Theoretical investigations of looping of a long chain polymer molecule in dilute solutions

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March 2021

Understanding the rate of polymer looping processes forms the basis of understanding several biochemical processes around us. The biological processes like primary folding pathways in proteins, in DNA looping and in cellular biology where a gene can be activated when a transcription factor bound far away from the promoter site is brought near the active site, RNA folding *etc.*, are mediated through the polymer looping process, which is the rate-determining step [1]. Hence, understanding the kinetics and dynamics of these simple events such as end-to-end relaxation of a freely suspended polymer chain inside solvents has thus become an important step towards understanding such processes in detail [2]. The statistical description of such processes captures a multitude of average properties of the polymer along with statistical variables like the survival probability, the rate of the reaction, the distribution of mean passage time profile, *etc.* [3]. For simplicity we consider the distribution of change in end-to-end distance resulting in different polymer configuration to be effective one-dimensional random walk problem [4, 5, 6, 7]. If the polymer molecule is immersed in solvent, a description of the end-to-end distribution can be obtained by using a Smoluchowski-like equation. In this equation, the end-to-end distribution of an isolated polymer reduces to the description of a particle moving under a parabolic potential. Ensuring the occurrence of reaction between two ends is modelled in the equation by adding a sink function which can be arbitrary positioned. This sink function results in decay of the survival probability of the un-reacted population. The region associated with the sink function is defined to have a finite strength which is more factual assumption and is closer to reality. All the existent analytical models used in understanding polymer looping problem considers perfectly absorbing boundary, which is equivalent to using a Dirac delta sink of infinite strength. In principle the sink function can range from a localized Dirac delta function to non-localized exponential and Gaussian function [8, 9, 10, 11]. We have used Dirac delta function of arbitrary strength to model the looping process [12]. Even there are cases where a Dirac delta function of time dependent sink strength is absolutely necessary for explaining the experimental data [13].

In reality the semi flexible nature of the bio-polymers is modelled by a fractional diffusion model, which represents a slower the dynamics of the looping process

[14]. Another general model is considering the process to be reversible which can be understood by using two state model [15, 16]. All models proposed above can also be used to understand the polymer un-looping process in solution [17]. Since many biomolecular events occurring in molecular aggregates and immunological systems, electrostatic steering in enzyme to ligand binding processes could be modelled by this type of equations, thus it is desirable to achieve a solution of this Smoluchowski-like equation with a sink of finite strength analytically in time and Laplace domain. Therefore, this thesis deals with developing different methods of solving the equation by analytical or semi-analytical approach.

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