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The Mean First Rotation Time of a planar polymer

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Abstract

We estimate here the mean first time, called the mean rotation time (MRT), for a planar polymer to wind around a point. The polymer is modeled as a collection of n rods, each of them parameterized by a Brownian angle. We are led to study the sum of i.i.d. exponentials with a one dimensional Brownian motion in the argument. We find that the free end of the polymer satisfies a novel stochastic equation with nonlinear time function. Finally, we obtain an asymptotic formula for the MRT, and the leading order term depends on \sqrt{n} and, interestingly, weakly on the initial configuration. Our analytical results are confirmed by Brownian simulations.

1 Introduction

The main focus of this paper is on some properties of a planar polymer motion and in particular, the mean time that a rotation is completed around a fixed point. This mean rotation time (MRT) provides a quantification for the transition between a free two dimensional Brownian motion to a restricted motion. To characterize this time, we shall use a simplified model

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of a polymer made by a collection of n two dimensional connected rods with Brownian random angle (Figure 1). To estimate the mean rotation time, we shall fix one end part of the polymer. We shall examine how the MRT depends on various parameters such as the diffusion constant, the number of rods or their length. Using some types of approximations and numerical simulations, the mean time for the two polymer ends to meet was estimated in dimension three [PZS96, WiF74].

Although the windings of a planar Brownian motion, that is the number of rotations around one point in dimension 2 or a line in dimension three and its asymptotic behavior has commonly been studied [ReY99, Spi58, PiY86, LeGY87, LeG90], very little is known about the mean time for a rotation to be completed for the first time. For an Ornstein-Uhlenbeck process, we recently [Vak10] estimated the first time that it hits the boundary of a given cone.

The paper is organized as followed: in section two, we present the polymer model. In section three, we study a sum of i.i.d. exponentials of one dimensional Brownian motions. Interestingly, using a Central Limit Theorem, we obtain a new stochastic equation for the limit process. This equation describes the motion of the free polymer end. In section four, we obtain the main result which is an asymptotic formula for the MRT $E[\tau_n]$ when the polymer is made of n rods of equal lengths l_0 with the first end fixed at a distance L from the origin and the Brownian motion is characterized by the diffusion constant D the rotational diffusion constant. We find that The MRT depends logarithmically on the initial configuration and for $nl_0 \gg L$ and $n \geq 3$, the leading order term is given by:

1.

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \left[2 \ln \left(\frac{\sum_{k=1}^n e^{\frac{i}{\sqrt{2D}} \theta_k(0)}}{\sqrt{n}} + O(1) \right) + Q \right],$$

where $(\theta_k(0), 1 \leq k \leq n)$ are the initial angles of the polymer and $Q = 9.56$,

2. for an initially stretched polymer,

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \ln n,$$

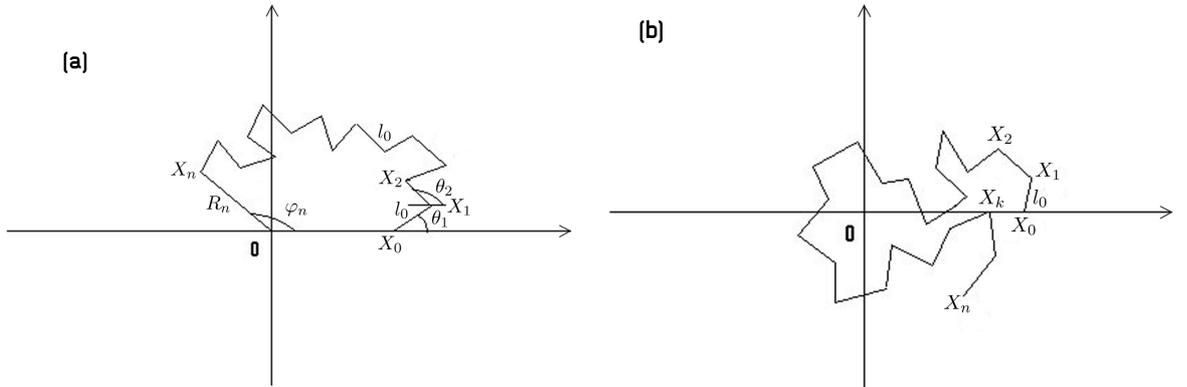


Figure 1: **Schematic representation of a planar polymer winding around the origin.**(a) A random configuration, (b) MRT when one of the beads reaches 2π .

3. for an average over uniformly distributed initial angles,

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \left[2 \ln \left(\frac{L}{l_0 \sqrt{n}} + O(1) \right) + Q \right].$$

We confirm our analytical results with Brownian simulations. Finally, in section five we discuss some related and open questions.

2 Stochastic modeling of a planar polymer

Various models are available to study polymers: the Rouse model consists of a collection of beads connected by springs, while more sophisticated models account for bending, torsion and specific mechanical properties [Rou53, SSS80, DoE94]. We shall consider here a very crude approximation where a planar polymer is modeled as a collection of n rigid rods, with equal fixed lengths l_0 of coordinates $(X_0, X_1, X_2, \dots, X_n)$ (Figure 1) in a framework with an origin $\mathbf{0}$. We shall fix one of the polymer end $X_0 = (L, 0)$ (where $L > 0$) on the x -axis. The dynamics of the i -th rod is characterized by its angle $\theta_i(t)$ with respect to the x -axis. The overall polymer dynamics is thus characterized by the angles $(\theta_1(t), \theta_2(t), \dots, \theta_n(t), t \geq 0)$. Due to the thermal collision in the medium, the angles are independent Brownian variables.

Thus, with $\stackrel{(law)}{=}$ denoting equality in law,

$$(\theta_i(t), i \leq n) \stackrel{(law)}{=} \sqrt{2D} (B_i(t), i \leq n) \Leftrightarrow \begin{cases} d\theta_1(t) = \sqrt{2D} dB_1(t) \\ d\theta_2(t) = \sqrt{2D} dB_2(t) \\ \vdots \\ d\theta_n(t) = \sqrt{2D} dB_n(t), \end{cases}$$

where D is the rotational diffusion constant and $(B_1(t), \dots, B_n(t), t \geq 0)$ is an n -dimensional Brownian motion (BM). The position of each rod can now be obtained as

$$\begin{cases} X_1(t) = L + l_0 e^{i\theta_1(t)} \\ X_2(t) = X_1(t) + l_0 e^{i\theta_2(t)} \\ \vdots \\ X_n(t) = X_{n-1}(t) + l_0 e^{i\theta_n(t)}. \end{cases} \quad (1)$$

In particular, the moving end is given by

$$X_n(t) = L + l_0 (e^{i\theta_1(t)} + \dots + e^{i\theta_n(t)}) = L + l_0 \sum_{k=1}^n e^{i\theta_k(t)} = L + l_0 \sum_{k=1}^n e^{i\sqrt{2D}B_k(t)}, \quad (2)$$

which can be written as

$$X_n(t) = R_n(t) e^{i\varphi_n(t)}, \quad (3)$$

and thus $\varphi_n(t)$ defines the rotation of the polymer with respect to the origin $\mathbf{0}$ and R_n is the associated distance.

Thus to compute the MRT, we shall study a sum of exponentials of Brownian motions, which usually leads to surprising computations [Yor01]. First, we scale the space and time variables as followed

$$\tilde{l} = \frac{L}{l_0} \quad \text{and} \quad \tilde{t} = \frac{t}{2D}. \quad (4)$$

equation (2) becomes

$$X_n(t) = \tilde{l} + \sum_{k=1}^n e^{i\tilde{B}_k(t)}, \quad (5)$$

where $(\tilde{B}_1(t), \dots, \tilde{B}_n(t), t \geq 0)$ is an n -dimensional Brownian motion (BM), and for $k = 1, \dots, n$, using the scaling property of Brownian motion, we have:

$$\tilde{B}_k(t) \equiv \frac{1}{\sqrt{2D}} B_k(t) \stackrel{(law)}{=} B_k\left(\frac{t}{2D}\right) = B_k(\tilde{t}).$$

From now on, we shall use B instead of \tilde{B} .

Before describing our approach, we shall now discuss the initial configuration of the polymer. The initial polymer configuration is given by

$$c_n \equiv \sum_{k=1}^n e^{i\theta_k(0)}, \quad (6)$$

where the initial angles $\theta_k(0)$ are such that the polymer has not already made a loop. After scaling, the initial configuration becomes

$$c_n = \sum_{k=1}^n e^{i\tilde{\theta}_k(0)}. \quad (7)$$

with

$$\tilde{\theta}_k(0) = \sqrt{2D} \theta_k(0). \quad (8)$$

From now on, we shall use $\theta_k(0)$ instead of $\tilde{\theta}_k(0)$. Any segment in the interior of the polymer can hit the angle 2π around the origin, but we will not consider this as a winding event, although we could and in that case, the MRT would be different. Rather, we shall only consider that given an initial configuration c_n , the MRT is defined as

$$MRT \equiv E\{\tau_n | c_n\} \equiv E[\tau_n], \quad (9)$$

where

$$\tau_n \equiv \inf\{t > 0, \varphi_n(t) = 2\pi \text{ or } -2\pi\}. \quad (10)$$

Thus, an initial configuration is not winding when

$$|\varphi_n(0)| < 2\pi. \quad (11)$$

Thus, we can define the winding event using a one dimensional variable only. In general, winding is a rare event and we expect that the MRT will depend crucially on the length of the polymer and will be quite long. Interestingly, the rotation is accomplished when the angle $\varphi_n(t)$ reaches 2π or -2π , but the distance of the free end point to the origin is not fixed, leading to a one dimensional free parameter space. This undefined position is in favor of a winding time that is not too large compared to any narrow escape problem where a Brownian particle has to find a small target in a confined domain [WaK93, PWPSK09, HoS04, SSHE06, SSH07, BKH07].

In this study, we will consider not only that the initial condition satisfies $|\varphi_n(0)| < 2\pi$, but we shall impose that $\varphi_n(0)$ is located far enough from 2π , to avoid studying any boundary layer effect, which would lead to a different MRT law. Indeed, starting inside the boundary layer for a narrow escape type problem leads to specific escape laws [SSHE06]. Given a small $\varepsilon > 0$ we shall consider the space of configurations Ω_ε such that $|\varphi_n(0)| < 2\pi - \varepsilon$. We shall mainly focus on the stretched polymer

$$(\theta_1(0), \theta_2(0), \dots, \theta_n(0)) = (0, 0, \dots, 0) \quad (12)$$

and thus $c_n = n > 0$ (in this case, $\varphi_n(0) = 0$). Finally, it is quite obvious that winding occurs only when the condition

$$nl_0 > L \quad (13)$$

is satisfied, which we assume all along.

The outline of our method is: first we show that the sum $X_n(t)$ converges (eq. (2)) and we obtain a Central Limit Theorem. Using Itô calculus, we study the sequence

$$\frac{1}{\sqrt{n}}\bar{X}_n(t) = \frac{1}{\sqrt{n}}[X_n(t) - E(X_n(t))]. \quad (14)$$

and prove that $X_n(t)$, for n large, converges to a stochastic process which is a generalization of an Ornstein-Uhlenbeck process (GOUP), containing a time dependent deterministic drift $c_n e^{-t}$. This GOUP is driven by a (local) martingale $(M_t^{(n)}, t \geq 0)$ that we further characterize. Interestingly, each

of the two cartesian coordinates of $(M_t^{(n)}, t \geq 0)$ converges to two independent Brownian motions with two different time scale functions. To obtain an asymptotic formula for the MRT, we show that in the long time asymptotic, where winding occurs, the GOUP can be approximated by a standard Ornstein-Uhlenbeck process (OUP). Using some properties of the GOUP [Vak10], we finally derive the MRT for the polymer which is the mean time that $\varphi_n(t) = 2\pi$ or -2π .

3 Properties of the free polymer end $X_n(t)$ using a Central Limit Theorem

In this section we study some properties of the free polymer end $\overline{X}_n(t)$. In particular, using a Central Limit Theorem, we show that the limit process satisfies a stochastic equation of a new type. To study the random part of $X_n(t)$, we shall remove from it its first moment and we shall now consider the asymptotic behavior of the drift-less sequence

$$\frac{1}{\sqrt{n}}\overline{X}_n(t) = \frac{1}{\sqrt{n}}[X_n(t) - E(X_n(t))]. \quad (15)$$

We start by computing the first moment $E(X_n(t))$. Because in relation (2), $(\theta_i(t), t \geq 0)$ are n independent identically distributed (iid) Brownian motions with variance $2D$, after rescaling, we obtain that

$$\begin{aligned} E(X_n(t)) &= E\left[\tilde{l} + \sum_{k=1}^n e^{iB_k(t)}\right] \\ &= \tilde{l} + \left(\sum_{k=1}^n E[e^{i(B_k(t)-B_k(0))}] E[e^{i(B_k(0))}]\right) \\ &= \tilde{l} + c_n e^{-\frac{t}{2}}. \end{aligned} \quad (16)$$

where c_n is defined by (7) and we have used that

$$E[e^{i(B_k(t)-B_k(0))}] = e^{-\frac{t}{2}} \quad (17)$$

We study the sequence (15) as follows:

$$\begin{aligned}\frac{1}{\sqrt{n}}\bar{X}_n(t) &= \frac{1}{\sqrt{n}} \left[\sum_{k=1}^n e^{iB_k(t)} - E \left(\sum_{k=1}^n e^{iB_k(t)} \right) \right] \\ &= \frac{1}{\sqrt{n}} \sum_{k=1}^n F_k(t),\end{aligned}\tag{18}$$

where $F_k(t) = e^{iB_k(t)} - E(e^{iB_k(t)})$. Applying Itô's formula to

$$Z_t^{(n)} = \frac{1}{\sqrt{n}} \sum_{k=1}^n F_k(t)\tag{19}$$

with $Z_0^{(n)} = 0$, we obtain that

$$\begin{aligned}Z_t^{(n)} &= \frac{i}{\sqrt{n}} \int_0^t \sum_{k=1}^n e^{iB_k(s)} dB_k(s) - \frac{1}{2\sqrt{n}} \int_0^t \sum_{k=1}^n (e^{iB_k(s)} - E(e^{iB_k(s)})) ds = \\ &= M_t^{(n)} - \frac{1}{2} \int_0^t Z_s^{(n)} ds,\end{aligned}\tag{20}$$

where

$$\begin{aligned}M_t^{(n)} &= \frac{1}{\sqrt{n}} i \int_0^t \sum_{k=1}^n e^{iB_k(s)} dB_k(s) \\ &= \frac{1}{\sqrt{n}} \int_0^t \sum_{k=1}^n (i \cos(B_k(s)) - \sin(B_k(s))) dB_k(s) \\ &= S_t^{(n)} + iC_t^{(n)}.\end{aligned}\tag{21}$$

We shall now study the asymptotic limit of the local martingale $M_t^{(n)}$ and summarize our result in the following theorem.

Theorem 3.1 *The sequence $(M_t^{(n)}, t \geq 0)$ converges in law to a Brownian motion in dimension 2, viewed at a nonlinear function of time. We obtain a convergence in law associated with the topology of the uniform convergence on compact sets of the functions in $C(\mathbb{R}_+, \mathbb{R}^2)$. More precisely,*

$$(S_u^{(n)}, C_u^{(n)}, u \geq 0) \xrightarrow[n \rightarrow \infty]{(law)} (\hat{\beta}_{\frac{1}{2} \int_0^u ds (1+e^{-2s})}, \tilde{\beta}_{\frac{1}{2} \int_0^u ds (1-e^{-2s})}, u \geq 0),\tag{22}$$

where $(\hat{\beta}_u, \tilde{\beta}_u, u \geq 0)$ are two independent Brownian motions.

Remark 3.2 *The approximation result of equation (22) is new and it shows that the sum of complex exponentials of i.i.d. Brownian motions can be approximated by a two dimensional Brownian motion, given at a time which is a nonlinear function different for each coordinate.*

The proof of Theorem 3.1 is given in Appendix A. We conclude that the sequence $M_t^{(n)}$ converges in law as

$$M_t^{(n)} \xrightarrow[n \rightarrow \infty]{(law)} \hat{\beta}_{\left(\frac{t}{2} + \frac{1-e^{-2t}}{4}\right)} + i\tilde{\beta}_{\left(\frac{t}{2} - \frac{1-e^{-2t}}{4}\right)}, \quad (23)$$

and we define $Z_t^{(n)}$, which generalizes a classical Ornstein-Uhlenbeck process. It is driven by $(M_t^{(n)}, t \geq 0)$ and is solution of

$$\begin{aligned} Z_t^{(n)} &= M_t^{(n)} - \frac{1}{2} \int_0^t Z_s^{(n)} ds \\ &= e^{-\frac{t}{2}} \int_0^t e^{\frac{s}{2}} dM_s^{(n)}. \end{aligned} \quad (24)$$

Corollary 3.3 *The sequence $Z_t^{(n)}$ converges*

$$\begin{aligned} Z_t^{(n)} &= e^{-\frac{t}{2}} \int_0^t e^{\frac{s}{2}} dM_s^{(n)} \\ &\xrightarrow[n \rightarrow \infty]{(law)} e^{-\frac{t}{2}} \left\{ \int_0^t e^{\frac{s}{2}} d\hat{\beta}_{\left(\frac{1}{2} \int_0^u ds (1+e^{-2s})\right)} + i \int_0^t e^{\frac{s}{2}} d\tilde{\beta}_{\frac{1}{2} \left(\int_0^u ds (1-e^{-2s})\right)} \right\} \\ &= e^{-\frac{t}{2}} \left\{ \int_0^t e^{\frac{s}{2}} \left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right) \right\}. \end{aligned} \quad (26)$$

From the identities (15), (16), (18), (20) and Theorem 3.1 we obtain the following expansion

$$\begin{aligned} X_n(t) &= \overline{X}_n(t) + E[X_n(t)] \\ &= \sqrt{n} Z_t^{(n)} + c_n e^{-\frac{t}{2}} + \tilde{l}, \end{aligned} \quad (27)$$

with $Z_t^{(n)}$ a GOUP driven by $M_t^{(n)}$ which is given by (23). From this expression for the sequence $X_n(t)$, and using the Ornstein-Uhlenbeck property

[ReY99], we have that

$$\begin{aligned}
X_n(t) &= \sqrt{n}Z_t^{(n)} + c_n e^{-\frac{t}{2}} + \tilde{l} \\
&= \sqrt{n} \left(\frac{\tilde{l}}{\sqrt{n}} + Z_t^{(n)} + \frac{c_n}{\sqrt{n}} e^{-\frac{t}{2}} \right) \\
&= \sqrt{n} \left(e^{-\frac{t}{2}} \left(\frac{\tilde{l}}{\sqrt{n}} + \int_0^t e^{\frac{s}{2}} dM_s^{(n)} \right) + \frac{c_n}{\sqrt{n}} e^{-\frac{t}{2}} \right) \\
&\stackrel{(law)}{\approx} \sqrt{n} e^{-\frac{t}{2}} \left(\tilde{c}_n + \left(\int_0^t e^{\frac{s}{2}} \left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right) \right) \right),
\end{aligned}$$

where

$$\tilde{c}_n \equiv \frac{\tilde{l}}{\sqrt{n}} + \frac{c_n}{\sqrt{n}}, \quad (28)$$

and $\tilde{l} = \frac{L}{l_0}$ is the rescaled distance of the fixed end from the origin $\mathbf{0}$ (l_0 is the fixed length of the rods), n is the number of rods/beads, and c_n is a constant depending on the initial configuration. Finally

$$X_n(t) \stackrel{(law)}{\approx} \sqrt{n} e^{-\frac{t}{2}} (\tilde{c}_n + I(t)), \quad (29)$$

where

$$I(t) = \left(\int_0^t e^{\frac{s}{2}} \left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right) \right). \quad (30)$$

4 Asymptotic expression for the MRT

Estimation of the MRT

We shall now study more precisely the different time scales of the two Brownian motions in (23) and in (30). We rewrite the expression (26) as:

$$Z_t^{(n)} \stackrel{(law)}{\underset{n:large}{\approx}} e^{-\frac{t}{2}} I(t), \quad (31)$$

where

$$I(t) = \int_0^t e^{\frac{s}{2}} \left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right). \quad (32)$$

In order to study $I(t)$, we decompose it into two integrals, the first one from 0 to t_1 and the second one from t_1 to t , where $t_1 = O\left(\frac{1}{t}\right)$.

We shall estimate each one for t large, hence $t_1 \rightarrow 0$ with $t_1 < t$, the regime for which the rotation will be accomplished. Thus:

$$I(t) = J^1(t_1) + J^2(t), \quad (33)$$

where:

$$J^1(t_1) \equiv \int_0^{t_1} e^{\frac{s}{2}} \left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right) \quad (34)$$

$$J^2(t) \equiv \int_{t_1}^t e^{\frac{s}{2}} \left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right). \quad (35)$$

We shall now estimate each integral separately. We shall use the notation $\langle \cdot \rangle$ for the quadratic variation: for a real-valued stochastic process M_t and for the sequence $\{\Delta_n\}$ of the subdivisions of an interval $[0, t]$, for every t , the quadratic variation is

$$\langle M, M \rangle_t = \lim_{|\Delta_n| \rightarrow 0} \sum_{k=1}^n (M_{t_k} - M_{t_{k-1}})^2.$$

More generally, the quadratic covariation of two real-valued stochastic processes M_t and N_t is defined by

$$\langle M, N \rangle_t = \lim_{|\Delta_n| \rightarrow 0} \sum_{k=1}^n (M_{t_k} - M_{t_{k-1}}) (N_{t_k} - N_{t_{k-1}}).$$

We shall use here the following notation: $\stackrel{L^2}{\approx}$ denotes an approximation in the L^2 -norm: Two stochastic processes $(W_t^{(1)}, t \geq 0)$ and $(W_t^{(2)}, t \geq 0)$ such that $W_t^{(1)} \stackrel{L^2}{\approx} W_t^{(2)}$ referees to $\lim_{t \rightarrow \infty} E \left[\left(W_t^{(1)} - W_t^{(2)} \right)^2 \right] = 0$. We shall now show that:

$$J^1(t_1) \stackrel{L^2}{\approx} \int_0^{t_1} e^{\frac{s}{2}} \left(d\hat{\beta}_s + i d\tilde{\beta}_{\frac{s}{2}} \right) \quad (36)$$

$$J^2(t) \stackrel{L^2}{\approx} \sqrt{\frac{1}{2}} \int_{t_1}^t e^{\frac{s}{2}} \underbrace{\left(d\hat{\beta}_s + i d\tilde{\beta}_s \right)}_{d\mathbb{B}_s} + O(1), \quad (37)$$

For that purpose, we start with the first integral. Using Burkholder-Davis-Gundy inequality (BDG) [ReY99, KaSh88], there exists a constant $0 < c_1 < \infty$ such that:

$$\begin{aligned}
& E \left[\left(J^1(t_1) - \int_0^{t_1} e^{\frac{s}{2}} \left(d\hat{\beta}_s + id\tilde{\beta}_{\frac{s}{2}} \right) \right)^2 \right] \\
& \equiv E \left[\left(\int_0^{t_1} e^{\frac{s}{2}} \left[\left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right) - \left(d\hat{\beta}_s + id\tilde{\beta}_{\frac{s}{2}} \right) \right] \right)^2 \right] \\
& = E \left[\left(\int_0^{t_1} e^{\frac{s}{2}} \left[d\hat{\beta}_{\left(\frac{1-e^{-2s}}{4} - \frac{s}{2}\right)} + i d\tilde{\beta}_{\left(-\frac{1-e^{-2s}}{4} + \frac{s}{2} - \frac{s^2}{2}\right)} \right] \right)^2 \right] \\
& \leq c_1 E \left[\left\langle \int_0^{t_1} e^{\frac{s}{2}} \left[d\hat{\beta}_{\left(\frac{1-e^{-2s}}{4} - \frac{s}{2}\right)} + i d\tilde{\beta}_{\left(-\frac{1-e^{-2s}}{4} + \frac{s}{2} - \frac{s^2}{2}\right)} \right] \right\rangle \right] \\
& = c_1 \left(\int_0^{t_1} e^s d \left(\frac{1-e^{-2s}}{4} - \frac{s}{2} \right) - \int_0^{t_1} e^s d \left(-\frac{1-e^{-2s}}{4} + \frac{s}{2} - \frac{s^2}{2} \right) \right) \\
& = c_1 \left(\int_0^{t_1} e^s d \left(\frac{1-e^{-2s}}{2} \right) - \int_0^{t_1} e^s ds + \int_0^{t_1} e^s d \left(\frac{s^2}{2} \right) \right) \\
& = c_1 \left(\int_0^{t_1} e^s (e^{-2s} + s - 1) ds \right) \\
& = c_1 \left(\int_0^{t_1} e^{-s} ds + \int_0^{t_1} s e^s ds - \int_0^{t_1} e^s ds \right) \\
& = c_1 (e^{-t_1} - 1 + t_1 e^{t_1} - 2e^{t_1} + 2) = O(t_1) \equiv O\left(\frac{1}{t}\right) \stackrel{t:large}{\approx} 0, \tag{38}
\end{aligned}$$

and for the second one:

$$\begin{aligned}
& E \left[\left(\left(J^2(t) - \sqrt{\frac{1}{2}} \int_{t_1}^t e^{\frac{s}{2}} \left(d\hat{\beta}_s + id\tilde{\beta}_s \right) \right) - O(1) \right)^2 \right] \\
& \leq E \left[\left(J^2(t) - \sqrt{\frac{1}{2}} \int_{t_1}^t e^{\frac{s}{2}} \left(d\hat{\beta}_s + id\tilde{\beta}_s \right) \right)^2 \right] + (O(1))^2 \\
& \leq O(1) + (O(1))^2 = O(1), \tag{39}
\end{aligned}$$

because there is a constant $0 < c_2 < \infty$ such that:

$$\begin{aligned}
& E \left[\left(J^2(t) - \sqrt{\frac{1}{2}} \int_{t_1}^t e^{\frac{s}{2}} \left(d\hat{\beta}_s + i d\tilde{\beta}_s \right) \right)^2 \right] \\
&= E \left[\left(J^2(t) - \int_{t_1}^t e^{\frac{s}{2}} \left(d\hat{\beta}_{\frac{s}{2}} + i d\tilde{\beta}_{\frac{s}{2}} \right) \right)^2 \right] \\
&\equiv E \left[\left(\int_{t_1}^t e^{\frac{s}{2}} \left[\left(d\hat{\beta}_{\left(\frac{s}{2} + \frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(\frac{s}{2} - \frac{1-e^{-2s}}{4}\right)} \right) - \left(d\hat{\beta}_{\frac{s}{2}} + i d\tilde{\beta}_{\frac{s}{2}} \right) \right] \right)^2 \right] \\
&= E \left[\left(\int_{t_1}^t e^{\frac{s}{2}} \left[d\hat{\beta}_{\left(\frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(-\frac{1-e^{-2s}}{4}\right)} \right] \right)^2 \right] \\
&\leq c_2 E \left[\left\langle \int_{t_1}^t e^{\frac{s}{2}} \left[d\hat{\beta}_{\left(\frac{1-e^{-2s}}{4}\right)} + i d\tilde{\beta}_{\left(-\frac{1-e^{-2s}}{4}\right)} \right] \right\rangle \right] \\
&= c_2 \left(\int_{t_1}^t e^s d \left(\frac{1-e^{-2s}}{4} \right) - \int_{t_1}^t e^s d \left(-\frac{1-e^{-2s}}{4} \right) \right) \\
&= c_2 \left(2 \int_{t_1}^t e^s \frac{1}{2} e^{-2s} ds \right) = c_2 \int_{t_1}^t e^{-s} ds \\
&= c_2 (e^{-t_1} - e^{-t}) = c_2 \left(e^{-O\left(\frac{1}{t}\right)} - e^{-t} \right) \stackrel{t: \text{large}}{\approx} O(1). \tag{40}
\end{aligned}$$

Thus:

$$I(t) \stackrel{L^2}{\approx} \int_0^{t_1} e^{\frac{s}{2}} \left(d\hat{\beta}_s + i d\tilde{\beta}_{\frac{s}{2}} \right) + \underbrace{\sqrt{\frac{1}{2}} \int_{t_1}^t e^{\frac{s}{2}} \left(d\hat{\beta}_s + i d\tilde{\beta}_s \right)}_{d\mathbb{B}_s} + O(1), \tag{41}$$

where $(\mathbb{B}_t = \hat{\beta}_t + i\tilde{\beta}_t, t \geq 0)$ is a 2-dimensional Brownian motion starting from 1.

We estimate now the contribution of each integral in (41). Using again Burkholder-Davis-Gundy inequality (BDG) [ReY99, KaSh88], there exists a

constant $0 < c_3 < \infty$ such that:

$$\begin{aligned}
E \left[\left(\int_0^{t_1} e^{\frac{s}{2}} \left(d\hat{\beta}_s + id\tilde{\beta}_{\frac{s^2}{2}} \right) \right)^2 \right] &\leq c_3 E \left[\left\langle \int_0^{t_1} e^{\frac{s}{2}} \left(d\hat{\beta}_s + id\tilde{\beta}_{\frac{s^2}{2}} \right) \right\rangle \right] \\
&= c_3 \left(\int_0^{t_1} e^s ds - \int_0^{t_1} e^s d\left(\frac{s^2}{2}\right) \right) \\
&= c_3 \left(\int_0^{t_1} e^s ds - \int_0^{t_1} s e^s ds \right) \\
&= c_3 \left((e^{t_1} - 1) - \left(t_1 e^{t_1} - \int_0^{t_1} e^s ds \right) \right) \\
&= c_3 \left((e^{t_1} - 1) - (t_1 e^{t_1} - e^{t_1} + 1) \right) \\
&= c_3 (2e^{t_1} - 2 - t_1 e^{t_1}). \tag{42}
\end{aligned}$$

For t large $\Rightarrow t_1 = O\left(\frac{1}{t}\right)$ small, and:

$$E [J^1(t_1)^2] \leq O(t_1) \equiv O\left(\frac{1}{t}\right),$$

and thus $J^1(t_1)$ is of order $O(t_1) \equiv O\left(\frac{1}{t}\right)$.

Asymptotic expression for the MRT

We shall now gather the expressions (33) and (42), with $t_1 = \frac{1}{t} \xrightarrow{t:large} 0$, to derive an asymptotic value for the MRT. First, we have that

$$I(t) \stackrel{L^2}{\approx} O(1) + \sqrt{\frac{1}{2}} \int_0^t e^{\frac{s}{2}} \left(d\hat{\beta}_s + i d\tilde{\beta}_s \right), \tag{43}$$

and from (29) and (31):

$$X_t^{(n)} \stackrel[n:large]{(law)}{\approx} \sqrt{n} Y_t^{(n)}, \tag{44}$$

where (we denote Y_t for $Y_t^{(n)}$)

$$Y_t \equiv e^{-\frac{t}{2}} \left(\tilde{c}'_n + \sqrt{\frac{1}{2}} \int_0^t e^{\frac{s}{2}} d\mathbb{B}_s \right), \tag{45}$$

and the sequence is

$$\tilde{c}'_n \equiv \frac{\tilde{l}}{\sqrt{n}} + \frac{c_n}{\sqrt{n}} + O(1), \quad (46)$$

where $\tilde{l} = \frac{l}{l_0}$ is the rescaled distance of the fixed end from the origin $\mathbf{0}$ (l_0 is the fixed length of the rods), n is the number of rods/beads, and $c_n \equiv \sum_{k=1}^n e^{i\theta_k(0)}$ is a constant depending on the initial configuration.

Changing time and expression of the MRT

We shall now apply successive changes of time to express the MRT. By changing the variables $u = \frac{s}{2}$ in (45) and by the scaling property of Brownian motion, we have

$$Y_t \equiv e^{-\frac{t}{2}} \left(\tilde{c}'_n + \sqrt{\frac{1}{2}} \int_0^{t/2} e^u d\mathbb{B}_{2u} \right) \stackrel{(law)}{=} e^{-\frac{t}{2}} \left(\tilde{c}'_n + \int_0^{t/2} e^u d\mathbb{B}_u \right).$$

Thus:

$$Y_{2t} \stackrel{(law)}{=} e^{-t} \left(\tilde{c}'_n + \int_0^t e^u d\mathbb{B}_u \right). \quad (47)$$

For $\lambda = 1$ and $z_0 = \tilde{c}'_n$, by Dambis-Dubins-Schwarz Theorem we have that [Vak10]:

$$Y_{2t} \stackrel{(law)}{=} e^{-t} (\mathbb{B}_{\alpha_t}), \quad (48)$$

where

$$\begin{aligned} \alpha_t &= \int_0^t e^{2s} ds = \frac{e^{2t} - 1}{2} \\ \Rightarrow \alpha^{-1}(t) &= \frac{1}{2} \ln(1 + 2t). \end{aligned} \quad (49)$$

By applying Itô's formula to (48), we obtain

$$dY_{2s} = -e^{-s} \mathbb{B}_{\alpha_s} ds + e^{-s} d(\mathbb{B}_{\alpha_s}).$$

We divide by Y_{2s} and we obtain:

$$\frac{dY_{2s}}{Y_{2s}} = -ds + \frac{d\mathbb{B}_{\alpha_s}}{\mathbb{B}_{\alpha_s}}.$$

Thus:

$$\operatorname{Im} \left(\frac{dY_{2s}}{Y_{2s}} \right) = \operatorname{Im} \left(\frac{d\mathbb{B}_{\alpha_s}}{\mathbb{B}_{\alpha_s}} \right),$$

which means that for the continuous winding process

$$\theta_t^Z \equiv \operatorname{Im} \left(\int_0^t \frac{dZ_s}{Z_s} \right), t \geq 0, \quad (50)$$

associated to a stochastic process Z , then

$$\theta_{2t}^Y = \theta_{\alpha_t}^{\mathbb{B}}.$$

Thus with relation (49), the first hitting times of the symmetric conic boundary of angle c

$$T_c^\theta \equiv \inf \{ t \geq 0 : |\theta_t^Y| = c \}, \quad (51)$$

and

$$T_{-c,c}^\theta \equiv \inf \{ t \geq 0 : |\theta_t^B| = c \} \quad (52)$$

for the Ornstein-Uhlenbeck process Y and for a Brownian motion B respectively satisfy

$$2T_c^\theta = \frac{1}{2} \ln (1 + 2T_{-c,c}^\theta). \quad (53)$$

Finally,

$$E [2T_c^\theta] = \frac{1}{2} E [\ln (1 + 2T_{-c,c}^\theta)] \quad (54)$$

$$= \frac{\ln 2}{2} + \frac{1}{2} E \left[\ln \left(T_{-c,c}^\theta + \frac{1}{2} \right) \right], \quad (55)$$

and equivalently:

$$E [T_c^\theta] = \frac{1}{4} E [\ln (1 + 2T_{-c,c}^\theta)] \quad (56)$$

$$= \frac{\ln 2}{4} + \frac{1}{4} E \left[\ln \left(T_{-c,c}^\theta + \frac{1}{2} \right) \right]. \quad (57)$$

Thus, by taking $c = 2\pi$, for n large, the mean time $E[\tau_n]$ that the polymer rotates around $\mathbf{0}$, is

$$E[\tau_n] \approx \frac{\sqrt{n}}{4} \left(\ln 2 + E \left[\ln \left(T_{-2\pi, 2\pi}^\theta + \frac{1}{2} \right) \right] \right). \quad (58)$$

By using the series expansion of $\log(1+x)$, we shall now estimate the second term:

$$\begin{aligned} E \left[\ln \left(T_{-c, c}^\theta + \frac{1}{2} \right) \right] - E \left[\ln (T_{-c, c}^\theta) \right] &= E \left[\ln \left(1 + \frac{1}{2T_{-c, c}^\theta} \right) \right] \\ &= \frac{1}{2} E \left[\frac{1}{T_{-c, c}^\theta} \right] - \frac{1}{8} E \left[\left(\frac{1}{T_{-c, c}^\theta} \right)^2 \right] + \dots \end{aligned}$$

Using the Laplace transform for the hitting time $T_{-c, c}^\theta$ of a Brownian motion

$$E \left[e^{-\frac{\lambda^2}{2} T_{-c, c}^\theta} \right] = \frac{1}{\cosh(\lambda c)}, \quad (59)$$

[ReY99] (Chapter II, Prop. 3.7) or [PiY03](p.298), we get

$$\begin{aligned} E \left[\frac{1}{T_{-c, c}^\theta} \right] &= \int_0^\infty dt E \left[e^{-t T_{-c, c}^\theta} \right] \stackrel{t=\frac{\lambda^2}{2}}{=} \int_0^\infty \lambda d\lambda \underbrace{E \left[e^{-\frac{\lambda^2}{2} T_{-c, c}^\theta} \right]}_{\frac{1}{\cosh(\lambda c)}} \\ &\stackrel{\lambda c = \mu}{=} \frac{1}{c^2} \int_0^\infty \frac{\mu d\mu}{\cosh(\mu)} = \frac{2}{c^2} \int_0^\infty \frac{\mu d\mu}{e^\mu (1 + e^{-2\mu})}, \end{aligned} \quad (60)$$

with:

$$\begin{aligned} \int_0^\infty \frac{\mu d\mu}{e^\mu (1 + e^{-2\mu})} &= \int_0^\infty \mu d\mu e^{-\mu} \sum_{n=0}^{+\infty} (-e^{-2\mu})^n \\ &= \sum_{n=0}^{+\infty} \int_0^\infty \mu d\mu (-1)^n e^{-(2n+1)\mu} \\ &= \sum_{n=0}^{+\infty} (-1)^n \frac{1}{(2n+1)^2} = \beta(2) = K, \end{aligned}$$

where $\beta(s)$ denotes Dirichlet's beta function which for $s = 2$ is equal to the Catalan's constant $K \approx 0.915965 \dots$. Similarly,

$$\begin{aligned}
E \left[\left(\frac{1}{T_{-c,c}^\theta} \right)^2 \right] &= \frac{1}{2\Gamma(2)} \int_0^\infty \lambda^3 \underbrace{E \left[e^{-\frac{\lambda^2}{2} T_{-c,c}^\theta} \right]}_{\frac{1}{\cosh(\lambda c)}} d\lambda \\
&\stackrel{\lambda c = \mu}{=} \frac{1}{2\Gamma(2)} \frac{1}{c^4} \int_0^\infty \frac{\mu^3 d\mu}{\cosh(\mu)} \\
&= \frac{1}{\Gamma(2)c^4} \int_0^\infty \mu^3 d\mu e^{-\mu} \sum_{n=0}^{+\infty} (-e^{-2\mu})^n \\
&= \frac{1}{\Gamma(2)c^4} \sum_{n=0}^{+\infty} \int_0^\infty \mu^3 d\mu (-1)^n e^{-(2n+1)\mu} \\
&= \frac{3!}{\Gamma(2)c^4} \sum_{n=0}^{+\infty} (-1)^n \frac{1}{(2n+1)^4} = \frac{6}{c^4} \beta(4). \quad (61)
\end{aligned}$$

Thus, for $c = 2\pi$, using formula (60) we obtain the numerical result

$$\frac{1}{2} E \left[\frac{1}{T_{-2\pi,2\pi}^\theta} \right] = \frac{1}{4\pi^2} K \approx 1.16 * 10^{-2},$$

and similarly using formula (61), we obtain

$$\frac{1}{8} E \left[\left(\frac{1}{T_{-2\pi,2\pi}^\theta} \right)^2 \right] = \frac{6}{8\pi^4} \beta(4) \approx 1.1925 * 10^{-4}.$$

Thus,

$$\frac{1}{8} E \left[\left(\frac{1}{T_{-2\pi,2\pi}^\theta} \right)^2 \right] \ll \frac{1}{2} E \left[\frac{1}{T_{-2\pi,2\pi}^\theta} \right],$$

and we can approximate:

$$E \left[\ln \left(T_{-2\pi,2\pi}^\theta + \frac{1}{2} \right) \right] \approx E \left[\ln (T_{-2\pi,2\pi}^\theta) \right] + \frac{1}{2} E \left[\frac{1}{T_{-2\pi,2\pi}^\theta} \right]. \quad (62)$$

To estimate the first moment of $\ln (T_{-c,c}^\theta)$, for an angle c , we use $(Z_t = Z_t^{(1)} + iZ_t^{(2)}, t \geq 0)$ a standard planar Brownian motion, starting from $\check{c}'_n + i0, \check{c}'_n > 0$,

where $(Z_t^{(1)}, t \geq 0)$ and $(Z_t^{(2)}, t \geq 0)$ are two independent linear Brownian motions, starting respectively from \tilde{c}'_n and 0. From the skew product representation [ReY99, Vak10] there is another planar Brownian motion $(\delta_u + i\gamma_u, u \geq 0)$ starting from $\log \tilde{c}'_n + i0$, such as:

$$\log |Z_t| + i\theta_t \equiv \int_0^t \frac{dZ_s}{Z_s} = (\delta_u + i\gamma_u) \Big|_{u=H_t \equiv \int_0^t \frac{ds}{|Z_s|^2}}, \quad (63)$$

and equivalently

$$\log |Z_t| = \delta_{H_t}; \quad \theta_t = \gamma_{H_t}. \quad (64)$$

Thus, with $T_{-c,c}^\gamma \equiv \inf \{t \geq 0 : |\gamma_t| = c\}$, because $\theta_{T_{-c,c}^\theta} = \gamma_{H_{T_{-c,c}^\theta}}$:

$$T_{-c,c}^\gamma = H_{T_{-c,c}^\theta},$$

hence $T_{-c,c}^\theta = H_u^{-1} \Big|_{u=T_{-c,c}^\gamma}$, where

$$H_u^{-1} \equiv \inf \{t : H_t > u\} = \int_0^u ds \exp(2\delta_s) \equiv A_u. \quad (65)$$

Hence, with $\delta_s = \log(\tilde{c}'_n) + \delta_s^{(0)}$, where $(\delta_s^{(0)}, s \geq 0)$ is another one-dimensional Brownian motion starting from 0, we obtain:

$$\begin{aligned} T_{-c,c}^\theta &= H^{-1}(T_{-c,c}^\gamma) \equiv \int_0^{T_{-c,c}^\gamma} ds \exp(2\delta_s) = (\tilde{c}')^2 \left(\int_0^{T_{-c,c}^\gamma} ds \exp(2\delta_s^{(0)}) \right) \\ &\equiv (\tilde{c}')^2 T_{-c,c}^{\theta(1)}, \end{aligned}$$

where $T_{-c,c}^{\theta(1)} \equiv \inf \{t \geq 0 : |\theta_t^Z| = c\}$ is the first hitting time of the symmetric conic boundary of angle c of a process Z starting from 1. Thus:

$$E [\ln (T_{-c,c}^\theta)] = 2 \ln(\tilde{c}') + E [\ln (T_{-c,c}^{\theta(1)})]. \quad (66)$$

The first moment of $\ln (T_{-c,c}^{\theta(1)})$ has the following integral representation ([Vak10] Prop. 2.9):

$$E [\ln (T_{-c,c}^{\theta(1)})] = 2F(c) + \ln(2) + c_E,$$

where

$$F(c) = \int_0^\infty \frac{dz}{\cosh\left(\frac{\pi z}{2}\right)} \ln(\sinh(cz)), \quad (67)$$

and $c_E \approx 0.577$ denotes Euler's constant.

Indeed, the skew product representation (64), for $t = T_{-c,c}^\theta$, yields: $H_{T_{-c,c}^\theta} = T_{-c,c}^\gamma \iff T_{-c,c}^\theta = A_{T_{-c,c}^\gamma}$, thus, for $\varepsilon > 0$:

$$E[(T_{-c,c}^\theta)^\varepsilon] - 1 = E\left[\left(A_{T_{-c,c}^\gamma}\right)^\varepsilon\right] - 1.$$

On the left hand side, we have

$$\frac{1}{\varepsilon} \left(E[(T_{-c,c}^\theta)^\varepsilon] - 1 \right) \equiv \frac{1}{\varepsilon} \left(E\left[e^{\varepsilon \ln(T_{-c,c}^\theta)} \right] - 1 \right) \xrightarrow{\varepsilon \rightarrow 0} E[\ln(T_{-c,c}^\theta)],$$

and on the right hand side, we use Bougerol's identity for $u = T_{-c,c}^\gamma$. This identity tells that for any fixed $u > 0$:

$$\sinh(\delta_u) \stackrel{(law)}{=} \hat{\delta}_{(A_u \equiv \int_0^u ds \exp(2\beta_s))},$$

with $(\hat{\delta}_t, t \geq 0)$ another Brownian motion, independent of δ . Hence, using the scaling property of Brownian motion, the density of $\delta_{T_{-c,c}^\gamma}$ [BiY87]:

$$h_{-c,c}(y) = \left(\frac{1}{2c}\right) \frac{1}{\cosh\left(\frac{y\pi}{2c}\right)} = \left(\frac{1}{c}\right) \frac{1}{e^{\frac{y\pi}{2c}} + e^{-\frac{y\pi}{2c}}},$$

and taking the limit for $\varepsilon \rightarrow 0$, we obtain (66). From (66), we finally obtain

$$E[\ln(T_{-c,c}^\theta)] = 2 \ln(\tilde{c}'_n) + 2F(c) + \ln(2) + c_E. \quad (68)$$

For $c = 2\pi$, we have $F(2\pi) \approx 3.8$. In Figure 2 we plot F with respect to the angle c . In summary, from (58), (62) and (68):

$$E[\tau_n] \approx \frac{\sqrt{n}}{4} (2 \ln(\tilde{c}'_n) + Q), \quad (69)$$

where

$$Q = 2F(2\pi) + 2 \ln 2 + c_E + \frac{1}{2} E\left[\frac{1}{T_{-2\pi,2\pi}^\theta}\right] \quad (70)$$

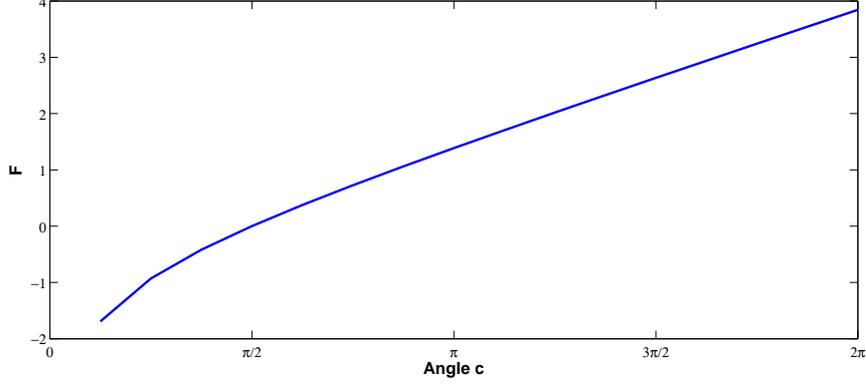


Figure 2: F as a function of the angle c .

is a constant with $F(2\pi) \approx 3.8$, $c_E \approx 0.577$, and $E \left[\frac{1}{T^{\theta_{-2\pi, 2\pi}}} \right] \approx 2.32 \cdot 10^{-2}$, thus

$$Q \approx 9.56. \quad (71)$$

For an initial configuration $c_n \equiv \sum_{k=1}^n e^{i\theta_k(0)}$

$$\tilde{c}'_n \approx \frac{\tilde{l}}{\sqrt{n}} + \frac{c_n}{\sqrt{n}} + O(1), \quad (72)$$

the MRT is given by the formula

$$E[\tau_n] \approx \frac{\sqrt{n}}{4} \left[2 \ln \left(\frac{\tilde{l}}{\sqrt{n}} + \frac{c_n}{\sqrt{n}} + O(1) \right) + Q \right]. \quad (73)$$

For a long enough polymer, such that $nl_0 \gg L \Rightarrow n \gg \tilde{l}$, so $\frac{\tilde{l}}{\sqrt{n}}$ is negligible with respect to $O(1)$, we obtain:

$$E[\tau_n] \approx \frac{\sqrt{n}}{4} \left[2 \ln \left(\frac{\sum_{k=1}^n e^{i\theta_k(0)}}{\sqrt{n}} + O(1) \right) + Q \right]. \quad (74)$$

Finally, using the unscaled variables (4), we obtain:

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \left[2 \ln \left(\frac{\sum_{k=1}^n e^{\frac{i}{\sqrt{2D}}\theta_k(0)}}{\sqrt{n}} + O(1) \right) + Q \right]. \quad (75)$$

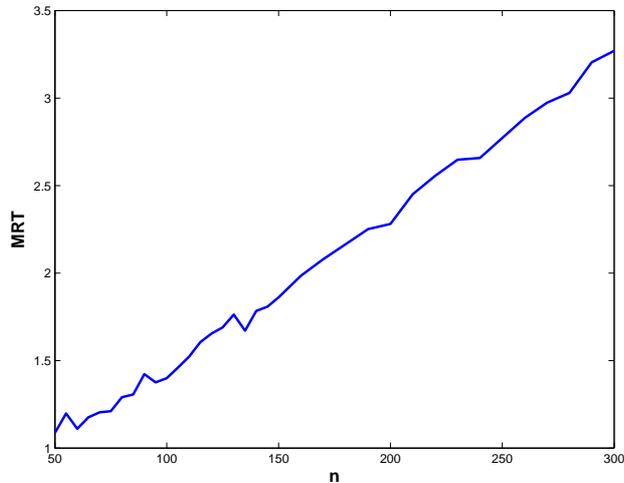


Figure 3: **MRT of the free polymer end as a function of the number of beads n (Brownian simulations).**

Expressions (74) and (75) show that the leading order term of the MRT depends through the log on the initial configuration, however this dependence is weak. The term of order $O(1)$ needs further investigation.

We consider now that the polymer is initially stretched, hence $c_n = n$. From (73), for a long enough polymer such that $nl_0 \gg L \Rightarrow n \gg \tilde{l}$, thus $\frac{\tilde{l}}{\sqrt{n}}$ and $O(1)$ are negligible with respect to \sqrt{n} , by using the unscaled variables (4), the MRT is approximately:

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} [\ln(n) + Q]. \quad (76)$$

In order to check the range of validity of formula (76), we run some Brownian simulations. In Figure 3, we simulated the MRT with a time step $dt = 0.01$ for $n = 50$ to 300 rods in steps of 5, and for each n , we took 300 samples and averaged over all of them. The parameters we chose are $D = 10$ the diffusion coefficient, $L = 0.3$ the distance from the origin $\mathbf{0}$ and $l_0 = 0.25$ the length of each rod and we chose for the initial condition a stretch polymer located on the half line $\mathbf{0}x$ (hence $c_n = L + nl_0$) $\theta_k(0) = 0, \forall k = (1, \dots, n)$ and then we computed the MRT $E[\tau_n]$. In Figure 4, we plot both the results from Brownian simulations and the formula (76). We considered values $n = 50$ from 300 rods in steps of 10, $D = 10$, $L = 0.3$, $l_0 = 0.25$, thus the condition

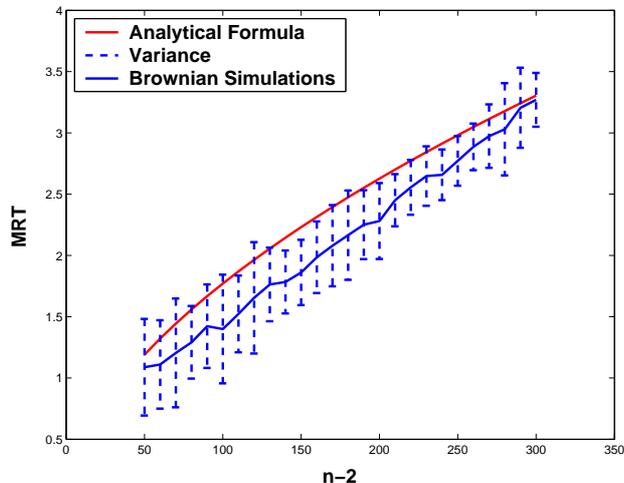


Figure 4: **Comparing the Analytical Formula and the Brownian simulations of the MRT.** The MRT of the polymer end is depicted with respect to the number of beads n .

$\sqrt{n} l_0 \gg L$ is satisfied. For each numerical computation, we performed 300 runs simulations with a time step $dt = 0.01$. By comparing the numerical simulations (Fig. 4), with the analytical formula for the MRT, we see an overshoot.

The straight initial configuration is no restriction to the generality of our study: we have that $c_n \leq n$ and the upper bound is achieved for a straight initial configuration. In Figure 5, we simulate the MRT $E[\tau_n]$ for both a random and a initially straight configuration (Brownian simulations with a time step $dt = 0.01$ for $n = 50$ to 300 rods in steps of 5, and for each n , we took 300 samples and averaged over all of them; the parameters we chose are $D = 10$ the diffusion coefficient, $L = 0.3$ the distance from the origin $\mathbf{0}$ and $l_0 = 0.25$).

Uniformly distributed initial angles

When the initial angles $(\theta_1(0), \theta_2(0), \dots, \theta_n(0))$ are uniformly distributed over $[0, 2\pi]$, by averaging over all the possible initial configurations, from (7), we

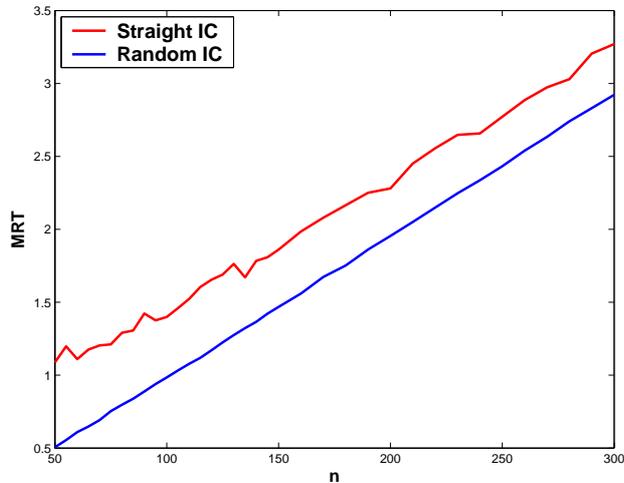


Figure 5: MRT of the free polymer end as a function of the number of beads n for the straight and for a random initial configuration (Brownian simulations).

obtain

$$\begin{aligned}
 E[X_n(0)] &\equiv E[\tilde{l} + c_n] = \tilde{l} + E\left[\sum_{k=1}^n e^{i\theta_k(0)}\right] \\
 &= \tilde{l} + E\left[\sum_{k=1}^n (\cos(\theta_k(0)) + i \sin(\theta_k(0)))\right] = \tilde{l}. \quad (77)
 \end{aligned}$$

Thus, the mean initial position for a bead is \tilde{l} and by using the unscaled variables (4) the MRT is given by

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \left[2 \ln \left(\frac{L}{l_0 \sqrt{n}} + O(1) \right) + Q \right]. \quad (78)$$

Remark 4.1 Formula (75) (or formulas (76) and (78)) provides the asymptotic expansion for the MRT when $\theta_1 \in \mathbb{R}_+$. In reality $\theta_1 \in [0, 2\pi]$, thus a better characterization is to estimate the MRT by using the probability density function for θ_1 in the one dimensional torus. By repeating the previous calculations, these formulas remain valid.

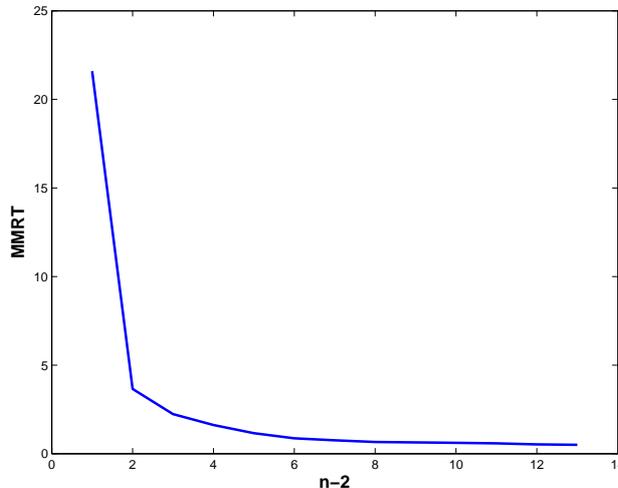


Figure 6: **Brownian simulations of the MMRT as a function of the number of beads $n - 2$ for $D = 10$.**

4.1 The Minimum Mean First Rotation Time

The Minimum Mean Rotation Time (MMRT) is the first time that any of the segments of the polymer loops around the origin,

$$MMRT \equiv \min_{E_n} E\{\tau_n | c_n\} \equiv E[\tau_{min}], \quad (79)$$

where E_n is the ensemble of rods such that can travel up to the origin. The MMRT is now a decreasing function of n . In Figure 6, we present some simulations for the MMRT as a function of n (100 simulations per time step $dt = 0.01$ with $n = 4$ to 15 rods and the diffusion constant $D = 10$, $L = 0.3$ the distance from the origin $\mathbf{0}$ and $l_0 = 0.25$ the length of each rod). The initial configuration is such that $|\varphi_n(0)| < 2\pi - \varepsilon$, e.g. the straight initial configuration: $\theta_k(0) = 0, \forall k = (1, \dots, n)$.

In Figure 7, we present some Brownian simulations for the MMRT as a function of D and of L (Figure 7(a) and Figure 7(b) respectively). L and l_0 satisfy the rotation compatibility condition $nl_0 > L$. $E[\tau_{min}]$ decreases with D and increases with the distance from the origin L .

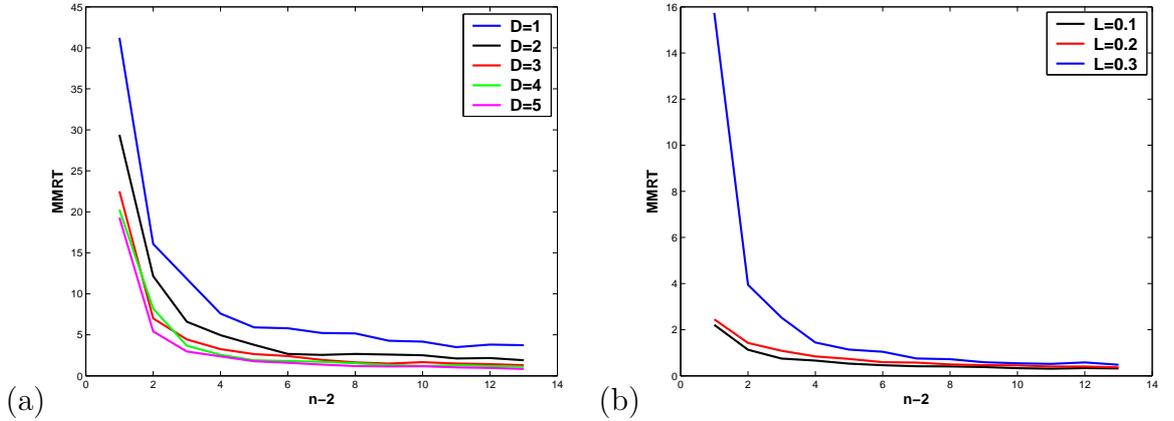


Figure 7: **Brownian simulations of the MMRT as a function of the number of beads $n - 2$.** (a) For several values of D with $L = 0.3$, (b) for several values of L with $D = 10$.

Initial configuration in the boundary layer

When the polymer is almost making a loop, we expect the MRT to have a different behavior. We look at this numerically, and we start with an initial polymer configuration in the boundary layer :

$$2\pi - \varepsilon \leq |\varphi_n(0)| < 2\pi.$$

where ϕ_n is defined in 3. The rotation of the polymer will be complete very fast and using Brownian simulations (100 runs per point with $n = 10$ rods and the diffusion constant $D = 1$, $L = 0.1$ the distance from the origin $\mathbf{0}$ and $l_0 = 0.2$ the length of each rod), we plotted in Figure 8 the results showing that when the initial total angle $\varphi_n(0)$ tends to 2π , the MRT tends to zero, the precise asymptotic remains to be completed. Numerically, we postulate that there is threshold for an initial total angle $|\varphi_n(0)| = \frac{\pi}{2}$. Before this value, the MRT seems independent from this angle, whereas for $|\varphi_n(0)| > \frac{\pi}{2}$, the MRT decreases to zero. However, this needs further investigation.

5 Discussion and conclusion

In the present paper, we studied the MRT for a planar polymer consisting of n rods of length l_0 . The first end is fixed at a distance L from the origin, while

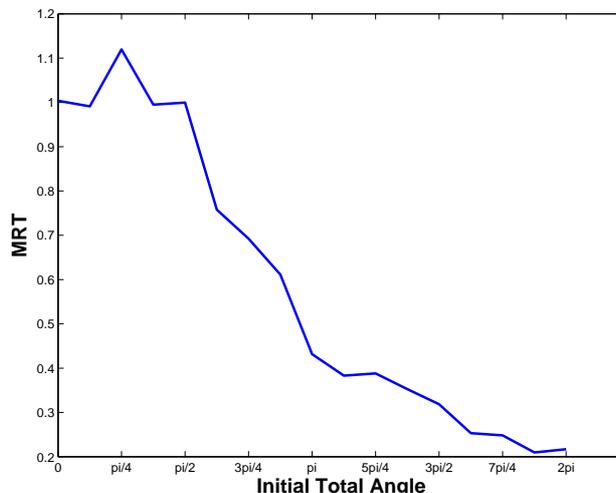


Figure 8: **Brownian simulations of the MRT as a function of the initial total angle $\varphi_n(0)$.**

the other end moves by Brownian motion. Interestingly, we have shown here that the motion of the free polymer end satisfies a new stochastic equation (27), containing a nonlinear time-dependent deterministic drift. When n is large, the limit stochastic equation is an Ornstein-Uhlenbeck process, with different time scales for each of the two coordinates.

We found that the MRT $E[\tau_n]$ actually depends on the initial configuration of the polymer. This result is in contrast with the small hole theory [HSS07, SSHE06, SSH06a, SSH06b, HoS04, WaK93, WHK93, SSH08] which shows that the leading order term of the MFPT for a Brownian particle to reach a small hole does not depend on the initial configuration. There are several reasons for such a difference. First, the position of the free moving end is a sum of i.i.d. variables and is not Markovian, which leads to a process with memory. Second, we may not be exactly in the context of a small hole, because the polymer completes a rotation when the free end reaches any point of the positif x-axis. In summary, for $nl_0 \gg L$, the leading order term of the MRT is given by

1.

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \left[2 \ln \left(\frac{\sum_{k=1}^n e^{\frac{i}{\sqrt{2D}} \theta_k(0)}}{\sqrt{n}} + O(1) \right) + Q \right],$$

where $(\theta_k(0), 1 \leq k \leq n)$ is the sequence of the initial angles and $Q = 9.56$,

2. for a stretched initial configuration

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \ln n,$$

3. for an average over uniformly distributed initial angles

$$E[\tau_n] \approx \frac{\sqrt{n}}{8D} \left[2 \ln \left(\frac{L}{l_0 \sqrt{n}} + O(1) \right) + Q \right].$$

As we have shown, these formula show very good agreement Brownian simulations (Fig. 4). The order one term $O(1)$ in cases 1 and 3 needs further investigation. There are several extension of this work: when the polymer has already made one loop, what is the probability to make a second loop before unwrapping and in that case, what is the MRT. How to extend such study in dimension 3.

Appendix

In the Appendix we prove Theorem 3.1. We use arguments coming from probability theory and we show the convergence of the sequence $(M_t^{(n)}, t \geq 0)$ to a Brownian motion in dimension 2, with different time scale functions.

A Proof of Theorem 3.1

To prove the theorem, we study each sequence $S_t^{(n)}$ and $C_t^{(n)}$ separately. The change of time comes from Dambis-Dubins-Schwarz Theorem and the scaling property of the Brownian motion [ReY99]. For a fixed time $t \geq 0$, we have

$$\begin{aligned}
 C_t^{(n)} &:= \frac{1}{\sqrt{n}} \int_0^t \sum_{k=1}^n \cos(B_k(s)) dB_k(s) \\
 &= \frac{1}{\sqrt{n}} \beta^{(n)} \left(\int_0^t \sum_{k=1}^n \cos^2(B_k(s)) ds \right) \\
 &= \tilde{\beta}^{(n)} \left(\frac{1}{n} \int_0^t \sum_{k=1}^n \cos^2(B_k(s)) ds \right) \quad , \tag{80}
 \end{aligned}$$

and

$$\begin{aligned}
 S_t^{(n)} &:= -\frac{1}{\sqrt{n}} \int_0^t \sum_{k=1}^n \sin(B_k(s)) dB_k(s) \\
 &= \frac{1}{\sqrt{n}} \hat{\beta}^{(n)} \left(\int_0^t \sum_{k=1}^n \sin^2(B_k(s)) ds \right) \\
 &= \hat{\tilde{\beta}}^{(n)} \left(\frac{1}{n} \int_0^t \sum_{k=1}^n \sin^2(B_k(s)) ds \right) \quad , \tag{81}
 \end{aligned}$$

where $(\beta_u, \hat{\beta}_u, \tilde{\beta}_u, \hat{\tilde{\beta}}_u, u \geq 0)$ are four independent Brownian motions. To study the limit of $(S_u^{(n)}, C_u^{(n)}, u \geq 0)$ and prove convergence in law, we shall show [Bil68, Bil78] or [ReY99] (Chapter XIII):

1. The convergence of the finite dimensional distributions and
2. the tightness of the sequence $(M_t^{(n)}, t \geq 0)$, where by definition, a sequence $(M_t^{(n)}, t \geq 0)$ of random variable is tight if, for all $\varepsilon > 0$, there exists a compact subset K such that $P(M_t^{(n)} \in K) > 1 - \varepsilon$ for all $n \geq 1$.

1. We consider two functions f, g and we study the characteristic function ($\forall \lambda, \mu \in \mathbb{R}$) (λ and μ could be omitted ($\lambda = \mu = 1$) as they don't play any role in the proof. However, it seems better to use them so as to have the general form of the characteristic function as known). We study now

$$E \left[e^{i \left(\lambda \int_0^\infty f(u) dS_u^{(n)} + \mu \int_0^\infty g(u) dC_u^{(n)} \right)} \right] = E \left[e^{i \left(\lambda \int_0^\infty f(u) dS_u^{(n)} + \mu \int_0^\infty g(u) dC_u^{(n)} \right)} \times \right. \\ \left. \times e^{\frac{1}{2} \left\langle \lambda \int_0^\cdot f(s) dS_s^{(n)} + \mu \int_0^\cdot g(s) dC_s^{(n)} \right\rangle_u - \frac{1}{2} \left\langle \lambda \int_0^\cdot f(s) dS_s^{(n)} + \mu \int_0^\cdot g(s) dC_s^{(n)} \right\rangle_u} \right]. \quad (82)$$

We know that since we have an exponential martingale [ReY99]

$$E \left[e^{i \left(\lambda \int_0^\infty f(u) dS_u^{(n)} + \mu \int_0^\infty g(u) dC_u^{(n)} \right) + \frac{1}{2} \left\langle \lambda \int_0^\cdot f(s) dS_s^{(n)} + \mu \int_0^\cdot g(s) dC_s^{(n)} \right\rangle_u} \right] = 1. \quad (83)$$

Moreover:

$$\left\langle \lambda \int_0^\cdot f(s) dS_s^{(n)} + \mu \int_0^\cdot g(s) dC_s^{(n)} \right\rangle_u = \\ = \lambda^2 \int_0^u f^2(s) d \langle S^{(n)} \rangle_s + \mu^2 \int_0^u g^2(s) d \langle C^{(n)} \rangle_s \\ + 2\lambda\mu \int_0^u f(s)g(s) d \langle S^{(n)}, C^{(n)} \rangle_s. \quad (84)$$

Using the Law of Large Numbers, with $\xrightarrow{(P)}$ denoting convergence in Probability,

$$\langle S^{(n)}, C^{(n)} \rangle_u = \frac{1}{n} \int_0^u \sum_{k=1}^n \sin(B_k(s)) \cos(B_k(s)) ds \\ \xrightarrow[n \rightarrow \infty]{(P)} \int_0^u E [\sin(B_1(s)) \cos(B_1(s))] ds \\ = 0. \quad (85)$$

Indeed, by the symmetry property of the Brownian motion $B_1 \stackrel{(law)}{=} -B_1$, thus: $E [\sin(B_1(s)) \cos(B_1(s))] = E [\sin(-B_1(s)) \cos(-B_1(s))]$ which yields:

$E [\sin(B_1(s)) \cos(B_1(s))] = 0$. Similarly, the Law of Large Numbers yields:

$$\begin{aligned} \langle S^{(n)} \rangle_u &= \frac{1}{n} \int_0^u \sum_{k=1}^n \sin^2(B_k(s)) ds \\ &\xrightarrow[n \rightarrow \infty]{(P)} \int_0^u E [\sin^2(B_1(s))] ds, \end{aligned} \quad (86)$$

and

$$\begin{aligned} \langle C^{(n)} \rangle_u &= \frac{1}{n} \int_0^u \sum_{k=1}^n \cos^2(B_k(s)) ds \\ &\xrightarrow[n \rightarrow \infty]{(P)} \int_0^u E [\cos^2(B_1(s))] ds. \end{aligned} \quad (87)$$

However

$$E [(\cos(B_1(s)) + i \sin(B_1(s)))^2] = E [\cos^2(B_1(s)) - \sin^2(B_1(s))],$$

as, once more by symmetry, $E [\sin(B_1(s)) \cos(B_1(s))] = 0$, and (recall that $\forall \lambda, E [e^{\lambda B(s)}] = e^{\frac{\lambda^2}{2}s}$):

$$E [(\cos(B_1(s)) + i \sin(B_1(s)))^2] = E [e^{2iB_1(s)}] = e^{-2s}.$$

Hence:

$$E [\cos^2(B_1(s))] - E [\sin^2(\sqrt{2D}B_1(s))] = e^{-2s},$$

and

$$E [\cos^2(B_1(s))] + E [\sin^2(B_1(s))] = 1.$$

We deduce:

$$E [\cos^2(B_1(s))] = \frac{1 + e^{-2s}}{2} \quad (88)$$

$$E [\sin^2(B_1(s))] = \frac{1 - e^{-2s}}{2}. \quad (89)$$

Thus:

$$\begin{aligned}
\langle S^{(n)} \rangle_u &= \frac{1}{n} \int_0^u \sum_{k=1}^n \sin^2(B_k(s)) ds \\
&\xrightarrow[n \rightarrow \infty]{(P)} \int_0^u E [\sin^2(B_1(s))] ds \\
&= \frac{1}{2} \int_0^u (1 - e^{-2s}) ds,
\end{aligned} \tag{90}$$

and

$$\begin{aligned}
\langle C^{(n)} \rangle_u &= \frac{1}{n} \int_0^u \sum_{k=1}^n \cos^2(B_k(s)) ds \\
&\xrightarrow[n \rightarrow \infty]{(P)} \int_0^u E [\cos^2(B_1(s))] ds \\
&= \frac{1}{2} \int_0^u (1 + e^{-2s}) ds.
\end{aligned} \tag{91}$$

Hence, from (82):

$$\begin{aligned}
&E \left[e^{i(\lambda \int_0^\infty f(u) dS_u^{(n)} + \mu \int_0^\infty g(u) dC_u^{(n)})} \right] \\
&\xrightarrow{n \rightarrow \infty} \exp \left(-\frac{\lambda^2}{2} \int_0^\infty f^2(u) \frac{1}{2} (1 - e^{-2u}) du - \frac{\mu^2}{2} \int_0^\infty g^2(u) \frac{1}{2} (1 + e^{-2u}) du \right) \\
&= E \left[e^{i\lambda \int_0^\infty f(u) dS_u} \right] E \left[e^{i\mu \int_0^\infty g(u) dC_u} \right],
\end{aligned} \tag{92}$$

which shows the convergence of the finite distributions.

2. In order to prove tightness, we shall use Kolmogorov's criterion: $(M_t^{(n)}, t \geq 0)$ is tight if, for every n , there exist positive constants α, β and c_4 such as:

$$E \left[\left| M_t^{(n)} - M_s^{(n)} \right|^\beta \right] \leq c_4 |t - s|^{1+\alpha}. \tag{93}$$

Indeed, Cauchy-Schwarz inequality yields

$$\begin{aligned}
E \left[\left| M_t^{(n)} - M_s^{(n)} \right|^\beta \right] &= E \left[\left| S_t^{(n)} + iC_t^{(n)} - S_s^{(n)} - iC_s^{(n)} \right|^\beta \right] \\
&\leq \left(E \left[\left| S_t^{(n)} - S_s^{(n)} \right|^{2\beta} \right] \right)^{1/2} \left(E \left[\left| C_t^{(n)} - C_s^{(n)} \right|^{2\beta} \right] \right)^{1/2}.
\end{aligned} \tag{94}$$

By using Burkholder-Davis-Gundy inequality (BDG) [ReY99, KaSh88], there exists a constant $0 < c_5 < \infty$ such that:

$$\begin{aligned} E \left[\left| S_t^{(n)} - S_s^{(n)} \right|^{2\beta} \right] &\leq E \left[\left(\sup_{u,v} |S_u^{(n)} - S_v^{(n)}| \right)^{2\beta} \right], \quad s < u, v < t \\ &\leq c_5 E \left[\left\langle S_t^{(n)} - S_s^{(n)} \right\rangle^\beta \right]. \end{aligned} \quad (95)$$

We have that:

$$\langle S^{(n)} \rangle_t = \frac{1}{n} \int_0^t \sum_{k=1}^n \underbrace{\sin^2(B_k(u))}_{\leq 1} du \leq t \quad (96)$$

$$\langle S^{(n)} \rangle_s = \frac{1}{n} \int_0^s \sum_{k=1}^n \underbrace{\sin^2(B_k(u))}_{\leq 1} du \leq s \quad (97)$$

$$\langle S_t^{(n)}, S_s^{(n)} \rangle = 0. \quad (98)$$

Thus,

$$\left(E \left[\left| S_t^{(n)} - S_s^{(n)} \right|^{2\beta} \right] \right)^{1/2} \leq c_5^{1/2} |t - s|^{\beta/2}. \quad (99)$$

Similar computations for $C^{(n)}$, lead to a constant $0 < c_6 < \infty$ such that:

$$\left(E \left[\left| C_t^{(n)} - C_s^{(n)} \right|^{2\beta} \right] \right)^{1/2} \leq c_6^{1/2} |t - s|^{\beta/2}. \quad (100)$$

From (94), (99) and (100) we deduce (93) for e.g. $\alpha = 1$, $\beta = 2$ and $c_4 = (c_5 c_6)^{1/2}$. So, we proved that $(M_t^{(n)}, t \geq 0)$ is tight.

Summarizing our results 1 and 2, we deduce that the sequences $(S_u^{(n)})$ and $(C_u^{(n)}, u \geq 0)$ are asymptotically independent and finally,

$$(S_u^{(n)}, C_u^{(n)}, u \geq 0) \xrightarrow[n \rightarrow \infty]{(law)} (\hat{\beta}_{\frac{1}{2}} \int_0^u ds (1+e^{-2s}), \tilde{\beta}_{\frac{1}{2}} \int_0^u ds (1-e^{-2s}), u \geq 0).$$

□

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