Entropic forces generated by grafted semiflexible polymers

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The entropic force exerted by the Brownian fluctuations of a grafted semiflexible polymer upon a rigid smooth wall are calculated both analytically and by Monte Carlo simulations. Such forces are thought to play an important role for several cellular phenomena, in particular, the physics of actin-polymerization-driven cell motility and movement of bacteria like Listeria. In the stiff limit, where the persistence length of the polymer is larger than its contour length, we find that the entropic force shows scaling behavior. We identify the characteristic length scales and the explicit form of the scaling functions. In certain asymptotic regimes we give simple analytical expressions which describe the full results to a very high numerical accuracy. Depending on the constraints imposed on the transverse fluctuations of the filament there are characteristic differences in the functional form of the entropic forces. In a two-dimensional geometry, the entropic force exhibits a marked peak.

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I. INTRODUCTION

In a cellular environment soft objects like membranes and polymers are subject to Brownian motion. As a result there are interactions between them which are entropic in origin, i.e. a consequence of constraints imposed on the Brownian fluctuations. For example, two parallel membranes repel each other entropically with a potential that falls off like a power law in the distance between them \cite{1}. Similarly, thermally fluctuating biopolymers like F-Actin and microtubules may exert entropic forces on membranes or some other obstacles; for an illustration see Fig.1. Though due to the same thermal fluctuations such forces have to be distinguished from forces obtained by pulling on a biopolymer \cite{2,3}. It will turn out that the force-distance curves of these two cases have no resemblance at all in a regime where thermal fluctuations play a role, which is generically the case for all cytoskeletal filaments. Both types of forces are thought to play a prominent role in cell motility and movement of pathogens like listeria monocytogenes, that propel itself through the cytoplasm of infected cells by constructing behind it a polymerized tail of cross-linked actin filaments \cite{4}. Similarly, in a crawling cell, the force generated from the growth of a collection of actin fibers is responsible for the protrusion of cell membrane, which are known as lamellipodia, filopodia, or microspikes according to their shapes \cite{5}. It seems that quite generally polymerizing networks of actin filaments are capable of exerting significant mechanical force, which are used by eukaryotic cells and their prokaryotic pathogens to change shape or move. One type of force is generated by fluctuating filaments at the leading edge of the network. The length of the thermally fluctuating parts of these polymers are typically 200 \textasciitilde 300nm, which is very short compared to their persistence length $\ell_p \approx 17\mu m$ \cite{6}, such that an analysis which considers these filaments as stiff seems appropriate.

In this paper we will not enter into the debate on the particular force generating mechanism responsible for all these different types of cell motility, but rather give a detailed analysis of the entropic forces which fluctuating stiff polymers exert on rigid walls. This may serve as important input for future molecular models of force generation in cellular systems.

Consider a semiflexible polymer with contour length $L$ and persistence length $\ell_p$ with one end fixed both in position and orientation to some rigid support (see Fig.1), e.g. the dense part of an actin gel. We choose coordinates such that the grafted end is at the origin with the tangent fixed parallel to the $z$-axis. Consider a rigid, smooth wall orthogonal to the $x$-$z$-plane at a distance $\zeta$ from the origin. Let $\vartheta$ be the angle between the $z$-axis and the normal $\hat{n}$ of the wall. If $\zeta$ is small enough, the wall will constrain the Brownian fluctuations of the poly-
mer leading to an increase in free energy with respect to the unconstrained polymer. On time scales larger than the equilibration time of the grafted polymer this results in an average force \( f \) exerted on the wall. Our goal is to calculate how the entropic force \( f \) depends on \( \zeta \) and \( \vartheta \) and the contour length \( L \) and the persistence length \( \ell_p \) of the polymer.

We will proceed as follows. The following Section III serves to introduce and discuss the various types of thermodynamic forces which can be generated by fluctuating semiflexible polymers. We will arrive at the conclusion that the entropic forces discussed above are closely related to the probability distribution of the free end of the clamped polymer. In Section III we start our analysis of entropic forces with a polymer grafted perpendicular to the wall. This chapter contains a definition of the wormlike chain model and the basic idea of our analytical calculations, which starting from the tip distribution calculates the restricted free energy and the entropic force. The analysis is complemented by Monte Carlo (MC) simulations, which both show the range of validity of the analytical results and the crossover from semiflexible to Gaussian chains. Details of the calculations are deferred to the Appendices A, B and C. Section IV treats the technically more complicated case of a polymer inclined at an angle \( \vartheta \) with respect to the wall. Here we obtain the entropic forces analytically up to the numerical evaluation of some integrals. For some asymptotic cases explicit analytical formula are again obtained. The MC simulations in this chapter are restricted to a parameter range which is close to the stiff limit, and mainly serve the purpose to define the range of applicability of the analytical results. Finally, in the conclusion we give a discussion of our main results.

II. ENTROPIC FORCES AND PROBABILITY DENSITIES

According to the wormlike chain model [7, 8], the elastic energy of a given configuration \( \mathbf{r}(s) \), parameterized in terms of the arc length \( s \in [0, L] \), is given by

\[
\beta H = \frac{\ell_p}{2} \int_0^L ds \left( \frac{\partial \mathbf{t}(s)}{\partial s} \right)^2.
\]

Here \( \mathbf{t}(s) = \partial \mathbf{r}(s)/\partial s \equiv \mathbf{t}(s) \) is the local tangent to the contour \( \mathbf{r}(s) \) and \( \ell_p = \kappa/k_B T \) is the persistence length with \( \kappa \) the polymer’s bending modulus, and \( \beta = 1/k_B T \). As the polymer is considered to be inextensible, we have \( |\mathbf{t}(s)| = 1 \) for all \( s \), i.e. the tangent vectors are restricted to the unit sphere.

In a cellular environment biopolymers are flexed by Brownian motion, i.e. they exhibit thermal fluctuations in their shape. This mere fact makes for a rich mechanical response genuinely different from its classical analogue, a rigid beam. Consider a polymer whose position (not its orientation) is fixed at one end and one is pulling on its other end, a typical situation encountered in an experiment using optical or magnetic tweezers. Then there is no unique force-distance relation. It actually matters whether one pulls at constant force \( f \) and measures the resulting average distance \( \langle r \rangle (f) \) or vice versa. Results for the constant force ensemble are thoroughly discussed in Ref.[2]. In a constant distance ensemble the probability density distribution of the end-to-end distance \( P(r) \) provides the necessary information. It defines a free energy \( F(r) = -k_B T \ln P(r) \) from which the average force may be derived by differentiation, \( \langle f \rangle (r) = -\partial F(r)/\partial r \).

Here we are interested in the force a fluctuating filament exerts on a rigid obstacle which is fixed in its position \( \mathbf{r}_x \). The polymer’s end facing the obstacle is considered as free to fluctuate and only its proximal end is fixed in position and orientation; see Fig.1. Since there are no direct forces between polymer and obstacle the force exerted on the wall is solely due to the steric constraints imposed on the filament. This suggests to use the term “entropic forces”, frequently used in analogous physical situations [12]. However, this should not leave the reader with the wrong impression that there are different physical origins for entropic forces and those discussed in the preceding paragraph. It is merely the type of “boundary condition” imposed on the thermal fluctuations which leads to their (drastically) different character.

For getting acquainted with the problem let us consider the simplest case, a grafted polymer whose one end and tangent is fixed such that it is oriented perpendicular to a smooth wall (Fig.1 with \( \vartheta = 0 \)). The presence of the wall allows only for those polymer configurations which are entirely in the halfspace to the left of the wall. Since we are mostly interested in stiff polymers (which have a low probability for back-turns) this restriction may be approximated as a constraint solely on the position of the polymer tip facing the wall, \( r_x(L) \leq \zeta \); later in Section IV C we will show some simulation data going beyond this approximation.

To derive the average force acting on the wall we consider a wall potential \( U(\zeta - r_x(L)) \) for the free polymer tip, which at the end of the calculation will be reduced to a hard wall potential. For now picture a steep potential which rises rapidly for \( r_x(L) \rightarrow \zeta \). Then, the ensemble average for the force the polymer tip excerts perpendicular to the wall reads

\[
\langle f_\parallel \rangle (\zeta) = \frac{1}{Z_\parallel (\zeta)} \int \mathcal{D}[\mathbf{r}(s)] e^{-\beta(H+U)} \frac{\partial U}{\partial r_x(L)}.
\]

Here the partition sum

\[
Z_\parallel (\zeta) = \int \mathcal{D}[\mathbf{r}(s)] e^{-\beta(H+U)}
\]

is a path integral over all polymer configurations compatible with the boundary conditions imposed on the distal and free end of the grafted polymer, where the measure is taken such that the partition sum without a constraining
wall \((U = 0)\) is normalized to 1. This is now a thermodynamic force. In an actual experiments it is obtained by a time average with an averaging time much larger than the equilibration time for the grafted polymer. This force would also be measured in an experiment where a large number of independent and identical polymers push against the same wall.

Since the wall potential depends only on the difference between the position of the polymer tip and the wall we may rewrite the entropic force in Eq. 4 as

\[
\langle f_\parallel \rangle(\zeta) = k_B T \frac{\partial}{\partial \zeta} \ln Z_\parallel(\zeta) .
\]

Upon defining a free energy of the confined polymer as

\[
\mathcal{F}_\parallel(\zeta) = -k_B T \ln Z_\parallel(\zeta) ,
\]

the entropic forces again reads as a spatial derivative of a free energy

\[
\langle f_\parallel \rangle(\zeta) = -\frac{\partial}{\partial \zeta} \mathcal{F}_\parallel(\zeta) .
\]

The physical interpretation of this free energy becomes clear as one goes to the hard wall limit. Then, the partition function reduces to

\[
Z_\parallel(\zeta) = \int D[r(s)] \Theta(\zeta - r_z(L)) e^{-\beta H} =: \langle \Theta(\zeta - r_z(L)) \rangle_0 ,
\]

where the subscript 0 indicates that the average is now taken with respect to the bending Hamiltonian only. The \(\Theta\)-function, defined such that \(\Theta(x) = 1\) for \(x > 0\) and zero elsewhere, indicates that only those configurations are counted with the position of the polymer tip to the left of the wall. Hence, as for the fixed distance ensemble in a pulling experiment, the free energy results from a quantity measuring the number of configurations obeying the imposed constraint, where each configuration is weighted by a Boltzmann factor for the bending energy.

It is useful to rewrite the partition function as

\[
Z_\parallel(\zeta) = \int_{-L}^{L} dz \Theta(\zeta - z) \langle \delta(z - r_z(L)) \rangle_0 = \int_{-L}^{\zeta} dz P_\parallel(z) ,
\]

where \(P_\parallel(z) = \langle \delta(z - r_z(L)) \rangle_0\) is the probability density to find the \(z\)-coordinate of the polymer’s free end at \(z\), irrespective of its transverse coordinates. It identifies the restricted partition sum as the cumulative distribution function corresponding to the probability density \(P_\parallel(z)\). One may then write the entropic force in the alternative form

\[
\langle f_\parallel \rangle(\zeta) = k_B T \frac{P_\parallel(\zeta)}{Z_\parallel(\zeta)} .
\]

Upon multiplying this formula by \(d\zeta\) it may be interpreted as follows. The work done on the wall upon displacing it by an infinitesimal distance \(d\zeta\) equals the thermal energy scale \(k_B T\) times a conditional probability \(P_{\parallel 0}(\zeta) d\zeta / Z_\parallel(\zeta)\), which measures the probability that the position of the polymer tip is within a distance \(d\zeta\) from the wall given that the polymer is in the left halfspace.

Since the probability density for the position of the polymer tip \(P(x, z)\) is actually a function of the position perpendicular and transverse to the wall, Eq. 9 immediately suggests that one could define a local entropic pressure. Indeed, upon generalizing the above arguments one may write

\[
p(x, \zeta) = \frac{-1}{Z_\parallel(\zeta)} \int D[r] \frac{\partial U}{\partial \zeta} \delta(x - r_\bot(L)) e^{-\beta(H + U)} = \frac{k_B T}{Z_\parallel(\zeta)} \frac{\partial}{\partial \zeta} \langle \Theta(\zeta - r_z(L)) \rangle_0 \delta(x - r_\bot(L))_0 = k_B T \frac{P(x, \zeta)}{Z_\parallel(\zeta)}
\]

for the entropic pressure, i.e. the force per unit area exerted locally at \(x\) on the wall. Again, the entropic force is given by the thermal energy scale times a conditional probability density, which now measures the probability of finding the polymer tip at a particular site \(x\) on the wall conditioned on the polymer configuration being to the left of the wall. Pictorially, one may say that the local pressure is given by \(k_B T\) times the number of “collisions” of the polymer with the wall per unit area, a reasoning which is frequently used in scaling analyses.

The total force is, of course, obtained by integrating over this local pressure, \(\langle f_\parallel \rangle(\zeta) = \int dx p(x, \zeta)\). In addition, one may now also define an entropic torque as has recently been done for a rigid rod facing a planar wall \[16\]; we leave this issue for future investigations.

Generalizing the above ideas suggests to introduce an effective local free energy per unit area as

\[
\mathcal{F}(x, \zeta) = -k_B T \int_\zeta^L dz \frac{P(x, \zeta)}{Z_\parallel(\zeta)} ,
\]

which is useful in applications where the obstacle is actually not rigid but soft with some internal elasticity, e.g. a membrane, whose dynamics is much slower than the equilibration time of the polymer. Then the elastic energy describing membrane bending and the above effective free energy may just be added to describe the combined system. Of course, such a description fails if time scales for the dynamics of both soft objects are comparable.

Our main conclusion in this section is that entropic forces generated by a grafted stiff polymer can be reduced to the calculation of the probability distribution of the polymer tip. For a polymer constrained to two dimensions this distribution function has been found to show quite interesting behavior such as bimodality in the
transverse displacement of the free end \[14\]. This pronounced feature of the distribution function has recently been rationalized upon exploiting an interesting analogy to a random walker in shear flow \[13\].

III. POLYMER ORTHOGONAL TO A WALL

In this section we are going to calculate the entropic force generated by a grafted polymer whose orientation is on average perpendicular to the wall. It illustrates the basic idea of our analytical calculations for the simplest geometry.

A. Weakly bending limit: mode analysis

In evaluating the distribution function analytically we restrict ourselves to the limit of a weakly bending filament. In other words, we consider the persistence length \( \ell_p \) to be large enough compared to the total contour length \( L \), such that the statistical weight of configurations with small sharp bends will be negligible. The key small dimensionless quantity will be the stiffness parameter

\[
\varepsilon = \frac{L}{\ell_p}
\]

and we will refer to the weakly bending limit also as the stiff limit.

For small \( \varepsilon \), the transverse components, \( t_x(s) \) and \( t_y(s) \), of the tangent vector \( t(s) \) will be small for all \( s \). While the condition \( |t(s)| = 1 \) would suggest a parameterization of \( t(s) \) in terms of polar coordinates or Euler angles, for reasons that will become apparent later we want to have independent variables that appear in a symmetric way in the integrand. Thus we choose to parameterize \( t \) by

\[
t = \frac{1}{\sqrt{1 + a_x^2 + a_y^2}} \begin{pmatrix} a_x \\ a_y \\ 1 \end{pmatrix},
\]

where we dropped all arguments \( s \) for brevity; the generalization to \( d \) spatial dimensions is obvious.

The boundary conditions at the ends of the polymer are

\[t(0) = (0, 0, 1)^T \quad \text{(clamped end)}, \quad (14a)\]
\[t(L) = (0, 0, 0)^T \quad \text{(free end)}. \quad (14b)\]

This translates into \( a(0) = (a_x(0), a_y(0))^T = (0, 0)^T \) and \( \dot{a}(L) = (\dot{a}_x(L), \dot{a}_y(L))^T = (0, 0)^T \). We thus can choose a Fourier representation, or in other words a normal mode decomposition

\[a_x(s) = \sum_{k=1}^{\infty} a_{x,k} \sin \left( \frac{\lambda_k s}{L} \right) \]

with eigenvalues

\[\lambda_k = \frac{\pi}{2} (2k - 1), \quad (16)\]

and Fourier (normal mode) amplitudes

\[a_{x,k} = \frac{2}{L} \int_0^L ds \, a_x(s) \sin \left( \frac{\lambda_k s}{L} \right), \quad (17)\]

and similar for \( a_y(s) \). To second order in the Fourier amplitudes the location of the end-point along the \( z \)-axis reads

\[r_z(L) = \int_0^L ds \, t_z(s) \]
\[\approx L - \frac{1}{2} \int_0^L ds \left[ a_x^2(s) + a_y^2(s) \right] \]
\[= L - \frac{L}{4} \sum_{k=1}^{\infty} [a_{x,k}^2 + a_{y,k}^2]. \quad (18)\]

Similarly, we find for the Hamiltonian to second order

\[
\beta H \approx \frac{\ell_p}{4L} \sum_{k=1}^{\infty} \lambda_k^2 [a_{x,k}^2 + a_{y,k}^2]. \quad (19)\]

B. Moment generating function

For calculating the probability density function \( P_{||}(z) \) we follow a procedure outlined in Ref. \[9\] and consider the moment generating function

\[
P_{||}(f) := \langle e^{-f(L-r_z(L))} \rangle_0 = \int_{-L}^{L} dz \, e^{-f(L-z)} P_{||}(z) = \int_0^{\infty} d\rho \, e^{-\rho \beta H} P_{||}(L - \rho). \quad (20)\]

Note that thermal averages have to be evaluated using the bare elastic free energy, Eq. \[1\]. Since for stiff chains configurations with large values for the stored length (“compression”) \( \rho = L - z \) are rather unlikely, we can extend the upper boundary of the integral in the last line of the preceding equation to infinity. This allows us to write the moment generating function as the Laplace transform of the distribution function \( P_{||}(z) \)

\[
P_{||}(f) = \int_0^{\infty} d\rho \, e^{-\rho \beta H} P_{||}(L - \rho). \quad (21)\]

For \( f = 0 \) the latter equation reduces to the normalization condition of the probability density function \( P_{||}(z) \) such that \( P_{||}(0) = 1 \).

Combining Eqs. \[18\] \[14\] and \[20\] the moment generating function can be put into the following path integral form

\[
P_{||}(f) = \int D[a(s)] \exp \left\{ -\frac{1}{2} \int_0^L ds \left[ \ell_p \dot{a}^2 + f a^2 \right] \right\}. \quad (22)\]
with the boundary conditions given by Eq. (13). This path integral is easily evaluated upon using the Fourier representation of the transverse tangent fields, Eq. (15), and noting that to harmonic order fluctuations in all transverse directions are statistically independent. We find in $d$ spatial dimensions

$$\mathcal{P}_\parallel(f) = \left(\int \prod_{k=1}^{\infty} \frac{d\alpha_k}{\mathcal{N}} \exp \left(-\frac{1}{4} \left[\frac{\lambda_k^2 \ell_p}{L} + fL \right] \alpha_k^2 \right) \right)^{(d-1)} = \prod_{k=1}^{\infty} \left(1 + \frac{fL^2}{\ell_p^2 \lambda_k^2} \right)^{-\frac{1}{2}d(1)},$$

where the normalization factor $\mathcal{N}$ of the path integral was chosen such that $\mathcal{P}_\parallel(0) = 1$. If $f \in \mathbb{R}_+$, the product may be rewritten as

$$\mathcal{P}_\parallel(f) = \left(\cosh \sqrt{\frac{fL^2}{\ell_p^2}} \right)^{-\frac{1}{2}d(1)}.$$

Note that the moment generating function, which also depends on the length scales $L$ and $\ell_p$, has the scaling form

$$\mathcal{P}_\parallel(f, L, \ell_p) = \tilde{\mathcal{P}}_\parallel(fL\parallel),$$

where we have defined the characteristic longitudinal length scale

$$L\parallel := \frac{L^2}{\ell_p}.$$

The formulas Eq. (23) and Eq. (24) are the basis for all subsequent calculations in this section, which are basically different forms of performing the inverse Laplace transform.

For future reference and comparison with the entropic forces we close this subsection with a discussion of the force-extension relation in the fixed force ensemble. It simply follows as the first moment of the moment generating function

$$\langle r_z(L) \rangle_f = L + \frac{\partial \ln \mathcal{P}_\parallel(f)}{\partial f} = L \left(1 - \frac{L(d-1) \coth \sqrt{fL\parallel}}{4\ell_p} \right),$$

where $f$ is the external force in units of the thermal energy $k_B T$. In the limit of small external forces this reduces to

$$\langle r_z(L) \rangle_f = L \left[1 - \frac{d-1}{4} L \frac{1}{\ell_p} + \frac{d-1}{12} \left(\frac{L}{\ell_p}\right)^2 fL \right],$$

which identifies $L\parallel$ as $4/(d-1)$ times the equilibrium stored length due to thermal fluctuations. We also recover the effective linear spring coefficient $k_\parallel = 12\ell_p^2/(d-1)k_B TL^4$, which was previously calculated in Ref. [15]. For strong stretching forces the extension saturates asymptotically as

$$\langle r_z(L) \rangle_f = L \left[1 - \frac{L(d-1)}{4 \ell_p \sqrt{fL\parallel}} \right].$$

In the limit of large compressional forces the weakly bending rod approximation breaks down and one has to use different approaches to evaluate the force-extension relation [10].

C. Probability density for the position of the polymer tip: analytical and MC results in 3d

We now return to the distribution function and the resulting entropic forces. Upon performing the inverse Laplace transform one gets (for details of the calculations see Appendix A 1)

$$\mathcal{P}_\parallel(z) = \frac{2}{L\parallel} \sum_{k=1}^{\infty} (-1)^{k+1} \lambda_k \exp \left[-\lambda_k^2 \frac{L - z}{L\parallel} \right].$$

Inspection of Eq. (30) immediately tells us that it can be written in scaling form

$$\tilde{\mathcal{P}}_\parallel(z, L, \ell_p) = L^{-1} \tilde{\mathcal{P}}_\parallel(\tilde{\rho}),$$

where we have made the dependence of the probability density on $L$ and $\ell_p$ explicit and introduced the scaling variable

$$\tilde{\rho} = \frac{L - z}{L\parallel}.$$

measuring the compression of the filament in units of $L\parallel$. This implies that data for the probability density of the polymer tip can be rescaled to fall on a scaling function $\tilde{\mathcal{P}}_\parallel(\tilde{\rho})$, shown as the solid curve in Fig. 2. Of course, since the analytical calculations are based on the mode analysis in the weakly bending limit such a universal scaling curve is obtained only for small enough stiffness parameters $\varepsilon$.

The probability density is strongly peaked towards full stretching, $\tilde{\rho} \to 0$, and falls off exponentially for large $\tilde{\rho}$, such that for $\tilde{\rho} \geq 0.3$

$$\tilde{\mathcal{P}}_\parallel(\tilde{\rho}) = \pi \exp \left(-\frac{1}{4} \pi^2 \tilde{\rho} \right)$$

is already an excellent approximation. The series expansion given by Eq. (30) converges well for all values of $z$ well below $L$, but its convergence properties become increasingly worse if $z$ approaches $L$. As detailed in Appendix A 2 one may also derive an alternative series representation of the tip distribution function which converges well close to full stretching

$$\tilde{\mathcal{P}}_\parallel(\tilde{\rho}) = \sum_{l=0}^{\infty} (-1)^l \sqrt{\frac{2l+1}{\pi \tilde{\rho}^2}} \exp \left[-\left(l + \frac{1}{2}\right)^2 \right].$$
Already the first term of Eq. (34)

\[ \hat{P}_\parallel(\hat{\rho}) = \frac{1}{\sqrt{\pi \rho^3}} \exp \left( -\frac{1}{4\hat{\rho}} \right), \]

(35)
gives an excellent fit for \( \hat{\rho} \leq 0.3 \). In particular, it captures the main feature of the distribution function, namely its maximum close to full stretching. The same approximate expression may also be obtained by evaluating the inverse Laplace transform using the method of steepest descent; see Appendix B. The asymptotic results given in Eq. (35) and Eq. (36) taken together give a representation of the scaling curve to a very high numerical accuracy. They are the analogues of the results found in Ref. 1 for a freely fluctuating filament; see also Ref. 11.

The MC data shown in Fig 2 have been obtained by using a standard algorithm for a discretized wormlike chain, similar to the one described in Ref. 4. As expected, the MC results agree very well with the analytical calculations for small values of \( \varepsilon \). From Fig 2 we can read off that the asymptotic stiff scaling regime remains valid up to stiffness parameters \( \varepsilon \approx 0.1 \); even for \( \varepsilon = 0.5 \) the shape of the scaling function resembles the MC data quite closely. As the polymer becomes more flexible the shape asymptotically becomes Gaussian; for \( \varepsilon = 3 \) a skew is still noticeable. Note that in the parameter range given in Fig 2 the width of the rescaled probability densities stays approximately the same and is hence well characterized by the longitudinal scale \( L_\parallel \).

D. Confinement free energy and entropic forces: 3d

Now we are in a position to calculate the restricted partition sum (cumulative probability distribution) \( Z_\parallel(\zeta) = \int_\zeta^{\infty} dz P_\parallel(z) \) by (formally) integrating the series expansion Eq. (30) term by term. This gives

\[ Z_\parallel(\zeta) = 1 - \int_\zeta^{\infty} dz P_\parallel(z) \]
\[ = 1 - 2 \sum_{k=1}^{\infty} (-1)^{k+1} \lambda_k^{-1} \left( 1 - e^{-\lambda_k^2(L-\zeta)/L_\parallel} \right) \]
\[ = 2 \sum_{k=1}^{\infty} (-1)^{k+1} \lambda_k^{-1} e^{-\lambda_k^2(L-\zeta)/L_\parallel}, \]

(36)

where in the first line we used the normalization of \( P_\parallel(z) \) and in the final line the identity

\[ \sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{2k - 1} = \frac{\pi}{4}. \]

(37)
The series expansion in Eq. (36) converges well for all values of \( \zeta \) well below \( L \). Alternatively, one may start from Eq. (34) and derive

\[ Z_\parallel(\zeta) = 1 + 2 \sum_{k=1}^{\infty} (-1)^{k} \text{erfc} \left( \frac{\lambda_k / \pi}{\sqrt{L - \zeta}/L_\parallel} \right), \]

(38)

which is well behaved for \( \zeta \) close to \( L \), and dominated by its first term. A second method to obtain Eq. (38) can be found in Appendix C.

From both series expansions it is evident that the restricted partition sum has the scaling property

\[ Z_\parallel(\zeta, L, \ell_p) = \tilde{Z}_\parallel(\tilde{\eta}), \]

(39)

where we have introduced the scaling variable

\[ \tilde{\eta} = \frac{L - \zeta}{L_\parallel}, \]

(40)

which measures the minimal stored length (compression) \( \eta = L - \zeta \) of the filament in units of \( L_\parallel \). The confinement free energy, \( \tilde{f}_\parallel(\tilde{\eta}) = -k_B T \ln \tilde{Z}_\parallel(\tilde{\eta}) \), corresponding to this partition function is shown in Fig 3. Again, the universal scaling function describes the MC data well for \( \varepsilon \leq 0.1 \). Note that for all values of \( \tilde{\eta} \) and the stiffness parameter \( \varepsilon \) the free energy is convex. This will turn out to be an important feature which distinguishes the 3d and 2d case.

Upon using Eq. (14) for the entropic force we find

\[ f_\parallel(\zeta) = \frac{k_B T}{L_\parallel} \frac{\tilde{P}_\parallel(\tilde{\eta})}{\tilde{Z}_\parallel(\tilde{\eta})}, \]

(41)

which immediately shows its scaling behavior and identifies \( k_B T/L_\parallel \) as the characteristic force scale. It is up to
a prefactor identical to the critical force

\[ f_c = \frac{\pi^2 \kappa}{4L^2} = \frac{\pi^2 k_B T}{4L_f} \]  

(42)

for the buckling instability of a classical Euler-Bernoulli beam [19]. It suggest to rewrite the entropic force as

\[ f_\parallel(\zeta, L, \ell_p) = f_c \tilde{f}_\parallel(\tilde{\eta}) , \]  

(43)

with the scaling function

\[ \tilde{f}_\parallel(\tilde{\eta}) := \frac{4}{\pi^2} \frac{\tilde{P}_\parallel(\tilde{\eta})}{Z_\parallel(\tilde{\eta})}. \]  

(44)

The analytical result for the scaling function \( \tilde{f}_\parallel(\tilde{\eta}) \), shown as the solid curve in Fig. 4, has several characteristic features. First of all, it is always monotonically increasing since the free energy is convex. For \( \tilde{\eta} \gtrsim 0.4 \), the scaling function is \( \tilde{f}_\parallel \approx 1 \) corresponding to \( f_\parallel \approx f_c \), i.e. a vanishing contribution of thermal fluctuations to the force. For smaller \( \tilde{\eta} \), corresponding to larger distances \( \zeta \) between the wall and the grafted end of the polymer, fluctuations reduce the force exerted on the wall by effectively shortening the polymer. For \( \zeta \to L \) (resp. \( \tilde{\eta} = 0 \)), the probability of the polymer to contact the wall becomes smaller and smaller until finally for \( \zeta = L \) only one configuration, namely the completely straight one, has \( r_\parallel(L) = 1 \). Hence the force must vanish for all \( \zeta \geq L \) (resp. \( \tilde{\eta} \leq 0 \)).

We have learned already in Section III C that there are excellent approximations to the scaling function for the probability density of the free polymer end for small values of the reduced stored length, Eq. (35). In the same way, the first term of Eq. (38) is an excellent approximation to the infinite series for \( \tilde{\eta} \ll 0.2 \). Thus we may write for the scaling function of the entropic force

\[ \tilde{f}_\parallel(\tilde{\eta}) = \frac{4 e^{-1/4\tilde{\eta}}}{\pi^{5/2} \tilde{\eta}^{3/2} (1 - 2 \text{erfc}(1/2\sqrt{\tilde{\eta}}))} \],  

(45)

which already describes most of the nontrivial shape of the scaling function. For \( \tilde{\eta} \gtrsim 0.2 \) it suffices to high accuracy to use the first two terms of Eq. (38), which gives

\[ \tilde{f}_\parallel(\tilde{\eta}) = \frac{1 - 3e^{-2\pi^2\tilde{\eta}}}{1 - \frac{1}{3} e^{-2\pi^2\tilde{\eta}}}. \]  

(46)

Upon inspection of Eq. (46) one may interpret the functional form of the entropic force as due to two effects. In the numerator we have the probability density for the position of the free end at the wall. This function shows a pronounced peak as one decreases the distance \( \zeta \) (resp. increases the scaling variable \( \tilde{\eta} \)). At the same time, the denominator, the cumulative distribution function, decreases with decreasing \( \zeta \). It is now a matter of how fast these changes occur what the ensuing shape of the scaling function for the entropic force will be. In the present case of a polymer in 3d the decrease in the cumulative distribution function seems to be fast enough to compensate the maximum in the probability density of the free polymer end such that the entropic force becomes a monotonically increasing function of \( \tilde{\eta} \).

From Fig. 4 one observes that the universal scaling curve is a lower bound to the MC data for all values of the stiffness parameter \( \varepsilon \). For fixed \( \varepsilon \) the entropic force always increases monotonically with increasing compression; for intermediate values \( \varepsilon \approx 2.5 \) there is a pronounced change in curvature at \( \tilde{\eta} \approx 0.25 \). For strong compression the results asymptote to the mechanical
limit \((k_B T = 0)\). This limit is not correctly reproduced within the harmonic approximation which gives
\[
 f_{\text{mech}}(\zeta) = f_c \Theta(L - \zeta),
\]
whereas the exact force-extension curve is a monotonous function in \(\zeta\) that is somewhat larger than \(f_c\) for \(\zeta < L\) and tends to \(f_c\) for \(\zeta \to L\).

One might finally ask, whether these entropic forces \(f_{\parallel}(\zeta)\) are related to the force extension relation discussed in section III B, \((r_z(L))_f = (r_z(L))_0 = k_{\parallel}^{-1} f + O(f^2)\) with \(k_{\parallel} = 6\kappa^2/k_B T L^4\). Rewriting these linear response result in scaling form we find,
\[
 f f_c = \frac{24}{\pi^2} \left( \eta - \frac{1}{2} \right). \tag{48}
\]
Comparing this with Fig.4 we see that the linear response result does not contain any information about the situation under investigation here. To the contrary, the initial rise of the force when \(\zeta\) becomes slightly smaller than \(L\) is highly nonlinear (see Eq. 15).

E. Distribution function and entropic forces: 2d

Analogous to the previous section the tip distribution function of a polymer confined to 2d, e.g. by two parallel glass plates, obeys a scaling law in the stiff limit
\[
 P_{\parallel}(z, L, \ell_p) = L_{\parallel}^{-1} \tilde{P}_{\parallel}(\tilde{\rho}) \tag{49}. \]
The scaling function may again be represented in terms of series expansions (see Appendix A 2). A series which converges well for small values of \(\tilde{\rho}\) reads
\[
 \tilde{P}_{\parallel}(\tilde{\rho}) = \sum_{i=0}^{\infty} \left( \frac{1}{i} \right) \frac{2i + 1}{\sqrt{2\pi} \tilde{\rho}^{3/2}} \exp \left[ -\frac{(l + \frac{1}{2})^2}{\tilde{\rho}} \right]; \tag{50}
\]
for an explicit formula for the binomial coefficient in Eq. 50 see Eq. A7. The scaling function, shown as the solid curve in Fig.6 has an overall shape which is quite similar to 3d with a pronounced maximum close to full stretching. The series approximations may again give useful approximate expressions for the shape. In the proximity of full stretching, the series given by Eq. 50 converges very fast such that already the first term
\[
 \tilde{P}_{\parallel}^{\langle}(\tilde{\rho}) = \frac{1}{8\pi \tilde{\rho}^{3/2}} \exp \left( -\frac{1}{16\tilde{\rho}} \right) \tag{51}
\]
is an excellent approximation for the whole series at least for \(\tilde{\rho} \leq 0.3\). As in 3d, a saddle point approximation also gives Eq. 51 (see Appendix B). Alternatively, as shown in Appendix A 2, one may derive a series expansion which converges well in the strong compression limit; see Eq. A11. For \(\tilde{\rho} \gtrsim 0.3\) it suffices to use the first term of this sum only which reads
\[
 \tilde{P}_{\parallel}^{>}(\tilde{\rho}) = \frac{\pi e^{-\pi^2/\tilde{\rho}/4}}{2\sqrt{2}} \left[ 1 + 1.5 e^{-5\pi^2/16} + 2 e^{-12\pi^2/16} + 2.5 e^{-21\pi^2/16} + 3 e^{-32\pi^2/16} \right]. \tag{52}
\]

Upon increasing the stiffness parameter the rescaled probability distribution deviates from the scaling function in the semiflexible limit and approaches a Gaussian. In contrast to 3d there is an intermediate parameter regime in the stiffness parameter where \(\tilde{P}_{\parallel}(\tilde{\rho})\) exhibits a marked shoulder. This feature of the distribution function has recently been identified and explained in terms of an interesting analogy with the physics of a random walker in shear flow [12].

Upon integrating Eq. 50 from \(-L\) to \(\zeta\) one obtains for the restricted partition sum
\[
 Z_{\parallel}(\zeta) = 1 - \sqrt{2} \sum_{k=0}^{\infty} \frac{(-1)^k (2k-1)!}{2^k k!} \frac{\text{erfc} \left( \frac{\lambda_{2k+1}}{2\sqrt{\eta}} \right)}{49}, \tag{53}
\]
with the same scaling variable \(\tilde{\eta}\) as in the previous section. Similarly, using Eq. A11 gives
\[
 Z_{\parallel}(\zeta) \approx \frac{1}{1.49} \sum_{k=0}^{\infty} \frac{(-1)^k 8^{k+1}}{k} \lambda_{2k+1}^{-1} e^{-\lambda_{2k+1}^2/4\tilde{\eta}} \tag{54}
\]
Hence, as in 3d, one finds for the free energy
\[
 F_{\parallel}(\zeta, L, \ell_p) = -k_B T \ln \tilde{Z}_{\parallel}(\tilde{\eta}) \tag{55}
\]
and the entropic force
\[
 f_{\parallel}(\zeta, L, \ell_p) = f_c \tilde{f}_{\parallel}(\tilde{\eta}) \tag{56}
\]
with the scaling function
\[
 \tilde{f}_{\parallel}(\tilde{\eta}) = \frac{4}{\pi^2} \frac{\tilde{Z}_{\parallel}(\tilde{\eta})}{\tilde{Z}_{\parallel}(\tilde{\eta})} \tag{57}
\]
and \(f_c = \pi^2 \kappa/4L^2\); see the solid curves in Fig.6 and Fig.7 for a plot of the scaling functions for the free energy and
indicated in the graph.

exhibits a change in curvature at \( \tilde{\eta} \). The results in 2d and 3d is that the effective free energy \( \epsilon \approx 5 \) as indicated in the graph.

The key difference between the results in 2d and 3d is that the effective free energy exhibits a change in curvature at \( \tilde{\eta} \approx 0.05 \) and as a result a pronounced peak in the entropic force. The peak is a pretty robust feature of the distribution function and vanishes only for very large values of \( \tilde{\eta} \).

In order to understand the physical origin of this peak it suffices to consider small values of \( \tilde{\eta} \). Then, using only the leading term of the series expansion Eq. (53), one obtains for the entropic force

\[
\tilde{f}_\parallel^<(\tilde{\eta}) = \frac{\sqrt{2} e^{-1/16\tilde{\eta}}}{\pi^{5/2} \tilde{\eta}^{3/2} (1 - \sqrt{2} \operatorname{erfc}[1/4\sqrt{\tilde{\eta}}])}.
\]

This has the same functional form as the corresponding expression in 3d, Eq. (55), but differs in some numerical factors. These differences can all be traced back to the strength \( \alpha \) of the essential singularity of the tip distribution function close to full stretching, \( \tilde{P}_\parallel(\tilde{\rho}) \propto \exp(-\alpha/\tilde{\rho}) \); compare Eq. (56) with Eq. (31). One may interpret this strength as a kind of phase space factor counting how fast the number of polymer configurations decreases as one approaches full stretching. It clearly shows that the maximum of the entropic force in 2d is of purely geometric origin. As an interesting consequence of this maximum one should note, that for most values of the reduced stored length \( \tilde{\eta} \) the entropic force exceeds the purely mechanical force given by the Euler buckling force.

**IV. GRAFTED POLYMER AT AN OBLIQUE ANGLE TO THE WALL**

The generic situation one encounters in a cellular system is that the polymer is inclined with respect to a membrane. Then we have to ask how the force derived above changes when the graft of the polymer is not orthogonal to the constraining wall but at some oblique angle \( \pi/2 - \vartheta \); see Fig. 8. Since the presence of the wall restricts the position of the polymer tip to

\[
r_z(L) \cos \vartheta + r_x(L) \sin \vartheta \leq \zeta
\]

one has to evaluate the restricted partition sum

\[
Z(\zeta, \vartheta) = \langle \Theta[\zeta - r_z(L) \cos \vartheta - r_x(L) \sin \vartheta] \rangle_0
= \int dx dz P(x, z) \Theta[\zeta - z \cos \vartheta - x \sin \vartheta]
\]

to find the entropic force.

**A. Probability distribution function of the tip**

This calculation requires the knowledge of the joint probability density of the tip

\[
P(x, z) := \langle \delta[r_x(L) - x] \delta[r_z(L) - z] \rangle_0.
\]

In Section III we have already analyzed the reduced distribution function \( P_\parallel(z) \) and found that its width is characterized by the scale \( L_\parallel = L^2/\ell_p \). Similarly, one can find an explicit expression for \( P_{\perp}(x) \) in harmonic approximation, where

\[
r_x(L) \approx \sum_{k=1}^{\infty} a_{x,k} \int_0^L ds \sin(\lambda_k s/L) = L \sum_{k=1}^{\infty} \lambda_k^{-1} a_{x,k}.
\]
and thus

$$P_\perp(x) = \int \frac{dq}{2\pi} e^{iqx} \left\langle \exp \left[ -i \frac{q}{2} \sum_{k=1}^\infty \frac{\lambda_k^{-1} a_{x,k}}{L} \right] \right\rangle$$

$$= \int \frac{dq}{2\pi} e^{iqx} \exp \left[ -\frac{q^2}{2} \sum_{k=1}^\infty \lambda_k^{-4} \right]. \quad (63)$$

With $\sum_{k=1}^\infty \frac{1}{(2k-1)^2} = \frac{\pi^4}{90}$, this gives a Gaussian dis-

tribution

$$P_\perp(x) = \frac{1}{\sqrt{2\pi L_\perp}} e^{-\frac{1}{2} x^2}, \quad (64)$$

where we have defined the characteristic transverse length scale

$$L_\perp = \sqrt{L^3/3\ell_p}. \quad (65)$$

Together with $L_\parallel$ these are the two length scales characterizing the width of the joint distribution function. This suggests to write the joint distribution function as

$$P(x, z, L, \ell_p) = \frac{1}{L_\parallel L_\perp} \tilde{P}(\tilde{x}, \tilde{z}) \quad (66)$$

in terms of dimensionless variables

$$\tilde{x} = \frac{x}{L_\perp}, \quad (67)$$

$$\tilde{z} = \frac{(L - z)}{L_\parallel}. \quad (68)$$

An explicit form of the joint distribution function can be calculated to harmonic order. For simplicity, we start with a polymer fluctuating only in the $x$-$z$-plane ($d = 2$). Then

$$P_2(x, z) = \int \frac{dq_x dq_z}{2\pi} e^{-i q_x z - i q_z x} \left\langle e^{i q_x r_x(L) + i q_z r_z(L)} \right\rangle_0$$

$$= \int \frac{dq_x dq_z}{2\pi} e^{i q_x (L - z) - i q_z x} \prod_k \left\langle \exp \left[ -1 \left( \frac{L q_z}{4} a_{x,k}^2 - \frac{L q_x}{\lambda_k} a_{x,k} \right) \right] \right\rangle$$

$$= \int \frac{dq_x dq_z}{2\pi} e^{i q_x (L - z) - i q_z x} \prod_k \sqrt{\frac{\lambda_k^2}{\lambda_k^2 + i q_z L_\perp}} \exp \left[ -\frac{3q_z^2 L_\perp^2}{\lambda_k^2 (\lambda_k^2 + i q_z L_\parallel)} \right]$$

$$= \frac{1}{L_\perp L_\parallel} \int \frac{dq_x dq_z}{2\pi} e^{i q_x \tilde{z} - i q_z \tilde{x}} \left( \prod_k \sqrt{\frac{1}{1 + i q_z \lambda_k^{-2}}} \right) \exp \left[ -\frac{3q_z^2}{2} \sum_k \lambda_k^2 \right]$$

$$= \frac{1}{L_\perp L_\parallel} \int \frac{dq_x dq_z}{2\pi} a_2(q_z) e^{i q_x \tilde{z} - i q_z \tilde{x}} \exp \left[ -\frac{3}{2} q_z^2 b(q_z) \right], \quad (69)$$

where for $z \in \mathbb{R}_+$ we have \[16\]

$$a_2(z) := \prod_k \sqrt{\frac{1}{1 + z \lambda_k^{-2}}} = \sqrt{\frac{1}{\cosh \sqrt{z}}}. \quad (70)$$

$$b(z) := 2 \sum_k \frac{1}{\lambda_k^2 (\lambda_k^2 + z)} = \sqrt{z} - \tanh \sqrt{z}. \quad (71)$$

For $d = 3$, the additional degrees of freedom associated with excursions in the $y$-direction lead to the replacement of $q_x a_x^2(k) + q_z a_z^2(k)$ by $q_x |a_x^2(k) + a_y^2(k)|$ which results in an additional factor of $\sqrt{1 + i q_z \lambda_k^{-2}}$ for each mode $k$. Thus, for general $d$, we have to replace $a_2(z)$ with

$$a_d(z) := \prod_k \left[ \frac{1}{1 + z \lambda_k^{-2}} \right]^{(d-1)/2}. \quad (72)$$

As $\Re[b(\bar{q}_z)] > 0$ for all $\bar{q}_z \in [-\infty, \infty]$, the Gaussian
integration over \( \tilde{q}_z \) in Eq. (69) can be performed by completing the square, such that

\[
\tilde{P}_d(\tilde{x}, \tilde{\rho}) = \int \frac{d\tilde{q}_z}{2\pi} e^{i\tilde{q}_z \tilde{\rho}} \frac{a_d(\tilde{q}_z)}{\sqrt{6\pi b(\tilde{q}_z)}} \exp \left[ -\frac{\tilde{x}^2 + \tilde{y}^2}{6b(\tilde{q}_z)} \right]. \tag{73}
\]

Along similar lines one may also calculate the full joint distribution function for a grafted polymer in \( d = 3 \),

\[
P_3(x, y, z) = \frac{1}{L^3 L\parallel} \int \frac{d\tilde{q}_z d\tilde{q}_y d\tilde{q}_x}{2\pi} a_3(\tilde{q}_z) \frac{a_3(\tilde{q}_y)}{6\pi b(\tilde{q}_x)} \exp \left[ -\frac{\tilde{x}^2 + \tilde{y}^2}{6b(\tilde{q}_x)} \right]
\]

\[
= \frac{1}{L^3 L\parallel} \tilde{P}_3(\tilde{x}, \tilde{y}, \tilde{\rho}). \tag{74}
\]

In addition to the poles of \( a_3(\tilde{q}_z) \) at \( \tilde{q}_z = 1\lambda_k^2 \) on the positive imaginary axis of the \( \tilde{q}_z \)-plane, the integrand also has singularities at the zeros \( 1\lambda_k^2 \) of \( b(z) \). Thus we continue by evaluating the integrals numerically.

### 1. Numerical evaluation of integrals

The integrand of Eq. (73) has no singularities on the real \( \tilde{q}_z \)-axis. Before attempting a numerical integration, we discuss the behavior of the different terms appearing in Eq. (73). For \( d = 3 \), we have

\[
a_3(z) = \prod_{k} \frac{1}{1 + z\lambda_k^2} = \frac{1}{\cosh \sqrt{z}}. \tag{75}
\]

For \( \tilde{q}_z \in \mathbb{R} \), the real and the imaginary part \( 1/\cosh \sqrt{u\tilde{q}_z} \) are respectively even and odd functions rapidly decaying in magnitude for \( \tilde{q}_z \rightarrow \pm \infty \). The real part of \( 1/b(\tilde{q}_z) \) is strictly positive and increasing with increasing \( |\tilde{q}_z| \). The imaginary part of \( 1/b(\tilde{q}_z) \) behaves asymptotically as \( 3 |b^{-1}(\tilde{q}_z)| \sim \tilde{q}_z \) leading to a second strongly oscillating contribution to the integrand of Eq. (73) besides \( \exp(\sqrt{u\tilde{q}_z}) \). In the interest of numerical stability of the integration, it is advantageous to rewrite the integrand appearing in Eq. (73) to

\[
\frac{1}{2\pi} e^{\sqrt{u}(\tilde{x}^2/6)} \frac{a_3(\tilde{q}_z)}{\sqrt{2\pi 3b(\tilde{q}_z)}} \exp \left[ -\frac{\tilde{x}^2}{6} (1/b(\tilde{q}_z) - 1) \right] \tag{76}
\]

for \( q \) larger than some fixed \( q_0 \).

### 2. Region of vanishing probability

Eq. (76) suggests that \( \tilde{\rho} = \tilde{x}^2/6 \) is a special situation. The probability density \( P(x, z) \) must vanish for points which are at distances greater than \( L \) from the graft: \( x^2 + z^2 \leq L^2 \). What does this translate to in the harmonic approximation? The largest value \( x^* \) of \( r_x(L) \) that can be obtained for a given value \( z^* \) of \( r_z(L) \) can be found from the variation of \( r_x(L) - \rho(z^* - r_z(L)) \) where \( \rho \) is a Lagrange multiplier. Using Eq. (18) and Eq. (22), this leads to \( a_{x,k} = a/\lambda_k \) where \( a \) is some number. We thus find

\[
x^* = L a \sum_{k=1}^{\infty} \lambda_k^{-2} = L a^2 \tag{77}
\]

and

\[
z^* = L - \frac{L}{4} a^2 \sum_{k=1}^{\infty} \lambda_k^{-2} = L - L a^2 \tag{78}
\]

resulting in

\[
\frac{L - z^*}{L} = \frac{1}{2} \left( \frac{x^*}{L} \right)^2. \tag{79}
\]

As \( L a^2 / L\parallel = 1/3 \), this is equivalent to

\[
\tilde{\rho}^* = \frac{1}{6} (\tilde{x}^*)^2. \tag{80}
\]

Hence \( \tilde{P}(\tilde{x}, \tilde{\rho}) \) has to vanish for \( \tilde{\rho} < \tilde{x}^2/6 \).

### 3. Results for the general distribution function

It is now straightforward to evaluate the integrals in Eq. (73) by some standard numerical method. The corresponding results are shown in Fig. 9 as contour plots of \( \tilde{P}(\tilde{x}, \tilde{\rho}) \) in \( d = 3 \) and \( d = 2 \), respectively. These analytical results compare very well with MC results for polymers with a stiffness parameter \( \varepsilon \leq 0.2 \); see a plot with \( \varepsilon = 0.1 \) in Fig. 10. There are deviations between the harmonic approximation and MC data for larger values of \( \varepsilon \) [14, 17, 20].

![FIG. 9: Contour plot of the probability density \( \tilde{P}(\tilde{x}, \tilde{\rho}) \) in \( d = 3 \) (top) and \( d = 2 \) (bottom).](image)
The density distribution essentially vanishes outside the parabola given by \( \bar{\rho} = \bar{x}^2/6 \), corresponding to the classical contour of the polymer in harmonic order. The main weight of \( \bar{\rho}(\bar{x}, \bar{\rho}) \) is concentrated close to this line, where the effect is stronger for \( d = 2 \). Profiles parallel to the \( \bar{\rho} \) direction are of a shape qualitatively similar to \( \bar{\rho}(\bar{\rho}) \) (Fig. 2) at least for small \( \bar{x} \). Profiles parallel to the \( \bar{x} \)-axis are not Gaussian. For small \( \bar{\rho} \lesssim 0.1 \), they are peaked at \( \bar{x} = 0 \) but unlike a Gaussian, they vanish for \( \bar{x}^2 > 6\bar{\rho} \). For larger \( \bar{\rho} \), they display a double-peaked shape. Both features would be completely missed by a factorization approximation \( \bar{\rho}(\bar{x}, \bar{\rho}) = \bar{\rho}(\bar{x})\bar{\rho}(\bar{\rho}) \). An elaborate discussion of the features of the distribution function in \( d = 2 \) and \( d = 3 \) as one increases the stiffness parameters or introduces some backbone elasticity will be the topic of a forthcoming publication.

The shape of the full joint probability distribution \( P_3(x, y, z) \) is best illustrated by plotting an isosurface, e.g. \( P_3(\hat{x}, \hat{y}, \bar{\rho}) = 0.1 \) as shown in Fig. 11. Due to rotational symmetry a density plot for \( P_3(x, y, z) \) may be obtained by rotating the contour plot of \( P_3(x, z) \) (Fig. 9) around the \( z \)-axis. Again MC and analytical results are identical for small \( \varepsilon \).

### B. Entropic forces: scaling functions

We are now in a position to evaluate the general expression Eq. (60) for the restricted partition sum. Before going into the details of the calculation it is instructive to have a look at the geometry of the problem in terms of the dimensionless variables \( \bar{x} \) and \( \bar{\rho} \). Recall that \( \bar{x} \) and \( \bar{\rho} \) are measuring the transverse displacement of the tip \( x \) and the stored length \( L - z \) in units of the characteristic transverse and longitudinal length scales, \( L_\perp \) and \( L_\parallel \), respectively. As can be inferred from Fig. 9 the wall crosses the \( \bar{x} \)- and \( \bar{\rho} \)-axis at

\[
\eta_\perp = \frac{L \cos \theta - \zeta}{L_\perp \sin \theta} \quad \text{and} \quad \eta_\parallel = \frac{L \cos \theta - \zeta}{L_\parallel \cos \theta},
\]

respectively; see Fig. 12. These are the two basic dimensionless variables characterizing the entropic forces exerted on the inclined wall. We also introduce the slope \( \mu = \tan \alpha \) of the constraining wall with respect to the \( \bar{x} \)-axis

\[
\mu = \frac{\eta_\parallel}{\eta_\perp} = \frac{L_\perp}{L_\parallel} \tan \vartheta = \frac{1}{\sqrt{3\varepsilon}} \tan \vartheta. \tag{82}
\]
As discussed above the finite length of the polymer gives a constraint on the reduced stored length \( \bar{\rho} \) such that it has to be larger than \( \bar{x}^2 / 6 \), i.e. above the parabola drawn in Fig.12. Hence, just the points on the constraining wall inside the parabola are accessible to the tip of the polymer. As one moves the wall further away from the grafted end, the number of contact points decreases and finally reduces to zero when the wall becomes tangent to the parabola. In this limit, where

\[
\eta_{||}^2 = -\frac{3}{2} \mu^2
\]

the force exerted on the wall vanishes.

We may now write the restricted partition sum in terms of the reduced stored length \( \eta_{||} \) and the slope of the wall \( \mu \)

\[
Z(\zeta, \vartheta) = \tilde{Z}(\eta_{||}, \mu),
\]

where

\[
\tilde{Z}(\eta_{||}, \mu) = \frac{1}{L^2} \tilde{Z}(\eta_{||}, \mu) = \frac{1}{2} \text{rfc} \frac{\eta_{||}}{2 \mu} \left( e^{\mu q} (a_3(q) e^{2 \xi(\mu q)^2 b(q)} - e^{\xi(\mu q)^2}) \right) - \int_0^\infty \frac{dq}{\pi q} \left( e^{\mu q} (a_3(q) e^{2 \xi(\mu q)^2 b(q)} - e^{\xi(\mu q)^2}) \right),
\]

as shown in Appendix D. The force is again found by taking the derivative of \( \eta_{||} \). The force increases monotonically in 2d and 3d. Whereas the force increases monotonically with increasing \( \delta \eta_{||} \) for 3d, it shows a pronounced maximum in 2d, the physical origin of which is the same as

\[
\delta f(\eta_{||}, \mu) = \frac{4}{\pi^2} \left( \eta_{||} - \eta_{||}^2 \right) \left( \eta_{||} + 3 \mu^2 / 2 \right)
\]

for \( \vartheta = 0 \). The maximum in 2d vanishes upon increasing \( \mu \), which can either be understood as an increase in the inclination angle or an increase in the persistence length; see Eq. (86).

For comparison MC data are given for a particular value of the stiffness parameter, \( \varepsilon = 0.1 \). In this stiff regime the analytical results compare very well with the MC data, except for large values in the stored length where the harmonic approximation is expected to become invalid.

In Fig. 13 the analytical results for the scaling function \( \tilde{f}(\eta_{||}, \mu) \) of the entropic force are shown as a function of \( \delta \eta_{||} = \eta_{||} - \eta_{||}^2 \), for a series of values for \( \mu \). Since we have subtracted off the critical value of the reduced stored length \( \eta_{||}^2 \), the forces vanish for \( \delta \eta_{||} \leq 0 \). There is a dramatic difference in the shape of the force-distance curves in 2d and 3d. Whereas the force increases monotonically with increasing \( \delta \eta_{||} \) for 3d, it shows a pronounced maximum in 2d, the physical origin of which is the same as

\[
\eta_{||} = \frac{k_B T}{L_\perp \sin \vartheta} f(\eta_{||}, \mu)
\]

(90)
where

\[ \tilde{f}(\eta, \mu) = \mu \frac{\pi^2}{4} \tilde{f}(\eta/\mu, \mu). \] (91)

Like in the previous scaling plot the force should vanish for \( \delta \eta_\parallel < 0 \), which in terms of \( \eta_\perp \) reads \( \eta_\perp < -\frac{3}{2} \mu \).

Again, there is a marked difference between 2d and 3d results; see Fig. 14. We also observe that the scaling function \( \tilde{f}(\eta, \mu) \) asymptotically approaches a limiting curve for \( \mu \to \infty \), which for a fixed value of \( \varepsilon \) corresponds to \( \vartheta \to \pi/2 \). It turns out, as we will show now, that this limiting behavior can well be explained within a factorization approximation \( P(x, z) \approx P_\parallel(z)P_\perp(x) \). Then, \( \mathcal{Z}(\zeta, \vartheta) \) simplifies to

\[ \mathcal{Z}(\zeta, \vartheta) = \int dz P_\parallel(z) \mathcal{Z}_\perp(\zeta \sin^{-1} \vartheta - z \cot \vartheta). \] (92)

FIG. 14: Scaling function \( \tilde{f}(\eta_\perp, \mu) \) in \( d = 3 \) (top) and \( d = 2 \) (bottom) for a series of values for \( \mu \) (solid lines). For large \( \mu \), the scaling function \( \tilde{f}(\eta_\perp, \mu) \) asymptotically converges to \( \tilde{f}_\perp(\eta_\perp) \) obtained within a factorization approximation. The MC data indicated by different symbols in the graphs are given for a fixed stiffness parameter \( \varepsilon = 0.1 \).

is the restricted partition sum for the transverse fluctuations. The longitudinal distribution function \( P_\parallel(z) \) is, for small \( L/\ell_p \), strongly peaked at \( z \approx L \) with a characteristic width of \( L_\parallel \), and \( \mathcal{Z}_\perp \) varies on the scale \( L_\perp \). Then, for \( \mu \gg 1 \), the width of the longitudinal distribution function is much smaller than the transverse restricted partition sum, such that the integration over \( P_\parallel \) can be approximated by \( \mathcal{Z}(\zeta, \vartheta) \approx \mathcal{Z}_\perp(\zeta - L \cos \vartheta \sin^{-1} \vartheta) \) which upon using that the transverse distribution function is a simple Gaussian, Eq. (64), results in

\[ \mathcal{Z}(\zeta, \vartheta) \approx \frac{1}{2} \text{erfc} \frac{\eta_\parallel}{\sqrt{2}} =: \tilde{\mathcal{Z}}_\perp(\eta_\parallel) \] (94)

This approximation fails when \( \mu \approx 1 \), which defines an angle

\[ \vartheta_c = \arctan(L_\parallel/L_\perp) \approx \sqrt{3L/\ell_p} \] (95)

well above which the factorization approximation is valid. The entropic force is then

\[ f(\zeta, \vartheta) = \frac{k_B T}{L_\perp \sin \vartheta} \tilde{f}_\perp(\eta_\parallel), \] (96)

where

\[ \tilde{f}_\perp(\eta_\parallel) = -\frac{\tilde{\mathcal{Z}}_\perp(\eta_\parallel)}{\mathcal{Z}_\perp(\eta_\parallel)} = \sqrt{\frac{2}{\pi}} \text{erfc}(\eta_\parallel/\sqrt{2}). \] (97)

This result for the scaling function of the entropic force is indicated as the thick solid line in Fig. 14. It becomes exact in the limit \( \vartheta = \pi/2 \), where starting from Eq. (96), one can integrate out the longitudinal coordinate to end up with

\[ \mathcal{Z}(\zeta, \pi/2) = \frac{1}{2} \text{erfc} \left( \frac{-\zeta}{\sqrt{2L_\perp}} \right). \] (98)

Finally, for large \( \zeta \), one recovers the linear response result \( f(\zeta, \pi/2) = 3\kappa \zeta/L^3 \).

If we compare the results of the factorization approximation for \( \vartheta > \vartheta_c \), Eq. (64) and Eq. (97), to Eq. (2) and Eq. (5) of Ref. [21], one realizes that they are almost identical up to the minor difference that Mogilner and Oster define their \( \kappa_0 \) to be \( 4\kappa/L^3 \) where it actually should be \( 3\kappa/L^3 \). The factor 4 in Ref. [21] instead of the correct value 3 is the result of assuming that the minimal energy configuration of a thin rod bent by application of a force to its non-grafted end has constant radius of curvature for small deflections, which is not the case. In fact, the boundary condition of the mechanical problem forces the curvature to vanish at the non-grafted end. In Ref. [21] the entropic force was calculated by taking into account transverse fluctuations of the grafted polymer.
only and completely disregarding any stored length fluctuations. Here, the factorization approximation, which treats longitudinal and transverse fluctuations as independent, gives the same result for inclination angles \( \vartheta > \vartheta_c \). The reason behind the validity of the asymptotic results, Eq. (96) and Eq. (97), is that the tip distribution function is much narrower in the longitudinal than the transverse direction for \( \vartheta \gg \vartheta_c \sim \sqrt{L/\ell_p} \). Hence the range of validity of the factorization approximation becomes larger as the polymers become stiffer. Of course, the analysis in Ref. [21] has to fail for small inclination angles since it does not account for stored length fluctuations at all. This is seen most dramatically for \( \vartheta = 0 \), where such an approximation would give no force at all in contrast to what we find in Section III.

C. Entropic forces: explicit results

The analysis in the previous section gives the full scaling picture for the entropic forces as a function of the scaling variables \( \eta_\parallel \) and \( \eta_\perp \). Here we discuss our findings in terms of the actual distance of the grafted end to the wall \( \zeta \), the inclination angle \( \vartheta \), and the stiffness parameter \( \varepsilon = L/\ell_p \), which may be more convenient for actual applications. Of course, the disadvantage of such a representation is that we now have to give the results for particular values of the stiffness parameter. In this section we also restrict ourselves to the discussion of filaments which are allowed to fluctuate in 3d.

In Figs. 15 and 16 the force \( f \) in units of the Euler buckling force \( f_c \) is shown as a function of \( \zeta \) (in units of the total filament length \( L \)) for a series of values of \( \vartheta \) and vice versa; the stiffness parameter has been taken as \( \varepsilon = 0.1 \). Recall that the angle \( \vartheta = 0 \) corresponds to a wall perpendicular to the orientation of the grafted end of the polymer, which has been discussed in detail in Section III. Upon increasing the inclination angle \( \vartheta \) the entropic force decreases for all given values of \( \zeta \). This is to be expected since the wall then cuts off less from the probability cloud of the polymer tip. For the same reason the forces also decrease with increasing \( \zeta \) for a given value of \( \vartheta \). The analytical results (solid lines) agree well with the MC data for not too small values of \( \zeta \). The deviations grow larger upon decreasing the distance between the wall and the grafted end. Then non-linear effects not taken into account by our weakly bending approximation set in.

In the limit as the inclination angle approaches \( \pi/2 \) it is certainly no longer justified to calculate the entropic force by assuming that only the polymer tip is not allowed to penetrate the membrane. Then, one has to take into account the fact that also the body of the polymer is constrained by the presence of the wall. Since this reduces the number of allowed polymer configurations even further this effect is expected to lead to an enhancement of the entropic force. Indeed this is the case, as one may infer from Fig. 17 where we show a comparison with MC simulation accounting for these constraints. One also notes that the enhancement of the entropic forces becomes largest as \( \vartheta \to \pi/2 \) and the distance between the wall and the grafted end becomes small; a full account of this effect will appear in Ref. [22].

Finally, we would like to compare our full results with the factorization approximation discussed in the previous section, Eq. (97), which when corrected for some minor factor is identical to the results given in Ref. [21]. The comparison is given in Fig. 18 for a stiffness parameter \( \varepsilon = 0.1 \). In the limit of large inclination angles well above \( \vartheta_c \approx 30^\circ \), there is excellent agreement between the factorization approximation and the full results for not too small values of \( \zeta \). As one approaches \( \vartheta_c \) the range of

FIG. 16: Analytical and MC simulation results for the entropic force \( f/f_c \) as a function of the inclination angle \( \vartheta \) (in degrees) for a series of distances to the wall \( \zeta/L = 0.99, 0.985, \ldots, 0.95 \).

FIG. 15: Analytical and MC simulation results for the entropic force \( f/f_c \) as a function of the distance of the grafted end from the wall \( \zeta/L \) for a series of inclination angles \( \vartheta = 17, \ldots, 89 \) with steps 9 (in degree).
validity of the factorization approximation shrinks and finally it becomes invalid for \( \vartheta < \vartheta_c \).

To illustrate the applicability of the factorization approximation let us take some examples. For the cytoskeletal filament F-actin with a contour length 100 nm and persistence length \( \ell_p = 15 \mu m \), the stiffness parameter becomes \( \varepsilon = 0.006 \) which gives \( \vartheta_c \approx 7.6^\circ \). Upon increasing the stiffness parameter to \( \varepsilon = 0.1 \), which amounts to changing the contour length to a value of \( L = 1.6\mu m \), the critical angle \( \vartheta_c \) increases to 28.7°.

V. SUMMARY AND CONCLUSIONS

In summary, we have presented analytical calculations and extensive Monte Carlo simulations for the entropic force \( f \) exerted by a grafted polymer on a rigid obstacle (wall). The scale for the magnitude of the entropic force is given by the Euler buckling force \( f_c \propto k_B T \ell_p / L^2 \). The stiffness parameter \( \varepsilon = L / \ell_p \) discerns the two universal regimes of a Gaussian chain (\( \varepsilon \gg 1 \)) and a semiflexible chain (\( \varepsilon \ll 1 \)). In this manuscript we have mainly focused on the stiff limit, where analytical calculations using a weakly bending rod approximation are possible. In comparing our results with Monte Carlo simulations we have found that the range of applicability of the results obtained in the stiff limit extend to stiffness parameters as large as \( \varepsilon = 0.1 \). Qualitatively the asymptotic results remain valid even up to \( \varepsilon = 1 \).

For the simplest possible geometry, where the polymer is perpendicular to the wall, located at a distance \( \zeta \) from the grafted end, our analytical calculations show that the entropic force obeys a scaling law in the stiff limit

\[
  f_{\parallel}(\zeta, L, \ell_p) = f_c \tilde{f}_{\parallel}(\tilde{\eta})
\]

with the scaling variable \( \tilde{\eta} = (L - \zeta) / L \) measuring the minimal compression of the filament in units of the longitudinal width of the tip distribution function \( L_{\parallel} = L^2 / \ell_p \), and \( f_c \) the Euler buckling force of a classical beam. For small values of the scaling variable we have derived a simple analytical expression, Eq. (99),

\[
  \tilde{f}_{\parallel}(\tilde{\eta}) = \frac{4}{\pi^{5/2}} \frac{\exp(-1/4\tilde{\eta})}{\tilde{\eta}^{3/2} \left[ 1 - 2erfc(1/2\tilde{\eta}) \right]}
\]

and a corresponding formula in 2d, Eq. (100), which describe the full scaling function to a high numerical accuracy for \( \tilde{\eta} \leq 0.2 \). For \( \tilde{\eta} \geq 0.2 \) there are equally simple expressions, as for example Eq. (101) for 3d. We expect these formulas to be useful for molecular models of cell motility. The shape of the scaling function shows dramatic differences between 2d and 3d, which are of geometric origin. In 3d the entropic forces always stay below the Euler buckling force. In contrast, in 2d it is larger than the mechanical limit for most of the parameter space and exhibits a pronounced maximum at small values of the scaling variable \( \tilde{\eta} \) before it steeply drops to zero as \( \zeta \to L \).

Extensive Monte Carlo simulations confirm these analytical results and show that their range of applicability is \( \varepsilon \leq 0.1 \). For larger values of the stiffness parameter there are clear deviations from the stiff scaling limit, which become qualitative for \( \varepsilon \geq 1 \). Features of the stiff limit, such as the maximum in the entropic force, are visible even for \( \varepsilon \) as large as 4.
For a polymer inclined at an angle $\vartheta$ with respect to the wall also the transverse width $L_{\perp} = \sqrt{L_y^2 / 3 \ell_{\rho}}$ of the tip distribution function plays a significant role; note that the ratio $L_{\parallel} / L_{\perp} = \sqrt{3 \varepsilon}$. The entropic force can now be written in the scaling form

$$f(\zeta, \vartheta; L, \ell_{\rho}) = f_{\varepsilon}(\vartheta) \tilde{f}(|\eta_{\parallel}|, \eta_{\perp}),$$

where $\eta_{\perp} = (L \cos \vartheta - \zeta) / (L_{\perp} \sin \vartheta)$, $\eta_{\parallel} = (L \cos \vartheta - \zeta) / (L_{\parallel} \cos \vartheta)$ and $f_{\varepsilon}(\vartheta) = f_{\varepsilon} / \cos \vartheta$. It turned out that a proper choice of scaling variables are $\mu = |\eta_{\parallel}| / \eta_{\perp} = (L_{\parallel} / L_{\perp}) \tan \vartheta$ and $\eta_{\parallel}$ or $\eta_{\perp}$ depending on whether the inclination angle is smaller or larger than a characteristic angle $\vartheta_{c} = L_{\parallel} / L_{\perp}$, i.e. $\mu_{c} = 1$. Upon increasing the inclination parameter $\mu$ the shape of the scaling function changes from a step-function-like form at $\mu = 0$ to a purely convex shape as $\mu \to \infty$. The limit $\mu \to \infty$ either corresponds to $\vartheta \to \pi / 2$ or for a fixed $\vartheta \neq 0$ to the stiff limit $\varepsilon \to 0$. For 2d, in addition, the maximum vanishes at $\mu \approx 0.6$.

In the limit of inclination angles which are much larger than the characteristic angle $\vartheta_{c}$, we have found that an approximation, Eq. \[17\] and Eq. \[18\], based on factorizing the joint probability distribution of the polymer tip gives an excellent asymptotic representation of the full analytical results:

$$f(\zeta, \vartheta) = \frac{k_{B} T}{L_{\perp} \sin \vartheta} \sqrt{\frac{2}{\pi}} \frac{e^{-\eta_{\perp}^{2} / 2}}{\text{erfc}(\eta_{\perp} / \sqrt{2})}.$$  \hspace{1cm} (102)

It is simpler than the full scaling form since it only depends on a single scaling variable. Up to minor factors this asymptotic formula for the entropic force is mathematically identical to the results found in Ref.\[21\], which was derived upon assuming that the tip of the polymer fluctuates perpendicular to its contour only. Since $\tan \vartheta_{c} \propto \sqrt{\varepsilon}$ the range of applicability of this results grows with increasing stiffness parameter. For example, $\vartheta_{c}$ equals approximately 30° and 10° for stiffness parameter $\varepsilon$ equal to 0.1 and 0.006, respectively. For $\vartheta \leq \vartheta_{c}$ the factorization approximation fails completely, since it gives an incorrect description of the longitudinal stored length fluctuations.

Then, a full analysis in terms of a two parameter scaling function is necessary.

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APPENDIX A: INVERSE LAPLACE

TRANSFORM OF THE MOMENT GENERATING

FUNCTION

In this appendix we collect our calculations of the inverse Laplace transform of the moment generating functions. This will give as two sets of series representations, which show good convergence properties either close to full stretching or for strong compression of the filament.

1. Series representation of the 3d tip distribution function for large stored length

Starting from the moment generating function $P_{\parallel}(f)$ one can calculate the distribution function $P_{\parallel}(z)$ by an inverse Laplace, i.e. an integral along the imaginary axis,

$$P_{\parallel}(z) = \int_{-i \infty}^{+i \infty} \frac{df}{2 \pi i} e^{f(z) - L_{\parallel}} P_{\parallel}(f).$$  \hspace{1cm} (A1)

Since the moment generating function

$$P_{\parallel}(f) = \prod_{k=1}^{\infty} \left(1 + \frac{4 f L_{\parallel}^{2} (2k - 1)^{2} \pi^{2}}{\ell_{\rho} (2k - 1)^{2} \pi^{2}}\right)^{-1}$$  \hspace{1cm} (A2)

has poles at $f_{k} = -\lambda_{k}^{2} L_{\parallel}^{2} / (2k - 1)^{2}$ with $k = 1, 2, 3, ...$ only along the negative real axis, standard residuum calculus gives

$$P_{\parallel}(f) = \sum_{k=1}^{\infty} \exp \left[-(L - z) \lambda_{k}^{2} \ell_{\rho} / L_{\parallel}^{2}\right] \prod_{l \neq k} \left(1 - \frac{(2k - 1)^{2}}{(2l - 1)^{2}}\right)^{-1} \left(\frac{L_{\parallel}^{2}}{\ell_{\rho} \lambda_{k}^{2}}\right)^{-1}$$  \hspace{1cm} (A3)

Using $\prod_{k=1}^{\infty} \left(1 - \frac{z^{2}}{(2k - 1)^{2}}\right) = \cos \left(\frac{\pi z}{2}\right)$ \[16\], the product term can be written as

$$\prod_{l \neq k} \left(1 - \frac{(2k - 1)^{2}}{(2l - 1)^{2}}\right)^{-1} = \lim_{k' \to k} \left(1 - \frac{(2k' - 1)^{2}}{(2k - 1)^{2}}\right) \prod_{l \neq k} \left(1 - \frac{(2k - 1)^{2}}{(2l - 1)^{2}}\right)^{-1} = \lim_{k' \to k} \left(1 - \frac{(2k' - 1)^{2}}{(2k - 1)^{2}}\right) \cos^{-1} \left(\frac{\pi}{2} (2k' - 1)\right) = \frac{2 (-1)^{k+1}}{\pi} \frac{2}{2k - 1} = 2 (-1)^{k+1} \frac{1}{\lambda_{k}}.$$  \hspace{1cm} (A4)
Hence we find

\[
P_\parallel(z) = 2L_-^{-1} \sum_{k=1}^{\infty} (-1)^{k+1} \lambda_k \exp \left[ -\lambda_k^2 (L - z)/L_\parallel \right]
\]  

(A5)

with the characteristic longitudinal length scale \(L_\parallel = L^2/\ell_p\).

2. Series representation for the tip distribution function close to full stretching: general \(d\)

We begin the analysis with the two-dimensional case, where

\[
P_\parallel(f) = \prod_{k=1}^{\infty} \left( 1 + \frac{f L_\parallel}{\lambda_k} \right)^{-1/2} = \sqrt{\frac{1}{\cosh \sqrt{fL_\parallel}}}.
\]  

(A6)

For the derivation of our first series representation we start from the product formula for the moment generating function. In this representation one has branch cuts on the negative real axis at \(\tilde{\rho} = f L_\parallel = -\lambda_k^2\) for \(k \in \mathbb{N}\). We now deform the contour in the complex plane such that we enclose the negative real axis. Then

\[
\tilde{P}_\parallel(\tilde{\rho}) = \int_{-\infty}^{+\infty} \frac{d\tilde{\rho} \tilde{P}_\parallel(\tilde{f})}{2\pi i} e^{i\tilde{\rho} \tilde{f}} = \int_{-\infty}^{0} \frac{d\tilde{\rho} \tilde{P}_\parallel(\tilde{f} - i\epsilon)}{2\pi i} e^{i\tilde{\rho} \tilde{f}} + \int_{0}^{+\infty} \frac{d\tilde{\rho} \tilde{P}_\parallel(\tilde{f} + i\epsilon)}{2\pi i} e^{i\tilde{\rho} \tilde{f}}
\]

where \(\epsilon \to 0\). To proceed we need to evaluate the product formula on the negative real axis. We find for \(x \in [2k + 1, 2k + 3]\)

\[
\lim_{\epsilon \to 0} \prod_{l=1}^{\infty} \int_{-\infty}^{+\infty} \frac{1}{1 - \frac{x^2 + \epsilon \cos x}{\lambda_l^2}} = (\mp 1)^k \frac{1}{\sqrt{\cos x}}
\]  

(A8)

Upon substituting \(y^2 = \tilde{f}\) this finally results in the series expansion

\[
\tilde{P}_\parallel(\tilde{\rho}) = 2 \sum_{n=0}^{\infty} (-1)^n \int_{\lambda_{2n+1}}^{\lambda_{2n+2}} dy \frac{y e^{-y^2 \tilde{\rho}}}{\sqrt{\cos y}}.
\]  

(A9)

For large values of \(\tilde{\rho}\), corresponding to a significant compression of the polymer, the integral is dominated by the contribution from the interval \([\pi/2, 3\pi/2]\), such that the leading factor will be proportional to \(\exp(-\pi^2 \tilde{\rho}/4)\). In order to evaluate \(\tilde{P}_\parallel(\tilde{\rho})\) further, we may average \(ye^{-y^2 \tilde{\rho}}\) over the interval and approximate the integral as

\[
\int_{\lambda_{2n+1}}^{\lambda_{2n+2}} dy \frac{y e^{-y^2 \tilde{\rho}}}{\sqrt{\cos y}} \approx \frac{1}{5} \sum_{m=4}^{8} \lambda_{2n+\frac{m}{2}} \exp \left[ -\lambda_{2n+\frac{m}{2}}^2 \tilde{\rho} \right] \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} dy \frac{dy}{\sqrt{\cos y}}
\]  

(A10)

such that we finally get

\[
\tilde{P}_\parallel(\tilde{\rho}) \approx \frac{1}{N} \sum_{n=0}^{\infty} (-1)^n \sum_{m=4}^{8} \lambda_{2n+\frac{m}{2}} \exp \left[ -\lambda_{2n+\frac{m}{2}}^2 \tilde{\rho} \right],
\]  

(A11)

where

\[
N^{-1} = \frac{2}{5\pi} \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} dy \frac{dy}{\sqrt{\cos y}} \approx 0.67.
\]  

(A12)

Next we drive a series representation suitable for small values of \(\tilde{\rho}\). We use that for \(f \in \mathbb{R}_+\) one has \(\cosh x = \frac{1}{2}(e^x + e^{-x})\) and the generalized binomial theorem, this can be expanded to give

\[
P_\parallel(f) = \frac{1}{\sqrt{\cosh \sqrt{fL_\parallel}}}.
\]  

(A13)

\[
P_\parallel(f) = \sqrt{2} \sum_{l=0}^{\infty} \left( \frac{-1}{l} \right)^{l+1/2} e^{-(2l+1/2) \sqrt{fL_\parallel}},
\]  

(A14)
which is a holomorphic function on \( \mathbb{C} \setminus \mathbb{R}_- \). Hence by the theorem of identity from complex calculus this formula remains valid \( \forall f \in \mathbb{C} \setminus \mathbb{R}_- \). Substituting \( y = \sqrt{fL} \) transforms Eq. (A1) to

\[
\tilde{P}_\parallel(\tilde{\rho}) = \int_{-\infty}^{\infty+i} \frac{dy}{\pi} e^{y^2 \tilde{\rho}} y \tilde{P}_\parallel(y^2).
\] (A15)

Inserting the series representation Eq. (A14) and using the integral representation

\[
D_1(z) = \sqrt{2\pi e^\frac{z^2}{2}} \int_{-\infty}^{\infty+i} ds \frac{1}{2\pi i} \exp\left[-zs + \frac{s^2}{2}\right]
\] (A16)

for the parabolic cylinder function \( \mathbf{16} \) as well as

\[
\left( -\frac{1}{2} \right) = (-1)^l \frac{(2l - 1)!!}{2^l!},
\] (A17)

where \( n!! = n(n-2)(n-4) \ldots \) yields

\[
\tilde{P}_\parallel(\tilde{\rho}) = \frac{1}{\sqrt{\pi \tilde{\rho}}} \sum_{l=0}^{\infty} (-1)^l \frac{(2l - 1)!!}{2^l!} \exp\left[-\frac{(l + \frac{1}{2})^2}{2 \tilde{\rho}}\right] D_1\left(\frac{2l + \frac{1}{2}}{\sqrt{2 \tilde{\rho}}}\right).
\] (A18)

With \( D_1(x) = xe^{-x^2/4} \) Eq. (A13) becomes Eq. (50).

Finally, all the calculations are easily generalized to general spatial dimensions \( d \). One finds the series representation

\[
\tilde{P}_\parallel(\tilde{\rho}) = 2^{d/2} \frac{1}{\sqrt{2\pi}} \sum_{l=0}^{\infty} \left( -\frac{1}{2} \right)^{(d-1)} \left( \frac{l + \frac{1}{2}}{\tilde{\rho}^{d/2}} \right) \exp\left[-\frac{(l + \frac{d-1}{2})^2}{\tilde{\rho}}\right]
\] (A19)

which is the fast converging for small \( \tilde{\rho} \).

**APPENDIX B: SADDLE POINT APPROXIMATION**

Starting from Eq. (A11) and introducing \( \delta = fL_\parallel \) gives

\[
P_\parallel(z) = \int_{-\infty}^{+\infty} \frac{df}{2\pi i} e^{fL_\parallel \delta} \cosh^{-1} \sqrt{fL_\parallel} = L_-^{-1} \int_{-\infty}^{+\infty} \frac{df}{2\pi i} \frac{2e^{f\delta}}{e^{\sqrt{f}} + e^{-\sqrt{f}}}.
\] (B1)

We are interested to the asymptotic result of the integral close to full stretching \( \tilde{\rho} \to 0 \). Upon substituting \( f = \xi/\tilde{\rho}^2 \) one finds

\[
P_\parallel(z) = \frac{2}{\tilde{\rho}^2 L_\parallel} \int_{-\infty}^{+\infty} d\xi \frac{\exp[f(\xi)/\tilde{\rho}]}{1 + \exp[-2\sqrt{\xi}/\tilde{\rho}]}
\] (B2)

where \( f(\xi) = \xi - \sqrt{\xi} \). Since the function \( f(\xi) \) has a global maximum at \( \xi_0 = 0.25 \) the main contribution to the integral in the limit \( 1/\tilde{\rho} \to \infty \) comes from the integration along the curve of steepest descent which passes through \( \xi_0 \). We need to find this curve such that \( 3[f(\xi)] = \text{constant} = 3[f(\xi_0)] = 0 \). We write \( \sqrt{\xi} = \sqrt{a}(1 + is) \) in terms of the curve parameter \( s \). Then the condition \( 3[f(\xi)] = 0 \) gives \( a = 1/4 \), and the curve of steepest descent is given in terms of \( \Re[\xi] = \frac{1}{2}(1 - s^2) \) and \( 3[\xi] = 2as \), which is a parabola parameterized by \( s \). The saddle point approximation amounts to a contour integral along this parabola, where \( f(\xi) = -(1 + s^2)/4 \), such that

\[
P_\parallel(z) = \frac{1}{L_\parallel \tilde{\rho}^2} \int_{-\infty}^{+\infty} ds \frac{1}{2\pi i} \exp\left[\frac{-s^2}{4\tilde{\rho}}\right] = \frac{1}{\sqrt{\sqrt{\pi \tilde{\rho}^3 L_\parallel}}} \exp\left[-\frac{1}{4\tilde{\rho}}\right].
\] (B3)

To the leading order in \( \tilde{\rho} \) we get

\[
P_\parallel(z) = \sqrt{\frac{\pi}{8\pi \tilde{\rho}^3 L_\parallel}} \exp\left[-\frac{1}{16\tilde{\rho}}\right].
\] (B5)

**APPENDIX C: JACOB TRANSFORMATION OF THE RESTRICTED PARTITION SUM \( \tilde{Z}_\parallel(\zeta) \)**

To unclutter the formulas in this section, we use the generic argument \( x \equiv \eta_\parallel \). \( \tilde{Z}_\parallel(x) \) can be written as

\[
\tilde{Z}_\parallel(x) = 2 \int_0^\infty dy \sum_{k=-\infty}^{\infty} (-1)^{k+1} \delta(y - \lambda_k) \frac{1}{y} e^{-\varphi y^2 x}
\] (C1)

where we defined

\[
\delta(y) := \sum_{k=-\infty}^{\infty} (-1)^{k+1} \delta(\lambda_k - y).
\] (C2)

Since \( \delta(y) \) is odd in \( y \) and has periodicity \( 2\pi \), we can expand it into a Fourier-sine-series:

\[
\delta(y) = \sum_{l=1}^{\infty} d_l \sin(ly)
\] (C3)
where
\[
d_t = \frac{2}{\pi} \int_0^\pi dy \delta(y) \sin(ly) = \frac{2}{\pi} \sin(l\pi/2) = \frac{2}{\pi} \begin{cases} 0 & \text{if } l \text{ is even} \\ (-1)^{(l-1)/2} & \text{if } l \text{ is odd} \end{cases}. \quad (C4)
\]
This results in
\[
\tilde{\delta}(y) = \frac{2}{\pi} \sum_{l=1}^\infty (-1)^{l+1} \sin((2l-1)y). \quad (C5)
\]
Inserting this into Eq. (C1) we find for \( \tilde{Z}_{\parallel}(x) \)
\[
\tilde{Z}_{\parallel}(x) = \frac{4}{\pi} \sum_{l=1}^\infty (-1)^{l+1} \int_0^\infty dy \, y^{-1} e^{-y^2x} \sin((2l-1)y). \quad (C6)
\]
The integral evaluates to \( \text{10} \) (with \( \mu = 0, \beta = x, \gamma = 2l-1 \))
\[
\int_0^\infty dy \, y^{-1} e^{-y^2x} \sin((2l-1)y) = \frac{(2l-1)e^{-(2l-1)^2/4x}}{2\sqrt{x}} \sqrt{\pi} \, _1F_1 \left( 1; \frac{3}{2}; \frac{(2l-1)^2}{4x} \right). \quad (C7)
\]
As the confluent hypergeometric function \( _1F_1(\alpha; \gamma; z) \) has the property \( \Phi(\alpha, \gamma; z) = e^z \Phi(\gamma - \alpha, \gamma; -z) \)
\( \text{10} \) we find with \( \text{10} \)
\[
\Phi \left( 1, \frac{3}{2}; z \right) = e^z \Phi \left( 1, \frac{3}{2}; -z \right) = \frac{\sqrt{\pi} e^z}{2\sqrt{\pi}} \text{erf}\sqrt{z}. \quad (C8)
\]
Our result for \( \tilde{Z}_{\parallel}(x) \) is thus
\[
\tilde{Z}_{\parallel}(x) = 2 \sum_{l=1}^\infty (-1)^{l+1} \text{erf} \frac{2l-1}{2\sqrt{x}}. \quad (C9)
\]
This still has problems for \( x \to 0 \) where \( \text{erf}(2l-1)/2\sqrt{x} \to 1 \). We can, however rewrite it to
\[
\tilde{Z}_{\parallel}(x) = 2 \sum_{l=1}^\infty (-1)^{l+1} + 2 \sum_{l=1}^\infty (-1)^l \text{erf} \frac{2l-1}{2\sqrt{x}}. \quad (C10)
\]
All convergence problems are now isolated in the first sum. As we know that \( \tilde{Z}_1(0) = 1 \) (compare Eq. \( \text{35} \)) we assign \( 2 \sum_{l=1}^\infty (-1)^{l+1} = 1 \) to finally find
\[
\tilde{Z}_{\parallel}(x) = 1 + 2 \sum_{l=1}^\infty (-1)^l \text{erf} \frac{2l-1}{2\sqrt{x}}. \quad (C11)
\]

### APPENDIX D: GRAFT-ANGLE-DEPENDENT FORCE

We evaluate the general expression Eq. \( \text{30} \) using the representation
\[
\Theta(x) = \lim_{\epsilon \to 0^+} \int dq \frac{e^{iqx}}{2\pi i q - i\epsilon} \quad (D1)
\]
of the step function \( \Theta(x) \). With Eq. \( \text{73} \) we find
\[
\tilde{Z}(\zeta, \vartheta) = \int dq \frac{e^{iq\zeta / \cos \vartheta - L_1}}{2\pi i q - i\epsilon} a_d(-i\eta) \exp \left[ -(qL_2 L_1^{-1} \tan \vartheta)^2 3b(-i\eta) / 2 \right] \quad (D2)
\]
where
\[
\tilde{Z}(\eta, \mu, \varphi, \zeta) = - \int dq \frac{e^{iq\zeta / \cos \vartheta - L_1}}{2\pi i q + i\epsilon} a_d(-i\eta) e^{-\frac{\eta^2 q^2 (L_2 - L_1) \tan \vartheta}{2}}. \quad (D3)
\]
Using the Dirac formula
\[
\frac{1}{q + i\epsilon} = \mathcal{P} \frac{1}{q} - i\pi \delta(q), \quad (D4)
\]
\( a_3(0) = 1, \, 3b(0) = 1 \) and the symmetry properties of \( a_3(iq) \) and \( b(iq) \), we find
\[
\tilde{Z}(\eta, \mu, \varphi, \zeta) = \frac{1}{2} - 2 \int_0^\infty dq \frac{1}{2\pi i q} \left( e^{iq\eta} a_3(iq) e^{-\frac{\eta^2 q^2 (L_2 - L_1) \tan \vartheta}{2}} \right) \quad (D5)
\]
The notation \( \mathcal{P} \) denoting the principal value has been dropped as the integrand is regular at \( q = 0 \). For large \( \mu \) and/or \( \zeta \), \( \tilde{Z}(\eta, \mu, \varphi, \zeta) \) vanishes. This means that the integral in Eq. \( \text{35} \) must approach 1/2. Subtracting the result of the numerically evaluating the non-vanishing integral from 1/2 strongly amplifies the unavoidable round-off error. We therefore rewrite Eq. \( \text{D5} \) to
\[
\tilde{Z}(\eta, \mu, \varphi, \zeta) = \frac{1}{2} + \mathcal{P} \int_0^\infty dq \frac{e^{iq\eta} a_3(iq)}{2\pi i q} e^{-\frac{q^2 3b(iq)}{2}} = \frac{1}{2} \text{erf} \frac{\eta}{\sqrt{2} \mu}. \quad (D7)
\]
where we used the identity
\[
\frac{1}{2} - \mathcal{P} \int_{-\infty}^\infty dq \frac{e^{iq\eta} a_3(iq)}{2\pi i q} e^{-\frac{q^2 3b(iq)}{2}} = \frac{1}{2} \text{erf} \frac{\eta}{\sqrt{2} \mu}. \quad (D7)
\]
As $\Im q^2 b(\imath q) \sim -q$ for large $|q|$, it is again advantageous to split the integrals at some $q_0$ and, for $q > q_0$, to rewrite the imaginary part appearing in the integrand of Eq. (D6) to

\[ \Im \left[ e^{\imath \eta \parallel + 3 \mu^2 / 2} \left( a_3(\imath q)e^{-\frac{3}{2} \mu^2 (q^2 b(\imath q) + \imath q)} - e^{-\frac{3}{2} \mu^2 (q^2 b(\imath q) + \imath q)} \right) \right] \]

(D8)

and the real part appearing in Eq. (D9) to

\[ \Re \left( e^{\imath \eta \parallel + 3 \mu^2 / 2} a_3(\imath q)e^{-\frac{3}{2} \mu^2 (q^2 b(\imath q) + \imath q)} \right) . \]

(D9)

In both cases the integrand is holomorphic for $\Im q < 0$. Hence the integrals vanish if $\delta \eta \parallel := \eta \parallel + 3 \mu^2 / 2 < 0$ which we already understood in the simple geometric picture of the problem.

Both integrals now vanish in the limit of large $\eta \parallel$ and have well-behaved integrands on $[0, \infty]$. The precision with which $\tilde{f}(\eta \parallel, \mu)$ can be calculated is, however, still limited by the relative error in evaluating the integrals. This relative error grows quickly with increasing $\eta \parallel$ limiting the range of $\eta \parallel$ over which $\tilde{f}(\eta \parallel, \mu)$ can be calculated reliably (note that the first term of Eq. (D8) vanishes with increasing $\eta \parallel$ as well).

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