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Multilayer Markov Chains with Applications to Polymers in Shear Flow

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We present an analysis of multilayer Markov chains and apply the results to a model of a tethered polymer chain in shear flow. We find that the stationary probability measure in the direction of the flow is nonmonotonic, and has several maxima and minima for sufficiently high shear rates. This is in agreement with the experimental observation of *cyclic dynamics* for such polymer systems. Estimates for the stationary variance and expectation value were obtained and showed to be in accordance with our numerical results.

KEY WORDS: multilayer Markov chain, polymer, shear flow, Ornstein Uhlenbeck process

1. INTRODUCTION

The *static* mechanical properties of DNA-molecules have been studied extensively since the 1960s. Analogies between random walks and polymer configurations have been exploited by a number of authors mostly in the case of static polymers. Although there are still unresolved problems for polymers tethered to a wall in equilibrium conditions,[(6)] the attention has shifted to polymers in flow conditions. Recently, a large number of studies about the interesting (stretching) *dynamics* that DNA chains, and polymer chains in general, can exhibit in (shear-)flow have recently appeared.[(1–4,7–10)] These investigations have revealed a host of interesting phenomena, such as molecular individualism,[(10)] tumbling,[(9)] and shear-enhanced

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fluctuations.[1] Apart from the experimental works, most efforts were made in the study of the flexible chains[2,4,7] with a finite length and in that of the wormlike chain model,[1,5] using either scaling approximations[3,8] or numerical simulations.[1] Here we follow a complementary approach and develop a general stochastic model, that consists of two coupled Markov processes: a driven process in the x- and an ordinary Ornstein-Uhlenbeck process in the y-direction. The model that we put forward is shown to give a good description of tethered polymers in shear flow. Moreover, besides being important for a tethered polymer in shear flow, the model has interesting mathematical properties that justify a detailed mathematical study.

We consider as a first model simple random walk with drift proportional to the height. In this model the random walk becomes transient as soon as the drift parameter is non-zero. We give precise estimates of the average position and the variance of the position as a function of time. The second model is more realistic, i.e., considers an underlying (e.g. harmonic) potential on which a drift in the x-direction, proportional to the height y is superimposed. This model is roughly speaking behaving as a random walk on a finite set, driven by a stationary Markov chain (what we call a multilayer Markov chain). We find that when the underlying potential is sufficiently increasing, a unique stationary measure exist. For the case of a harmonic potential, the probability density of this measure is calculated numerically and is shown to have multiple maxima when the drift κ is sufficiently strong. This can account for the experimentally observed cyclic dynamics of tethered DNA chains.

This paper is organized as follows. In Sec. 2 we introduce a simple random walk model with drift and show that for all $\kappa > 0$ this random walk is transient. Next in Sec. 3, we consider a driven random walk in a potential and show that under certain conditions this process has a unique stationary measure. The harmonic case is treated separately in Sec. 4. In Sec. 5, the numerical calculations and results for a harmonic potential are presented. Analytical results for two-layer Markov chains are derived in Sec. 6 and Sec. 7 is devoted to summary and discussion.

2. SIMPLE RANDOM WALK MODEL

In this section we consider the continuous-time random walk on $\mathbb{Z}^2$, with jump rates given by

$$\begin{aligned} r((x, y), (x+1, y)) &= e^{\kappa |y|} \\ r((x, y), (x-1, y)) &= 1 \\ r((x, y), (x, y+1)) &= 1 \\ r((x, y), (x, y-1)) &= 1 \end{aligned} \tag{2.1}$$

In words, this means that at height y, the walker drifts to the right at rate $e^{\kappa|y|}$, all other jump rates are one. The following representation of this random walk is useful. For every $y \in \mathbb{Z}$ we consider a rate one Poisson process N_t and an independent Poisson process with rate $e^{\kappa|y|}$, notation N_t^y. Let S_t denote the position of the continuous time simple random walk (with jump rate 1) starting at the origin at time t. Let τ_k, $k \in \mathbb{N}$ denote the successive jump times of this random walk S_t. Then, for the process (X_t, Y_t), defined by the rates (2.2) and starting at the origin, we have that Y_t is distributed as S_t, and conditioned on $\{S_t : t \geq 0\}$, X_t equals

$$X_t = \sum_{k:\tau_{k+1}\leq t} N^{S_{\tau_k}}_{\tau_{k+1}-\tau_k} - N_{\tau_{k+1}-\tau_k} = \int_0^t \left(dN_s^{S_s} - dN_s\right) \tag{2.2}$$

The following proposition is a consequence of this representation.

Proposition 2.1. *Denote $\lambda(x) = e^{\kappa|x|}$. For the conditional expectation we have*

$$\mathbb{E}\{X_t \mid S_s, s \leq t\} = \sum_{k:\tau_{k+1}\leq t} (\lambda(S_{\tau_k}) - 1)(\tau_{k+1} - \tau_k) = \int_0^t (\lambda(S_s) - 1)\, ds \tag{2.3}$$

For the conditional variance we have

$$V(X_t \mid S_s, s \leq t) = \left(\sum_{k:\tau_{k+1}\leq t} (\lambda(S_{\tau_k}) - 1)(\tau_{k+1} - \tau_k)\right)^2 = \int_0^t (\lambda(S_s) + 1)\, ds \tag{2.4}$$

Proof: The first equality in both formulas follows from (2.2), the independence of the increments in the sum, and the independence of N_t^y from N_t. The second equality is immediate since τ_k are the jump-times of $\{S_t : t \geq 0\}$ □

Taking expectations over S_t (always denoted by $\tilde{\mathbb{E}}_x$, where $x \in \mathbb{Z}$ is the starting point), then gives the following:

Proposition 2.2. *With the notation of Proposition 2.1 we have*

$$\mathbb{E}(X_t) = \int_0^t \tilde{\mathbb{E}}_0(e^{\kappa|S_s|} - 1)\, ds = 2\int_0^t \tilde{\mathbb{E}}_0(e^{\kappa S_s} - 1)I(S_s > 0))\, ds \tag{2.5}$$

and

$$V(X_t) = \int_0^t \tilde{\mathbb{E}}_0(e^{\kappa|S_s|} + 1)\, ds = 2\int_0^t \tilde{\mathbb{E}}_0(e^{\kappa S_s} + 1)I(S_s > 0)) + 2\int_0^t \tilde{\mathbb{E}}_0(I(S_s = 0)\, ds \tag{2.6}$$

As a consequence we have the following estimates

1. *For the expectation:*

$$\frac{e^{2t\sinh^2(\kappa/2)}-1}{\sinh^2(\kappa/2)} - 2t \le \mathbb{E}_0(X_t) \le \frac{e^{2t\sinh^2(\kappa/2)}-1}{\sinh^2(\kappa/2)} - 2t + \min\left\{\frac{4}{3}\kappa t^{3/2}, 2t\right\} \tag{2.7}$$

2. *For the variance:*

$$\frac{e^{2t\sinh^2(\kappa/2)}-1}{\sinh^2(\kappa/2)} + 2t \le V(X_t) \le \frac{e^{2t\sinh^2(\kappa/2)}-1}{\sinh^2(\kappa/2)} + 6t \tag{2.8}$$

Proof: (2.5) and (2.6) follow immediately from Proposition 2.1 and the symmetry of the simple random walk $S_t = -S_t$ (in distribution). Write

$$\begin{aligned}
\mathbb{E}_0(X_t) &= \int_0^t \tilde{\mathbb{E}}_0(e^{\kappa|S_s|}-1)\,ds \\
&= 2\int_0^t \tilde{\mathbb{E}}_0\left((e^{\kappa S_s}-1)(I(S_s>0))\right)ds \\
&= 2\int_0^t \tilde{\mathbb{E}}_0(e^{\kappa S_s}-1)ds - 2\int_0^t \tilde{\mathbb{E}}_0((e^{\kappa S_s}-1)(I(S_s\le 0)))ds \\
&= \left(\frac{2(e^{t(\cosh\kappa-1)}-1)}{\cosh\kappa-1} - 2t\right) + \epsilon_t
\end{aligned} \tag{2.9}$$

with

$$\epsilon_t = (-2)\int_0^t \tilde{\mathbb{E}}_0((e^{\kappa S_s}-1)(I(S_s\le 0)))ds \tag{2.10}$$

and where we used the identity

$$\tilde{\mathbb{E}}_0(e^{\kappa S_t}) = \mathbb{E}(\cosh\kappa)^{N_t}) = \exp\left(t(\cosh\kappa-1)\right) \tag{2.11}$$

where the second expectation is over the Poisson process only. Now estimate

$$\begin{aligned}
|\tilde{\mathbb{E}}_0((e^{\kappa S_s}-1)I(S_s\le 0))| &= \tilde{\mathbb{E}}_0\left|\left(\left(\kappa\int_{S_s}^0 e^{\xi\kappa}d\xi\right)I(S_s\le 0)\right)\right| \\
&\le \kappa\tilde{\mathbb{E}}_0(|S_s|I(S_s\le 0)) \le \kappa\sqrt{\tilde{\mathbb{E}}_0\left(S_s^2\right)} \\
&= \kappa\sqrt{s}
\end{aligned} \tag{2.12}$$

This gives

$$\epsilon_t \leq \frac{4}{3}\kappa t^{3/2} \tag{2.13}$$

On the other hand, we have the simple estimate

$$0 \leq \epsilon_t \leq 2t \tag{2.14}$$

Combination of (2.9), (2.10), (2.13), and (2.14) gives the estimate for $\mathbb{E}(X_t)$. The estimation of the variance goes along the same line and is left to the reader. □

Another consequence of the representation (2.2) is the fact that we can couple the processes with $\kappa < \kappa'$ such that $X_t \leq X'_t$ for all $t > 0$, with probability one in the coupling. This means that there exists a process (the so-called "coupled process" or "coupling") $\{(\tilde{X}_t, \tilde{X'}_t) : t \geq 0\}$ with first marginal $\tilde{X}_t = X_t$ in distribution and second marginal $\tilde{X'}_t = X'_t$ in distribution, and such that $\tilde{X}_t \leq \tilde{X'}_t$ for all $t > 0$, with probability one.

Indeed, the Poisson process $N_t^{S_t}$ has intensity $\lambda(S_t)$, which is a monotonically increasing function of κ. In fact we have more, as is formulated in the following theorem.

Theorem 2.1. *Suppose $f \leq g$ are two strictly positive functions on $\mathbb{Z}$. Define the rates*

$$\begin{aligned} r_f((x, y), (x + 1, y)) &= f(y) \\ r_f((x, y), (x - 1, y)) &= 1 \\ r_f((x, y), (x, y + 1)) &= 1 \\ r_f((x, y), (x, y - 1)) &= 1 \end{aligned} \tag{2.15}$$

and analogously for r_g. Then for the corresponding random walks (X_t^f, Y_t^f), (X_t^g, Y_t^g) there exists a coupling (X_t^1, Y_t^1), (X_t^2, Y_t^2) such that $X_t^1 \leq X_t^2$ for all t, $Y_t^1 = Y_t^2$ for all t with probability one.

Proof: As before, let S_t denote simple random walk in continuous time. Suppose that $f \leq g$ are strictly positive functions on $\mathbb{Z}$, and denote by $N^f(S_s)_s$ (resp. $N^g(S_s)_s$ the jump process with compensator $\int_0^s f(S_s)\, ds$ (resp. $\int_0^s g(S_s)\, ds$). Since the compensators dominate each other, there exists a coupling such that $N^f(S_s)_s \leq N^g(S_s)_s$ with probability one. This coupling then defines the coupling of the theorem via the representation (2.2). □

As a consequence we have

Theorem 2.2. *For all $\kappa > 0$, the random walk (X_t, Y_t) with rates (2.2) is transient.*

Proof: Replace the rates by r_f, where $f(x) = 0$ for $x = 0$ and $f(x) = e^\kappa$ for $x \neq 0$. By Theorem 2.1, it suffices to see that for this random walk (with rates r_f), $X_t \to \infty$ almost surely. The only (minor) complication with this random walk is that its drift is zero on the X-axis, on all other horizontal lines the drift is bounded from below by a strictly positive constant. So, let τ_n, $n \in \mathbb{N}$ denote the successive times at which the random walk is on the X-axis. If this is a finite sequence, then there is nothing to prove, because if the walk leaves the X-axis it has a drift bounded from below. Since upon an excursion in the upper-halfplane say the drift is bounded from below, we have

$$\mathbb{E}\big(X_{\tau_n} - X_{\tau_{n+1}} | X_{\tau_n}\big) > c$$

where $c > 0$ does not depend on n. Therefore $X_{\tau_n} \to \infty$ as $n \to \infty$, which gives $X_t \to \infty$ almost surely in the process with rates r_f. □

As a final result in this section, the following proposition shows that in the current model, the "polymer" will be more and more stretched in the X direction. Remember that in (X_t, Y_t), Y_t is behaving as the continuous-time simple random walk S_t.

Proposition 2.3. *For all $t > 0$, there exists $\alpha_t > 0$ not depending on κ such that*

$$\mathbb{E}_0\left(\frac{X_t}{1 + S_t^2}\right) \geq (e^\kappa - 1)\alpha_t \tag{2.16}$$

Proof: Denote $\lambda(x) = e^{\kappa|x|}$. From (2.3) we obtain

$$\begin{aligned}\mathbb{E}_0\left(\frac{X_t}{1 + S_t^2}\right) &= \mathbb{E}_0\left(\frac{\int_0^t (\lambda(S_s) - 1)ds}{1 + S_t^2}\right)\\ &\geq (e^\kappa - 1)\mathbb{E}_0\left(\frac{(\int_0^t I(S_s \neq 0))}{1 + S_t^2}\right)\end{aligned} \tag{2.17}$$

□

3. POSITIVE RECURRENT RANDOM WALK CASE

In the random walk model of Sec. 2, the polymer can become arbitrary long. A more realistic situation is met when the polymer has some equilibrium length.

This means that the "unperturbed process," corresponding to $\kappa = 0$ is a random walk with some reversible equilibrium distribution.

More precisely, we choose the following rates.

$$\begin{aligned} r^{\kappa}_{\beta}((x, y), (x + 1, y)) &= e^{-\beta(V^{\kappa}_y(x+1) - V^{\kappa}_y(x))} \\ r^{\kappa}_{\beta}((x, y), (x - 1, y)) &= e^{-\beta(V^{\kappa}_y(x-1) - V^{\kappa}_y(x))} \\ r^{\kappa}_{\beta}((x, y), (x, y + 1)) &= e^{-\beta(V(y+1) - V(y))} \\ r^{\kappa}_{\beta}((x, y), (x, y - 1)) &= e^{-\beta(V(y-1) - V(y))} \end{aligned} \tag{3.1}$$

Where we choose

$$V^{\kappa}_y(x) = V^0(x - \kappa|y|) \tag{3.2}$$

In words, V is the potential governing the Y-motion, and V^0 is the potential governing the X-motion at ground level $y = 0$.

The presence of $\kappa > 0$ induces a shift in the equilibrium position of the potential V^0, depending on the height y.

This is the general picture which we consider in this section: the Y-process is a reversible Markov chain with some equilibrium potential $V : \mathbb{Z} \to \mathbb{R}$. At height y, the X-process moves as a reversible Markov chain with equilibrium potential $V^0(\cdot - \kappa|y|)$, i.e., the "original" equilibrium potential V^0 shifted over $\kappa|y|$. In principle the potentials for the Y-motion and X-motion can be different. A simple and natural choice is the harmonic potential

$$V^0(x) = \frac{x^2}{2}, \quad V(y) = \frac{y^2}{2}$$

For technical reasons we will treat this case in continuous space, and deal in this section with potentials $V(y)$ that increase faster as $y \to \infty$. In the following section we will consider the harmonic case in continuous space context.

The presence of the shifts in the potential landscape of the X-process as soon as $\kappa \neq 0$ is responsible for the breaking of detailed balance, i.e., as soon as $\kappa \neq 0$, the process (X_t, Y_t) does not have a reversible measure.

Remember however that the the jumps in the y direction have a rate that does not depend on x. This is a key simplifying property which leads to the following.

Proposition 3.1. *Let Y_t denote the process with generator*

$$\begin{aligned} L_2 f(y) = e^{-\beta(V(y+1) - V(y))}&(f(y + 1) - f(y)) \\ &+ e^{-\beta(V(y-1) - V(y))}(f(y - 1) - f(y)) \end{aligned}$$

Then process (X_t, Y_t) with rates (3.1) has Y_t as second marginal. In particular, if Y_0 is distributed according to the stationary distribution of the Y process $\mu(y) = e^{-\beta y^2/2}$, then Y_t is a stationary process with single time marginals μ.

Proof: Let $f(x, y) = \varphi(y)$ be a function depending on y only. Let L^κ_β be the generator corresponding to the rates r^κ_β. We then have

$$Lf = L_2\varphi \tag{3.3}$$

which is once again a function of y only. Therefore, iterated application of L give

$$\mathbb{E}_{(x,y)} f(X_t, Y_t) = (e^{tL_2}\varphi)(y) \tag{3.4}$$

□

The picture of (X_t, Y_t) is the following: we have the autonomous random walk Y_t with equilibrium distribution μ, and in between two successive jumps of this random walk, the X process is a random walk with equilibrium distribution depending on the height y, with average equilibrium position $\kappa|y|$. Let us make this more precise and give an explicit formula for the conditional expectation of increments of the X process (which is not a Markov process). We introduce the notation $c^+_y(x)$ resp. $c^-_y(x)$ for the rate to jump in the plus resp. minus direction for the random walk with rates $r^\kappa_\beta((x, y), (x+1, y))$, $r^\kappa_\beta((x, y), (x-1, y))$. This is a random walk ξ^y_t on $\mathbb{Z}$ where *y acts as a parameter in the rates*. As long as in process (X_t, Y_t), Y_t does not jump, i.e, $Y_t = y$, X_t is evolving as this random walk with rates $c^+_y(x)$ resp. $c^-_y(x)$. We denote by L_y the generator of this process, i.e.,

$$L_y f(x) = c^+_y(x)(f(x+1) - f(x)) + c^-_y(x)(f(x-1) - f(x)) \tag{3.5}$$

Let $Y_n, n \in \mathbb{N}$, $\tau_n, n \in \mathbb{N}$ denote successive jump times and positions at the jump times $(T_n = T_{\tau_n})$ of the (autonomous) random walk Y_t. Let us denote $X_n = X_{\tau_n}$. Then *conditioned on* Y, τ, X_n is a Markov process with

$$\mathbb{E}(X_n - X_{n-1}|X_{n-1}, Y, \tau) = \mathbb{E}^y_{X_{i-1}} \int_{\tau_{i-1}}^{\tau_i} \left(c^+_{Y_{i-1}}\left(\xi^y_{s-\tau_{i-1}}\right) - c^-_{Y_{i-1}}\left(\xi^y_{s-\tau_{i-1}}\right)\right)$$

where $\mathbb{E}^y_{X_{i-1}}$ denotes expectation over the random walk with rates $c^+_y(x)$, $c^-_y(x)$ starting from X_{i-1}. Remember that τ_i are the jump times of Y_t. Therefore, conditioned on the positions $\{Y_n : n \in \mathbb{N}\}$, the increments $\tau_i - \tau_{i-1}$ are i.i.d. exponential random variables with parameter $\lambda = \lambda(Y_{i-1})$, where

$$\lambda(y) = e^{-\beta(V(y+1)-V(y))} + e^{-\beta(V(y-1)-V(y))}$$

is the total jump rate at height y. Therefore we can take the expectation over τ variables in (3.6), and obtain

$$\mathbb{E}(X_i - X_{i-1} \big| X_{i-1} = x, Y) = \mathbb{E}_x^{Y_{i-1}} \left(\int_0^\infty e^{-\lambda(Y_{i-1})s} \big(\big(c^+_{Y_{i-1}} - c^-_{Y_{i-1}} \big) \big(\xi^y_s \big) \big) \right) \quad (3.6)$$

This leads then to the following

Proposition 3.2. *Suppose Y_t is distributed according to its stationary measure μ. Let X_n denote the position of the X coordinate of (X_t, Y_t) at the moment of the n-th jump of Y_t. Then we have the following formula*

$$\begin{aligned} \mathbb{E}[X_n - X_{n-1} \big| X_{n-1}] &= \sum_y \mu(y) \mathbb{E}^y_{X_{n-1}} \int_0^\infty e^{-\lambda(y)s} (c^+_y - c^-_y) \big(\xi^y_s \big) \\ &= \sum_y \mu(y) (\lambda(y) - L_y)^{-1} (c^+_y - c^-_y)(X_{n-1}) \quad (3.7) \end{aligned}$$

Proof: This follows from taking the expectation over the stationary process Y in (3.6). □

3.1. Stationary Measure

In this subsection we prove that if the potential V governing the Y-motion is increasing fast enough as $y \to \infty$ then there exists a unique stationary measure for the process (X_t, Y_t) with generator corresponding to the rates (3.1).

Theorem 3.1. *Choose $V^0(x) = \frac{1}{2}x^2$ and suppose that for some $\epsilon > 0$*

$$\sum_y e^{\beta\kappa^2(1+\epsilon)|y|^2} e^{-\beta V(y)} < \infty \quad (3.8)$$

Then the process (X_t, Y_t) has a unique stationary measure μ with finite exponential moments for both x and y coordinate, i.e., for all $s, t \in \mathbb{R}$,

$$\sum_{x,y} \mu(x, y) e^{tx+sy} < \infty \quad (3.9)$$

Proof: We make a process with rates $\tilde{r}$ having a unique *reversible measure* such that at every site (x, y) the drift towards $(x + 1, y)$ is bigger than in the process with rates (3.1). This is clearly *sufficient*. Indeed, if the process with rates (3.1) had no stationary measure, then the only reason is that the X-coordinate would drift to $+\infty$, which is not possible if such a domination with a reversible process can be obtained. Indeed, in that case we can couple the processes with rates (3.1) and $\tilde{r}$ such that in the first process the number of jumps in the positive x direction is almost surely smaller than in the second process, i.e., if both processes start at the same location, in the coupling $X_t^{(1)} \leq X_t^{(2)}$ for all $t > 0$, with probability one. Therefore, a stationary measure exists, and the uniqueness follows from irreducibility. The auxiliary process with rates $\tilde{r}$ corresponds to a potential $\mathcal{B}$ which satisfies

$$\mathcal{B}(x+1, y) - \mathcal{B}(x, y) \leq 2(-\kappa|y| + x) \tag{3.10}$$

ensuring the domination of the rate to jump in the positive x direction:

$$r_\beta((x, y), (x+1, y)) \leq \tilde{r}((x, y), (x+1, y)) := e^{-\frac{1}{2}(\beta(\mathcal{B}(x+1,y)-\mathcal{B}(x,y)))}$$

So a possible choice is

$$\mathcal{B}(x, y) = \mathcal{B}(0, y) - 2\kappa|y|x + (x+1)^2 \tag{3.11}$$

where

$$\mathcal{B}(0, y) = V(y)$$

is the potential governing the y-motion. In that case, using (3.8), we obtain

$$\begin{aligned} Z := \sum_{x,y} e^{-\beta\mathcal{B}(x,y)} &= \sum_y e^{-\beta V(y)} \sum_x e^{-\beta(x+1)^2 + 2\kappa\beta|y|x} \\ &\leq C(\epsilon, \beta) \sum_y e^{-\beta V(y)} e^{\beta\kappa^2(1+\epsilon)|y|^2} < \infty \end{aligned} \tag{3.12}$$

Therefore, $\mu(x, y) = \frac{e^{-\beta\mathcal{B}(x,y)}}{Z}$ is a reversible probability measure for the walk with rates $\tilde{r}$.

To see (3.9), remark that for $t = 0$, this is clear since the Y-marginal of the stationary measure is $e^{-\beta(y)}$, whereas for $s = 0$ it follows from (3.11), $\mu(x, y) = e^{-\beta\mathcal{B}(x,y)}/Z$ and the property $X_t^{(1)} \leq X_t^{(2)}$ for all $t > 0$ with probability one in the coupling. □

Remark 3.1. If (3.8) is not satisfied, then there does not exist a potential $\mathcal{B}$ such that the rates (3.1) can be dominated by the reversible rates $\tilde{r}$. Indeed, such a potential should satisfy

$$\mathcal{B}(x+1, y) - \mathcal{B}(x, y) \leq 2(-\kappa|y| + x)$$

and $V(0, y) = V(y)$, which implies that

$$\sum_y e^{-\beta V(y)} \sum_x e^{-\beta\mathcal{B}(x,y)} = \infty$$

This does however not exclude the possibility that the process with rates (3.1) still has a stationary (non-reversible) measure.

4. HARMONIC CASE

For the case of a quadratic potential $V(y) = y^2$, we can apply Theorem 3.1 only if $\kappa \leq 1$. Therefore, in order to cover also the other values of κ, in this section we describe this case in continuous space, i.e., using stochastic differential equations. This in contrast to the discrete random walk case has the advantage of giving more explicit formulas. The equations are

$$\begin{aligned} dX_t &= -(X_t - \kappa |Y_t|)\, dt + dB_t \\ dY_t &= -Y_t dt + dB'_t \end{aligned} \tag{4.1}$$

where B and B' are independent Brownian motions. In words this means that Y_t is an Ornstein-Uhlenbeck (OU) process corresponding to the quadratic potential $V(y) = y^2$. Given $Y_t = y$, X_t moves as a OU-process corresponding to the quadratic potential $V_y(x) = (x - \kappa|y|)^2$. Using (4.1) and Ito's formula, we obtain,

$$\mathbb{E} f(X_t) - \mathbb{E} f(X_0) = -\int_0^t \mathbb{E}(f'(X_s)(X_s - \kappa|Y_s|))\, ds + \frac{1}{2}\int_0^t f''(X_s)\, ds \tag{4.2}$$

It is then a simple exercise to see that

$$\mathbb{E}_{(0,0)}(X_t) = \kappa e^{-t} \int_0^t e^s \mathbb{E}_0 |Y_s| ds \tag{4.3}$$

where the expectation $\mathbb{E}_0$ is over the Y-process only, and $\mathbb{E}_{(0,0)}$ denotes expectation in the process (X_t, Y_t) starting from $(0, 0)$. This formula shows that the expectation of X_t is uniformly bounded in time and increases linearly with κ. Therefore, this process has a stationary distribution $\mu(dxdy)$ with

$$\int x\mu(dxdy) = \lim_{t\to\infty} \mathbb{E}_{(0,0)}(X_t) = \kappa \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} |y| e^{-y^2} dy = \frac{\kappa}{\sqrt{\pi}} \tag{4.4}$$

where we used that $e^{-y^2}/\sqrt{\pi}$ is the unique stationary distribution of the Y-process.

For the n-th moment, $n \geq 2$, we obtain the following recursion from (4.2):

$$\mu(x^n) - \kappa\mu(|y|x^{n-1}) - \frac{1}{2}(n-1)\mu(x^{n-2}) = 0 \tag{4.5}$$

Using Hölder's inequality with $p = n/(n-1)$, $q = n$, this leads to

$$\mu(x^n) - \kappa m_n^{1/n} \mu(x^n)^{\frac{n-1}{n}} - \frac{1}{2}(n-1)\mu(x^{n-2}) \leq 0 \tag{4.6}$$

where $m_n = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} |y|^n e^{-y^2}$ are the stationary moments of the OU-process. For $n = 2$, this leads to the following inequality for the stationary variance of x

$$0 \leq \mu(x^2) - \mu(x)^2 \leq \frac{1}{2} + \kappa^2\left(\frac{1}{4} - \frac{1}{\pi}\right) + \frac{\kappa}{4}\sqrt{\kappa^2 + 8} \tag{4.7}$$

5. NUMERICAL RESULTS

In this section we will present numerical results of the investigations of the random walk with rates given by Eqs. (2.2). We numerically solve for the Markov process that is generated by these rates, starting at $t = 0$ in $(x_0, y_0) = (0, 0)$. We use an alternating direction implicit (ADI) algorithm to guarantee stability and second order accuracy in the time-step. In the ADI-algorithm for the numerical solution of the Markov process with rates (2.2) we set the time step $\Delta t = 10^{-4}$. In Fig. 1(a), we present the probability measure for $\kappa = 0$, and $\beta = 1$, that is, there is no flow and the average chain length squared, given by the total variance in x and y: $\mathbb{E}(X_t^2 + Y_t^2)$, ≈ 1. Of course, the probability measure μ is symmetric in both x- and y- directions and hence $\mathbb{E}(X_t) = \mathbb{E}(Y_t) = 0$. In Fig. 1(b) the probability measure for $\kappa = 8.0$ is shown. Here we see a clear asymmetry arising, which is due to the shear force that is pushing the polymer chain on average to the right. For each layer, there is a probability for the end of the polymer chain to occupy in that layer a position with x-coordinate X. The maximum probability, however, is dependent on the y-coordinate of the chain end. An interesting question is now in what way $\mathbb{E}(X_t)$ depends on the shear rate κ and to what kind of second moments the probability distribution gives rise to. In Fig. 2 the x-position of the chain end is depicted as a function of κ. It is seen to increase approximately linearly with κ. This linear scaling of $\mathbb{E}(X_t)$ with κ was also derived in Sec. 4 in the continuous case. This scaling relation can physically be explained as follows. The average

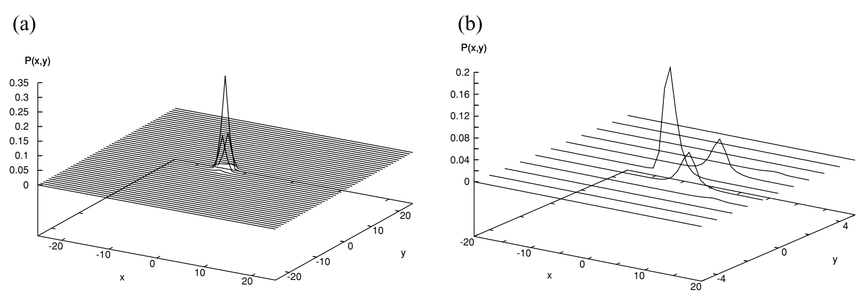

Fig. 1. A three-dimensional plot of the probability measure $\mu(x, y) = P(x, y)$ for $\beta = 1.0$ and $\kappa = 0$ (Gaussian symmetric shape) in (a) and $\beta = 1.0$ and $\kappa = 8.0$ in (b). In (b) the maxima in the probability density shift to higher values of x for larger values of y.

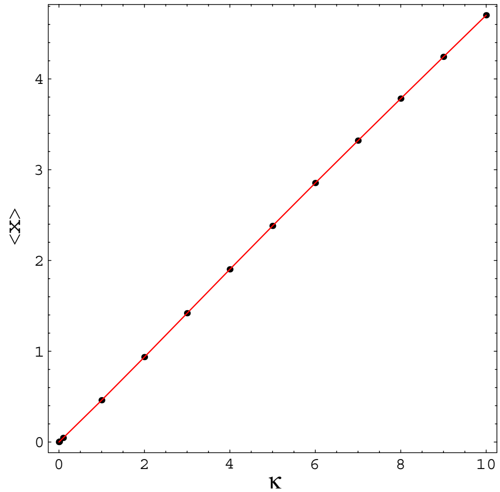

Fig. 2. (color online) For fixed $\beta = 1$, and varying shear rates κ, $\mathbb{E}(X_t) = \langle x(t) \rangle$ of the process with rates (2.2) is depicted. A linear increase of $\langle x(t) \rangle$ with κ is manifest.

y-coordinate of chain end $\mathbb{E}(Y_t) = 0$ and the deviations around $y = 0$ do not depend on κ. This implies that the time spent in a particular layer does not depend on κ. So if the shear rate is increased, this implies that the chain end will feel a "force" that is proportional to κ, because the distribution over the different layers is independent of κ. The only consequence of the larger value of κ is the greater extension of the polymer chain.

A more interesting quantity is the variance of the probability density function in the x-direction. As noted before, the variance in the y-direction is always constant and its value is given by the variance in the x-direction for $\kappa = 0$ and equals 0.49. The variance in the x-direction $\mathbb{E}(X_t^2)$ is shown in Fig. 3 as a solid curve with dots denoting the computer simulation results. To illustrate that the variance increases more rapid than quadratically with κ, we plotted a parabola that fits quite well to the curve for small values of κ, but is clearly seen to deviate significantly from the numerically obtained curve for larger values of κ. This behavior of the variance as a function of κ illustrates that the coupling between the Markov processes in the x- and y-direction can lead to non-trivial behavior and indeed greatly enhanced fluctuations. This has in fact also been observed in experiments by Doyle *et al.*[1] and was heuristically explained in Refs. 3 and 7.

An even better understanding of this phenomenon is obtained if the reduced probability measure in the x-direction, that is, $\mu_X(x) = \int_{-\infty}^{\infty} \mu(x, y)\, dy$, is investigated. In Fig. 4, we present $\mu_X(x)$, for three different values of κ. From Fig. 4 the non-monotonicity of the $\mu_X(x)$ is conspicuous. For small values of the shear

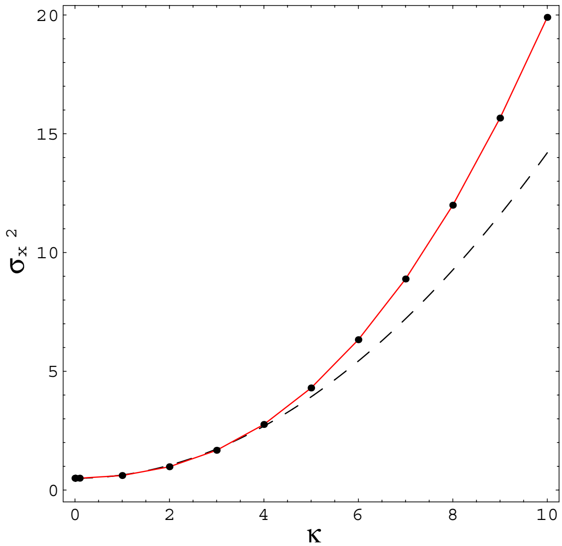

Fig. 3. (color online) The variance in the x-direction is plotted, manifest is that it is systematically above its mean square quadratic fit.

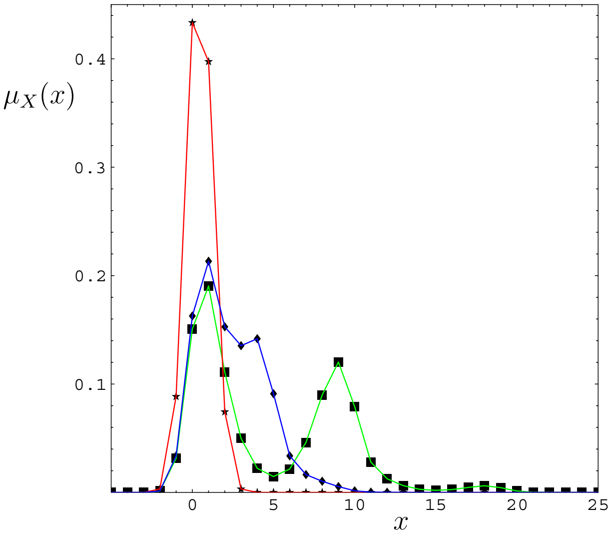

Fig. 4. (color online) The reduced probability in the x-direction $\mu_X(x)$ for three different values of κ. The stars correspond to $\kappa = 1.0$, the diamonds to $\kappa = 5$, and the squares to $\kappa = 10.0$. For larger values of κ multiple maxima in $\mu_X(x)$ develop.

rate κ, we observe a shift and an asymmetry in the measure as compared to the $\kappa = 0$ result. For higher values of κ we find that the stationary probability measure develops a "hole" in the distribution and for still higher values of κ subsequently several maxima and minima are displayed. These results strongly suggest a physical scenario that is in correspondence with the findings of Refs. 1, 3, 7 about the cyclic dynamics of tethered DNA chains in shear flow. There it was reported that a tethered DNA chain exhibits large fluctuations in chain length in the direction of the shear velocity. Furthermore, it was observed that the angle between the polymer chain and the wall shows more or less periodic variations. Our model gives an explanation for the observed large temporal fluctuations in terms of a probability of the chain end to be at a specific position x. There are certain regions where the chain end can be found with rather high probability. The chain end will then make jumps between these high probability regions with certain rates. This offers an explanation for the large chain end excursions and the corresponding length fluctuations that are typically seen in the experiments.

6. GENERAL STRUCTURE AND SIMPLE EXAMPLES

6.1. A Four State Example

In our process (X_t, Y_t), Y_t is an autonomous Markov chain with a known stationary distribution, and X_t is driven by the state of Y_t. As soon as Y_t is a non-trivial (reversible) Markov chain, and X_t depends in a non-trivial way on the state Y_t, then the resulting process will loose its reversibility. In this section we give simple examples of such a process in which we can explicitly compute the stationary distribution, and in particular see that non-trivial currents arise as soon as Y_t is a non-trivial process.

In the simplest set-up, both X and Y have two possible states. For the (X, Y)-process, we then choose the transition rates $c((00), (10)) = c((10), (00)) = 1$, and $c((01), (11)) = e^\kappa$ and $c((11), (10)) = 1$. An elementary computation gives the stationary measure μ of the corresponding continuous time Markov chain (X_t, Y_t):

$$\begin{aligned}
\mu(\{(0,0)\}) &= \frac{3+e^\kappa}{10+6e^\kappa} \\
\mu(\{(0,1)\}) &= \frac{2}{5+3e^\kappa} \\
\mu(\{(1,0)\}) &= \frac{1+e^\kappa}{5+3e^\kappa} \\
\mu(\{(1,1)\}) &= \frac{3e^\kappa+1}{10+6e^\kappa}
\end{aligned} \tag{6.1}$$

The marginal distribution of Y is of course $\mu(Y = 1) = \mu(Y = 0) = 1/2$, but as soon as $\kappa \neq 0$ this stationary distribution μ is not reversible, as can be seen e.g.

from the expectation of the stationary current over the bond $(01) - (11)$:

$$\mu(J_0) = \mu(00) - \mu(10) = \frac{e^\kappa - 1}{10 + 6e^\kappa} = -\mu(J_1) = \mu(01)e^\kappa - \mu(11)$$

In the limit $\kappa \to \infty$ the current saturates at the value $1/6$. For the stationary expectation of the x-coordinate we find

$$\mu(X) = \lim_{t\to\infty} \mathbb{E}_{(x,y)}(X_t) = \frac{1}{2} + \frac{e^\kappa - 1}{5 + 3e^\kappa} \tag{6.2}$$

The eigenvalues of the generator are, in decreasing order:

$$\begin{aligned}\lambda_1 &= 0\\ \lambda_2 &= -2,\\ \lambda_3 &= \frac{1}{2}(-5 - e^\kappa + \sqrt{4 + (e^\kappa - 1)^2}),\\ \lambda_4 &= \frac{1}{2}(-5 - e^\kappa - \sqrt{4 + (e^\kappa - 1)^2})\end{aligned} \tag{6.3}$$

Remark that, although the generator is not symmetric, all eigenvalues are real and negative, and the speed of relaxation to equilibrium is *speeded up* by the introduction of non-zero κ, i.e., the eigenvalues λ_3, λ_4 are decreasing functions of κ, with $\lambda_3 \to -3$, $\lambda_4 \to -\infty$ as $\kappa \to \infty$.

In particular, for the autocorrelation function we have

$$\mathbb{E}_\mu\left((X_t - \mu(X))(X_0 - \mu(X))\right) = C_1 e^{-2t} + C_2 e^{\lambda_3 t} + C_3 e^{\lambda_4 t} \leq C e^{-2t} \tag{6.4}$$

with the inequality uniformly in κ. The constants C_1, C_2, C_3 can be computed explicitly from the eigenvectors which are given by (in the order corresponding to (6.3):

$$\begin{aligned}\mathbf{e_1} &= \left(\frac{3 + e^\kappa}{1 + 3e^\kappa}, \frac{4}{1 + 3e^\kappa}, \frac{2 + 2e^\kappa}{1 + 3e^\kappa}, 1\right)\\ \mathbf{e_2} &= (-1, 0, 0, 1)\\ \mathbf{e_3} &= (q_1, -1, -q_1, 1)\\ \mathbf{e_4} &= (q_2, -1, -q_2, 1),\end{aligned} \tag{6.5}$$

where q_1 and q_2 are given by

$$\begin{aligned}q_1 &= \frac{2(2 + \sqrt{5 - 2e^\kappa + e^{2\kappa}})}{3 + e^{2\kappa} + \sqrt{5 - 2e^\kappa + e^{2\kappa}} + e^\kappa\sqrt{5 - 2e^\kappa + e^{2\kappa}}},\\ q_2 &= \frac{2(-2 + \sqrt{5 - 2e^\kappa + e^{2\kappa}})}{-3 - e^{2\kappa} + \sqrt{5 - 2e^\kappa + e^{2\kappa}} + e^\kappa\sqrt{5 - 2e^\kappa + e^{2\kappa}}}.\end{aligned} \tag{6.6}$$

6.2. General Two Layer Case

We continue with $Y_t \in \{0, 1\}$ but allow now for X_t to take values in a general finite set $\{x_1, \dots, x_n\}$. We will show that the marginals on a single layer can be obtained as the stationary distribution of an "effective" Markov generator which is a non-trivial combination of the generators on both levels. For the Y_t process we still take independent flips between zero and one, at rate 1. The generator of (X_t, Y_t) then has a two-block structure

$$\mathbf{L}(A, B) = \begin{pmatrix} A - I & I \\ I & B - I \end{pmatrix} \tag{6.7}$$

where the identity parts correspond to the flips $0 \to 1$, i.e., transitions $(x_i, 0) \to (x_i, 1)$ or $(x_i, 1) \to (x_i, 0)$ (which occur at rate one by hypothesis), and where A, B are the generators of the Markov process corresponding to the states 0, 1 of the Y process. The stationary measure can then be written as (μ, ν), where μ, resp. ν is the marginal of the first $Y = 0$ resp. second $Y = 1$ layer. It satisfies the equation

$$\begin{aligned} \mu(A - I) + \nu &= 0 \\ \mu + \nu(B - I) &= 0 \end{aligned} \tag{6.8}$$

This leads to

$$\begin{aligned} \mu &= \nu(I - A)^{-1} \\ \mu &= \nu(I - B) \end{aligned} \tag{6.9}$$

which gives

$$\nu((I - A)^{-1} - (I - B)) = 0 \tag{6.10}$$

This equation expresses that ν is the stationary measure of the process with "effective generator"

$$\mathcal{L}(A, B) = (I - A)^{-1} - (I - B) = B + \int_0^\infty e^{-t}(S_A(t) - I) \tag{6.11}$$

where $S_A(t) = e^{At}$ is the semigroup corresponding to the generator A. Remark that since A, B are generators, $\mathcal{L}(A, B)$ is also a generator (since powers of generators are generators and sums of generators are generators). Similarly, μ is the stationary measure of the process with generator $\mathcal{L}(B, A) = A + \int_0^\infty e^{-t}(S_B(t) - I)$. Remark that if $A = B$, then the stationary measure of $\mathcal{L}(A, B)$ coincides with the stationary measure of the process with generator A. Indeed let μ_A denote the stationary measure of the process with generator A then $\mu_A A = 0 = \mu_A(S_A(t) - I)$ and hence $\mu_A \mathcal{L}(A, A) = 0$. So in that case $(\mu, \nu) = \frac{1}{2}(\mu_A, \mu_A)$. Summarizing, we obtained

Theorem 6.1. *Let (X_t, Y_t) be the continuous time Markov chain with generator (6.7), and (μ, ν) its stationary measure. Then μ, resp. ν is the stationary measure of the process with generator (6.11). If $A = B$, then $(\mu, \nu) = \frac{1}{2}(\mu_A, \mu_A)$, where μ_A is the stationary measure of the process with generator A.*

This theorem shows that the marginals of a multilayer Markov process can be reduced to the computation of the stationary distribution of "effective Markov chains" which arise from the generators $A_1, \ldots, A_n$ of the generators for given layers by a sequence of operations $\mathcal{L}(\cdot, \cdot)$, $\mathbf{L}(\cdot, \cdot)$.

7. DISCUSSION

We have addressed the issue of a tethered polymer in shear flow that is described by coupled multilayer Markov chains. We prove that for such a system a unique stationary measure exists, when the end point of the chain moves in potential that is quadratic in the x and y directions or stronger. Estimates for the $\mathbb{E}(X_t)$ and the variance of X_t were derived. Moreover, we calculated the stationary measure in the case of a harmonically bound chain numerically. The probability measure $\mu_X(x)$ that we obtained exhibits the interesting feature that it is nonmonotonic, but has multiple maxima. This surprising fact accounts very well for the cyclic dynamics that is typically observed in systems in which a tethered DNA chain is subjected to shear flow with a sufficiently high shear rate. Moreover, we have demonstrated that the stationary probability measure can in fact be calculated exactly for a number a *finite state* driven Markov processes. Such an approach may be useful for other systems than polymers, which can also be described by driven Markov processes. Our approach to the tethered chain problem illustrates how the stochastic view point may lead to new insights about familiar problems in the dynamics in of polymer chains.

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