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Pressure induced by thermal fluctuation of an elastic filament confined within a narrow channel

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ABSTRACT

Consider a flexible macro-molecule that is immersed in water at or above room temperature. As a result of thermal motion within the water, the filament is driven to undergo random fluctuations in shape. These fluctuations are a consequence of uncoordinated motion of water molecules. If the range of filament motion is restricted by nearby surfaces, the phenomenon becomes more complex. In this study, it is presumed that the filament is restricted to lie within a plane so that the motion is two dimensional. Furthermore, the range of the planar motion of the filament is confined to the region between inflexible straight boundaries lying in the plane of motion. A result of thermal fluctuation of the filament is that, when in close proximity to a boundary, a normal pressure is induced between the filament and that confining boundary. In the present development, frictional interaction of the filament with either confining boundary is presumed to be negligible. The goal is to determine the dependence of the induced pressure on the separation distance between the confining boundaries in terms of prevailing thermal conditions and physical characteristics of the system.

1. Introduction

Under conditions of thermodynamic equilibrium, a gas that is confined within a very stiff container exerts a steady pressure on the container walls. Each gas molecule moves along a sequence of randomly oriented straight line paths at a speed determined by the prevailing temperature. In its travels, any individual molecule rebounds elastically from collisions with the container surface, implying the existence of an impulsive normal force exerted by the surface on each molecule as it rebounds; frictional interaction is presumed to be negligible. Over time, the collective effect of many molecules moving in this way is perceived as a steady pressure on the container inner surface or on any other exposed surface. The same physical effect prevails for other types of confined “fluids” under conditions in which gravitational effects are negligible.

At a somewhat larger scale, suppose that a flexible macro-molecule, perhaps a strand of actin or a synthetic polymer, is immersed in warm water and that it undergoes thermal fluctuations in shape in the region between relatively stiff confining surfaces. It can be anticipated that an interaction force or pressure is induced between the filament and any confining surface. However, due to the size and elasticity of such a molecule, the generation of a confining pressure is not as simple as it is for the case of a gas. In this report, we consider the circumstance of confinement of a long flexible molecule immersed in water. Such a molecule is viewed as a filament that is in its undeformed reference configuration when straight and that is capable of elastic bending into the range of large deflection response. The focus of this development is on the pressure induced on a particular flat confining surface that restricts the range of thermally induced motion of the filament.

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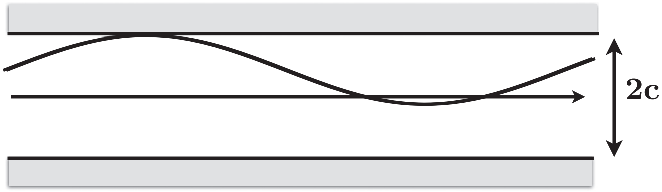

Fig. 1. A representative segment of a flexible filament confined within the channel of width $2c$. The elastic bending energy of the filament is zero when it is straight, and a means of determining the elastic bending energy for an arbitrary configuration is outlined in the text.

A number of experimental studies of filament fluctuations in a thermal environment have been reported in the literature. Perhaps the earliest direct experimental observations of a flexible actin filament confined within a channel were reported by Choi et al. (2005), providing among the earliest observations of persistence length and other characteristic of confined flexible strands. Chen and Sullivan (2006) were among the first to carry out experiments on the fluctuation of a filament confined between nominally rigid plates. In reporting results, they focused on the tangent–tangent correlations along individual filaments. In a different direction, Wang et al. (2010) observed filament migration within a polymer entanglement and deduced the effective confining potential guiding the motion under those circumstances. In a third experimental study, Burkhardt et al. (2010) observed fluctuation of a polymer filament in a circular channel and discussed the observed behavior in the context of scaling rules as they are thought to apply for long, tightly bound filaments.

It is noted in passing that phenomena of this general kind are often analyzed by means of Monte Carlo or similar methods. However, with a few minor simplifications, the present system is shown to yield to a simple and relatively transparent strategy for analysis.

2. The material model

A physical model for large amplitude planar motion of such a filament is adapted to the circumstances presumed here, following the development reported by Jonsdottir and Freund (2014). Planar motion is understood to imply that all filament nodes are constrained to move within a single plane. Specifically, consider a continuous filament of length L with uniform elastic bending modulus B along its length. Following the classical theory of elastic bending, the bending modulus is the ratio of the bending moment acting across a particular filament normal cross-section to the local curvature of the line of centroids of the uniform cross-sections of the filament (Fig. 1).

The analysis is simplified significantly if, instead, a model filament is considered that is composed of n links, each of very small length $b=L/n$. The links themselves undergo no deformation. The value of n is large enough so that $b \ll L$ and the value $n=1000$ is chosen here. The links are numbered left-to-right from 1 to 1000. Adjacent links are joined end-to-end with an elastic bending element of rotational stiffness κ that acts across the joint and that resists an increase in magnitude of the relative orientation at each link-to-link junction. The physical dimensions of κ , the joint bending stiffness, are force $\times$ length. If the orientation difference between a pair of adjacent links is given by the angle θ then the energy stored in the junction between them is $\frac{1}{2}\kappa\theta^2$. If it is required that the total energy stored in a semi-circular filament is the same for either a continuous or a segmented filament, it is found that κ must have the value B/b.

3. Analysis

It is evident that, for a fixed value of L, the quality of the approximation improves as n becomes larger. The analysis is carried out for the value $n=1000$. It is noted that, as the value of n increases, the shape of the segmented filament becomes ever closer to a smooth shape with a continuously turning tangent. For purposes of numerical simulation of fluctuations of filaments, this approach with a segmented filament is simple to implement, even for the case of deflections with magnitude well beyond the range of small deformation. In addition, it is noted that any stable moment versus curvature relationship, either linear or nonlinear, can be adopted to represent the elastic response of the filament without adding complexity to the calculation. For example, it might be assumed that the bending stiffness κ depends on the magnitude of θ nonlinearly. For present purposes, it is assumed that κ has the constant value B/b deduced from the continuous bending stiffness as indicated above.

4. Filament energy

As the filament deforms due to thermal excitation, it can take on any configuration among an enormous number of admissible configurations. For example, suppose that a filament contains 1000 links, each of length b. Further, suppose that the links are assigned number labels from 1 to 1000 along the filament, and the nodes between the links, as well as the endpoints, are assigned number labels from 1 to 1001. Then link $(j-1)$ is joined to link j at node j; the end nodes 1 and 1001