



On chirality and length-dependent potentials in polymer entanglements

C.C. Bernido^{a,*}, M.V. Carpio-Bernido^a, J.B. Bornales^b

^a *Research Center for Theoretical Physics, Central Visayan Institute Foundation, Jagna, Bohol 6308, Philippines*

^b *Physics Department, MSU-Iligan Institute of Technology, Iligan City 9200, Philippines*

Received 14 September 2004; received in revised form 3 March 2005; accepted 4 March 2005

Available online 23 March 2005

Communicated by C.R. Doering

Abstract

The lineal structure of an entangled polymer of length L is simulated by a potential, $V = \dot{f}(s)\vartheta$, where, $\dot{f} = df/ds$, $0 \leq s \leq L$, and $f(s)$ a modulating function. Entanglement probabilities calculated for two cases, (a) $f(s) = k \cos(vs)$, and (b) $f(s) = ks^p$, show a significant influence of chirality or “handedness”.

© 2005 Elsevier B.V. All rights reserved.

PACS: 82.35.Lr; 36.20.Ey; 87.15.He; 87.15.Cc

Keywords: Coiling probabilities; Chirality

1. Introduction

The presence of chirality, or “handedness”, in substances at the molecular level has been a puzzling issue in biochemistry. It is known, for instance, that amino acids in the proteins of living organisms are of the “left-handed” kind, and that all the chiral sugars in carbohydrates are “right-handed”. The chirality of amino acids, in turn, manifests in the handedness

of the helical structures of the proteins they form. To what extent chirality influences the folding and unfolding of macromolecules is a question worth investigating. Moreover, the process in which information contained in the constituent units is used to form the three-dimensional structure of the macromolecule also requires elucidation. This would allow us to understand better how the amino acid sequence on most proteins determines its globular shape, or the way in which a protein chain folds up, in order to carry out its biological function. It appears instructive, therefore, to look at physical models which can incorporate some of the curious characteristics observed in a macromolecule such as,

* Corresponding author.

E-mail address: cbernido@mozcom.com (C.C. Bernido).

- (1) the ability of a macromolecule to use the one-dimensional sequence of data in its repeating units to influence its globular structure, and,
- (2) the way in which chirality can influence the three-dimensional structure of a polymer.

We study these features in this Letter by considering the process in which a polymer winds around another polymer [1–4]. We simulate the data contained in the repeating units of the entangled polymer by using a potential of the form, $V = f(s)\vartheta$, where $f = df/ds$, and ϑ is an angular variable about the z -axis. Here, $f(s)$ is a modulating function where, $0 \leq s \leq L$, and L is the length of the polymer. In particular, we look at two cases (a) $f(s) = k \cos(vs)$, and (b) $f(s) = ks^p$, where k is a positive constant and $p = \pm 1, \pm 2, \pm 3, \dots$. We shall also see that for any modulating function $f(s)$, the “handedness” of the winding polymer has a significant effect on the entanglement probabilities.

2. Brief review of a generic case

Let us take a polymer which entangles around a straight polymer oriented along the z -axis. To evaluate the entanglement probabilities, one can consider a projection of the entangled polymer on the plane perpendicular to the z -axis. A topologically equivalent situation, however, is to consider the entangled polymer to lie on the plane. If we now take the intersection of the straight polymer with the plane to be at the origin, the entangled polymer on the plane can be viewed as a two-dimensional random walk [2]. We can then investigate the various configurations of the random walk on the plane which starts at \mathbf{r}_0 and ends at \mathbf{r}_1 , in the presence of a singularity at the origin where the straight polymer is located. The various paths of the random walk can go around the origin clockwise or counterclockwise giving rise to an interesting problem with topological constraints. Employing polar coordinates $\mathbf{r} = (r, \vartheta)$ for this problem, Edwards [2] used the Wiener representation of the random walk in which the probability is represented by,

$$P(\mathbf{r}_1, \mathbf{r}_0) = \int \exp\left[-\frac{1}{l} \int_0^L (d\mathbf{r}/ds)^2 ds\right] \mathcal{D}^2[\mathbf{r}], \quad (2.1)$$

where the integral is taken over all paths $\mathbf{r}(s)$ such that $\mathbf{r}(0) = \mathbf{r}_0$ and $\mathbf{r}(L) = \mathbf{r}_1$. Here, we represent the polymer as consisting of N freely hinged individual molecules, each of length l such that $L = Nl$. In view of the point singularity, a set of topologically equivalent configurations can be characterized by a winding number n , where $n = 0, \pm 1, \pm 2, \dots$, indicating the number of times the polymer turns around the straight polymer intersecting the plane at the origin ($n \geq 0$, signifies n turns counterclockwise, and $n \leq -1$ means $|n + 1|$ turns clockwise).

Since we are interested in the number of possible windings around the origin that the polymer on the plane undergoes, we can simplify the calculation by fixing the radial variable to $r = R$, i.e., $\mathbf{r} = (R, \vartheta)$, and use ϑ to track the number of turns, clockwise or counterclockwise, around the origin. We note that a fixed radial part describes the entanglement scenario in the low temperature limit [4] for any polymer interaction potential $V(r)$ which has a minimum at some value $r = R$. This is what we refer to as the generic case where Eq. (2.1) reduces to,

$$P(\vartheta_1, \vartheta_0) = \int \exp\left[-\frac{1}{l} \int_0^L R^2 \left(\frac{d\vartheta}{ds}\right)^2 ds\right] \mathcal{D}[R d\vartheta], \quad (2.2)$$

with, $\vartheta_1 = \vartheta(L)$ and $\vartheta_0 = \vartheta(0)$. This was evaluated in Ref. [1] using white noise analysis with the result,

$$P(\vartheta_1, \vartheta_0) = \sum_{n=-\infty}^{+\infty} P_n, \quad (2.3)$$

where P_n is the probability function for polymer configurations which entangle n times around the origin given by,

$$P_n = \sqrt{R^2/lL\pi} \exp[-(R^2/lL)(\vartheta_0 - \vartheta_1 + 2\pi n)^2]. \quad (2.4)$$

An application of Poisson’s sum formula also gives the total probability function,

$$\begin{aligned} P(\vartheta_1, \vartheta_0) &= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \exp[-im(\vartheta_0 - \vartheta_1) - m^2(lL/4R^2)]. \end{aligned} \quad (2.5)$$

Note that the m in Eq. (2.5) is not anymore the winding number n of Eq. (2.3). Setting $\vartheta_0 = \vartheta_1$ for an

Download English Version:

<https://daneshyari.com/en/article/9868190>

Download Persian Version:

<https://daneshyari.com/article/9868190>

[Daneshyari.com](https://daneshyari.com)