundary, respectively. We will be interested in the span of fluctuations

of the polymer away from the boundary, characterized by the length scale Δ . Specifically, following a note by one of us [15], we argue that Δ in the curved boundary case is determined by the non-local competition between entropy loss when polymer is tightly confined in a narrow strip of width Δ along the surface, and entropy loss of its stretching beyond imposed necessity by making a wider detour around the obstacle. Our analysis reveals the universal scaling, $\Delta \sim R^\beta$, as a function of R with the KPZ growth exponent $\beta = 1/3$, while the correlation length S^* at which the chain experiences curvature of the disk scales as $S^* \sim R^{1/z}$ with the KPZ dynamic exponent $z = 3/2$. Simulations of this system reveal that the one-point distribution of typical fluctuations can be well described by the squared Airy law, connecting our polymer problem in 2D with the (1+1)D Ferrari-Spohn universality class [10, 16].

Strikingly, we found that this KPZ-like behavior is valid not only for a Gaussian polymer (which is like a regular random walk), but for a polymer with an arbitrary fractal dimension $D_f = 1/\nu$, where ν is the usual metric exponent of the mean-square end-to-end distance against the number of monomers $\langle R^2 \rangle \sim b^2 N^{2\nu}$, where b is the (Kuhn) monomer length scale. The examples, in addition to the usual Gaussian $\nu = 1/2$, include self-avoiding polymers in 2D, $\nu = 3/4$ [17], in 3D (if the ring is wound around a cylinder), $\nu \approx 0.588$ [18]; annealed branched polymers, $\nu = 1/4$ [19] without or $\nu \approx 7/13$ with excluded volume [20]; one ring in a 3D melt of other unconcatenated rings, $\nu = 1/3$ [21, 22]; polymers with quadratic non-local Hamiltonian producing subdiffusive fractal paths with arbitrary $\nu \leq 1/2$ [23, 24].

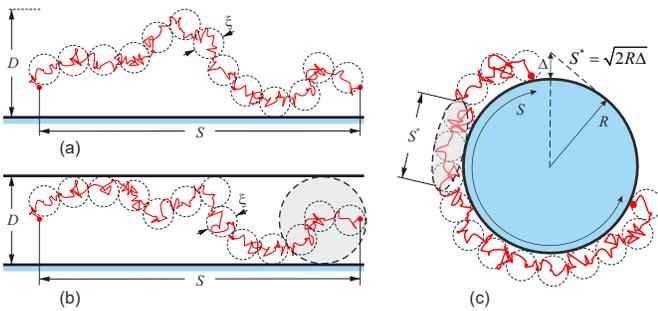


Figure 1. Stretching of a polymer chain in a flat (left) or curved (right) geometry. In each case, chain is represented as a train of Pincus blobs. (a): the polymer is stretched above a planar boundary and fluctuates at distance D in the perpendicular direction; (b): the polymer is additionally confined within distance $\Delta \ll D$ above the surface, and Pincus blobs are combined as “super-blobs” (grey ball). (c): the polymer is stretched around a circular boundary of radius R . End-to-end distance along the surface in all cases is fixed, $S \gg bN^\nu$.

II. PATH STRETCHING IN EMPTY SPACE OR ALONG A FLAT BOUNDARY

As a worm-up and for future reference, consider a chain of $M \gg 1$ monomers with the fractal dimension $D_f = 1/\nu$ and let it be stretched along a flat boundary, with end-to-end distance fixed at $S \gg bM^\nu$. As shown in Fig. 1(a), the chain looks like a train of blobs of size g each. Chain statistics is unaffected inside the blob, i.e. $\xi = bg^\nu$, and the train of blobs is stretched, meaning that $S = \frac{M}{g}\xi$. Simple algebra then gives $g = (Mb/S)^{1/(1-\nu)}$ and $\xi = b(Mb/S)^{\nu/(1-\nu)}$. These blobs generalize the classical “Pincus blobs” [25] for arbitrary ν , except our problem is not formulated in terms of stretching force, but in terms of fixed end-to-end distance, $S \gg bM^\nu$.

Free energy of chain stretching, F_{str} , is about $k_B T$ per blob:

$$\frac{F_{\text{str}}}{k_B T} \sim \frac{M}{g} = \left(\frac{S}{bM^\nu} \right)^{\frac{1}{1-\nu}}. \quad (1)$$

The statistics of chain of blobs in the direction perpendicular to the surface is Gaussian (compare, e.g., with the similar conclusion for self-avoiding polymers in [26, Equation 1.50]), its spread is, therefore,

$$D = \left(\frac{M}{g} \right)^{1/2} \xi = bM^\nu \left(\frac{bM^\nu}{S} \right)^{\frac{2\nu-1}{2(1-\nu)}}. \quad (2)$$

If a chain is additionally confined within a layer of width $\Delta \ll D$ as depicted in Fig. 1(b), then, considering “super-blobs” of G Pincus blobs each (see Fig. 1(b)), such that $\xi G^{1/2} = \Delta$, we can find the confinement free energy as $k_B T$ per super-blob:

$$\frac{F_{\text{conf}}}{k_B T} = \frac{M}{gG} = \frac{b^2 M^{2\nu}}{\Delta^2} \left(\frac{bM^\nu}{S} \right)^{\frac{2\nu-1}{1-\nu}} \quad (3)$$

An interesting observation is that size D perpendicular to stretching (see (2)) is a *decreasing* function of elongation S only for $\nu > 1/2$, while for $\nu < 1/2$ it is an *increasing* function. In other words, the “subdiffusive” polymers with $\nu < 1/2$ behave as a substances with a negative Poisson ratio: upon stretching they swell in perpendicular direction. Clearly, this is because fractal polymers with $\nu < 1/2$ have some negative correlations between monomers. These correlations are destroyed by stretching which leads to chain’s “releasing”.

III. PATH STRETCHING ALONG A CURVED SURFACE: FREE ENERGY AND ELLIPTIC BLOBS

Let us keep ends of a chain of N monomers at distance S away along a surface of a cylinder of radius R – see Fig. 1(c). We assume the chain is stretched, i.e. $S \gg aN^\nu$, however we do not impose any relation between S and R . Clearly, $S > 2\pi R$ means wrapping around the cylinder. Free energy of such a chain consists of two contributions. The first one describes chain stretching to the distance $\frac{S}{2\pi R}(R + \Delta)$; the corresponding free energy is given by (1), by replacing $M \rightarrow N$ and $S \rightarrow S(1 + \Delta/R)$. The second term corresponds the polymer confining in a strip of the width Δ , and it is given by (3), with similar replacement $M \rightarrow N$. Overall, variational free energy becomes

$$\frac{F_{\text{circ}}}{k_B T} \propto \left(\frac{S}{bN^\nu} \frac{R + \Delta}{R} \right)^{\frac{1}{1-\nu}} + \frac{b^2 N^{2\nu}}{\Delta^2} \left(\frac{bN^\nu}{S} \right)^{\frac{2\nu-1}{1-\nu}} \quad (4)$$

This free energy is the extension of Eq. (2) in the Comment [15]. Assuming $\Delta \ll R$, we can linearize the first term and then minimize this free energy to get

$$\frac{\Delta}{bN^\nu} = \left(\frac{R}{bN^\nu} \right)^{\frac{1}{3}} \left(\frac{bN^\nu}{S} \right)^{\frac{2\nu}{3(1-\nu)}} \quad (5)$$

It is instructive to re-derive (5) in a different way. Given the chain is localized in a strip of width Δ , curvature of the underlying surface becomes relevant only at scales exceeding $S^* = (R\Delta)^{1/2}$ (see Fig. 1(c)). We call chain section covering distance S^* “an elliptic blob”. To find the number of monomers in elliptic blob, N^* , we can use the result (2), with the replacement $D \rightarrow \Delta$ and $S \rightarrow S^*$. The train of elliptic blobs is fully stretched around the curved boundary, hence their number is $N/N^* \sim S/S^*$. A few lines of algebra based on this relation yield the previously obtained answer (5). Simultaneously, we get the expressions for cross-over scale S^* at the given R :

$$S^*/bN^\nu = (R/bN^\nu)^{\frac{2(1-\nu)}{3-2\nu}}. \quad (6)$$

Our results (2) for effectively flat surface at $S < S^*$ and (5) for the curved one at $S > S^*$ are collected in Fig.

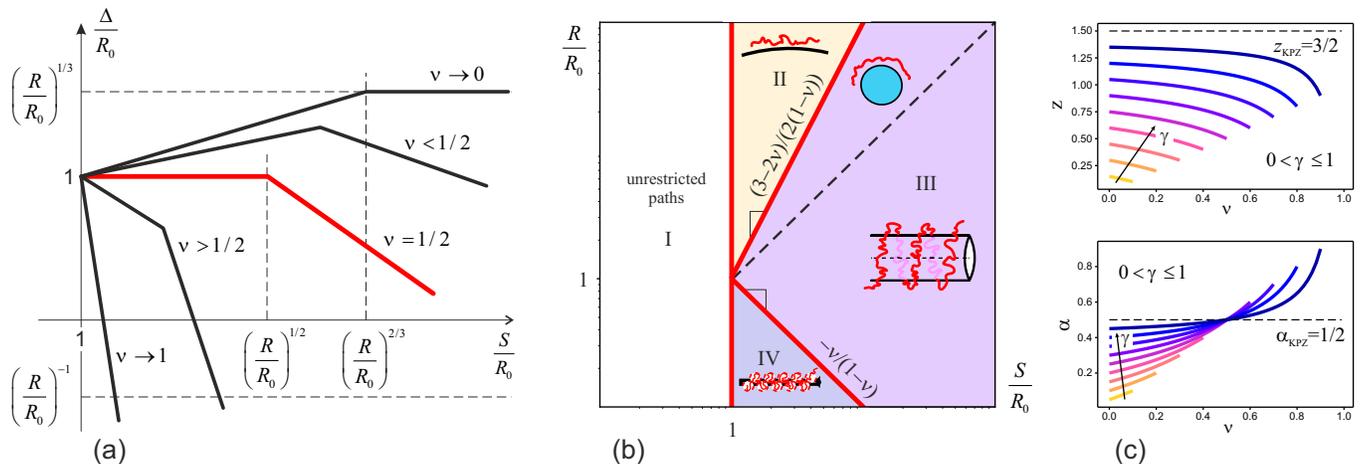


Figure 2. (a): Polymer chain spread, Δ , away from a cylindrical surface as a function of curvilinear distance between chain ends S , for a variety of ν values (or fractal dimensions $D_f = 1/\nu$). All distances measured relative to the unperturbed coil size $R_0 = bN^\nu$. (b): Four regimes of fluctuations for various values of disc radius R and end-to-end distance S . Regime II corresponds to effectively flat barrier, while regime IV is for an obstacle thinner than one Pincus blob. The most interesting is regime III, it corresponds to the stretched polymer on the essentially curved barrier. The dashed line highlights winding around the cylinder. (c): Exponents z (upper) and α (bottom) as the functions of $\nu < \gamma$ for different values of γ . The increase of γ from $\gamma = 0.1$ (yellow) to $\gamma = 0.9$ (dark blue) is shown by arrows on both diagrams. Limiting KPZ values corresponding to $\gamma = 1$ are marked by black dashed lines.

2(a). There, we plot Δ/bN^ν as a function of stretching $S/bN^\nu > 1$ for a variety of ν values, $\nu \in (0, 1)$. In particular, at $\nu < 1/2$, the behavior $\Delta(S)$ is non-monotonic: Δ increases at modest S , because stretching destroys negative correlations, while at larger S the curvature of the underlying disc takes over and forces Δ to decrease again. Thus, for "subdiffusive" paths the negative Poisson ratio flips its sign to the positive at stretching S^* when the boundary becomes substantially curved. A curious fact is that at the specific value $\nu = 1/3$ (which corresponds to a sort of a crumpled statistics) the non-monotonous dependence $\Delta(S)$ comes back to the starting value $\Delta/bN^\nu \sim 1$ exactly when S becomes of the order of disc radius, R , i.e. when chain is forced to make about one full turn around the disc.

Another way to summarize our results is given in the Fig. 2(b) in terms of four distinct regimes in the space of two dimensionless control parameters, namely, the amount of stretching S and radius of the disc R , both scaled by the unperturbed coil size, S/bN^ν and R/bN^ν :

$$\frac{\Delta}{bN^\nu} = \begin{cases} 1, & \text{Regime I} \\ (S/bN^\nu)^{-\frac{2\nu-1}{2(1-\nu)}}, & \text{Regime II} \\ (R/bN^\nu)^{\frac{1}{3}} (S/bN^\nu)^{-\frac{2\nu}{3(1-\nu)}}, & \text{Regime III} \\ (S/bN^\nu)^{-\frac{\nu}{1-\nu}}, & \text{Regime IV} \end{cases} \quad (7)$$

The first regime (I) deals with the free unrestricted polymers with $S < bN^\nu$; for them, fixation of ends only marginally affects the statistics, $\Delta \sim bN^\nu$. The second (II) and the third (III) regimes correspond to stretched polymers above effectively flat (2) and curved (5) boundaries, respectively. The most interesting regime, where

the span of fluctuations is R -dependent, is the regime (III); remarkably, in this regime the dependence $\Delta(R) \propto R^{1/3}$ turns out to be independent on ν .

When the cylinder radius becomes as small as the Pincus blob size, $R \sim \xi$, so does the elliptic blob, $S^* \sim \xi$, and the crossover to regime IV occurs. Clearly, in this regime every Pincus blob "hugs" around the entire cylinder and, thus, $\Delta = \xi \geq R$,¹. In terms of the winding number, n , the regime IV corresponds to $n > (S/bN^\nu)^{1/(1-\nu)} \gg 1$. In this regard, it is tempting to compare regime IV of winding around a thin cylinder with winding around a zero-width line topological obstacle studied earlier [5–9]. In that case, $\Delta \sim bN^\nu$, with only weak dependence on winding number n (see formula (48) in the work [9], which is exact for $\nu = 1/2$). Since physical obstacle is always not purely topological, but also geometrical with some finite radius R , our present work allows to clarify the applicability conditions of the result of [9]: $2\pi Rn \ll bN^\nu$.

Our results can be generalized for the chain stretched around a smooth barrier of varying curvature, e.g., around an ellipse (see Fig. A1). Clearly, varying curvature determines the local size of the elliptic blob, S^* , while the Pincus blob size ξ and the number of monomers therein, g , would be invariant. As a result, the spread in the radial direction to the barrier at each point τ adopts the following universal form (see Appendix A1 for deriva-

¹ Note that (5) is not valid in this regime, since the Pincus blob ξ exceeds the size of the elliptic blob S^* .

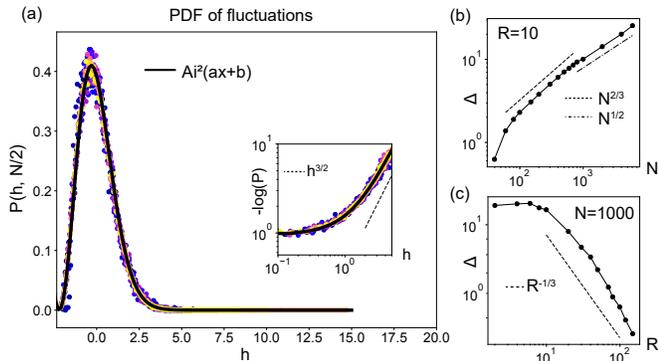


Figure 3. Molecular dynamics simulations of a stretched polymer of length N over a disc of radius R , in the units of monomer size b . (a): Probability density distribution $P(h, N/2)$ of scaled variable $h = (r - \Delta)/\sigma(r)$, where $\sigma(r)$ is the standard deviation of radial excursions r of the median monomer $N/2$ above the disk of radius $R = 10$. The collapse is shown for different polymer length $N = 80, 100, 200, 300, 400, 500, 600, 700, 800, 1000$, each coded by individual color. The black thick line is the best fit by the squared Airy function with the parameters $a \approx 0.7$, $b \approx -0.8$, properly normalized. The inset shows the tail of $-\log P(h, N/2)$. (b): Typical excursions as a function of N at the fixed disk size, $R = 10$. (c): Typical excursions as a function of R at the fixed polymer length, $N = 1000$.

tion details):

$$\Delta(\tau) = (R(\tau)\xi^2)^{1/3} \quad (8)$$

where $R(\tau)$ describes the local radius of curvature at point τ .

In order to validate the scaling results we have performed molecular dynamics simulations of the chains stretched around the disk (see Appendix A4 for details). Namely, we have considered a situation, in which the ends of an ideal chain are fixed at $S = \pi R$. According to (5), theoretical predictions for that case are:

$$\Delta = \begin{cases} N^{2/3} R^{-1/3} b^{4/3} & \text{“stretched”, } \Delta < R \\ N^{1/2} b & \text{“unperturbed”, } \Delta > R \end{cases} \quad (9)$$

As we see from Fig. 3(b) and (c) the span of fluctuations in both sets of simulations perfectly agrees with the predictions (9). We further compute the distribution of the scaled excursions for the stretched chain at various N , see Fig. 3(a). As one can infer from this plot, the distributions remarkably collapse on the squared Airy function, which also describes the one-point distribution of fluctuation in the Ferrari-Spohn process, i.e. constrained (1+1)D random paths above the semicircle [10, 14, 16].

IV. DISCUSSION

One of the most striking of our results is that the dependence of the typical fluctuations in the curved regime on the disc radius, R , can be written as $\Delta = R^\beta f(S, N, b, \nu)$ with $\beta = 1/3$ being the 1D KPZ *growth* exponent. Thus, it is tempting to look for a mapping between our problem and KPZ and to interpret R as time, t , in the associated stochastic growth problem. To see how it works, let us set $S = N^\gamma b \gg N^\nu b$, i.e. consider $\nu < \gamma < 1$. As (5) suggests, in the limit $\gamma \rightarrow 1$ typical fluctuations Δ are controlled by R only

$$\Delta = b(R/b)^\beta, \quad (10)$$

for $R < R^*$, where $R^* = b(S/b)^z$ is the crossover radius, below which a polymer with $N = (S/b)^{1/\gamma}$ monomers experiences curvature of the disk, and z reads

$$z(\gamma, \nu) = \frac{3\gamma - 2\nu\gamma - \nu}{2\gamma(1 - \nu)} \rightarrow 3/2, \quad \gamma \rightarrow 1. \quad (11)$$

The crossover, described by the 1D KPZ *dynamic* exponent, $z = 3/2$, (11) corresponds to the boundary between flat (II) and curved (III) regimes in Fig. 2(b). In the flat regime (II), $R > R^*$, the typical fluctuations do not depend on R and are described by the stretching S only, $\Delta = b(S/b)^\alpha$, where α reads

$$\alpha(\gamma, \nu) = 1 - \frac{\gamma - \nu}{2\gamma(1 - \nu)} \rightarrow \frac{1}{2}, \quad \gamma \rightarrow 1, \quad (12)$$

yielding the 1D KPZ *roughness* exponent $\alpha = 1/2$. In Fig. 2(c) we demonstrate the dependence of the exponents z and α on ν at different values of γ . As an intrinsic property of the “full stretching” limit, the curves $z(\nu), \alpha(\nu)$ become flat upon the increase of γ , approaching their respective 1D KPZ values.

Importantly, the implications of the $\gamma \rightarrow 1$ limit above can be realized for any other γ , but the chain should be renormalized to the Pincus blobs. Indeed, under the change $N \rightarrow N/g, b \rightarrow \xi$ a two-dimensional walk becomes effectively (1+1)D and, therefore, it naturally inherits all the scalings of the “full stretching” limit

$$\begin{cases} \Delta_{\text{curved}} = \xi(R/\xi)^\beta, & S > S^* \\ S^* = \xi(R/\xi)^{1/z} \\ \Delta_{\text{flat}} = \xi(S/\xi)^\alpha, & S < S^* \end{cases} \quad (13)$$

where $\xi = \xi(N, S)$ plays a role of a new coarse-grained monomer. Note that (13) holds for any fractal dimension of the polymer: upon stretching the correlations induced by fractality are destroyed at scales larger than the Pincus blob size, ξ . This effect is already observed in the classical stretching in the flat regime (II). However, at scales larger than S^* universal curvature-induced correlations get developed, featuring the KPZ exponent $\beta = 1/3$.

From representation (13) it is evident that after proper renormalization *any* fractal walk in two dimensions above the disk can be self-consistently described by the set of KPZ exponents. The curvature-induced correlation length of the two-dimensional path $S^* \sim R^{2/3}$ has the physical meaning of the elliptic blob, i.e. the scale at which the walk stays effectively flat. The flat regime of the chain is characterized by insufficiently strong curvature of the disk and, in turn, corresponds to large time scales of the KPZ growth in a finite system. However, as our simulations suggest, the distribution of typical fluctuations in the polymer problem is given by the squared Airy function, which is different from the Tracy-Widom distribution of the KPZ process (though the tails, $\sim \exp(-ch^{3/2})$, are equivalent, see the inset in 3(a)). In fact, this is a well-known consequence of the impermeability of the boundary, playing a role of the "mean-field" for a more complex system of many non-intersecting ("vicious") (1+1)D Brownian walks, the top of which is known to belong to the KPZ universality class (see the flowchart Fig. A3 and further discussion in Appendix A3). Replacing all such walks (but the top one) with the circular boundary we arrive at the Ferrari-Spohn model, for which the squared Airy behaviour for the one-point distribution has been established. Therefore, we conjecture that the (1+1)D representation (13) of the two-dimensional stretched polymers belong to the Ferrari-Spohn universality class.

Another interesting connection of our problem is revealed by looking at free energy (4) for the specific case when $\nu = 1/2$ and radius has specific value $R = S^2/bN$ (indicated by a dashed blue line on Fig. S2). Along this line, free energy reads $\frac{F_{\text{circ}}}{k_B T} \sim \frac{\Delta}{b} + \frac{b^2 N}{\Delta^2}$, which can be interpreted by noticing that $W(N) = \max_{\Delta} \exp\left(-\frac{\Delta}{b} - \frac{b^2 N}{\Delta^2}\right)$ is the probability for a random walker with diffusivity b^2/π^2 to survive during time N on the line with randomly Poisson positioned traps with density $1/b^2$. This is classical Balagurov-Vaks problem [27], and its solution $W(N) \sim e^{-\text{const } N^{1/3}}$ is controlled by the optimal interval between the traps, Δ . In the Appendix A2 we develop this connection in greater details along with the review of several relations to other known problems and models in statistical physics.

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APPENDIX

In this Appendix we first generalize our results about stretching polymer around a circular disc and consider stretching it around an ellipse or another convex barrier. Then, we re-formulate our problem and establish its connection to the problems of random walks in the space with Poisson-distributed traps. Further, we speculate about other connections of our problem across the fields. Finally, at the end, we describe technical details of polymer simulations used in our work.

A1. STRETCHING OF A POLYMER AROUND AN ELLIPTIC (OR ANOTHER CONVEX) BARRIER

Let us return to Eq. (4) in the main text. We offer here a slightly different view on it. Let us start from a scaling derivation of Pincus blobs. Clearly, the quantity ξ is a correlation length. Given that there is only one macroscopic length scale for an unrestricted coil, $R_F = bN^\nu$, correlation length in case when two ends stay at distance S apart, must obey the scaling $\xi = R_F \phi(S/R_F)$, where the behavior of scaling function $\phi(x)$ is as follows: $\phi(x) \sim 1$ when $x \ll 1$, while $\phi(x) \sim x^\mu$ when $x \gg 1$ with some critical exponent μ . The latter must be chosen such that for $S \rightarrow bN$ the blob size is reduced to (Kuhn) monomer size b . The following equation with $\mu = \nu/(1-\nu)$, provides the requested behavior:

$$\xi = R_F \left(\frac{R_F}{S} \right)^{\frac{\nu}{1-\nu}} \quad (\text{A-1})$$

If the chain is stretched by force rather than by fixing end-to-end distance, then $\xi = k_B T/f$, so ξ can be viewed as a proxy for the stretching force.

Now, we return to the equation (4) of the main text and re-write it as follows:

$$\begin{aligned} \frac{F_{\text{circ}}}{k_B T} &\sim \left(\frac{S}{bN^\nu} \frac{R+\Delta}{R} \right)^{\frac{1}{1-\nu}} + \frac{b^2 N^{2\nu}}{\Delta^2} \left(\frac{bN^\nu}{S} \right)^{\frac{2\nu-1}{1-\nu}} \\ &\sim \left(\frac{S}{bN^\nu} \right)^{\frac{1}{1-\nu}} \frac{\Delta}{R} + \frac{b^2 N^{2\nu}}{\Delta^2} \left(\frac{bN^\nu}{S} \right)^{\frac{2\nu-1}{1-\nu}} \\ &\sim \frac{S}{\xi} \left(\frac{\Delta}{R} + \frac{\xi^2}{\Delta^2} \right). \end{aligned} \quad (\text{A-2})$$

In the last transformation, we expressed free energy in terms of blob size, ξ . Minimization of this free energy with respect to Δ yields the result

$$\Delta \sim (R\xi^2)^{1/3} \quad (\text{A-3})$$

Of course, this result is entirely equivalent to our previous formula (5) in the main text for the curved surface.

Quite remarkable fact is that this result does not involve ν at all. In terms of ξ (or stretching force) there is no dependence on ν .

The result (A-3) allows us to consider stretching a polymer around a bumpy surface whose curvature changes from place to place, for instance, around an ellipse or around other convex curve with slowly changing curvature as shown in Fig. A1.

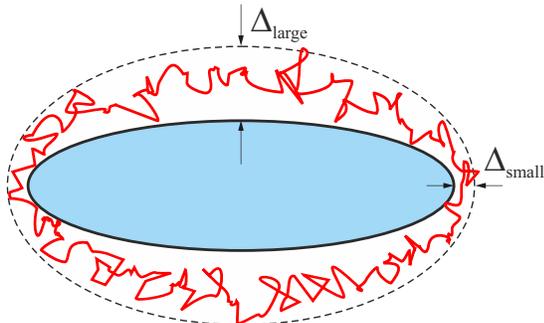


Figure A1. Polymer chain stretched around an ellipse.

Since tension force is the same everywhere along the polymer, so is the blob size ξ . Therefore, if curvature radius is different in different places (while changing slowly, over length scales much larger than ξ), the factor S/ξ in (A-2), which signals additivity of the free energy on the blob level, can be replaced by the integral along S with “density” $1/\xi$:

$$\frac{F}{k_B T} = \int_0^S \frac{dx}{\xi} \left[\frac{\Delta(x)}{R(x)} + \frac{\xi^2}{\Delta^2(x)} \right], \quad (\text{A-4})$$

providing the result

$$\Delta(x) \sim (R(x)\xi^2)^{1/3}. \quad (\text{A-5})$$

These results apply of course only to the case of everywhere convex impermeable boundary, because if some parts are concave, the stretched polymer will take a straight shortcut.

A2. STRETCHING FREE ENERGY MINIMIZATION FROM AN “OPTIMAL FLUCTUATION” PERSPECTIVE

The purpose of this section is to establish the connection between our polymer stretching problem and classical Balagurov-Vaks (BV) problem of random walks on the line with randomly distributed traps [27] (see also later more detailed treatment by Donsker and Varadhan [28]). To see the connection with the stretched polymers, let us return again to formula (4) in the main text and re-write it by assuming, as in the main text, $S = bN^\gamma$, with $\gamma < 1$. Power γ can be viewed as a proxy of the distance

S , characterizing the stretching degree. Furthermore, we can also say $S = R\theta$, where θ is the corresponding angle, $\theta < 2\pi$ (or $\theta > 2\pi$) correspond to less than one (or more than one) full turns around the cylinder; in the latter case, $\theta/2\pi$ is the winding number. In terms of γ and θ , the two terms of free energy read

$$\begin{aligned} \frac{F_{\text{circ}}}{k_B T} &\sim \frac{\Delta}{R} N^{\frac{\gamma-\nu}{1-\nu}} + \frac{b^2}{\Delta^2} N^{1+\frac{(1-\gamma)(2\nu-1)}{1-\nu}} \\ &= N^{\frac{(1-\gamma)(2\nu-1)}{1-\nu}} \left[\theta N^{-\frac{(1-\gamma)(3\nu-1)}{1-\nu}} \frac{\Delta}{b} + \frac{b^2}{\Delta^2} N \right]. \end{aligned} \quad (\text{A-6})$$

This result has a transparent connection with BV problem in two cases. First, if the chain is strongly stretched such that $\gamma \rightarrow 1^-$, such that $1 - \gamma \ll 1/\ln N$. In that case,

$$\frac{F_{\text{circ}}}{k_B T} \sim \theta \frac{\Delta}{b} + \frac{b^2}{\Delta^2} N. \quad (\text{A-7})$$

for arbitrary ν . Second, if $\nu = 1/2$ and $\theta = N^{1-\gamma}$, in that case

$$\frac{F_{\text{circ}}}{k_B T} \sim \frac{\Delta}{b} + \frac{b^2}{\Delta^2} N; \quad (\text{A-8})$$

this latter case corresponds to $\nu = 1/2$ of the polymer. In this case mapping to Balagurov-Vaks is realized along the line $R = bN^{2\gamma-1}$, which can be also presented as

$$R/R_0 = \frac{1}{\sqrt{N}} (S/R_0)^2. \quad (\text{A-9})$$

The behavior (A-9) is illustrated by the dashed blue line in the $R-S$ diagram, Fig. A2. Interestingly, the slope of this line coincides with the slope of the boundary between flat (II) and curved (III) regimes in the particular case of $\nu = 1/2$. However, note that the coefficient in (A-9) is N -dependent. Therefore, the mapping to BV in the second case (A-8) might be realized only for particular value of N , provided a pair of values $(R/R_0, S/R_0)$ on this diagram.

While in the first case (A-7) the BV mapping is realized in the whole area of the curved regime III, in the second case (A-8) it is not. Along the BV lines of constant N in Fig. A2 the stretching parameter γ changes, and the extremities of these lines provide respective bounds to γ . As Fig. A2 suggests, the stretching must be strong enough, $\gamma > 2/3$, otherwise one enters the regime IV of weak fluctuations. On the other hand, it is evident that as long as a BV polymer, being wrapped over cylinder many times, is forced to make a single turn only, $R/R_0 \rightarrow S/R_0$, the stretching attains its asymptotic limit, $\gamma \rightarrow 1$. This rhymes well with the behavior of the winding number in the second case $\theta = N^{1-\gamma} \gg 1$ for $\gamma < 1$. Thus, the region of less than one turn, i.e. between the dashed black line and the boundary II-III, is forbidden for the BV polymers, unless they are fully stretched (the first case).

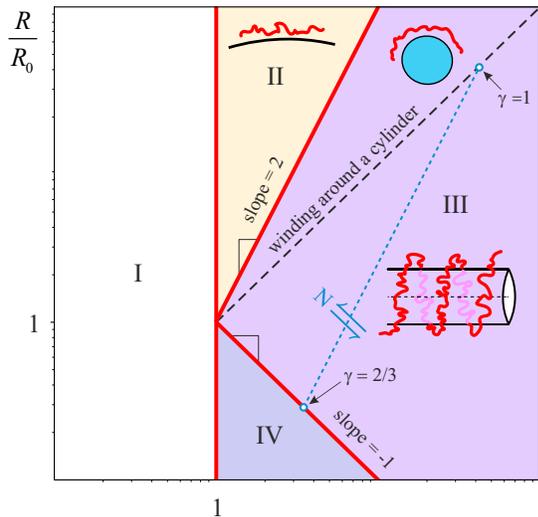


Figure A2. The same diagram as Fig.2(b) in the main text to demonstrate the place of Balagurov-Vaks problem (dashed blue line) in the context of 2D stretched polymer chains. The slopes between the regimes are computed for the particular value of $\nu = 1/2$. The arrows correspond to two values of the stretching parameter, $\gamma = 2/3$ and $\gamma = 1$, between which the mapping to Balagurov-Vaks can be realized for any N .

Let us remind the Balagurov-Vaks setting. Consider an auxiliary 1D problem of random walks on the line with Poisson-distributed absorbing traps. Let n_{tr} be the average density of traps on the line. Following Balagurov and Vaks [27], we are interested in the probability $W(N)$ for the walker to survive during “time” N (assuming “diffusivity” is equal to b^2/π^2), i.e. with the probability that until time N the walker does not encounter any trap. The probability to have an interval Δ between nearest neighboring Poisson-distributed traps is equal $\exp(-n_{\text{tr}}\Delta)$. On the other hand, the probability to survive for a “long time” $N \gg \Delta^2/b^2$ between absorbing (Dirichlet) boundary conditions on both ends of the interval Δ is estimated as $\exp(-b^2N/\Delta^2)$. The total survival probability is controlled by the Lifshitz’s “optimal fluctuation” [29], i.e., by finding such an interval Δ that maximizes the product of the two above mentioned factors:

$$W(N) \sim \max_{\Delta} \left[e^{-n_{\text{tr}}\Delta - b^2N/\Delta^2} \right]. \quad (\text{A-10})$$

The connection with (A-7) is now obvious, and θ/b plays the role of traps density, $n_{\text{tr}} = \theta/b$. Clearly, (A-8) (which is restricted to $\nu = 1/2$ and special value of R) corresponds to trap density just $n_{\text{tr}} = 1/b$. Note that the derivation of the BV survival probability has relied on the assumption $Nb^2 \gg \Delta^2$, i.e. a the walk between the neighboring traps is constrained. For the case of $\nu = 1/2$ this is equivalent to $R/R_0 \ll (S/R_0)^2$ in the polymer problem, which forbids flat geometry. As can be seen from Fig. A2, this condition is well satisfied.

Maximization of the expression (A-10) yields

$W(N) \sim \exp\left(-\text{const } b^{2/3} n_{\text{tr}}^{2/3} N^{1/3}\right)$, which is exactly the Balagurov-Vaks answer [27] for the 1D survival probability of the unbiased random walk of time N in the Poissonian array of traps. Due to the analogy, we can call the minus logarithm of the survival probability the “trap free energy”² (dropping from now on the $k_B T$ factor): $-\ln W(N) = F_{\text{trap}} \sim \theta^{2/3} N^{1/3}$. The minimal value of the polymer free energy is given by the same formula $F_{\text{circ}} \sim \theta^{2/3} N^{1/3}$.

Interestingly, the equivalent to (A-10) weight was maximized in [30] for computation of the correlation function of a polymer chain confined in a gel matrix. In that case the linear term was played by the confinement free energy inside a mesh (generating the exponential distribution of the chain segments lengths), while the quadratic term corresponded to the Rouse relaxation time of each chain segment within the mesh.

In both polymer and BV problem there is in general also the leading extensive term, proportional to N . In BV problem, it is due to a constant bias, c , superimposed on the symmetric random walk. In polymer problem it is a constant energy per every monomer (e.g., a bond energy). In both cases, therefore,

$$\begin{aligned} F_{\text{trap}} &\sim cN + (bn_{\text{tr}})^{2/3} N^{1/3} \quad \text{and} \\ F_{\text{circ}} &\sim cN + \theta^{2/3} N^{1/3}, \end{aligned} \quad (\text{A-11})$$

free energies are given by identical expressions, albeit with different physical interpretation of the parameters.

The Legendre transform from N to a conjugate variable, λ , realized via the inverse Laplace transform of the survival probability $W(N) = \exp(-F_{\text{trap}})$ or of the partition sum for a polymer $\exp(-F_{\text{circ}})$, gives the spectral density, $\rho(\lambda)$ (see [31] for more detail):

$$\begin{aligned} \rho(\lambda) &\propto \frac{1}{2\pi i} \int_{\varepsilon-i\infty}^{\varepsilon+i\infty} e^{-cN - \theta^{2/3} N^{1/3}} e^{N\lambda} dN \\ &\propto \exp\left[-\theta/\sqrt{c-\lambda}\right]. \end{aligned} \quad (\text{A-12})$$

A3. POLYMER STRETCHING ABOVE A DISC IN A BROADER CONTEXT

Having established the connection of our polymer problem with that of random walks between traps, we now switch to even further connections to a range of other problems and models. To facilitate the discussion, we outline it in the flowchart of mutually related ideas presented in Fig. A3.

² To be specific, we stick to the first case of strong stretching, $\gamma \rightarrow 1$, (A-7)

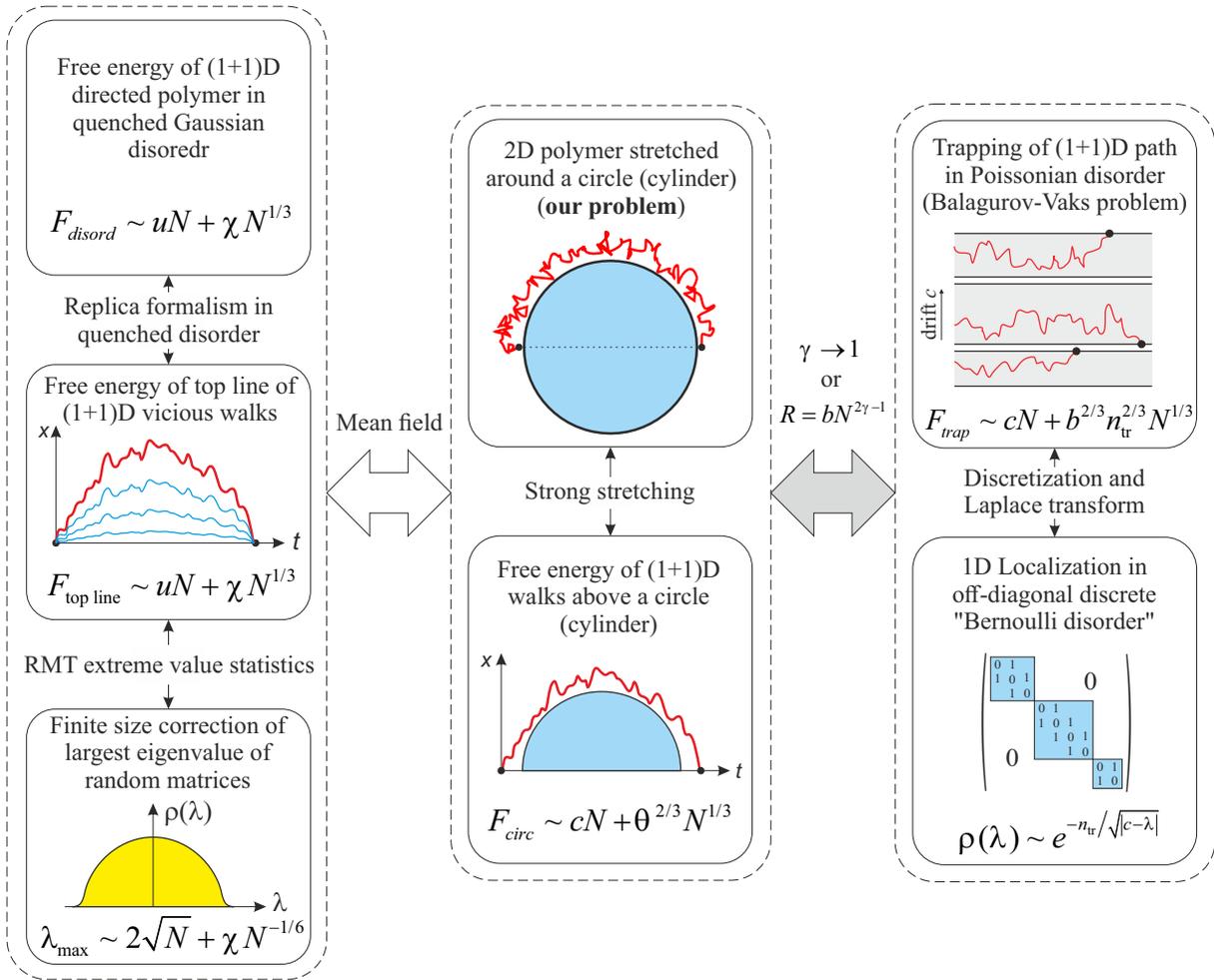


Figure A3. Flowchart of logical connections: place of our “2D polymer stretching above a curved boundary” problem in the context of other models and systems in statistical physics. **Central column** – 2D polymer (*top*) and (1+1)D polymer (*bottom*) are equivalent in the strong stretching regime, with free energy $F_{circ} \simeq cN + \theta^{2/3} N^{1/3}$. **Right column** – polymer problem in the proper limit maps onto biased Brownian motion in an array of Poisson distributed traps (*top*), or, equivalently, related to the spectrum of the off-diagonal random Bernoulli matrix (*bottom*). **Left column** – curved polymer stretching problem is a mean field approximation for the top line in the system of (1+1)D vicious (mutually non-intersecting) walks (*center*), which is in turn related to either directed polymer in Gaussian disorder (*top*) and to the maximal eigenvalue statistics in the spectrum of random matrices (*bottom*). The common motif is the $N^{1/3}$ scaling of the subleading correction term that controls relevant physics in all cases.

The central rectangle in Fig. A3 shows our problem and its limiting regime $\gamma \rightarrow 1^-$ of strong stretching (as a reminder, stretching of a polymer is characterized by the curvilinear end-to-end distance which we write in terms of γ as $S = bN^\gamma$). Minimal value of polymer free energy, as discussed before, is given by $F_{circ} \sim cN + \theta^{2/3} N^{1/3}$, where θ is the winding number, related to the radius of the void, $R = S/\theta$. The sublinear in N term of free energy represents the curvature-induced finite-size correction.

The right rectangle in the same Fig. A3 depicts the group of problems related to BV model of 1D random walk in the array of Poisson distributed traps, as reviewed in the previous section. In particular, the bottom panel of

the right rectangle schematically depicts the (biased) BV model [27]. There, we show pictorially a set of randomly positioned traps - thick lines parallel to the time axis. Within each interval between traps, the walker moves randomly under some constant bias c until it hits one of the boundaries for the first time. The connection to our polymer problem is highlighted by the “free energy” expression (A-11), in which trap density is related to the winding angle θ for the polymer.

In the upper panel on the right hand side we have drawn the typical three-diagonal random matrix with Bernoulli disorder. Its connection with BV model and, therefore, its relation to our polymer-around-a-cylinder problem can be understood by the following simple cal-

culuation. Let $\rho(\lambda)$ be the spectral density of ensemble of large tridiagonal symmetric matrices, A_N , with the bimodal (Bernoulli) distribution of sub-diagonal matrix elements $a_{j,j\pm 1} = \{0, 1\}$ as shown below:

$$A_N = \begin{pmatrix} 0 & \varepsilon_1 & 0 & \cdots & 0 \\ \varepsilon_1 & 0 & \varepsilon_2 & & \\ 0 & \varepsilon_2 & 0 & & \\ \vdots & & & & \\ 0 & & & \varepsilon_{N-1} & \\ & & \varepsilon_{N-1} & 0 & \end{pmatrix} \quad (\text{A-13})$$

where

$$\varepsilon_x = \begin{cases} 1 & \text{with probability } p \\ 0 & \text{with probability } 1 - p \end{cases} \quad (\text{A-14})$$

The matrix A_N at each $\varepsilon_x = 0$ splits into regular (gapless) three-diagonal ‘‘cage’’ of some random size D , each can be viewed as a transition matrix of a discrete random walk in the cage D . The probability to find such a cage is $Q(D) = p^D$. The spectral density $\rho(\lambda)$ of ensemble of matrices A_N has been exhaustively analyzed in [32, 33] and the tail of $\rho(\lambda)$ near the spectral edge $\lambda \rightarrow \lambda_{\max} = 2$ reads:

$$\rho(\lambda) \propto \exp \left[-\frac{\pi \ln p}{\sqrt{|2 - \lambda|}} \right] \quad (\text{A-15})$$

Obviously, $\rho(\lambda)$ in (A-15) is the same spectral density as in (A-12) for properly adjusted drift c and trap density n_{tr} .

Thus, the close similarity between central and right rectangles in the flowchart in Fig. A3 justifies our claim that nontrivial stretched exponent $1/3$ appearing for the random walk or a stretched polymer near the curved boundary points to the intimate connection with stretched exponent for survival probability of (1+1)D trapping problem in the Poissonian disorder.

The left rectangle highlights the known relation between the ground state free energy, F_{disord} of (1+1)D directed polymer in quenched Gaussian disorder [34] (upper panel) and the statistics of the top line in the ensemble of (1+1)D ‘‘vicious’’ random walks [35] (central panel). Let us note, that the last problem has also the interpretation (after proper rescaling by \sqrt{N}) in terms of the largest eigenvalue λ_{\max} of the Gaussian ensemble of random matrices. Since the same scaling (subject to numerical factors) is valid for both Gaussian Orthogonal (GOE), and Gaussian Unitary (GUE) ensembles, we do not specify here which particular ensemble is considered. At the spectral edge λ_{\max} has the finite-size corrections in N ($N \gg 1$): $\lambda_{\max} \sim 2\sqrt{N} + \chi N^{-1/6}$, where χ is N -independent and is distributed according to the Tracy-Widom law which takes slightly different forms for GOE and GUE.

The arrow ‘‘Mean field’’ designates the mean-field approximation of the many-body system of vicious walks, in which the influence of all trajectories lying below the topmost one, are replaced by the impermeable circular boundary, [16]. Note that finite-size corrections to the free energies, F_{disord} and F_{upper} , have the same scaling as the one for F_{circ} : in all cases the corresponding finite-size sublinear in N terms are of order of $N^{1/3}$.

We should emphasize that the above mentioned similarity, however attractive, is not complete. Although valid on averages, it cannot be extended on distributions: the partition functions of a polymer in quenched Gaussian disorder and fluctuations of the topmost vicious walks have the Tracy-Widom distribution, while the constrained random walk above the boundary is given by squared Airy function [14, 16]. Here we report the equivalent squared Airy PDF of fluctuations in the stretched polymer problem at various degrees of stretching (Fig. 3(a) in the main text). Apparently, this difference in distribution is the consequence of the fact that we have replaced the true many-body system (such as vicious walks) by its one-body mean-field analog.

To summarize, scaling analysis of a polymer strongly stretched around a cylinder reveals an unusual behavior of free energy $F_{\text{circ}} \sim cN + \theta^{2/3}N^{1/3}$ that points to an array of deep connections with a variety of problems in equilibrium and non-equilibrium statistical physics and random matrix theory, ranging from KPZ to Balagurov-Vaks problem, Lifshitz tails, Andresen localization, vicious random walks, etc. Although some of the arguments in the last section have intentionally tentative, hypothetical, and sometimes even speculative character, it seems to us that together they paint an exciting picture.

A4. DETAILS OF POLYMER SIMULATIONS

Simulations of stretched trajectories are done using polychrom module (available at <https://github.com/open2c/polychrom>), a wrapper around the open source GPU-assisted molecular dynamics package OpenMM [36]. A chain with phantom beads in simulations is supposed to model the ideal Gaussian chain with the fractal dimension $D_f = 2$. The chain is equipped with harmonic bonds of the following energy

$$U_{\text{bond}} = \frac{3}{2a^2} \sum_{i=1}^{N-1} (r_{i,i+1} - l_b)^2 \quad (\text{A-16})$$

where $a = 0.06$ is the standard deviation of the monomer-to-monomer distance, $r_{i,i+1} = |\mathbf{r}_{i+1} - \mathbf{r}_i|$; the equilibrium bond length is $l_b = 1$.

The cylindrical barrier for the chain is aligned along the z -axis, having the infinite length and the radius R in the $x - y$ plane. In order to prohibit the chain entering the area constrained by the cylinder, the following

soft repulsive potential of strength $k_{\text{cyl}} = 5$ is introduced when the chain crosses the disk boundary

$$U_{\text{cyl}} = k_{\text{cyl}} \sum_{i=1}^N \mathcal{H} \left[R - \sqrt{x_i^2 + y_i^2} \right] \left(R - \sqrt{x_i^2 + y_i^2} \right)^2 \quad (\text{A-17})$$

with $\mathcal{H}[\cdot]$ being the Heaviside step function. This potential has been further smoothed in simulations close to the vicinity of the boundary by means of a small parameter inserted under the root. Also, in order to keep the chain ends at the distance $S = \pi R$ apart, we additionally tether the end beads $\mathbf{r}_1, \mathbf{r}_N$ at two points on the diam-

eter by springs of strength $k_{th} = 100$ at a small distance $\delta = 0.1 < \Delta$ from the disk surface.

The chain of length N is initialized with a random walk configuration and equilibrated for a Rouse time τ_R in the potentials above. Computation of the Rouse time in simulations has been performed using the dynamics-based estimate for the microscopic Rouse time τ_0 , then $\tau_R = \tau_0 N^2$. This is done in separate short-time runs, in which the transition time τ_0 from the ballistic to Rouse behaviour of the mean-squared displacement of one monomer $r_0^2(t)$ is computed.

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