

SINGLE POLYMER DYNAMICS IN RANDOM FLOW

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The character of turbulence in dilute polymer solutions differs substantially from that in classical Newtonian fluids. The ability of polymers to change drastically the large-scale statistics of turbulent flows has many important applications, the most popular being the drag reduction (see, e.g., Ref. [1]). Though, the interaction between elastic degrees of freedom of polymers and kinetics degrees of freedom of the flow is still an problem. The stretching of a single polymer molecule by a non-homogeneous flow is then the first issue to address.

Polymers are long elastic chains of simple molecules called monomers. In the equilibrium configuration they have a compact globular form, while once placed in a non-homogeneous flow, they can be considerably stretched by the velocity gradients and become strongly elongated. The relative intensity of elastic relaxation and stretching is measured by the Weissenberg number Wi , which is the product of the typical relaxation time of the polymer and the characteristic velocity gradient. With increasing Weissenberg number, a sharp transition from the coiled equilibrium state to the highly stretched state was observed since 1974 in shear [2] and hyperbolic flows [3]. Recently, the coil-stretch transition has been investigated by S. Gerashchenko *et al.* in 3D random flows, which is the relevant case for practical applications [4]. Experimental results are in good accordance with theoretical [5-7] and numerical [8-9] predictions for dumbbell-like models.

We study the dynamics of a single polymer molecule passively transported by a smooth random flow. The polymer is described by an elastic dumbbell. The random flow belongs to the Batchelor-Kraichnan statistical ensemble, the main assumption being a zero correlation time [10]. Despite the unphysical character of such hypothesis, this model allows a fully analytic treatment of the problem and captures the basic aspects of polymer stretching by random flows. Asymptotic results for this model were already obtained by Chertkov [5] and Thiffeault [7]. Here we present the exact solution and compare theoretical results with numerical simulations for the 2D Navier-Stokes (NS) flow.

Elastic dumbbell models and Batchelor-Kraichnan flow

The polymer is modeled as two rigid beads joined by an elastic spring. The separation vector between the beads, \mathbf{R} , obeys the stochastic ordinary differential equation (for an introduction to elastic dumbbell models see Ref. [11])

$$d\mathbf{R} = (\mathbf{R} \cdot \nabla \mathbf{v}) dt - f(R) \frac{\mathbf{R}}{\tau} dt + \sqrt{\frac{2R_0^2}{\tau}} d\mathbf{w}, \quad (1)$$

where \mathbf{w} is a standard Brownian motion accounting for thermal noise, τ is the relaxation time of the dumbbell in the absence of flow, and R_0 is its equilibrium length. The function $f(R)$ specifies the elastic properties of the polymer. We shall consider two main cases:

$$\left\{ \begin{array}{l} \text{the Hookean dumbbell: } f(R) = 1; \\ \text{the FENE dumbbell: } f(R) = (1 - R^2/R_m^2)^{-1}. \end{array} \right.$$

In the former case the elastic force is linear. In the latter case, the elastic force diverges as the elongation reaches the maximum length of the polymer, R_m . The norm of the vector \mathbf{R} is a measure of the elongation of the molecule; we are interested in the statistics of the elongation when \mathbf{v} is a fixed random flow.

Within the Batchelor-Kraichnan model, the velocity field is a Gaussian random field on \mathbb{R}^d with zero mean and second-order correlation [10]

$$\langle \Delta v_i(\mathbf{x}, t) \Delta v_j(\mathbf{x} + \mathbf{r}, t') \rangle = D_1 [(d+1)\delta_{ij} r^2 - 2r_i r_j] \delta(t - t'),$$

where $\Delta v_i(\mathbf{x}, t) = v_i(\mathbf{x}, t) - v_i(0, t)$ and the constant D_1 determines the intensity of turbulent fluctuations. The flow is smooth, incompressible, and statistically invariant with respect to translations, rotations and reflections. The maximum Lyapunov exponent of this flow has a Gaussian distribution with mean value $\lambda = D_1 d(d-1)$ and variance $\Delta = 2\lambda d$ [10].

When the flow belongs to the aforementioned statistical ensemble it is possible to derive a closed one-dimensional Fokker-Planck equation for the probability density function (pdf) of R averaged over the realizations of the velocity field, $P(R, t)$ (for details we refer the reader to Refs. [12,13]):

$$\partial_t P = \partial_R [K_1(R)P] + \partial_R^2 [K_2(R)P]. \quad (2)$$

The drift and diffusion coefficients have a non trivial dependence on R :

$$K_1(R) = \left[\frac{\Delta}{2} + \lambda - \frac{f(R)}{\tau} \right] R + \frac{R_0^2 (d-1)}{\tau R} \quad \text{and} \quad K_2(R) = \frac{\Delta}{2} R^2 + \frac{R_0^2}{\tau}.$$

Equation (2) is solved with reflecting boundary conditions, that is the probability does not flow outside the domain of definition.

Hookean dumbbell model

The solution of Eq. (2) depends on the form the function f . We begin with the simplest case where the elastic force is supposed to be linear, i.e. $f(R) = 1$. This model is appropriate for elongations much smaller than the maximum length of the polymer.

Coiled state In random flows the Weissenberg number is defined as $Wi = \lambda\tau$. When Wi is smaller than one, the pdf of the elongation has a stationary limit independent of time and the initial condition [12]:

$$P_{st}(R) = N_1 R^{d-1} \left(1 + \frac{Wi R^2}{d R_0^2} \right)^{-(\alpha+d)/2}$$

where N_1 is the normalization constant and $\alpha = 2(\tau^1 - \lambda)/\Delta = d(1 - Wi)/Wi$. The pdf of the elongation: (a) scales as R^{d-1} for R much larger than R_0 ; (b) has a maximum in the neighborhood of the equilibrium size R_0 ; (c) has a power-law tail $R^{-\alpha}$ with positive α for R much larger than R_0 . Properties b) and c) are in accordance with the prediction of Balkovsky *et al.* for general random flows [6] and with numerical simulations [8-9] and experiments [4]. For small Wi , the majority of polymers are in the equilibrium configuration. When Wi approaches one, the scaling exponent α decreases. Consequently, the right tail of P_{st} raises, the number of diverging moments $\langle R^n \rangle$ increases, and the fraction of polymers that are highly elongated gets larger.

Starting from an initial condition picked on R_0 , the initial distribution relaxes to P_{st} . The typical relaxation time T can be computed from the spectrum of the Fokker-Planck operator which defines Eq. (2) [12]:

$$T/\tau = \begin{cases} \frac{1}{2} [1 - (d+2)Wi/d]^{-1} & 0 \leq Wi \leq d/(d+4) \\ 4Wi/[d(1-Wi)^2] & d/(d+4) \leq Wi < 1. \end{cases}$$

As Wi approaches one, the relaxation time diverges quadratically. Therefore, in this range experimental measures turn out to be delicate due to the long time needed to reach the stationary regime.

Stretched state When Wi exceeds one, the scaling exponent α becomes

negative and P_{st} is no longer integrable: the system does not reach a stationary state and polymers become more and more elongated with time. Therefore, the critical Wi for the Hookean dumbbell model in the δ correlated flow is $Wi = 1$. This is in agreement with the general prediction of Balkovsky *et al.* [6] and the experiments performed by Gerashchenko *et al.* [4].

In the stretched state, all the moments of R grow exponentially in time with an order-dependent exponent [5,12]

$$\langle R^n \rangle \approx R_0^n e^{n\Delta(2n-\alpha)t}.$$

The time-dependent pdf of the elongation, therefore, is intermittent in time and exhibits multiscaling.

To validate the theoretical analysis for the δ correlated model, we performed numerical simulations of Eq. (1). The flow has been obtained from the 2D NS equations, as described in Ref. [14]. In Fig. 1 we show the pdf of polymer elongation in the coiled state. This reaches a stationary form characterized by a peak in the neighborhood of R_0 and by power-law tails both for small and large elongations, in agreement with the predictions of the δ correlated model. Above the coil-stretch transition, the pdf becomes unstationary and polymers get more and more elongated (see Fig. 1).

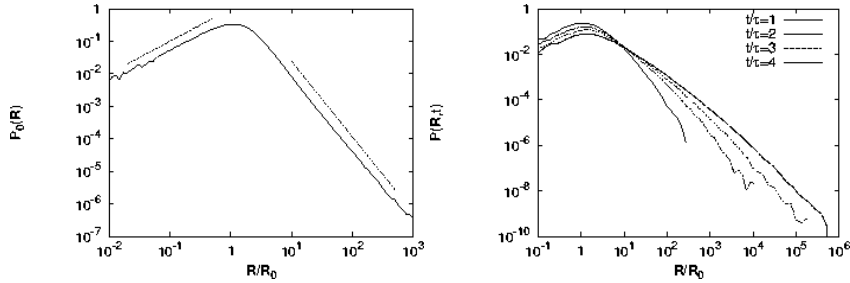


Fig. 1. Numerical simulations for the 2D NS flow. **Right:** Stationary pdf of the elongation in the coiled state ($Wi = 0.4$). The straight lines denotes the power laws R and $R^{1-\alpha}$ with $\alpha=1.32$. **Left:** time evolution of the pdf of the elongation in the stretched state ($Wi = 1.6$).

FENE dumbbell model

For elongations comparable with the maximum length of the polymer, non-linear effects should be taken into account and the elastic force should be modified to introduce the finite extensibility of the molecule. Within the FENE (finite extensible nonlinear elastic) dumbbell model, the function f takes the

form: $f(R) = (1 - R^2/R_m^2)^{-1}$. Thus, the elastic force diverges when R tends to the maximum length R_m .

The FENE model admits a stationary solution for all Wi [13]:

$$P_{st}(R) = N_2 R^{d-1} \left(1 + \frac{Wi}{d} \frac{R^2}{R_0^2}\right)^{-\gamma} \left(1 - \frac{R^2}{R_m^2}\right)^{\gamma}$$

where $\gamma = R_m^2 / (2R_0^2 + 2Wi R_m^2 / d) \approx d/2 Wi^{-1}$ and N_2 is the normalization constant and. The large- R behavior is the one predicted by Thiffeault [7]: the stationary pdf has a power-law tail for R much larger than R_0 and vanishes for $R = R_m$.

The position of the maximum of P_{st} , R , determines the fraction of polymers that are highly stretched. When $Wi < 1$, R is of the order of R_0 and the majority of polymers are in coiled state. With increasing Wi , the most probable elongation grow slowly until Wi exceeds one. Then, a sharp transition occurs to the strongly stretched state and elongations of the order of R_m become highly probable (see Fig. 2).

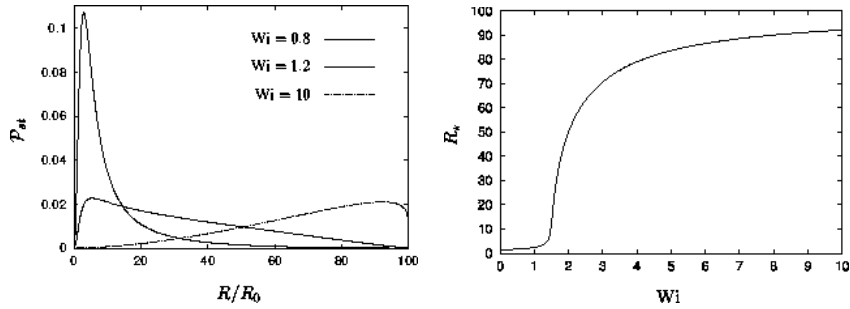


Fig. 2. Batchelor-Kraichnan flow. Left: stationary pdf of polymer elongation for the 3D FENE model at different Weissenberg numbers Wi . Right: most probable elongation R^* as a function of Wi ($R_m/R_0 = 100$).

Conclusions

We have investigated the dynamics of polymers in smooth random flows in a simplified model where a polymer molecule is described by an elastic dumbbell and the flow belongs to the Batchelor-Kraichnan statistical ensemble. We have computed the exact form of the stationary pdf of the elongation both for the Hookean model and the FENE model. Besides, in the linear case we have derived the typical time of relaxation to the stationary regime as a function of

the Weissenberg number. The computation of the relaxation time-scale for the FENE dumbbell is still an on-going work.

As confirmed by numerical simulations for the Hookean dumbbell in the 2D NS flow, the qualitative aspects of polymer dynamics in random flows are well captured by the elastic dumbbell model in the Batchelor-Kraichnan flow. Numerical simulations for the FENE model are more difficult since the elastic force diverges for $R = R_m$. It would be interesting to implement an integration scheme in order to compare theoretical results for the FENE model with numerical simulations for more realistic flows.

Finally, our analysis may be extended to more complete models, like the Rouse model [11], which take into account all the linear modes of oscillation of the polymer and describe the evolution of its shape.

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References

- 1] A. Gyr and H. W. Bewersdorff, *Drag Reduction of turbulent flows by additives*, Kluwer Academic Publishers, Dordrecht, 1995.
- 2] P. G. DeGennes, *J. Chem. Phys.*, 1974, **60**, 5030.
- 3] T. T. Perkins, D. E. Smith, and S. Chu, 1997, *Science*, **276**, 2016.
- 4] S. Gerashchenko, C. Chevillard, and V. Steinberg, 2004, *Phys. Rev. Lett.*, to be published (arXiv:nlin.CD/0404045).
- 5] M. Chertkov, *Phys. Rev. Lett.*, 2000, **84**, 4761.
- 6] E. Balkovsky, A. Fouxon, and V. Lebedev, *Phys. Rev. Lett.*, 2000, **84**, 4765.
- 7] J.-L. Thiffeault, *Phys. Lett. A*, 2003, **308**, 445.
- 8] B. Eckhardt, J. Kronjäger, and J. Schumacher, 2002, *Comput. Phys. Comm.*, **147**, 538.
- 9] G. Boffetta, A. Celani, and S. Musacchio, 2002, *Phys. Rev. Lett.*, **91**, 034501.
- 10] G. Falkovich, K. Gaw?dzki, and M. Vergassola, 2001, *Rev. Mod. Phys.*,

73, 913.

11] R. B. Bird, O. Hassager, R. C. Armstrong, and C. F. Curtiss, *Dynamics of Polymers, Kinetic Theory*, vol. II, Wiley, New York, 1977.

12] A. Celani, S. Musacchio, and D. Vincenzi, 2004, *J. Stat. Phys.*, to be published.

13] D. Vincenzi, 2004, *Appl. Math. Lett.*, submitted.

14] G. Boffetta, A. Celani, S. Musacchio, and M. Vergassola, 2002, *Phys. Rev. E*, **66**, 026304.