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Constrained random-force model for weakly bending semiflexible polymers

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The random-force (Larkin) model of a directed elastic string subject to quenched random forces in the transverse directions has been a paradigm in the statistical physics of disordered systems. In this Brief Report, we investigate a modified version of the above model where the total transverse force along the polymer contour and the related total torque, in each realization of disorder, vanish. We discuss the merits of adding these constraints and show that they leave the qualitative behavior in the strong stretching regime unchanged, but they reduce the effects of the random force by significant numerical prefactors. We also show that a transverse random force effectively makes the filament softer to compression by inducing undulations. We calculate the related linear compression coefficient in both the usual and the constrained random-force model.

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The random-force model was introduced by Larkin as a short-distance approximation to study the effect of a quenched random potential on the Abrikosov lattice [1,2]. Because of its simplicity (the relevant functional integrals are Gaussian), it admits exact solutions and has become a paradigm in the physics of disordered elastic manifolds [3]. In a recent publication [4], we used it to analytically investigate the effect of a quenched disordered environment on a strongly stretched wormlike chain. Of course, the randomness that biopolymers are subject to in the cellular environment is much more complicated [5,6], but this model yields some very simple analytical results for the weakly bending case.

The random-force model is mathematically well defined and its analysis is valid. However, its relevance to experimental measurements is obscured by the fact that the distribution of quenched disorder includes realizations of the random force which have nonzero total force along the polymer contour. The total transverse force in any given experiment is either zero or nonzero and, irrespective of the size of the polymer, these two distinct possibilities persist and do not average. One can show, using the central limit theorem, that the variance of the total transverse force, in the limit of long contour length L, scales as $\sim L$. This is a manifestation of lack of self-averaging, and the disorder-averaged value of an observable is not expected to coincide with the outcome of a single measurement in a long filament. Moreover, we should consider two distinct scenarios in a stretching experiment. In the first, the end points of the polymer are fixed in space and absorb (balance) both the total force and torque that the polymer feels. A net transverse random force will have a macroscopically manifest effect on the conformation of the polymer, as shown in Fig. 1. It will also be experienced by the end-point clamps. The same is true for a net torque. In the second scenario, the polymer ends are free to equilibrate in the random potential, and the net force and torque identically vanish. Averaging over all possible random-force realizations could be misleading in the case of vanishing net force or torque. These observations motivate us to study a modified version of the random-force model which includes the constraint of vanishing total force along the polymer contour in every single realization of the quenched disorder [7]. We also consider the additional constraint prescribed by the condition of mechanical equilibrium: that the total torque on the polymer in every single realization of the quenched disorder vanishes. The only effect of such a random force is the deformation of the polymer through random undulations. A quenched transverse random force could also result from the interaction of a stretched semiflexible random polyampholyte with a transverse electric field (assuming screened intrapolymer interactions). It is known that the constraint of global neutrality may affect the behavior of a random polyampholyte [8]. This provides further motivation for studying the constrained random-force model.

We consider a weakly bending wormlike chain of total contour length L in $1+1$ dimensions parametrized by the displacement $y(s)$ perpendicular to the aligning direction (x), where s is the arc length along the polymer contour. An axial force pair f is applied at its end points in the x direction, and a spatially varying random linear force density $g(s)$ is applied along the polymer contour in the transverse direction. The elastic energy functional is given by

$$\mathcal{H}_g[y(s)] = \frac{\kappa}{2}\int_0^L ds\,\left(\frac{\partial^2 y(s)}{\partial s^2}\right)^2 - \int_0^L ds\, g(s)y(s) + \frac{1}{2}f\int_0^L ds\,\left(\frac{\partial y(s)}{\partial s}\right)^2 - fL, \tag{1}$$

where κ is the bending rigidity related to the persistence length L_p via $\kappa = \frac{1}{2}L_p k_B T$, $f > 0$ corresponds to stretching, and $f < 0$ corresponds to compression along the filament axis.

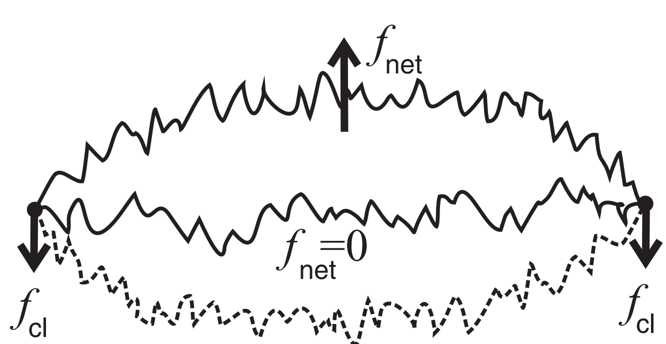

FIG. 1. An unconstrained random linear force density includes realizations with a finite net transverse force balanced by the clamps. Such a net force yields an overall bend in addition to the microscopic undulations.

The first term in the right-hand side (rhs) of Eq. (1) penalizes bending, the second term expresses the interaction with the transverse random force, and the remaining two express the interaction with the stretching force $(-f[x(L)-x(0)])$. $g(s)$ acts as quenched disorder. Its probability distribution is given by

$$\mathcal{P}[g(s)] \sim \int_{-\infty}^{+\infty} d\lambda \, \exp\left[i\lambda \int_0^L ds\, g(s)\right] \times \int_{-\infty}^{+\infty} d\mu \, \exp\left[i\mu \int_0^L ds\, s\, g(s)\right] \times \exp\left[-\int_0^L ds\, \frac{(g(s))^2}{2\Delta_g}\right]. \quad (2)$$

This is Gaussian at any arc-length position s with variance Δ_g, modified by the constraint of zero total force, which is expressed by the integral over λ using the Fourier representation of the Dirac δ function, and the constraint of zero total torque, which is expressed by the integral over μ. For the sake of simplicity, we consider hinged-hinged boundary conditions:

$$y(0) = y(L) = 0, \quad \partial_s^2 y(s)|_{s=0} = \partial_s^2 y(s)|_{s=L} = 0. \quad (3)$$

The force-extension relationship is obtained from

$$\overline{\langle x(L)\rangle} = L - \frac{1}{2}\int_0^L ds\, \overline{\left\langle \left(\frac{\partial y(s)}{\partial s}\right)^2 \right\rangle}, \quad (4)$$

where $\langle \cdots \rangle$ and $\overline{(\cdots)}$ denote thermal and disorder averages, respectively. The boundary conditions of Eq. (3) allow us to to expand $y(s)$ in a series of sines:

$$y(s) = \sum_{l=1}^{\infty} A^{(l)} \sin\left(\frac{l\pi}{L}s\right). \quad (5)$$

We calculate disorder-averaged correlators using the replica method as in Ref. [4]:

$$\overline{\langle A^{(l)}A^{(m)}\rangle} = \lim_{n\to 0} \frac{k_BT}{n} \sum_{a=1}^{n} (C^{-1})_{aa}^{(lm)}, \quad (6)$$

where

$$C_{ab}^{(lm)} = \chi_l{}^{-1}\delta_{ab}\delta_{lm} - \frac{L\Delta_g}{2k_BT}\left(\delta_{lm} - \frac{8}{\pi^2}\frac{1}{lm} - \frac{8}{\pi^2}\frac{(-1)^{l+m} - (-1)^l + 2(-1)^m}{lm}\right)\mathbf{1}_{ab}, \quad (7)$$

$$\chi_l = \frac{2}{L(\kappa(l\pi/L)^4 + f(l\pi/L)^2)}, \quad (8)$$

$\mathbf{1}_{ab}$ being an $n \times n$ matrix with all of its elements equal to 1, and

$$(C^{-1})_{ab}^{(lm)} \underset{n\to 0}{\longrightarrow} \delta_{lm}\left(\chi_l\delta_{ab} + \chi_l^2 \frac{L\Delta_g}{2k_BT}\mathbf{1}_{ab}\right) - \frac{4L\Delta_g}{\pi^2 k_BT} \times \left(\frac{\chi_l\chi_m}{lm} + \chi_l\chi_m \frac{(-1)^{l+m} - (-1)^l + 2(-1)^m}{lm}\right)\mathbf{1}_{ab}. \quad (9)$$

The first term in the rhs of Eq. (9) is related to the usual random-force model, whereas the remaining terms express the contribution of the constraints.

In the absence of the zero-torque constraint [that is, without the second factor in the rhs of Eq. (2)], Eqs. (7) and (9) become

$$C_{ab}^{(lm)} = \chi_l{}^{-1}\delta_{ab}\delta_{lm} - \frac{L\Delta_g}{2k_BT} \times \left(\delta_{lm} - \frac{2}{\pi^2}\frac{(-1+(-1)^l)(-1+(-1)^m)}{lm}\right)\mathbf{1}_{ab} \quad (10)$$

and

$$(C^{-1})_{ab}^{(lm)} \underset{n\to 0}{\longrightarrow} \delta_{lm}\left(\chi_l\delta_{ab} + \chi_l^2\frac{L\Delta_g}{2k_BT}\mathbf{1}_{ab}\right) - \frac{L\Delta_g}{\pi^2 k_BT}\chi_l\chi_m\frac{(-1+(-1)^l)(-1+(-1)^m)}{lm}\mathbf{1}_{ab}, \quad (11)$$

respectively.

In the strong stretching regime, which is defined by $f \gg \kappa/L_p^2$ for filaments with $L \gg L_P$ or $f \gg \kappa/L^2$ for filaments with $L_p \gg L$, we obtain

$$\overline{\langle x(L)\rangle} = L - \frac{k_BTL}{4\sqrt{\kappa f}} - \frac{1}{30}\frac{\Delta_g L^2}{f^2}. \quad (12)$$

The last term in the rhs of the above equation is the decrease in the end-to-end distance due to the undulations caused by the transverse random force. In the usual (unconstrained) random-force model, the numerical prefactor of that term is $\frac{1}{12}$ [9]. The zero-total-force constraint merely reduces this prefactor to $\frac{1}{24}$, and adding the zero-total-torque constraint further reduces it to $\frac{1}{30}$.

We also investigate the effect of the constraints on the pulling-force response of the width of the transverse undulations (mean square transverse displacement at the midpoint) of the stretched wormlike chain. In the strong stretching regime, we obtain

$$\overline{\left\langle \left(y\left(s=\frac{L}{2}\right)\right)^2\right\rangle} = \frac{1}{4}\frac{Lk_BT}{f} + \frac{1}{96}\frac{\Delta_g L^3}{f^2}. \quad (13)$$

In a similar fashion as with the force-extension response, the zero-total-force constraint reduces the effect of the random force, which is expressed by the last term, by a factor of $\frac{1}{2}$ (it changes the numerical prefactor from $\frac{1}{48}$ to $\frac{1}{96}$). The zero-total-torque constraint does not affect the width of transverse fluctuations. We point out, however, that these simple results Eqs. (12) and (13) hold only in the strong stretching regime. For arbitrary stretching force f, the difference between the usual and the constrained-random-force model is more complicated and depends on the system size (L) as can be seen from Eq. (9).

A wormlike chain at zero temperature does not yield to a small axial compressional force below the critical buckling value [10,11]. At any finite temperature, however, thermally induced undulations smooth out the buckling and give rise to a *linear* response for small compressional forces [12]. A quenched disordered environment induces similar undulations and therefore a similar contribution to the linear response coefficient. We consider the constrained random-force model as a simple model for the quenched disordered environment. Assuming $f < 0$ (compression) and $L_p \gg L$, we obtain the average projected length of the filament in the direction of the compressing force to leading (linear) order in $|f|$:

$$\overline{\langle x(L)\rangle} = L - \frac{1}{12}\frac{k_B T L}{\kappa} - \frac{1}{180}\frac{k_B T L^4}{\kappa^2}|f| - \frac{31}{302400}\frac{\Delta_g L^6}{\kappa^2} - \frac{67}{3326400}\frac{\Delta_g L^8}{\kappa^3}|f|. \quad (14)$$

The first line of Eq. (14) expresses the contribution of the thermally induced undulations, whereas the second reflects the effect of the transverse random force. Both contributions modify the classical Euler behavior of an elastic rod before buckling. This second line becomes

$$-\frac{1}{1890}\frac{\Delta_g L^6}{\kappa^2} - \frac{1}{9450}\frac{\Delta_g L^8}{\kappa^3}|f|$$

in the usual (unconstrained) random-force model and

$$-\frac{13}{120960}\frac{\Delta_g L^6}{\kappa^2} - \frac{37}{1814400}\frac{\Delta_g L^8}{\kappa^3}|f|$$

if we add the zero-total-force constraint (without the zero-total-torque constraint). In contrast to the nonlinear stretching response Eq. (12), where the contribution of the random-force undulations decreases relative to that of their thermal counterpart as the pulling force increases, in the linear compressional response the the two contributions enter on equal footing. We point out that the thermal and the quenched-disorder contributions differ qualitatively as far as their dependence on the filament parameters (bending stiffness κ and total contour length L) is concerned. This difference in principle could be useful to probe the existence of nonthermal lateral random forces on compressed microtubules in the cellular environment. For $f = 0$ and $T = 0$, a filament of fixed bending stiffness tends to crumple under the load of the random forces as its size L increases. This is typical of the Larkin model, and it remains unaffected by the zero-total-force and zero-total-torque constraints. Of course, within the context of our weakly bending approximation, we can only identify a tendency toward crumpling and not an actual transition.

In this Brief Report, we have investigated a modification of the random-force model which excludes realizations of disorder with a nonvanishing total force and a nonvanishing total torque. These are non-self-averaging contributions. We have calculated the force-extension response of a wormlike chain and the width of its transverse undulations in the strong stretching regime using this modified model. We have also calculated the linear compressional response using both the usual and the constrained random-force model. We have shown that the constraints leave the calculated behavior qualitatively unchanged but they reduce the effect of the random forces by significant numerical prefactors. The dependence of the disorder-induced contribution on the size of the system (L), which grows in the thermodynamic limit, suggests that the random-force model, even in its modified version, is inherently non-self-averaging. It would be interesting to calculate how the constraints discussed here would modify the free-energy-distribution functions analyzed in Ref. [3]. Although in this work we deal with a weakly bending wormlike chain, our analysis of the vanishing total force and torque constraints also holds in other applications of the random-force model (e.g., flux lines in type II superconductors or liquid crystals in random media [13]).

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