

Persistence length of semiflexible polymers and bending rigidity renormalization

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Abstract. – The persistence length of semiflexible polymers and one-dimensional fluid membranes is obtained from the renormalization of their bending rigidity. The renormalized bending rigidity is calculated using an exact real-space functional renormalization group transformation based on a mapping to the one-dimensional Heisenberg model. The renormalized bending rigidity vanishes exponentially at large length scales and its asymptotic behaviour is used to define the persistence length. For semiflexible polymers, our result agrees with the persistence length obtained using the asymptotic behaviour of tangent correlation functions. Our definition differs from the one commonly used for fluid membranes, which is based on a perturbative renormalization of the bending rigidity.

Introduction. – Thermal fluctuations of two-dimensional fluid membranes and one-dimensional semiflexible polymers or filaments are governed by their bending energy and can be characterized using the concept of a *persistence length* L_p . In the absence of thermal fluctuations at zero temperature, fluid membranes are planar and filaments are straight because of their bending rigidity. Sufficiently large and thermally fluctuating membranes or filaments lose their planar or straight conformation. Only subsystems of size $L \ll L_p$ appear rigid and maintain an average planar or straight conformation with a preferred normal or tangent direction, respectively. Larger membranes or filaments of sizes $L \gg L_p$, on the other hand, appear flexible. In the “semiflexible” regime for which L is smaller than or comparable with L_p , the statistical mechanics is governed by the competition of the thermal energy T and the bending rigidity κ . Experimental values for the persistence length of one-dimensional biological filaments vary from 50 nm for double-stranded DNA [1], 10 μm for actin filaments [2,3] up to the mm-range for microtubules [2]. The persistence lengths of two-dimensional fluid membranes composed of lipid bilayers are typically much larger than experimental length scales.

For semiflexible polymers with one internal dimension, L_p is usually defined by the characteristic length scale for the exponential decay of the two-point correlation function between unit tangent vectors \mathbf{t} along the polymer. A continuous model for an inextensible semiflexible polymer of contour length L is the wormlike chain (WLC) model [4]. In the WLC model the polymer is parametrized by its arc length s ($0 < s < L$) and the polymer contour is completely

determined by the field $\mathbf{t}(s)$ of unit tangent vectors. The Hamiltonian is given by the bending energy

$$\mathcal{H}\{\mathbf{t}(s)\} = \frac{\kappa_0}{2} \int_0^L ds (\partial_s \mathbf{t})^2, \quad \text{with } \mathbf{t}^2(s) = 1, \quad (1)$$

where κ_0 is the (unrenormalized) bending rigidity of the model. For a WLC embedded in d spatial dimensions, the tangent correlation function is found to be [5]

$$\langle \mathbf{t}(s) \cdot \mathbf{t}(s') \rangle = e^{-|s-s'|/L_p}, \quad \text{with } L_p = \frac{2}{d-1} \frac{\kappa_0}{T}, \quad (2)$$

where T is the temperature in energy units.

For fluid membranes with two internal dimensions, the analogous quantity is the correlation function of normal vectors. An approximate result has been given in ref. [6], but a rigorous treatment is missing due to the more involved differential geometry. Surfaces cannot be fully determined by specifying an arbitrary set of normal vectors, but have to fulfill additional compatibility conditions in terms of the metric and curvature tensors, the equations of Gauss, Mainardi and Codazzi, which ensure their continuity. Implementations of these constraints lead to a considerably more complicated field theory than (1) describing a two-dimensional fluid membrane in terms of its normal and tangent vector fields [7].

For fluid membranes, an alternative definition of the persistence length L_p has been given, which is linked to the effect of κ -renormalization. The mode coupling between thermal shape fluctuations of different wave lengths modifies the large scale bending behavior, which can be described by an effective or *renormalized* bending rigidity κ . The renormalized κ has been calculated using different perturbative renormalization group (RG) approaches [8–13]. The results are still controversial: Several authors [8–11] find a thermal softening of the membrane with increasing length scales, but differing prefactors, whereas Pinnow and Helfrich [13] obtained the opposite result. Furthermore, different definitions of the persistence length are considered in these approaches: In refs. [9–11], L_p is identified with the length scale, where the renormalized bending rigidity κ vanishes, while Helfrich and Pinnow defined L_p via the averaged absorbed area [8, 13].

In this letter, we obtain an exact real-space RG scheme for the bending rigidity of a semiflexible polymer or a one-dimensional fluid membrane, which allows us to define the persistence length as the characteristic decay length of the renormalized bending rigidity.

In principle, a perturbative result for the effective κ can be deduced from the RG analysis of the one-dimensional nonlinear σ -model, which is equivalent to the WLC Hamiltonian (1). After a Wilson-type momentum-shell RG analysis, one obtains the effective rigidity (see, *e.g.*, refs. [14])

$$\frac{\kappa(\Lambda)}{T} = \frac{\kappa_0}{T} \left[1 - \frac{T}{\kappa_0} \frac{d-2}{\pi} \left\{ \frac{1}{\Lambda} - \frac{1}{\Lambda_0} \right\} + \mathcal{O}(T^2/\kappa_0^2) \right], \quad (3)$$

which depends on the momentum Λ . The parameter $\kappa_0 = \kappa(\Lambda_0)$ is the “bare” coupling taken at the high momentum cut-off $\Lambda_0 = \pi/b_0$, which is given by a “lattice spacing” or bond length b_0 . Using also $\Lambda = \pi/\ell$ we obtain the renormalized $\kappa = \kappa(\ell)$ as a function of the length scale ℓ . Following the procedure previously used for membranes, the persistence length can be defined via

$$\kappa(L_p) \equiv 0 \quad \text{and, thus, } L_p \simeq \frac{\pi^2}{d-2} \frac{\kappa_0}{T}. \quad (4)$$

For the case of the polymer in the plane, the Hamiltonian simplifies to a free or Gaussian field theory such that $\kappa = \kappa_0$ is unrenormalized to all orders in κ_0/T and, thus, L_p as defined via $\kappa(L_p) \equiv 0$ would become infinitely large.

A similar perturbative momentum-shell RG procedure is possible in the so-called Monge parametrization of a weakly bent semiflexible polymer, analogous to the RG analysis for two-dimensional membranes [9]. Then the polymer is parametrized by its projected length x with $0 < x < L_x$, where L_x is the fixed projected length of the semiflexible polymer while its contour length becomes a fluctuating quantity. The renormalized $\kappa = \kappa(\ell_x)$ becomes a function of the projected length scale ℓ_x , which complicates a comparison with the result (3), which was derived in an ensemble of fixed contour length. Using the analogous criterion $\kappa(L_p) = 0$ we obtain $L_p \simeq 2\pi^2\kappa_0/(3d-1)T$ within the Monge parametrization.

A comparison of the RG results from the non-linear σ -model, see eq. (4), and the one obtained in the Monge parametrization with eq. (2) shows that the RG results for the persistence length L_p are not compatible with the definition using the tangent correlation function. This raises the general question which of the definitions should be preferred.

In this work we concentrate on a discrete description for semiflexible polymers, which is equivalent to the one-dimensional classical Heisenberg model. The advantage of this model is that the κ -renormalization as well as the tangent correlation function are exactly computable in arbitrary dimensions d . Consequently a direct comparison of the persistence length determined via κ -renormalization and via the tangent correlation function is possible. We introduce this model in the next section. The κ -renormalization is carried out in a similar fashion as is commonly used for Ising-like spin systems. In contrast to the nonlinear σ -model, we find nontrivial results for $\kappa(\ell)$ both in two and in three dimensions. As expected for an exact result, $\kappa(\ell)$ is always positive and approaches zero only asymptotically. Finally, we analyze the large scale behavior of $\kappa(\ell)$ leading to a power series of exponentials with the same decay length as obtained for the tangent-tangent correlations. We define this length scale to be the persistence length of the polymer.

Theoretical model. – A discretization of the WLC Hamiltonian (1) should preserve its local inextensibility. In addition, we want to use a discretized Hamiltonian which is locally invariant with respect to full rotations of single tangents \mathbf{t}_i —in addition to the global rotational symmetry of the polymer as a whole. A suitable discrete model is an inextensible semiflexible chain model as given by [15]

$$\mathcal{H}\{\mathbf{t}_i\} = \frac{\kappa_0}{b_0} \sum_{i=1}^M (1 - \mathbf{t}_i \cdot \mathbf{t}_{i-1}), \quad \text{with } \mathbf{t}_i^2 = 1, \quad (5)$$

with M bonds or chain segments of fixed length b_0 . The semiflexible chain model is equivalent to the one-dimensional classical Heisenberg model (except for the first term, which represents a constant energy term) describing a one-dimensional chain of classical spins.

The partition sum reads

$$\mathcal{Z}_M = \left(\prod_{j=0}^M \int d\mathbf{t}_j \right) \exp[-\mathcal{H}\{\mathbf{t}_j\}/T] = \left(\prod_{j=0}^M \int d\mathbf{t}_j \right) \prod_{i=1}^M T_{i,i-1}, \quad (6)$$

where we have introduced the transfer matrix

$$T_{i,i-1} = \exp[-K_0(1 - \mathbf{t}_i \cdot \mathbf{t}_{i-1})], \quad \text{with } K_0 \equiv \kappa_0/b_0T. \quad (7)$$

We can parametrize the scalar product of unit tangent vectors using the azimuthal angle difference $\Delta\theta_{i,i-1}$ as $\mathbf{t}_i \cdot \mathbf{t}_{i-1} = \cos(\Delta\theta_{i,i-1})$. Then the transfer matrix can be expanded as

$$T_{i,i-1} = \sum_{m=-\infty}^{\infty} \lambda_m^{(0)} e^{im\Delta\theta_{i,i-1}}, \quad \lambda_m^{(0)}(K_0) = e^{-K_0} I_m(K_0) \quad (8a)$$

in two dimensions and

$$T_{i,i-1} = \sum_{l=0}^{\infty} (2l+1) \lambda_l^{(0)} P_l(\cos \Delta\theta_{i,i-1}), \quad \lambda_l^{(0)}(K_0) = \sqrt{\frac{\pi}{2K_0}} e^{-K_0} I_{l+1/2}(K_0) \quad (8b)$$

in three dimensions, where $I_k(x)$ denotes the modified Bessel function of the first kind and $P_l(x)$ the Legendre polynomials [16]. In the following, the sums $\sum_{m=-\infty}^{\infty}$ for $d = 2$ and $\sum_{l=0}^{\infty} (2l+1)$ for $d = 3$ are abbreviated by $\sum_n^{(d)}$.

For simplicity, we restricted our analysis to $d = 2$ and $d = 3$ spatial dimensions, but our results can easily be generalized to arbitrary dimensions d : The transfer matrix is then expanded in Gegenbauer polynomials and the eigenvalues $\lambda_l^{(0)}$ are proportional to modified Bessel functions $I_{l+d/2-1}(K_0)$.

The partition sum and tangent-tangent correlations may be calculated exactly for open and periodic boundary conditions as was done, *e.g.*, in $d = 3$ by Fisher [17] and Joyce [18]. For arbitrary dimension d , the tangent-tangent correlation for open boundary conditions is simply

$$\langle \mathbf{t}(0) \cdot \mathbf{t}(L) \rangle = \left[\lambda_1^{(0)}(K_0) / \lambda_0^{(0)}(K_0) \right]^{L/b_0}, \quad (9)$$

which reduces in the continuum limit of small b_0 or large K_0 to (2).

Renormalization procedure. – The real-space functional RG analysis for the semiflexible chain (5) proceeds in close analogy to the one-dimensional Heisenberg model [19] and similarly to the Ising-like case where the \mathbf{t}_i 's are confined to discrete values [20]. Similar real-space functional RG methods have also been used to study wetting transitions or the unbinding transitions of strings [21, 22]. In each RG step, every second tangent degree of freedom is eliminated. We introduce a general transfer matrix

$$T_{i,i-1} = \exp[h(\mathbf{t}_i \cdot \mathbf{t}_{i-1}, K)], \quad (10)$$

where $h = h(u, K)$ defines an *arbitrary* interaction function depending on the scalar product of adjacent tangents $u = \mathbf{t}_i \cdot \mathbf{t}_{i-1}$ and the parameter K . We start the RG procedure with an initial value $K = K_0$ and an initial interaction function $h(u, K) = -K(1-u)$, see eq. (7). Also for an arbitrary interaction function $h(u, K)$ we can expand the transfer matrix in the same sets of functions as in (8), which defines eigenvalues $\lambda_m = \lambda_m(K)$ in 2d and $\lambda_l = \lambda_l(K)$ in 3d. Initially, these eigenvalues are given by $\lambda_m(K) = \lambda_m^{(0)}(K)$ and $\lambda_m(K) = \lambda_l^{(0)}(K)$, see (8).

Integration over one intermediate tangent \mathbf{t}' between \mathbf{t} and \mathbf{t}'' defines a recursion formula resulting in a new interaction function $h' = h'(u, K)$ and an energy shift g' by

$$\exp[h'(\mathbf{t} \cdot \mathbf{t}'', K) + g'(K)] = \int d\mathbf{t}' \exp[h(\mathbf{t} \cdot \mathbf{t}', K) + h(\mathbf{t}' \cdot \mathbf{t}'', K)], \quad (11)$$

where the energy shift g' is determined by the condition that $h'(1, K) = h(1, K) = 0$, *i.e.*, the energy is shifted in such a way that the interaction term is zero for a straight polymer. This leads to

$$\exp[g'(K)] = \int d\mathbf{t} \exp[2h(\mathbf{t} \cdot \mathbf{t}', K)]. \quad (12)$$

The recursions (11) and (12) are exact and can be used to obtain an exact RG relation for the eigenvalues $\lambda_k^{(N)}$ after N RG recursions,

$$\lambda_k^{(N+1)} = \left[\lambda_k^{(N)} \right]^2 / \left\{ \sum_n^{(d)} \left[\lambda_n^{(N)} \right]^2 \right\} = \left[\lambda_k^{(0)} \right]^{2^N} / \left\{ \sum_n^{(d)} \left[\lambda_n^{(0)} \right]^{2^N} \right\}. \quad (13)$$

In general, the new and old interactions $h'(u, K)$ and $h(u, K)$ will differ in their functional structure. Thus the renormalization of the parameter K cannot be carried out in an exact and simple manner as for one-dimensional Ising-like models with discrete spin orientation [20]. The only fixed point function of the recursion (11) is independent of u , *i.e.*, $h^*(u, K) = 0$ because of $h^*(1, K) = 0$. This result, together with the condition $h'(1, K) = 0$, which is imposed at every RG step, suggests that the function $h'(u, K)$ can be approximated by a *linear* function

$$h'(u, K) \simeq -K'(K)(1 - u) \quad \text{for } u = \mathbf{t} \cdot \mathbf{t}'' \simeq 1, \quad (14)$$

as long as the scalar product $u = \mathbf{t} \cdot \mathbf{t}''$ is close to one, *i.e.*, sufficiently close to the straight configuration. This approximation should improve when the whole function $h'(u, K)$ becomes small upon approaching the fixed point $h^*(u, K) = 0$ after many iterations, *i.e.*, on large length scales. Using the approximation (14), $K'(K)$ is defined by the slope of $h'(u, K)$ at $u = 1$,

$$K'(K) \equiv \left. \frac{dh'(u, K)}{du} \right|_{u=1} = \left. \frac{d}{du} \exp[h'(u, K)] \right|_{u=1}, \quad \text{with } u = \mathbf{t} \cdot \mathbf{t}'' \quad (15)$$

Equivalently, one could expand the explicit expression for $h'(x, K)$ given by (11) and the right-hand side of (14) for small tangent angles and compare the coefficients. In order to extract the renormalized bending rigidity κ' from the result for K' , one has to take into account that K' also contains the new bond length $b' = 2b$, which increases by a factor of 2 at each decimation step. Therefore,

$$\kappa'(K) = 2bT K'(K). \quad (16)$$

Using this procedure we can calculate the renormalized bending rigidity κ_N after N RG recursions in 2d and 3d starting from the exact RG recursions (13) for the eigenvalues. Inserting the renormalized eigenvalues into (8), taking the derivative according to (15) and applying the rescaling (16) finally yields the result

$$\frac{\kappa_N}{\kappa_0} = \frac{2^N}{K_0} \left\{ \sum_n^{(d)} [\lambda_n^{(0)}(K_0)]^{2^N} A_n^{(d)} \right\} / \left\{ \sum_n^{(d)} [\lambda_n^{(0)}(K_0)]^{2^N} \right\}, \quad (17)$$

with $A_n^{(2)} \equiv n^2$ and $A_n^{(3)} \equiv \frac{1}{2}n(n+1)$. In the following we will interpret κ_N as a continuous function $\kappa(\ell)$ of the length scale ℓ by replacing the rescaling factor $2^N = b_N/b_0$ by the continuous parameter ℓ/b_0 .

Persistence length. – The sums in the expressions for the effective bending rigidity (17) can be computed numerically. Figure 1 displays the results for $\kappa(\ell)/\kappa_0$ as a function of ℓ/b_0 for $K_0 = 1000$ and in 2d and 3d. The value $K_0 = 1000$ is appropriate for a semiflexible polymer with $\kappa_0/T = 10 \mu\text{m}$ and a bond length $b_0 = 10 \text{ nm}$, which is close to experimental values for F-actin [2,3]. For DNA, appropriate values are $\kappa_0/T \simeq 50 \text{ nm}$ and $b_0 \simeq 0.3 \text{ nm}$ and, thus, $K_0 \simeq 150$.

As long as ℓ is small, κ decays almost linearly in $d = 3$, which is also in qualitative agreement with the result (3) from the RG of the nonlinear σ -model. For $d = 2$ the decay is much slower at small length scales, but, in contrast to the non-linear σ -model where κ is *not* renormalized. This qualitative difference is due to the following important difference between the Heisenberg and the nonlinear σ -model: Parametrizing the WLC model (1) via tangent angle leaves only quadratic terms $\propto (\Delta\theta_{i,i-1})^2$, whereas the discrete semiflexible chain (5) gives terms $\propto 1 - \cos(\Delta\theta_{i,i-1})^2$, which represent the full expansion of the cosine and obey the local invariance under full rotations.

As ℓ increases $\kappa(\ell)$ approaches zero only asymptotically. Therefore, the definition of the persistence length as length scale where the renormalized κ vanishes, $\kappa(L_p) = 0$ —which is

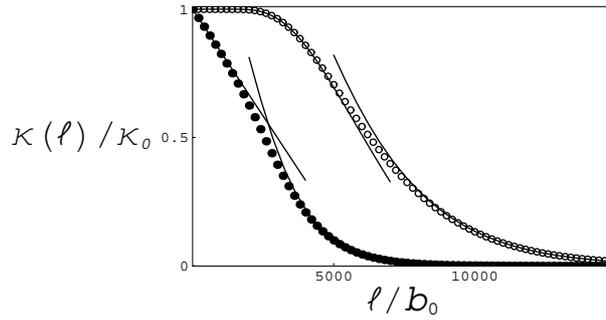


Fig. 1 – Renormalized bending rigidity $\kappa(\ell)/\kappa_0$ as a function of the length scale $\ell/b_0 = 2^N$ for $K_0 = 1000$ for $d = 2$ (\circ) and $d = 3$ (\bullet) according to the recursion relation (17). The lines show the asymptotic behavior for $\ell \gg \kappa_0/T$ and $\ell \ll \kappa_0/T$ according to eqs. (18) and (20), respectively.

usually used for fluid membranes— would always give an *infinite* result. We propose not to ask at which length scale the renormalized κ reaches zero, but rather *how* it reaches zero. For $\ell \geq b_0 K_0 = \kappa_0/T$ the sums in (17) converge fast and one has to include only the first few terms for accurate results. In fact, one can replace the Bessel functions contained in the eigenvalues $\lambda_k^{(0)}$, see (8), by their asymptotic form $I_k(x) \approx (x/2\pi)^{-1/2} \exp[x - (k^2 - 1/4)(2x)^{-1}]$ for large x [16]. This is justified for sufficiently large $K_0 \gtrsim 100$, which is fulfilled by semiflexible polymers like F-actin ($K_0 \simeq 1000$) or DNA ($K_0 \simeq 150$). Using this asymptotics we find $(\lambda_m^{(0)}(K_0))^{\ell/b_0} \sim e^{-m^2 \ell/2b_0 K_0}$ for $d = 2$ and $(\lambda_l^{(0)}(K_0))^{\ell/b_0} \sim e^{-l(l+1)\ell/2b_0 K_0}$ for $d = 3$. Moreover, we may expand (17) as a power series in $e^{-\ell T/\kappa_0}$ and obtain

$$\begin{aligned} \kappa(\ell)/\kappa_0 &\approx (\ell T/\kappa_0) \left(2e^{-\ell T/2\kappa_0} - 4e^{-\ell T/\kappa_0} + 8e^{-3\ell T/2\kappa_0} - \dots \right) \quad \text{for } d = 2, \\ \kappa(\ell)/\kappa_0 &\approx (\ell T/\kappa_0) \left(3e^{-\ell T/\kappa_0} - 9e^{-2\ell T/\kappa_0} + 42e^{-3\ell T/\kappa_0} - \dots \right) \quad \text{for } d = 3. \end{aligned} \tag{18}$$

The characteristic length scales in the expansions are $2\kappa_0/T$ in $d = 2$ and κ_0/T in $d = 3$, which are, therefore, a natural definition for the persistence length L_p . For general dimensionality d , the exponent of the first term is determined by the order of the Bessel function appearing in the eigenvalue. Thus the RG calculation leads to a persistence length

$$L_p = \frac{2\kappa_0}{T(d-1)}, \tag{19}$$

which agrees exactly with the result (2) based on the tangent correlation function.

Our definition based on the large-scale asymptotics of the exact RG flow is qualitatively different from the definition (4) used in perturbative RG calculations. While the result (3) from the nonlinear σ -model is only valid for small length scales $\ell \ll \kappa_0/T$, where $\kappa(\ell)$ is close to κ_0 , the expansion (18) describes the region $\ell \gg \kappa_0/T$. Indeed, taking the expansion of (17) for $\ell \ll \kappa_0/T$, that is

$$\begin{aligned} \kappa(\ell)/\kappa_0 &\approx 1 - (8\pi^2 \kappa_0/\ell T) e^{-2\pi^2 \kappa_0/\ell T} + \mathcal{O}(\ell e^{-4\pi^2 \kappa_0/\ell T}) \quad \text{for } d = 2, \\ \kappa(\ell)/\kappa_0 &\approx 1 - (\ell T/6\kappa_0) - \mathcal{O}(\ell^2 T^2/\kappa_0^2) \quad \text{for } d = 3, \end{aligned} \tag{20}$$

and defining L_p by the exponential decay length in two dimensions, respectively, by the linear term in three dimensions leads to a persistence length, which is considerably bigger than the value (19) found above. Hence it is not surprising that the two computations (3) and (18) yield different results. The slow exponential decay in the expansion (20) for $d = 2$ is reminiscent of the non-renormalization of κ in the non-linear σ -model, see eq. (3), and leads to a “plateau” in the numerical result for $\kappa(\ell)/\kappa_0$ for $\ell \ll \kappa_0/T$ in fig. 1.

Conclusion. – In conclusion we have presented a definition of the persistence length L_p of a semiflexible polymer or one-dimensional fluid membrane based on the large scale behaviour of the RG flow of the bending rigidity κ , as obtained from a functional real-space RG calculation. Our result (19) for L_p generalizes the conventional definition based on the exponential decay of a particular two-point tangent correlation function and gives identical results for L_p , thus justifying past experimental and theoretical work based on this conventional definition. The RG flows (17) or (18) allow us to follow the behaviour of a semiflexible polymer from a stiff polymer on short length scales to an effectively flexible polymer on large length scales quantitatively as a function of the length scale. On large length scales, our functional RG gives qualitatively different results from perturbative RG techniques, which have been used for the closely related problem of fluid membranes [8–13] and which we also applied to the one-dimensional semiflexible polymer. The generalization of our renormalization approach to two-dimensional fluid membranes is complicated by the more involved differential geometry of these two-dimensional objects and remains an open issue for future investigation. In analogy with our results for one-dimensional polymers and filaments as described here, we expect that a proper definition of the persistence length for two-dimensional fluid membranes again requires the asymptotic RG flow on large length scales which remains to be determined.

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