Fluctuation theorems for discrete kinetic models of molecular motors

Alessandra Faggionato\textsuperscript{1} and Vittoria Silvestri\textsuperscript{2}

\textsuperscript{1} Dipartimento di Matematica, Università di Roma ‘La Sapienza’, P.le Aldo Moro 5, 00185 Roma, Italy
\textsuperscript{2} Statistical Laboratory, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WB, United Kingdom
E-mail: faggiona@mat.uniroma1.it and V.Silvestri@maths.cam.ac.uk

Received 17 January 2017
Accepted for publication 15 March 2017
Published 13 April 2017

Abstract. Motivated by discrete kinetic models for non-cooperative molecular motors on periodic tracks, we consider random walks (also not Markov) on quasi one dimensional (1d) lattices, obtained by gluing several copies of a fundamental graph in a linear fashion. We show that, for a suitable class of quasi-1d lattices, the large deviation rate function associated to the position of the walker satisfies a Gallavotti–Cohen symmetry for any choice of the dynamical parameters defining the stochastic walk. This class includes the linear model considered in Lacoste et al (2008 \textit{Phys. Rev. E} 78 011915). We also derive fluctuation theorems for the time-integrated cycle currents and discuss how the matrix approach of Lacoste et al (2008 \textit{Phys. Rev. E} 78 011915) can be extended to derive the above Gallavotti–Cohen symmetry for any Markov random walk on \(\mathbb{Z}\) with periodic jump rates. Finally, we review in the present context some large deviation results of Faggionato and Silvestri (2017 \textit{Ann. Inst. Henri Poincaré} \textbf{53} 46–78) and give some specific examples with explicit computations.

Keywords: large deviations in non-equilibrium systems, molecular motors
1. Introduction

Molecular motors are special proteins able to convert chemical energy coming from ATP-hydrolysis into mechanical work, allowing numerous physiological processes such as cargo transport inside the cell, cell division, muscle contraction [20]. They are able to produce directed transport in an environment in which the fluctuations due to thermal noise are significant, achieving nonetheless an efficiency even higher than the one
of macroscopic motors. In addition synthetic molecular motors have been obtained and their improvements are under continuous investigation [16].

Molecular motors have been extensively studied both theoretically and experimentally (see [21, 26, 34, 35, 37] and references therein). We focus here on the large class of molecular motors (e.g. conventional kinesin) which work non-cooperatively and move along cytoskeletal filaments [20]. Keeping in mind the polymeric structure of these filaments, two main models have been proposed. In the so called Brownian ratchet model [21, 34] the dynamics of the molecular motor is given by a one-dimensional diffusion in a spatially periodic potential randomly switching its shape (indeed, along its mechanochemical cycle the molecular motor can be strongly or weakly bound to the filament, thus leading to a change in the interaction potential). The other paradigm [17, 18, 22–26, 40], on which we concentrate here, is given by continuous time random walks (CTRW), along with a quasi one dimensional (quasi-1d) lattice obtained by gluing several copies of a fundamental graph in a linear fashion. CTRWs are thought in the Montroll–Weiss sense [32], and are also known as semi-Markov processes satisfying the condition of direction-time independence in the physical literature [41], as well Markov renewal processes in the mathematical one [5].

The above fundamental graph used to build a quasi-1d lattice is a finite connected graph $G$ with two marked vertices $\varpi, \varpi'$ (see figure 1, left). For simplicity we assume that $G$ has no multiple edges or self-loops. The associated quasi-1d lattice $\mathcal{G}$ is then obtained by gluing several copies of $G$, identifying the $\varpi'$-vertex of one copy to the $\varpi$-vertex of the next copy (see figure 1, right). Given a vertex $v$ in $G$ and $n \in \mathbb{Z}$, we write $v^{(n)}$ for the corresponding vertex in the $n$th copy of $G$ in $\mathcal{G}$. Since $v^{(n-1)} = v^{(0)}$, to simplify the notation we denote such a vertex by $v^{(n)}$ throughout. Each site $v^{(n)}$ corresponds to a spot in the $n$th monomer of the polymeric filament to which the molecular motor can bind. The other vertices $v^{(n)}$ describe intermediate conformational states that the molecular motor achieves by conformational transformations, modeled by jumps along edges in $\mathcal{G}$. Note the periodicity of the quasi-1d lattice $\mathcal{G}$.

The evolution of the molecular motor is described by a CTRW $(X_t)_{t \geq 0}$, taking values in the vertex set of the quasi-1d lattice $\mathcal{G}$. Once arrived at vertex $x$, $X_t$ waits a random time with distribution $\psi_x$ (that we assume to have finite mean) and then jumps to a neighboring vertex $y$ in $\mathcal{G}$ with probability $p(x, y) > 0$. We assume that $\psi_x$ and $p(x, y)$ exhibit the same periodicity of $\mathcal{G}$. In what follows, we call dynamical characteristics the above data $\psi_x, p(x, y)$.

**Warning 1.1.** In the degenerate case that $\psi_x$ is a delta measure, e.g. $\psi_x$ equals $\delta_1$, the above CTRW reduces to the so-called discrete time random walk. We do not restrict to

https://doi.org/10.1088/1742-5468/aa6731
distributions $\psi_x$ having a probability density w.r.t. the Lebesgue measure, so that $\psi_x$ can be composed by some delta measure as well.

We remark that when $\psi_x$ is the exponential distribution with mean $1/\lambda(x)$, then the resulting CTRW is Markov and its density distribution $P_z(t) := P(X_t = x)$ satisfies the Fokker–Planck equation

$$\frac{\text{d}}{\text{d}t} P_z(t) = \sum_y r(y, x) P_z(t) - \sum_y r(x, y) P_z(t), \quad r(a, b) := \lambda(a)p(a, b).$$

In what follows, we assume that the random walk starts at $x_0$, i.e. $X_0 = x_0$.

As observed in [40], the above formalism allows us to treat at once several specific examples analyzed in the literature. For example, when the fundamental graph is given by a finite linear chain with $N$ vertices, we recover a CTRW on $\mathbb{Z}$ with nearest-neighbor jumps and $N$-periodic dynamical characteristics [17, 18]. Supported by experimental results, CTRWs on more complex quasi-1d lattices have been considered in the biophysics literature [9, 22] (see figure 2 for two examples).

Calling $V$ the set of vertices of the fundamental graph $G$, for $n \in \mathbb{Z}$ we define the $n$th cell as the set of vertices in $G$ of the form $v^{(n)}$ with $v \in V \setminus \{\sigma\}$ (for example, in figure 1 the 0th cell is given by $\{a^{(0)}, b^{(0)}, c^{(0)}, v^{(0)}\}$). Our aim is to investigate large fluctuations and associated symmetries of the cell process $(N_t)_{t \geq 0}$ defined as $N_t = n$ if $X_t$ belongs to the $n$th cell, i.e. if $X_t = v^{(n)}$ for some $v \in V \setminus \{\sigma\}$. Trivially, the cell process determines the position of the molecular motor along the filament apart from an error of the same order of the monomer size, which is negligible when analyzing velocity, Gaussian fluctuations and large deviations.

As shown in [13], the cell process admits a limit velocity $v_{\lim}$ (i.e. $N_t/t \to v_{\lim}$ almost surely) and has Gaussian fluctuations. A large deviation principle is proved in [14] (see section 5 for more details). We call $I : \mathbb{R} \to [0, +\infty]$ the associated large deviation function:

$$\mathbb{P}(N_t \approx n t) \sim e^{-I(n)t}, \quad t \gg 1.$$  

In the last decades some general principles, called fluctuation theorems and common to out-of-equilibrium systems, have been formulated and intensively studied first for dynamical systems and then also for stochastic processes (see for example [2, 4, 6, 7, 10, 15, 27, 33, 38]). For stochastic systems, they often correspond to relations of the form $J(\vartheta) = J(-\vartheta) - c\vartheta$, or similar, $c$ being a constant and $J$ being the rate function of an observable changing sign under time inversion. These last relations are also called Gallavotti–Cohen type symmetries, shortly GC symmetries in what follows. Fluctuations theorems have also been investigated for small systems such as molecular motors [1, 12, 14, 28–31, 37], and GC symmetries (in particular, for the velocity) have been obtained for some special models. In particular, in [28, 29, 31], the authors derive a GC symmetry for the rate function of the velocity of a molecular motor described by a generic Markov CTRW on $\mathbb{Z}$ with nearest-neighbor jumps and dynamical characteristics of periodicity.

Figure 2. Parallel chains model (left), divided-pathway model (right).
two, which corresponds to (1) with \( r(a, b) \) of the following form: \( r(a, a \pm 1) = \xi_{\pm} \) if \( a \) is even and \( r(a, a \pm 1) = \zeta_{\pm} \) if \( a \) is odd, for generic constants \( \xi_{\pm}, \zeta_{\pm} > 0 \). This GC symmetry for the velocity reads

\[
I(\vartheta) = I(-\vartheta) - c\vartheta, \quad \vartheta \in \mathbb{R},
\]

(3)

\( I \) being the rate function of the cell process modulo rescaling by the length of monomers in the polymeric filaments. For the above 2-periodic Markov CTRW it holds

\[
c = \frac{1}{2} \ln \frac{\xi_{\pm}}{\zeta_{\pm}}.
\]

Since the above CTRW with period 2 is a simplified model for the motion of real molecular motors, a natural question concerns the validity of (3) for a larger class of CTRWs, or even for all possible CTRWs on quasi-1d lattices. For Markov CTRWs we have shown in [14] that (3) is not universal, and in fact (3) is only universal in the subclass of 1d lattices whose fundamental graph \( G \) is \((\underline{v}, \bar{v})\)-minimal in the following sense: there exists a unique self-avoiding path \( \gamma \) in \( G \) from \( v \) to \( \bar{v} \). An example of \((\underline{v}, \bar{v})\)-minimal graphs \( G \) is given in figure 3. Note that the graphs \( G \) associated to the quasi-1d lattices in figure 2 are not \((\underline{v}, \bar{v})\)-minimal.

We can now recall the characterization provided in [14]:

**Theorem 1 ([14]).** Suppose that \( X_t \) is a Markov CTRW on the quasi-1d lattice \( G \), in particular it has exponentially distributed waiting times and transition rates \( r(\cdot, \cdot) \) as in (1). Then the following holds:

(i) If \( G \) is \((\underline{v}, \bar{v})\)-minimal, then the cell process \( N_t \) satisfies the GC symmetry

\[
I(\vartheta) = I(-\vartheta) - \Delta \vartheta, \quad \forall \vartheta \in \mathbb{R},
\]

(4)

where

\[
\Delta = \ln \frac{r(z_0, z_1)r(z_1, z_2) \cdots r(z_{n-1}, z_n)}{r(z_1, z_0)r(z_2, z_1) \cdots r(z_n, z_{n-1})}
\]

(5)

and \((z_0, z_1, z_2, \ldots, z_{n-1}, z_n), \) with \( z_0 = v \) and \( z_n = \bar{v} \), is the unique self-avoiding path from \( v \) to \( \bar{v} \) in \( G \).

(ii) Vice versa, if \( G \) is not \((\underline{v}, \bar{v})\)-minimal, then the set of transition rates \( r(\cdot, \cdot) \) for which the GC symmetry (4) holds for some \( \Delta \) (which can depend on \( r(\cdot, \cdot) \)) has zero Lebesgue measure.
It is simple to verify (see section 6) that the GC symmetry (3) can be satisfied for very special choices of the jump rates when $G$ is not $(\mathcal{G}, \sigma)$-minimal. In this case, due to the above theorem, a small perturbation of these rates typically breaks the GC symmetry.

We point out that in [13] the GC symmetry for the LD rate function of the cell process is analyzed for a larger class of random processes, having a suitable regenerative structure. Moreover, it has been proved (see theorems 4 and 8 in [13]) that the GC symmetry (3) holds if and only if $X_{S_1}$ and $S_1$ are independent, where the random time $S_1$ is defined as $S_1 := \inf\{t \geq 0 : X_t \in \{x^{(1)}, x^{(2)}\}\}$. For the Markov random walk on a linear chain this independence had been pointed out already in [8] (see remark 5.3).

We also point out the above theorem 1 is related to the theorem on page 584 of [3] (see also the discussion on cycle currents in section 4). On the other hand, in the derivation of the equivalence stated in that theorem, some additional arguments are necessary to get the difficult implication.

The aim of the present work is the following: (a) extend theorem 1-(i) to generic CTRWs (i.e. non Markov) and give some sufficient condition assuring the GC symmetry (3) for non $(\mathcal{G}, \sigma)$-minimal fundamental graphs (see section 2.1), (b) derive fluctuation theorems for time-integrated cycle currents in the case of generic CTRWs and $(\mathcal{G}, \sigma)$-minimal fundamental graphs and, as a consequence, recover the GC symmetry (3) independently from [14] (see section 2.2), (c) extend the matrix approach outlined in [28] to Markov CTRWs on general linear chain models, getting also the GC symmetry (4) (see section 2.3), (d) give a short presentation of some results of [14] in a less sophisticated language (see section 5), (e) give specific examples with explicit computations (see sections 6–9).

2. Main results

In this section we present our main results, postponing their derivation to the next sections and to the appendixes.

2.1. Extension of theorem 1-(i) to generic CTRWs

We consider generic CTRWs on $\mathcal{G}$, i.e. also non Markov. As a first result we give a sufficient condition assuring that the GC symmetry (3) holds for some constant $\Delta$ (for a sufficient and necessary condition see criterion 1 in appendix A). This condition is trivially satisfied in $(\mathcal{G}, \sigma)$-minimal graphs $\mathcal{G}$, thus leading to the extension of theorem 1-(i) to non Markov CTRWs.

**Theorem 2.** Consider a generic CTRW $(X_t)_{t \geq 0}$ on the quasi-1d lattice $\mathcal{G}$ with dynamical characteristics $p(x, y)$ and $\psi_x$. Then the cell process $N_t$ satisfies the GC symmetry (4) for some constant $\Delta$ if

$$\prod_{i=0}^{m-1} p(x_i, x_{i+1}) = e^{\Delta} \prod_{i=0}^{m-1} p(x_{i+1}, x_i)$$

(6)
for any self-avoiding path \((x_0, x_1, \ldots, x_m)\) from \(v\) to \(\bar{v}\) in the fundamental graph \(G\) \((x_0 = v, x_m = \bar{v})\).

As a consequence, if \(G\) is \((v, \bar{v})\)-minimal, then the cell process \(N_t\) satisfies the GC symmetry (4) where now

\[
\Delta = \ln \frac{p(z_0, z_1)p(z_1, z_2) \cdots p(z_{n-1}, z_n)}{p(z_1, z_0)p(z_2, z_1) \cdots p(z_n, z_{n-1})}
\]

(7)

and \((z_0, z_1, z_2, \ldots, z_{n-1}, z_n)\), with \(z_0 = v\) and \(z_n = \bar{v}\), is the unique self-avoiding path from \(v\) to \(\bar{v}\) in \(G\).

Note that for Markov CTRWs expressions (5) and (7) indeed coincide.

The theorem is a immediate consequence of criterion 1 discussed in appendix A.

Remark 2.1. When considering discrete time RWs (recall warning 1.1) it is possible to exhibit examples of fundamental graphs \(G\) which are not \((v, \bar{v})\)-minimal and such that the GC symmetry (3) holds for any choice of the jump probabilities \(p(x, y)\). We refer to section 7 for an example.

To see where condition (6) comes from, for each \(n \in \mathbb{Z}\) define \(T_n\) as the first time the cell process \(N_t\) reaches the cell \(n\), i.e. \(T_n := \inf \{t \geq 0 : N_t = n\}\). Recall that \(X_0 = v^{(0)}\), hence \(T_0 = 0\). As discussed in section 5, the sequences \((T_{\pm n})_{n \geq 1}\) satisfy a LDP with speed \(n\) and rate function

\[
J_\pm(\vartheta) := \sup_{\lambda \in \mathbb{R}} \{\lambda \vartheta - \log \varphi_\pm(\lambda)\}
\]

(8)

where \(\varphi_\pm(\lambda) = \mathbb{E}(e^{\lambda T_{\pm 1}} \mathbb{I}(T_{\pm 1} < \infty))\). Moreover, for large times \(t\) it holds

\[
e^{-tI(\vartheta)} \sim \mathbb{P}\left(\frac{N_t}{t} \approx \vartheta\right) \approx \mathbb{P}(T_{\vartheta^{|\vartheta|}} \approx t) \approx \mathbb{P}\left(\frac{T_{\vartheta^{|\vartheta|}}}{|\vartheta|} \approx \frac{1}{|\vartheta|}\right) \sim e^{-t|\vartheta|J_+(|\vartheta|)}
\]

where in the last term one has to choose \(J_+\) if \(\vartheta > 0\) and \(J_-\) if \(\vartheta < 0\). As a consequence we get

\[
I(\vartheta) = \begin{cases} \vartheta J_+(1/|\vartheta|) & \text{if } \vartheta > 0, \\ |\vartheta| J_-(1/|\vartheta|) & \text{if } \vartheta < 0. \end{cases}
\]

Hence, given \(\vartheta > 0\), using (8) we get

\[
I(\vartheta) - I(-\vartheta) = -c \vartheta \quad \Leftrightarrow \quad \vartheta J_+(\frac{1}{\vartheta}) - \vartheta J_-(\frac{1}{\vartheta}) = -c \vartheta
\]

\[
\Leftrightarrow \quad J_+(\vartheta) = J_-(\vartheta) - c
\]

\[
\Leftrightarrow \quad \varphi_+(\lambda) = e^c \varphi_-(\lambda).
\]

This shows that the GC symmetry of \(I\) reduces to the proportionality of

\[
\varphi_+(\lambda) = \mathbb{E}(e^{\lambda T_1} \mathbb{I}(T_1 < \infty)) = \sum_\gamma e^{\lambda T_1(\gamma)} \mathbb{P}(\gamma)
\]

(9)

\(\lfloor x \rfloor\) denotes the integer approximation of number \(x\).
and

\[ \varphi(\lambda) = \mathbb{E}(e^{\lambda T_\gamma} \mathbb{1}(T_\gamma < \infty)) = \sum_{\gamma} e^{\lambda T_\gamma} \mathbb{P}(\gamma), \]

(10)

where \( \gamma \mapsto \gamma^t \) is a suitable bijection on the path space (discussed in appendix A). Condition (6) corresponds to a ‘pairwise proportionality’ between \( e^{\lambda T_\gamma} \mathbb{P}(\gamma) \) and \( e^{\lambda T_\gamma} \mathbb{P}(\gamma^t) \), thus implying the proportionality of (9) and (10), and therefore the GC symmetry. In appendix A we reformulate in a more geometric way the proportionality of (9) and (10). By the above discussion, this formulation is equivalent to the GC symmetry, and this is indeed the content of criterion 1 in appendix A.

### 2.2. GC symmetries for cycle currents

As next result we show that, for \((\underline{x}, \underline{\sigma})\)-minimal fundamental graphs, the GC symmetry (3) is indeed a special case of a fluctuation theorem for cycle currents (see e.g. [2, 4, 11, 12]). As a consequence we give, among others, an alternative derivation of (3) for \((\underline{x}, \underline{\sigma})\)-minimal fundamental graphs, which is based on cycle theory and does not use preliminary facts from [14] as the above cited criterion 1.

We present here our result giving more details and precise definitions in section 4. To this aim, we assume \( \mathcal{G} \) to be \((\underline{x}, \underline{\sigma})\)-minimal and we denote by \( \tilde{\mathcal{G}} \) the new finite graph obtained from \( \mathcal{G} \) by gluing together \( \underline{x} \) and \( \underline{\sigma} \) in a single vertex called \( \underline{x} \) (see figure 4).

We denote by \( \mathcal{C}_1 \) the cycle in \( \tilde{\mathcal{G}} \) corresponding to the unique self-avoiding path \((z_0, z_1, \ldots, z_n)\) from \( \underline{x} \) to \( \underline{\sigma} \) in \( \mathcal{G} \), and we call \( \mathcal{C}_2, \ldots, \mathcal{C}_m \) the other cycles in \( \tilde{\mathcal{G}} \) which form, together with \( \mathcal{C}_1 \), a cycle basis according to Schnackenberg’s construction. We also define the affinity \( \mathcal{A}(\mathcal{C}) \) of a cycle \( \mathcal{C} \) as

\[ \mathcal{A}(\mathcal{C}) := \ln \prod_{i=0}^{k-1} \frac{p(x_i, x_{i+1})}{p(x_{i+1}, x_i)} = \frac{x_0 - x_k}{x_0 - x_k}, \]

(11)

Due to the periodicity of the dynamical characteristics, the CTRW \( X_t \) naturally induces a CTRW \( Y_t \) on \( \tilde{\mathcal{G}} \). We then consider the path in \( \tilde{\mathcal{G}} \) given by the vertices visited by \( Y \) up to time \( t \) and complete it to get a cycle \( \mathcal{C}_t \) in \( \tilde{\mathcal{G}} \), e.g. by adding an extra path of minimal length ending at the initial point. Finally we decompose the random cycle \( \mathcal{C}_t \) in the above cycle basis: \( \mathcal{C}_t = \sum_{i=1}^m a_i(t) \mathcal{C}_i \). The random coefficients \( a_i(t) \)’s are also called time-integrated cycle currents, and for them we derive in appendix B the following fluctuation theorems:

**Figure 4.** The fundamental graph \( \mathcal{G} \) and the associated graph \( \tilde{\mathcal{G}} \) obtained by gluing \( \underline{x} \) and \( \underline{\sigma} \).
**Theorem 3.** Suppose that $G$ is $(\mathcal{F}, \mathcal{P})$-minimal and let $(X_t)_{t \geq 0}$ be a generic CTRW on the associated quasi-1d lattice $G$. Then the random vector $\frac{1}{t}(a_1(t), a_2(t), \ldots, a_m(t))$ satisfies a LDP with speed $t$ and good\(^4\) rate function $\mathcal{I}$. Calling $\mathcal{I}(\vartheta_1, \vartheta_2, \ldots, \vartheta_m)$ the associated rate function, roughly we have

$$
\mathbb{P} \left[ \frac{1}{t}(a_1(t), \ldots, a_m(t)) \approx (\vartheta_1, \ldots, \vartheta_m) \right] \sim e^{-t \mathcal{I}(\vartheta_1, \vartheta_2, \ldots, \vartheta_m)}. \quad (12)
$$

Moreover the following GC symmetries hold:

$$
\mathcal{I}(\vartheta_1, \vartheta_2, \ldots, \vartheta_m) = \mathcal{I}(-\vartheta_1, -\vartheta_2, \ldots, -\vartheta_m) - \sum_{i=1}^{m} \vartheta_i \mathcal{A}(C_i), \quad (13)
$$

$$
\mathcal{I}(\vartheta_1, \vartheta_2, \ldots, \vartheta_m) = \mathcal{I}(\vartheta_1, -\vartheta_2, \ldots, -\vartheta_m) - \sum_{i=2}^{m} \vartheta_i \mathcal{A}(C_i), \quad (14)
$$

$$
\mathcal{I}(\vartheta_1, \vartheta_2, \ldots, \vartheta_m) = \mathcal{I}(-\vartheta_1, \vartheta_2, \ldots, \vartheta_m) - \vartheta_1 \mathcal{A}(C_i). \quad (15)
$$

As a consequence, the LD rate function $I(\vartheta)$ of the cell process introduced in (2) fulfills the GC symmetry

$$
I(\vartheta) = I(-\vartheta) - \mathcal{A}(C_i) \vartheta, \quad \forall \vartheta \in \mathbb{R}. \quad (16)
$$

Let us also remark that for Markov CTRWs the symmetry (16) reduces to (4), since $\mathcal{A}(C_i) = \Delta$.

For Markov CTRWs [12], but also for a larger class of CTRWs, one can show that the function

$$
Q(\lambda_1, \lambda_2, \ldots, \lambda_m) := \lim_{t \to \infty} -\frac{1}{t} \ln \mathbb{E} \left[ e^{-\sum_{i=1}^{m} \lambda_i a_i(t)} \right], \quad (\lambda_1, \lambda_2, \ldots, \lambda_m) \in \mathbb{R}^m
$$

is well posed and it holds

$$
\mathcal{I}(\vartheta_1, \vartheta_2, \ldots, \vartheta_m) := \sup_{(\lambda_1, \lambda_2, \ldots, \lambda_m) \in \mathbb{R}^m} \left\{ -\sum_{i=1}^{m} \vartheta_i \lambda_i + Q(\lambda_1, \lambda_2, \ldots, \lambda_m) \right\}. \quad (17)
$$

Moreover, via Legendre transform, the above identities (13)–(15) correspond respectively to the following (18)–(20):

$$
Q(\lambda_1, \lambda_2, \ldots, \lambda_m) = Q(\mathcal{A}(C_1) - \lambda_1, \mathcal{A}(C_2) - \lambda_2, \ldots, \mathcal{A}(C_m) - \lambda_m), \quad (18)
$$

$$
Q(\lambda_1, \lambda_2, \ldots, \lambda_m) = Q(\mathcal{A}(C_1) - \lambda_1, \mathcal{A}(C_2) - \lambda_2, \ldots, \mathcal{A}(C_m) - \lambda_m), \quad (19)
$$

$$
Q(\lambda_1, \lambda_2, \ldots, \lambda_m) = Q(\mathcal{A}(C_1) - \lambda_1, \mathcal{A}(C_2) - \lambda_2, \ldots, \mathcal{A}(C_m) - \lambda_m). \quad (20)
$$

\(^4\) ‘Good’ means that the level sets of $\mathcal{I}$ are compact

https://doi.org/10.1088/1742-5468/aa6731

9
2.3. Derivation of the GC symmetry (4) for Markov CTRWs on the linear chain by the matrix approach

When the CTRW on the quasi-1d lattice $G$ is Markov, then the LD rate function $I$ of the cell process $N_t$ can be expressed as the Legendre transform of the maximal eigenvalue of a suitable matrix depending by a scalar parameter. In [13, theorem 3] a general formula is derived by generalizing the matrix approach used in [28].

We restrict here to Markov CTRWs on a linear chain and show how one can derive the GC symmetry (4) by the matrix approach. To make the discussion self-contained we briefly recall how to express the LD rate function in terms of the above maximal eigenvalue. To this aim let $G$ be the linear chain graph of figure 5, i.e. $G = (V, E)$ with $V = \{0, 1, \ldots, N\}$, $E = \{(x, x + 1), x = 0, \ldots, N - 1\}$ and $y = 0$, $\bar{\sigma} = N$. If $G$ denotes the associated quasi-1d lattice, then $G$ can be identified with $\mathbb{Z}$ with periodic jump rates. We therefore take $\mathbb{Z}$ to be the vertex set of $G$, and denote by $\xi_{x}^\pm$, $x \in \mathbb{Z}$, the rate associated to the edge $(x, x \pm 1)$. Finally, set $r(x) = \xi_{x}^+ + \xi_{x}^-$. Then the Markov CTRW $X_t$ waits at $x$ an exponentially distributed time of mean $1/r(x)$, and then jumps to either $x + 1$ or $x - 1$ with probability $\xi_{x}^+/r(x)$ and $\xi_{x}^-/r(x)$ respectively. Note that $\xi_{x}^\pm = \xi_{x+N}^\pm$ and $r(x) = r(x+N)$ for any $x \in \mathbb{Z}$ and that the constant $\Delta$ in (5) is now given by $\Delta = \ln \frac{\xi_{0}^+ \xi_{1}^- \cdots \xi_{N-1}^+}{\xi_{0}^- \xi_{1}^+ \cdots \xi_{N-1}^-}$.

Let us first consider the case $N \geq 3$. Given $\lambda \in \mathbb{R}$, we introduce the $N \times N$ matrix $\mathcal{A}(\lambda)$, defined as follows for $0 \leq i, j \leq N - 1$:

$$
\mathcal{A}(\lambda)_{i,j} = \begin{cases} 
-\lambda & \text{if } i = j, \\
\xi_{j}^{+} & \text{if } 0 < i < N - 1, \ j = i - 1, \\
\xi_{j}^{-} & \text{if } 0 < i < N - 1, \ j = i + 1, \\
\xi_{0}^{+} e^{-\lambda} & \text{if } i = N - 1, \ j = 0, \\
\xi_{N-1}^{-} e^{\lambda} & \text{if } i = 0, \ j = N - 1, \\
0 & \text{otherwise.}
\end{cases}
$$

For example, for $N = 3$ we have

$$
\mathcal{A}(\lambda) = \begin{pmatrix}
-\lambda & \xi_{1}^{-} & \xi_{2}^{+} e^{\lambda} \\
\xi_{0}^{+} & -\lambda & \xi_{2}^{-} \\
\xi_{0}^{-} e^{-\lambda} & \xi_{1}^{+} & -\lambda
\end{pmatrix}.
$$
Following the approach of [28] for the 2-periodic linear model, we introduce the function
\[ F(x, \lambda, t) := \sum_{k \in \mathbb{Z}} e^{\lambda k} \mathbb{P}(X_t = x + kN) = \mathbb{E}[e^{\lambda N} \mathbb{I}(X_t = x + N_0 N)], \]

where, we recall, \( N_0 \) is the cell number of \( X_t \). By the Markov property of \( X_t \) we have
\[ \partial_t F(x, \lambda, t) = \xi^+_1 F(x, \lambda, t) + \xi^-_{x+1} F(x+1, \lambda, t) - r(x) F(x, \lambda, t). \]
Using that \( F(-1, \lambda, t) = e^{\lambda} F(N-1, \lambda, t) \) and \( F(N, \lambda, t) = e^{-\lambda} F(0, \lambda, t) \), we conclude that
\[ \partial_t F(x, \lambda, t) = \sum_{0 \leq y \leq N-1} A(\lambda)_{x,y} F(y, \lambda, t), \quad 0 \leq x \leq N - 1, \] (22)

and therefore
\[ F(x, \lambda, t) = \sum_{0 \leq y \leq N-1} [e^{\lambda \Lambda(\lambda)}]_{x,y} F(y, \lambda, 0). \]
When \( N = 2 \), (22) remains valid with \( A(\lambda) \) defined as
\[ A(\lambda) = \begin{pmatrix} -r(0) & \xi^+_1 e^{\lambda} + \xi^-_1 \\ \xi^+_0 + \xi^-_0 e^{-\lambda} & -r(1) \end{pmatrix} \]

Since on the other hand \( \mathbb{E}(e^{\lambda N}) = \sum_{0 \leq x \leq N-1} F(x, \lambda, t) \), the Perron–Frobenius theorem gives
\[ \mathbb{E}(e^{\lambda N}) \approx e^{\lambda \Lambda(\lambda)}, \quad \Lambda(\lambda) := \max\{\Re(\gamma) : \gamma \text{ eigenvalue of } A(\lambda)\}. \] (23)

By Gärtner–Ellis theorem, the cell process satisfies a LD principle with rate function \( I \) given by
\[ I(\vartheta) = \sup_{\lambda \in \mathbb{R}} \{ \vartheta \lambda - \Lambda(\lambda) \}, \quad \vartheta \in \mathbb{R}. \] (24)

Having (24) the GC symmetry (4) follows from the equality
\[ \Lambda(\lambda) = \Lambda(-\Delta - \lambda), \quad \lambda \in \mathbb{R}, \] (25)

with \( \Delta \) defined according to (5). This is in turn a consequence of the following result:

**Proposition 2.2.** Let \( \Delta = \ln \frac{\xi^+_1 \xi^-_1 \cdots \xi^+_x}{\xi^-_1 \xi^-_2 \cdots \xi^-_{x-1}} \). Then there exists an invertible matrix \( U \) such that
\[ U^{-1} A(\lambda) U = A^T(-\Delta - \lambda) \quad \forall \lambda \in \mathbb{C}, \] (26)

\( A^T(-\Delta - \lambda) \) being the transpose of \( A(-\Delta - \lambda) \). In particular, for the linear chain graph identity (25) is satisfied as well as the GC symmetry (4).

It is known that any square matrix \( A \) is similar to its transpose \( A^T \) [39], i.e. \( \exists \) an invertible matrix \( U \) such that \( U^{-1} A U = A^T \). Hence, once proved (26), one immediately gets that \( A(\lambda) \) and \( A(-\Delta - \lambda) \) have the same spectrum and therefore the conclusion of the proposition becomes trivial by the above discussion.

---

5 \( \Re(x) \) denotes the real part of the complex number \( x \).
2.4. Further results

Four specific examples are discussed in sections 6–9. We briefly comment on them. The derivation of theorem 1-(ii), given in [14], is mathematically involved. On the other hand, in section 6 we consider a parallel chains model (whose fundamental graph is not \((\mathring{v}, \mathring{\tau})\)-minimal) and show by direct computations that usually the GC symmetry (3) is not satisfied. In particular, we recover in a specific example the content of theorem 1-(ii). In section 7, by considering discrete time RWs (recall warning 1.1), we exhibit an example of fundamental graph \(G\) which is not \((\mathring{v}, \mathring{\tau})\)-minimal and such that the GC symmetry (3) holds for any choice of the jump probabilities \(p(x, y)\). Finally, in sections 8 and 9 we consider spatially homogeneous CTRWs on \(\mathbb{Z}\) with waiting times having respectively exponential and gamma distribution, and compute explicitly several quantities related to large deviations introduced in section 5 (in particular, the LD rate function for the hitting times and the LD rate function for the cell process).

2.5. Outline of the paper

As already pointed out, a crucial feature of the CTRWs on quasi-1d lattices is a regenerative structure (several results of [14] are indeed valid for stochastic processes exhibiting such a regenerative structure, not necessarily CTRWs). We explain this regenerative structure in section 3. In section 5 we recall the main results of [14] applied to the present context, while in section 4 we recall some basic facts on cycle currents and discuss in detail the objects involved in the cycle fluctuation theorems stated in theorem 3. Some of these results will be used in our proofs. In sections 6–9 we discuss the above mentioned example. Appendices [castelluccio_proof]A–[GC_extra_matrix]C will be devoted to the derivation of theorem 2, theorem 3 and proposition 2.2 respectively. Finally, appendix D contains some minor technical facts.

3. Regenerative structure and skeleton process

In this section we explain the regenerative structure behind the CTRWs on \(\mathcal{G}\). To this aim we introduce a coarse-grained version of \(X_n\) called skeleton process \((X^*_n)_{n \geq 0}\) with values in \(\mathbb{Z}\). More precisely, we set \(X^*_n = n\) if \(v^{(n)}\) is the last vertex of the form \(v^{(k)}\) visited by \((X_n)_{0 \leq n \leq t}\) (see the example in figure 6). In the applications to molecular motors, the skeleton process contains all the relevant information, since it allows to determine the position of the molecular motor up to an error of the same order of the monomer size.

Figure 6. Example of a trajectory \((X_t)_{t \geq 0}\) and the associated trajectory \((X^*_t)_{t \geq 0}\) referred to the quasi-1d lattice \(\mathcal{G}\) of figure 1.

https://doi.org/10.1088/1742-5468/aa6731
Fluctuation theorems for discrete kinetic models of molecular motors

13https://doi.org/10.1088/1742-5468/aa6731

J. Stat. Mech. (2017) 043206

Note that \(|N_t - X_t^*| \leq 1\), and therefore the skeleton process and the cell process have the same asymptotic behaviour and large deviations.

The technical advantage of dealing with the skeleton process instead of the cell process comes from the following regenerative structure. Consider the sequence \(S_1 < S_2 < \ldots\) of jump times for the skeleton process \(X_t^*\), set \(S_0 := 0\), call \(S_i := S_i - S_{i-1}\) the inter-arrival times and \(w_i := X_{S_i}^* - X_{S_{i-1}}^* \in \{-1, +1\}\) the jumps of the skeleton process (see figure 7).

By our assumptions on \(X_t\), we get that the sequence \((w_i, \tau_i)_{i \geq 1}\) is given by independent and identically distributed random vectors and it fully characterizes the skeleton process itself.

4. Time integrated cycle currents and affinity

In this section we restrict to \((\gamma, \sigma)\)-minimal fundamental graphs \(G\) and apply the cycle theory (see e.g. [2, 4, 11, 12]) to formulate fluctuation theorems for cycle currents also for non-Markovian CTRW (see theorem 3).

Let \(G\) denote a new finite graph obtained from \(G\) by gluing together \(y\) and \(\sigma\) in a single vertex called \(v_s\) (see figure 4). We denote by \(\pi : G \rightarrow \tilde{G}\) the natural graph projection (see figure 8) and introduce the projected process \(Y_t := \pi(X_t)\) having values in \(\tilde{G}\).

As explained in formula (29) below, one can recover the asymptotic behavior of the skeleton process \(X_t^*\) (and therefore of the cell process \(N_t\)) by analyzing the currents of the projected process \(Y_t\).

Let us briefly recall some concepts from cycle theory (see e.g. [2, 6, 12, 36]). A cycle \(C\) in \(\tilde{G}\) is described by a path \((x_0, x_1, \ldots, x_k)\) along edges of \(\tilde{G}\) such that \(x_0 = x_k\). Given a cycle \(C\) and two neighboring vertices \(x, y\) in \(\tilde{G}\), we define \(N_{x,y}(C)\) as the number of appearances of the string \((x, y)\) in \(C\) minus the number of appearances of the string \((y, x)\) in \(C\) (i.e. the number of jumps from \(x\) to \(y\) minus the number of jumps from \(y\) to \(x\) performed by the cycle \(C\)). We can make the cycle space into a real vector space by considering formal linear combinations of cycles and using the identification

\[
\sum_{i=1}^{m} a_i C_i = \sum_{j=1}^{k} b_j C_j
\]

whenever \(\sum_{i=1}^{m} a_i N_{x,y}(C_i) = \sum_{j=1}^{k} b_j N_{x,y}(C_j)\) for any neighboring vertices \(x, y\).

To the path \(\gamma = (z_0, z_1, \ldots, z_n)\) we associate the cycle \((v_s, z_1, z_2, \ldots, z_{n-1}, v_s)\) in the graph \(\tilde{G}\). Let us now fix a cycle basis \(C_1, C_2, \ldots, C_m\) in \(\tilde{G}\) with \(C_1 = (v_s, z_1, z_2, \ldots, z_{n-1}, v_s)\).
This can be done according to Schnackenberg’s construction as follows. We take a spanning tree (i.e. a subgraph of \( \tilde{G} \) without loops which contains all vertices of \( \tilde{G} \)) containing the linear chain \( (v, z_1, z_2, \ldots, z_{n-1}) \). Given an edge \( \{x, y\} \) in \( \tilde{G} \) not belonging to the spanning tree, there exists a unique self-avoiding cycle \( C \) (apart from orientation and starting point) in the graph obtained by adding the edge \( \{x, y\} \) to the spanning tree. Just take one \( C \), fixing arbitrarily orientation and starting point. The collection of cycles obtained by varying the edge \( \{x, y\} \) in this procedure forms a cycle basis. Note that this basis contains the cycle \( (v, z_1, z_2, \ldots, z_{n-1} \ast) \), which is indeed associated to the edge \( \{x, y\} \) (see figure 9). Note also that, since \( G \) is \( (\varphi, \pi) \)-minimal, the cycle \( C_1 \) has no edge in common with \( C_2, \ldots, C_m \).

We can finally define the affinity \( \mathcal{A}(C) \) of a cycle \( C \). To this aim recall that the CTRW is defined in terms of the dynamical characteristics \( \psi \) and \( p(x, y) \) and that we are considering also non Markov CTRWs. Note that the jump probabilities \( p(\cdot, \cdot) \) defined on \( G \) can be projected on the graph \( \tilde{G} \) without any ambiguity since we are assuming \( n \geq 3 \) (see figure 10 for an example). Finally, recall the definition of cycle affinity \( \mathcal{A}(C) \) (see (11)).

Let us now go back to the dynamics. Since \( X_0 = x^{(0)} \) we have \( Y_0 = v_0 \) (recall that \( Y_t = \pi(X_t) \)). We now associate to each trajectory \( (X_s)_{s \in [0,t]} \) a cycle \( C_t \) in \( \tilde{G} \) as follows. Consider the projected path \( (Y_s)_{s \in [0,t]} \). If \( Y_t = Y_0 = v_0 \), then \( C_t \) is given by the string of vertices visited by \( (Y_s)_{s \in [0,t]} \), taken in chronological order. If \( Y_t \neq Y_0 \), then we complete the above string by adding a path in \( \tilde{G} \) from \( Y_t \) to \( v_0 \) (this additional path depends only
on $Y_t$: the same final point $Y_t$, the same additional path). Finally, we take the decomposition of the random cycle $C_t$ in our fixed basis, i.e.

$$C_t = \sum_{i=1}^{m} a_i(t) C_i.$$ (28)

The fundamental link between the above construction and the original skeleton process is given by the following formula:

$$|X_t - a_1(t)| \leq 1.$$ (29)

This is obtained observing that, since the graph $G$ is $(\gamma, \tau)$-minimal, it holds $N_{v_1, z_1}(C_t) = \delta_{1, 1}$ (and therefore $N_{v_1, z_1}(C_t) = a_1(t)$ by (28)), and that $N_{v_1, z_1}(C_t)$ differs from $X_t$ by at most 1.

Having clarified the content of theorem 3, we refer to appendix B for its proof.

5. Previous results on the asymptotic velocity and large deviations

In this section we review some results of [13, 14]. We point out that a key ingredient in their derivation has been the regenerative structure discussed in section 3. In sections 8 and 9 we will discuss specific random walks for which the LD rate functions entering in theorem 4 below can be computed. On the other hand, theorem 5 below will be very useful in the rest of the paper.

Recall that $X_0 = \mathcal{Z}^{(0)}$ and that (see section 3) $S_1$ denotes the first jump time for the skeleton process $X^*_t$, i.e.

$$S_1 := \inf\{t \geq 0 : X_t \in \{\mathcal{Z}^{(0)}, \mathcal{Z}^{(1)}\}\}.$$ (30)

Recall also that we have assumed that all the waiting times of $X_t$ have finite mean, i.e. $\psi_{s_t}$ has finite mean for all vertices $x$ in $G$. It is then simple to show that $\mathbb{E}(S_1) < \infty$. As derived in [13], since $\mathbb{E}(S_1) < \infty$, almost surely the skeleton process and therefore also the cell process admit an asymptotic velocity:

$$\lim_{t \to \infty} \frac{N_t}{t} = \lim_{t \to \infty} \frac{X^*_t}{t} = \frac{\mathbb{P}(X^*_{S_1} = 1) - \mathbb{P}(X^*_{S_1} = -1)}{\mathbb{E}(S_1)} =: v_{\text{lim}}.$$ (31)
We refer the interested reader to [13] for what concerns the Gaussian fluctuations of $X^*$. In the rest of this section we concentrate on large deviations.

**Theorem 4 ([14]).** Call $T_n$ the first time the skeleton process hits $n \in \mathbb{Z}$, i.e.

$$T_n := \inf\{ t \geq 0 : X^*_t = n \} \in [0, +\infty].$$

Then the following holds:

(i) As $n \to \pm \infty$ the random variables $T_{\pm n}/n$ satisfy a LDP with speed $n$ and convex rate function

$$J_\pm(u) := \sup_{\lambda \in \mathbb{R}} \{ \lambda u - \ln \varphi_\pm(\lambda) \}, \quad u \in \mathbb{R},$$

where

$$\varphi_\pm(\lambda) := \mathbb{E}(e^{\lambda T_\pm(1)(T_{\pm 1} < \infty)}) \in (0, +\infty), \quad \lambda \in \mathbb{R}.$$  

(ii) As $t \to +\infty$, the random variables $X^*_t/t$ and $N_t/t$ satisfy a LDP with speed $t$ and good and convex rate function $I$ given by

$$I(\vartheta) = \begin{cases} \vartheta J_+(1/\vartheta) & \text{if } \vartheta > 0, \\ |\vartheta| J_-(1/|\vartheta|) & \text{if } \vartheta < 0, \end{cases}$$

and $I(0) = \lim_{\vartheta \to 0} I(\vartheta)$.

Roughly, we have

$$\mathbb{P}\left( \frac{T_{\pm n}}{n} \approx u \right) \sim e^{-nJ_\pm(u)}, \quad \mathbb{P}\left( \frac{N_t}{t} \approx \vartheta \right) \sim e^{-tI(\vartheta)}, \quad \mathbb{P}\left( \frac{X^*_t}{t} \approx \vartheta \right) \sim e^{-tI(\vartheta)}$$

for $n, t$ large, respectively.

It is useful for applications to reduce the computation of $\varphi_\pm$ to the one of simpler functions. The following characterization of $\varphi_\pm$ is provided in [14], proposition 4.3. Recall the definition of $S_1$ given in (30), and let $f_\pm : \mathbb{R} \to (0, +\infty]$ be defined by

$$f_\pm(\lambda) := \mathbb{E}(e^{\lambda S_1}(X^*_{S_1} = \pm 1)) \in (0, +\infty].$$

Then the functions $\varphi_\pm(\lambda)$ in (34) satisfy

$$\varphi_\pm(\lambda) = \frac{1 - \sqrt{1 - 4f_-(\lambda)f_+(\lambda)}}{2f_+(\lambda)}$$

for $\lambda \leq \lambda_c$, where $\lambda_c \in [0, +\infty)$ is the unique value of $\lambda$ such that $f_-(\lambda)f_+(\lambda) = 1/4$, while $\varphi_\pm(\lambda) = +\infty$ for $\lambda > \lambda_c$.

In addition to theorem 1 the following characterization of the GC symmetry for the cell process is provided in [14, theorem 4, 8]:

---

The rate function $I$ is good in the sense that $\{ \vartheta : I(\vartheta) \leq a \}$ is compact, for any $a \in \mathbb{R}$.
Theorem 5 ([14]). The following facts are equivalent:

(i) For some \( c \in \mathbb{R} \) the GC symmetry \( I(\vartheta) = I(-\vartheta) - c\vartheta \) holds for all \( \vartheta \in \mathbb{R} \);
(ii) The random variables \( X_{S_i} \) and \( S_1 \) are independent.
(iii) The functions \( \varphi_\lambda(\lambda) \) and \( \varphi_\lambda(\lambda) \) are proportional, i.e. \( \exists C > 0 \) such that \( \varphi_\lambda(\lambda) = C \varphi_\lambda(\lambda) \) for all \( \lambda \leq \lambda_c \).

Moreover, when (i), (ii) hold it must be \( c = \ln \frac{P(X_{S_i} = 1)}{P(X_{S_i} = -1)} = \ln C \).

Remark 5.1. As a byproduct of theorem 5 with theorem 2 (or, equivalently, with (16) in theorem 3) the independence stated in theorem 5-(ii) holds for any \((\psi, \sigma)\)-minimal fundamental graph.

Remark 5.2. Note that, by (37), Item (iii) is equivalent to the proportionality of \( f_\lambda(\lambda) \) and \( f_\lambda(\lambda) \), which is often easier to check. Indeed, for \( \lambda \leq \lambda_c \), \( \varphi_\lambda(\lambda) = C \varphi_\lambda(\lambda) \) if and only if \( f_\lambda(\lambda) = C f_\lambda(\lambda) \).

Remark 5.3. Consider a CTRW \( X \) on \( \mathbb{Z} \) with \( N \)-periodic rates. Since the fundamental graph is given by a finite linear graph and is therefore \((\psi, \sigma)\)-minimal, we know that the GC symmetry of theorem 5-(i) is satisfied (see theorems 2 and 3). As byproduct with theorem 5 we get in particular that the time needed by \( X \) to hit the set \( \{-N, N\} \) does not depend on which site is visited when first arriving in \( \{-N, N\} \). This property was already derived in [8] for CTRWs on \( \mathbb{Z} \) with \( N \)-periodic rates.

6. Example: violation of GC symmetry with a non \((\psi, \sigma)\)-minimal fundamental graph

Considering a Markov CTRW, the violation of the GC symmetry for almost any choice of jump rates in the case of non \((\psi, \sigma)\)-minimal fundamental graphs has a non trivial derivation, based on complex analysis [14]. We discuss here an example, given by a parallel-chains model [22], confirming the thesis.

Let us consider the fundamental graph \( G \) in figure 11 (left), in which to each pair of neighbouring vertices we have assigned a positive rate in \( \{\xi^\pm_\alpha, \xi^\pm_\eta, \eta^\pm_\sigma, \eta^\pm_\eta\} \). The associated quasi-1d lattice is represented in figure 11 (right).

Let \( X_t \) denote the Markov CTRW on \( G \) with periodic jump rates induced by \( G \). Finally, let \( N_t \) and \( X^*_t \) denote the cell process and skeleton process associated to \( X_t \).

By theorem 4, as \( t \to +\infty \), the random variables \( N_t/t \) and \( X^*_t/t \) satisfy a LDP with speed \( t \) and rate function \( I \), defined in (35). Since the fundamental graph \( G \) is not \((\psi, \sigma)\)-minimal, we aim to show that \( I \) satisfies the GC symmetry (3) only for a set of transition rates \( \{\xi^\pm_\alpha, \xi^\pm_\eta, \eta^\pm_\sigma, \eta^\pm_\eta\} \) of zero Lebesgue measure in \([0, \infty)^8\). According to theorem 5, to this end it suffices to show that \( \varphi_\lambda(\lambda) \) and \( \varphi_\lambda(\lambda) \) are not proportional for almost any choice of the jump rates.
The computation of the ratio $\frac{\phi(\lambda)}{\lambda}$ can be reduced to a single cell analysis as follows. Let $J_1$ be the first time that the process $X_t$, starting at $v_0$, reaches $v_1$ after performing at least one jump, and set

$$J_1 := \mathbb{E}(\lambda^{-1} f(X^s_{J_1} = \pm 1)).$$

One can check that $\frac{\phi(\lambda)}{\lambda}$ if and only if $\frac{\tilde{f}_+}{\lambda} = \mathbb{E}(\lambda^{-1} f(X^s_{J_1} = \pm 1))$ (see the beginning of appendix A for more details). The advantage of introducing the auxiliary functions $\tilde{f}_\pm(\lambda)$ is that in the present parallel chain model they are simple to compute.

Let $\tau_1, \tau_2$ denote the first and second jump time of the process $X_t$ respectively, and observe that

$$\{X_{J_1} = 1\} = \{X_\tau = a^{(0)}, X_\tau = a^{(1)}\} \cup \{X_\tau = b^{(0)}, X_\tau = b^{(1)}\},$$

$$\{X_{J_1} = -1\} = \{X_\tau = a^{(-1)}, X_\tau = a^{(-1)}\} \cup \{X_\tau = b^{(-1)}, X_\tau = b^{(-1)}\}.$$

Hence, for $\lambda < \Psi_0, \Psi_a, \Psi_b$, it holds

$$\mathbb{E}(\lambda^{-1} f(X^s_{J_1} = 1)) = \sum_{z = a^{(0)}, b^{(0)}} \mathbb{E}(\lambda^{(\tau + \eta)} f(X_\tau = z, X_\tau = v^{(1)})) = \frac{\xi_0^+ \xi_a^+}{(\Psi_0 - \lambda)(\Psi_a - \lambda)} + \frac{\eta_0^+ \eta_b^+}{(\Psi_0 - \lambda)(\Psi_b - \lambda)},$$

where we have set $\Psi_0 := \xi_0^+ + \xi_a^+ + \eta_0^+ + \eta_a^+, \Psi_a := \xi_a^+ + \xi_b^+, \Psi_b := \eta_a^+ + \eta_b^+$, and used that the waiting times at $v^{(0)}, a^{(0)}, b^{(0)}$ are exponentially distributed with inverse mean $\Psi_0, \Psi_a, \Psi_b$, respectively. If $\lambda$ is non smaller than $\Psi_0, \Psi_a, \Psi_b$, then the expectation $\mathbb{E}(\lambda^{-1} f(X^s_{J_1} = 1))$ diverges.

Repeating the same procedure for $\mathbb{E}(\lambda^{-1} f(X^s_{J_1} = -1))$ we end up with

$$\tilde{f}_\pm(\lambda) = \begin{cases} \frac{\xi_0^+ \xi_a^+}{(\Psi_0 - \lambda)(\Psi_a - \lambda)} + \frac{\eta_0^+ \eta_b^+}{(\Psi_0 - \lambda)(\Psi_b - \lambda)} & \text{if } \lambda < \Psi_0, \Psi_a, \Psi_b, \\ +\infty & \text{otherwise.} \end{cases}$$

We take the quotient to test proportionality. After a short calculation we find for $\lambda < \Psi_0, \Psi_a, \Psi_b$:

$$\frac{\tilde{f}_+(\lambda)}{\tilde{f}_-(\lambda)} = \frac{\xi_0^+ \xi_a^+ \Psi_b + \eta_0^+ \eta_b^+ \Psi_a - \lambda (\xi_0^+ \xi_a^+ + \eta_0^+ \eta_b^+)}{\xi_0^+ \xi_a^+ \Psi_b + \eta_0^+ \eta_b^+ \Psi_a - \lambda (\xi_0^+ \xi_a^+ + \eta_0^+ \eta_b^+)}.$$
This is equal to a constant (independent of \( \lambda \)) if and only if
\[
\det \begin{pmatrix}
\xi_0^+ \xi_a^- + \eta_0^+ \eta_b^- & - (\xi_0^+ \xi_a^- + \eta_0^- \eta_b^+)
\xi_a^- \xi_b^+ + \eta_0^- \eta_b^- & - (\xi_a^- \xi_b^+ + \eta_0^+ \eta_b^-)
\end{pmatrix} = 0
\] (38)
i.e. if and only if \((\Psi_0 - \Psi_0)(\xi_0^+ \xi_a^- \eta_a^- \eta_b^- - \xi_0^- \xi_a^+ \eta_a^+ \eta_b^+) = 0\). Note that the second term vanishes if and only if \(\xi_a^- \xi_b^+ = \eta_0^- \eta_b^+\), and therefore (38) only holds on a set of jump rates of zero Lebesgue measure. We conclude that for almost all choices of the jump rates the functions \(\tilde{f}_+\) and \(\tilde{f}_-\) are not proportional, and therefore the GC symmetry (3) is violated.

7. Example: non \((v, \bar{v})\)-minimal fundamental graph \(G\) where the GC symmetry (3) holds for any discrete time RW

We take the fundamental graph \(G\) exactly as in section 6. Moreover, we take \(\psi_z = \delta_1\), hence the random walk jumps at each integer time. Now take \(\{\xi_a^+, \xi_a^-, \eta_0^+, \eta_0^-\}\) to be jump probabilities: \(\xi_0^+ + \xi_0^- + \eta_0^- = 1\), \(\xi_a^+ + \xi_a^- = 1\) and \(\eta_0^+ + \eta_0^- = 1\). As discussed in the previous section, to prove that the GC symmetry (3) is satisfied for any choice of the jump probabilities, it is enough to show that \(\tilde{f}_+ (\lambda) = C \tilde{f}_- (\lambda)\). In this case (see theorem 5 and remarks 5.2) and (3) is satisfied with \(c = \ln C\). Since trivially
\[
\tilde{f}_+ (\lambda) = e^{2\lambda (\xi_0^+ \xi_a^- + \eta_0^+ \eta_b^-)}, \quad \tilde{f}_- (\lambda) = e^{2\lambda (\xi_a^- \xi_b^+ + \eta_0^- \eta_b^+)},
\]we conclude that (3) is always satisfied with \(c = \ln \frac{\xi_a^+ \xi_b^+ + \eta_0^- \eta_b^+}{\xi_a^- \xi_b^- + \eta_0^+ \eta_b^+}\).

8. Example: homogeneous CTRW on \(\mathbb{Z}\) with exponentially distributed waiting times

In this section we consider the simplest possible \((v, \bar{v})\)-minimal fundamental graph \(G\), given by only two vertices \(v, \bar{v}\), connected by an edge. We assign rate \(p \in (0, 1)\) to the oriented edge \((v, \bar{v})\) and rate \(q = 1 - p\) to the reverse edge \((\bar{v}, v)\), as represented in figure 12.

Let \(X_t\) be a Markov CTRW (with rates \(p, q\)) on the associated quasi-1d lattice \(G\), whose vertex set we identify with \(\mathbb{Z}\). Then \(X_t\) waits at each location an exponentially distributed time of mean 1, and then jumps either to the right or to the left with probability \(p\) and \(q\) respectively. Note that in this case the skeleton process \(X_t^*\) coincides with the random walk \(X_t\).

Our aim here is to implement theorem 4 and derive explicit expressions for the LD rate functions \(J_\pm\) of the hitting times and for the LD rate function \(I\) of the cell process.

As usual we take \(X_0 = 0\). Then, as it is well known and can be also recovered from the formulas in [13], the asymptotic velocity and diffusion coefficients of \(X_t\) are respectively given by \(v_{\text{lim}} = p - q\) and \(\sigma^2 = 1\). Moreover, by theorem 4, as \(t \to \infty\) the process
$X_t / t$ satisfies a LDP with speed $t$ and good and convex rate function $I$. In this section we show how $I$ can be computed using our approach.

Recall that $S_1$ denotes the first jump time for the skeleton process, which in this case coincides with the first jump time of $X_t$. Then the functions $f_\pm$ defined in (36) are given by

$$f_+(\lambda) = \mathbb{E}(e^{\lambda S_1} \mathbb{1}(X_{S_1} = 1)) = \begin{cases} \frac{p}{1 - \lambda}, & \lambda < 1 \\ +\infty, & \text{otherwise.} \end{cases}$$

$$f_-(\lambda) = \mathbb{E}(e^{\lambda S_1} \mathbb{1}(X_{S_1} = -1)) = \begin{cases} \frac{q}{1 - \lambda}, & \lambda < 1 \\ +\infty, & \text{otherwise.} \end{cases}$$

Hence, $f_+(\lambda)f_-(\lambda) = 1/4 \iff \lambda = 1 - 2\sqrt{pq} =: \lambda_c$. Moreover, by (37), for $\lambda \leq \lambda_c$ we have

$$\varphi_+(\lambda) = \frac{1 - \lambda - \sqrt{(1 - \lambda)^2 - 4pq}}{2q}, \quad \varphi_-(\lambda) = \frac{1 - \lambda - \sqrt{(1 - \lambda)^2 - 4pq}}{2p} = \frac{q}{p} \varphi_+(\lambda),$$

otherwise $\varphi_\pm(\lambda) = \infty$. It follows that $\ln \varphi_+(\lambda) = \ln \varphi_-(\lambda) - (\ln q/p)$ which, together with (33), gives $J_+(\vartheta) = J_-(\vartheta) + (\ln q/p)$ for all $\vartheta \in \mathbb{R}$. This implies that the rate function $I(\vartheta)$ satisfies the GC symmetry $I(\vartheta) = I(-\vartheta) = c\vartheta$, the constant $c$ being indeed $\ln q/p$ (which we already knew from theorem 1).

In order to compute $I$, we note that

$$\frac{d}{d\lambda} \ln \varphi_\pm(\lambda) = \vartheta \text{ for } \vartheta > 0,$$

we find $\hat{X}_\pm(\vartheta) = 1 - \frac{1}{\vartheta} \sqrt{1 + 4pq\vartheta^2}$ for $\vartheta > 0$, $J_+^\vartheta(\vartheta) = +\infty$ otherwise. This also gives us an explicit expression for $J_+(\vartheta) = J_+(\vartheta) - (\ln q/p)$. Note that $\lim_{\vartheta \to 0} J_+(\vartheta) = +\infty$ and $J_+$ has a critical point (i.e. with vanishing derivative) at $\vartheta = \frac{1}{\sqrt{1 - 4pq}}$ which is infinite if and only if $p = q = 1/2$. When finite, $\frac{1}{\sqrt{1 - 4pq}}$ is a point of minimum for $J_+$. Recalling the definition of the rate function $I$ given in (35), then, we conclude that $I$ is finite for all $\vartheta \in \mathbb{R}$ and

$$I(\vartheta) = 1 - \sqrt{\vartheta^2 + 4pq} - \vartheta \ln(\sqrt{\vartheta^2 + 4pq} - \vartheta) + \vartheta \ln(2q).$$
Finally, we point out that, since

$$-\vartheta \ln(\sqrt{\vartheta^2 + 4pq} - \vartheta) + \vartheta \ln(2q) = \vartheta \ln(\sqrt{\vartheta^2 + 4pq} + \vartheta) - \vartheta \ln 2p,$$

formula (39) matches equation (10.6) in [6].

Some plots of the above rate functions are given in figure 13.

9. Example: homogeneous CTRW on $\mathbb{Z}$ with Gamma-distributed waiting times

In this section we again consider the very simple fundamental graph $G$ in figure 12, together with the associated quasi-1d lattice $\mathcal{G}$. This time, on the other hand, we assume that the CTRW $X_t$ on $\mathcal{G}$ waits at each location $x \in \mathbb{Z}$ a Gamma-distributed random time (non exponential) and then jumps to either $x+1$ or $x-1$ with probability $p$ and $q = 1 - p$ respectively.

Note that again $X_t$ coincides with the associated skeleton process $X^s_t$. Moreover, since the waiting times are not exponentially distributed, the process is not Markovian. Our aim here it to implement theorem 4 and derive explicit expressions for the LD rate.
functions $J_{\pm}$ of the hitting times and for the LD rate function $I$ of the cell process. This can indeed be achieved when the waiting times have distribution Gamma($2, \gamma$) for some $\gamma > 0$.

Assume $X_0 = 0$ as usual, and note that $S_1$ introduced in (30) equals the first jump time of the process $X_t$. We first assume that $S_1 \sim \text{Gamma}(\nu, \gamma)$ for some parameters $\nu, \gamma > 0$, which means that the probability density function of $S_1$ is of the form $f(t) \propto t^{\nu-1}e^{-\gamma t}$ for $t > 0$. Moreover, it holds $\mathbb{E}(e^{\lambda S_1}) = \left(1 - \frac{\lambda}{\gamma}\right)^{-\nu}$ for $\lambda < \gamma$, $\mathbb{E}(e^{\lambda S_1}) = \infty$ otherwise. Note that if $\nu = 1$ we are back to exponential holding times of parameter $\gamma$.

Recall that, according to (35) in theorem 4, $I(\vartheta)$ for $\vartheta > 0$ can be deduced from the hitting times rate function $J_{\pm}$, defined in (33) as

$$J_{\pm}(u) := \sup_{\lambda \in \mathbb{R}} \{\lambda u - \ln \varphi_\pm(\lambda)\}. \quad (40)$$

The other branch of $I$ is then easily obtained by mean of the GC symmetry (see theorem 2 or (16) in theorem 3).

In order to compute $J_{\pm}$ we observe that, using the independence of $S_1$ and $X_{S_1}$ (which is a byproduct of e.g. theorems 2 with 5), for $\lambda < \gamma$ we have

$$f_{\pm}(\lambda) = \mathbb{E}(e^{\lambda S_1})\mathbb{P}(X_{S_1} = 1) = p \left(1 - \frac{\lambda}{\gamma}\right)^{-\nu},$$

$$f_{\pm}(\lambda) = \mathbb{E}(e^{\lambda S_1})\mathbb{P}(X_{S_1} = -1) = q \left(1 - \frac{\lambda}{\gamma}\right)^{-\nu}.$$

Solving $f_{\pm}(\lambda)f_{\pm}(\lambda) = 1/4$, then, we find $\lambda_c = \gamma(1 - (4pq)^{1/2\nu})$ and, by (37),

$$\varphi_\pm(\lambda) = \frac{1 - \sqrt{1 - 4f_{\pm}(\lambda)f_{\pm}(\lambda)}}{2f_{\pm}(\lambda)} = \frac{\left(1 - \frac{\lambda}{\gamma}\right)^{-\nu} - \sqrt{\left(1 - \frac{\lambda}{\gamma}\right)^{2\nu} - 4pq}}{2q}$$

for $\lambda \leq \lambda_c$, $\varphi_\pm(\lambda) = \infty$ otherwise.

Let us now compute the supremum in (40). According to (35) we are only interested in $J_{\pm}(u)$ for $u > 0$, that we assume throughout. Observe that the supremum can be restricted to $\lambda \leq \lambda_c$, since $\ln \varphi_\pm = \infty$ otherwise. Moreover, for $\lambda < \lambda_c$ we can differentiate the argument, to find that the supremum is attained at $\lambda(u)$ solution of $\varphi'_\pm(\lambda) = u\varphi_\pm(\lambda)$. Since

$$\varphi'_\pm(\lambda) = \frac{1}{2q} \left(-\frac{\nu}{\gamma}(1 - \frac{\lambda}{\gamma})^{\nu-1} \left[1 - \frac{\left(1 - \frac{\lambda}{\gamma}\right)^{\nu}}{\sqrt{\left(1 - \frac{\lambda}{\gamma}\right)^{2\nu} - 4pq}}\right]\right),$$

the equation $\varphi'_\pm(\lambda) = u\varphi_\pm(\lambda)$ reads

$$u\sqrt{\left(1 - \frac{\lambda}{\gamma}\right)^{2\nu} - 4pq} = \nu \left(1 - \frac{\lambda}{\gamma}\right)^{\nu-1}.$$
This can be explicitly solved for \( \nu = 2 \), to get

\[
\lambda(u) = \gamma \left[ 1 - \frac{1}{u} \sqrt{\frac{2}{\gamma^2} + \frac{4}{\gamma^4} + 4puq^4} \right].
\]  

(41)

From now on we assume \( \nu = 2 \). Plugging (41) back into (40), we find

\[
J_+(u) = u\lambda(u) - \ln \varphi_+(\lambda(u)) = \gamma u \left[ 1 - \frac{1}{u} \sqrt{\frac{2}{\gamma^2} + \frac{4}{\gamma^4} + 4puq^4} \right] \]

\[
-\ln \left[ \frac{1}{u} \left( \frac{2}{\gamma^2} + \sqrt{\frac{4}{\gamma^4} + 4puq^4} \right) \right] - \frac{2}{\gamma u^2} \left[ \frac{2}{\gamma^2} + \sqrt{\frac{4}{\gamma^4} + 4puq^4} \right] + \ln(2q).
\]

Using now that \( I(u) = uJ_+(1/u) \) for \( u > 0 \) by (35), we conclude that

\[
I(u) = \gamma \left[ 1 - u \sqrt{\frac{2}{\gamma^2} + \frac{4}{\gamma^4} + \frac{4pq}{u^4}} \right] - u\ln \left[ u^2 \left( \frac{2}{\gamma^2} + \sqrt{\frac{4}{\gamma^4} + \frac{4pq}{u^4}} \right) \right] - \frac{2u^2}{\gamma} \sqrt{\frac{2}{\gamma^2} + \sqrt{\frac{4}{\gamma^4} + \frac{4pq}{u^4}}} + u\ln(2q)
\]

for \( u > 0 \). Using the GC symmetry (16), which reads

\[
I(-u) = I(u) - u\ln(q/p),
\]

we also obtain \( I(u) \) for \( u < 0 \). Finally, \( I(0) = \lambda_c = \gamma(1 - \sqrt[4]{4pq}) \).

A plot of the above rate function is given in figure 14.
Acknowledgments

V Silvestri thanks the Department of Mathematics in University ‘La Sapienza’ for the hospitality and support. She also acknowledges the support of the UK Engineering and Physical Sciences Research Council (EPSRC) grant EP/H023348/1 for the University of Cambridge Centre for Doctoral Training, the Cambridge Centre for Analysis.

Appendix A. Derivation of criterion 1 implying theorem 2

Recall that $X_0 = y^{(0)}$. We define $J_1$ as the first time that, after at least one jump, the random walk visits again a state of the form $v^{(k)}$, i.e.

$$J_1 := \inf \{ t > 0 : X_t \in \{ y^{(1)}, y^{(0)} v^{(1)} \} \}$$

Moreover, we set

$$\tilde{f}_\pm (\lambda) := \mathbb{E}(e^{\lambda t} \mathbb{I}(X_t \in \{ y^{(\pm)} \})), \quad f_0 (\lambda) := \mathbb{E}(e^{\lambda t} \mathbb{I}(X_t \in y^{(0)})).$$

Due to [13, lemma 9.1] the following holds (recall (36)): if $\tilde{f}_0 (\lambda) < 1$, then

$$f_+ (\lambda) = \frac{\tilde{f}_+ (\lambda)}{1 - \tilde{f}_0 (\lambda)}, \quad f_- (\lambda) = \frac{\tilde{f}_- (\lambda)}{1 - \tilde{f}_0 (\lambda)}.$$  \hspace{1cm} (A.1)

Moreover, if $\tilde{f}_0 (\lambda) \geq 1$, then $f_+ (\lambda) = f_- (\lambda) = +\infty$.

As a byproduct with theorem 5 and remark 5.2 we conclude that the GC symmetry (4) is satisfied for some constant $\Delta$ if and only if $f_+ (\lambda) = e^{\Delta f_- (\lambda)}$ for all $\lambda \leq \lambda_c$, and therefore if and only if $\tilde{f}_+ (\lambda) = e^{\Delta \tilde{f}_- (\lambda)}$ for all $\lambda \leq \lambda_c$.

Given an integer $m \geq 1$, let $\mathcal{A}_m$ be the family of strings $(x_0, x_1, \ldots, x_m)$ such that $x_0 = y, x_m = \bar{y}, (x_i, x_{i+1})$ is an edge of the fundamental graph $G$ for all $0 \leq i < m$ and $x_i \in V \setminus \{ y, \bar{y} \}$ for all $0 < i < m$. We call $\mathcal{A}_m^*$ the family of sequences satisfying the same properties as above when exchanging the role of $y$ and $\bar{y}$.

Recall that $\psi_x$ is the law of the waiting time at $x$. We set

$$\phi_x (\lambda) := \int e^{\lambda t} \psi_x (dt)$$

for its Laplace transform. Then we can write

$$\tilde{f}_\pm (\lambda) = \sum_{m=1}^{\infty} \sum_{(x_0, x_1, \ldots, x_m) \in \mathcal{A}_m} \prod_{i=0}^{m-1} p(x_i, x_{i+1}) \prod_{i=0}^{m-1} \phi_{x_i} (\lambda).$$  \hspace{1cm} (A.2)

A similar expression holds for $\tilde{f}_- (\lambda)$, with $\mathcal{A}_m$ replaced by $\mathcal{A}_m^*$.

Given $\gamma = (x_0, x_1, \ldots, x_m)$ we set

$$R_\gamma := \prod_{i=0}^{m-1} p(x_i, x_{i+1}), \quad S_\gamma (\lambda) = \prod_{i=1}^{m-1} \phi_{x_i} (\lambda).$$

Note that the product in $S_\gamma (\lambda)$ starts from $i = 1$, hence all sites $x_i$ appearing in the product belong to $V \setminus \{ y, \bar{y} \}$. By mean of this notation we can write
Due to the previous observations, the GC symmetry (4) is satisfied for some constant $\Delta$ if and only

$$\sum_{m=1}^{\infty} \sum_{\gamma \in A_m} R_\gamma S_\gamma(\lambda) = e^\Delta \sum_{m=1}^{\infty} \sum_{\gamma \in A_m^*} R_\gamma S_\gamma(\lambda), \quad \lambda Y \leq \lambda_c. \quad (A.4)$$

Given $\gamma = (x_0, x_1, \ldots, x_m) \in A_m$ we write $\tilde{\gamma}$ for the loop-erased version of $\gamma$ (see figure A1 taken from [13]). We recall that $\tilde{\gamma}$ is obtained by erasing all the loops of $\gamma$ in chronological order. More precisely, consider the following algorithm. Set $i_0 := 0$ and, once defined $i_0, i_1, \ldots, i_k$, set $r := k$ if $i_k = m$, otherwise (if $i_k < m$) set

$$i_{k+1} := \max\{ j : i_k \leq j < m \text{ and } x_j = x_u \} + 1$$

(recall that $\gamma \in A_m$ visits $\sigma$ only as last point $x_m = \sigma$). Then the loop-erased version of $\gamma$ is given by $\tilde{\gamma} = (x_{i_0}, x_{i_1}, \ldots, x_{i_k})$. Since $\gamma \in A_m$ it must be $\tilde{\gamma} \in A_r$. Note that

$$R_\gamma = R_\gamma R_\gamma^{\text{loop}}, \quad R_\gamma^{\text{loop}} := \prod_{k=0}^{r-1} \prod_{i=k}^{i_{k+1}-2} p(x_i, x_{i+1}), \quad (A.5)$$

with the convention that $\prod_{i=k}^{i_{k+1}-2} p(x_i, x_{i+1}) = 1$ if $i_{k+1} = i_k + 1$ ($R_\gamma^{\text{loop}}$ is the contribution to $R_\gamma$ given by factors associated to the edges inside the loops, see figure A1).

We write $\gamma^{\dagger}$ for the path in $A_m^*$, going from $\sigma$ to $\gamma$ and obtained from $\gamma$ by reversing the order out of the loops and keeping the same order in the loops (see figure A1). More precisely, with the notation introduced above, it holds

$$\gamma^{\dagger} = (x_{i_0}, \ast \ast \ast, x_{i_{k-2}}, \ast \ast \ast, x_{i_1}, \ast \ast \ast, x_{i_0}).$$

where the pieces marked by $\ast \ast \ast$ are determined as follows. Take $k : 1 \leq k \leq r$. If $i_k = i_{k-1} + 1$, then the piece $'x_{i_k}, \ast \ast \ast, x_{i_{k-1}}'$ is indeed simply $'x_{i_k}, x_{i_{k-1}}'$. If $i_k > i_{k-1} + 1$, then the piece $'x_{i_k}, \ast \ast \ast, x_{i_{k-1}}'$ is given by $'x_{i_k}, x_{i_{k-1}} = x_{i_{k-1}} x_{i_{k-1}+1}, x_{i_{k-1}+2}, \ldots, x_{i_{k-1}} = x_{i_{k-1}}'$.

We note that the transformation $\gamma \mapsto \gamma^{\dagger}$ is an involutive bijection from $A_m$ to $A_m^*$ and that

$$\overline{(\gamma)}^{\dagger} = (\overline{\gamma})^{\dagger}, \quad R_\gamma^{\text{loop}} = R_\gamma^{\text{loop}}, \quad S_\gamma(\lambda) = S_\gamma(\lambda). \quad (A.6)$$
The above identities, together with (A.4) and (A.5), imply the following criterion:

**Criterion 1.** The GC symmetry (4) is satisfied for some constant $\Delta$ if and only if

$$\sum_{m=1}^{\infty} \sum_{\gamma \in \mathcal{A}_m} R^{\text{loop}}_\gamma (R_{\gamma} - e^{\Delta} R_{\gamma'}) S_{\gamma}(\lambda) = 0$$

(A.7)

for $\lambda \leq \lambda_c$. In particular, (4) is satisfied for some constant $\Delta$ if it holds $R_\gamma = e^{\Delta} R_{\gamma'}$ for any loop-free path $\gamma$ from $\nu$ to $\nu'$.

The above criterion is similar to criterion 1 in [14, section 9] and the derivation of criterion 1 is indeed inspired by [14, section 9].

If $G$ is $(\nu, \nu')$-minimal, then trivially the above criterion implies that (4) is satisfied with $\Delta$ given by (7).

**Appendix B. Derivation of theorem 3**

Recall that $\tilde{G}$ denotes the projected graph $\pi(G)$ as in figure 10, and $Y_t = \pi(X_t)$ is the projection of $X_t$ onto $\tilde{G}$.

The first part of the theorem up to (13) is known (see [11, section 8] and the theorem on [4, page 7]). Equation (15) is a byproduct of (13) and (14). Finally, since $I(\theta) = \inf_{\theta_2, \ldots, \theta_m} I(\theta, \theta_2, \ldots, \theta_m)$ by the contraction principle, the symmetry (16) follows trivially from (15).

It therefore remains to prove (14). To this aim recall that $(z_0, z_1, \ldots, z_n)$ denotes the unique self-avoiding path from $z_0 = \nu$ to $z_n = \nu'$ in $G$. A path $(x_{\lambda}, \lambda \in [0, l])$ on $\tilde{G}$, starting at $v$, makes excursions outside the set $\{v, z_1, \ldots, z_{n-1}\}$. Since $G$ is $(\nu, \nu')$-minimal, the graph $\tilde{G}$ is given by the cycle $C_1$ to which subgraphs $G_1, G_2, \ldots, G_l$ are attached in such a way that $C_1$ and $G_i$ share a unique vertex (see figure 4). We consider the transformed path $\Gamma((x_{\lambda}, \lambda \in [0, l]))$ where each excursion is replaced by a time inversion as follows. Suppose that at time $s_0$ the path $(x_{\lambda}, \lambda \in [0, l])$ enters some subgraph $G_i$ and it exits at some time $t_0 > s_0$. Then we replace the excursion $(x_{\lambda}, s_0 \leq \lambda \leq t_0)$ with the excursion $(x_{\lambda}, s_0 \leq \lambda \leq t_0)$, apart from some modifications at the jump times in order to have a càdlàg path at the end. To give a precise definition, call $v$ the unique vertex in common between $G_i$ and $\tilde{G}$. Then $x_{s_0} = x_{t_0} = v$. Let us suppose that during the excursion the path visits (in chronological order) the vertices $y_0, y_1, \ldots, y_{r-1}, y_r$ where $y_0 = y_r = v$, and that it remains at site $y_m$ a time $\tau_m$ for any $m = 0, 1, \ldots, r$. Note that it must be $t_0 = s_0 + \tau_0 + \tau_1 + \cdots + \tau_r$. Then we replace the excursion $(x_{\lambda}, s_0 \leq \lambda \leq t_0)$ by the path that visits (in chronological order) the vertices $y_0, y_1, \ldots, y_{r-1}, y_0$ with consecutive waiting times given by $\tau_r, \tau_{r-1}, \ldots, \tau_1, \tau_0$ (i.e. at time $s_0$ the new path is at $v = y_r$, where it remains for a time $\tau_r$, then the new path jumps to $y_{r-1}$ where it remains for a time $\tau_{r-1}$ and so on until jumping to $y_0 = v$ where it remains for a time $\tau_0$ and finally leaves the subgraph $G_i$ at time $s_0 + \tau_r + \tau_{r-1} + \cdots + \tau_1 + \tau_0 = t_0$.

Since $\Gamma$ is an involution, it is simple to compute the Radon–Nykodim derivative $dP/dQ$. We claim that

https://doi.org/10.1088/1742-5468/aa6731
Fluctuation theorems for discrete kinetic models of molecular motors

\[ \frac{dP}{dQ}(\{x_s\}_{s=0}^{t}, t) = \frac{dP(\{x_s\}_{s=0}^{t}, t)}{dP(\Gamma(\{x_s\}_{s=0}^{t}, t))} = e^{\sum_{i=2}^{m} a_i(t) A(C_i) + O(1)} \]  \quad (B.1)

where \( a(t) \) refers to the cycle \( C_t \) associated to the path \( \{x_s\}_{s=0}^{t} \).

To check the above formula suppose for simplicity that \( x_0 = x_1 = \ast \) (hence \( \{x_s\}_{s=0}^{t} \) visits (in chronological order) the sites \( w_0, w_1, \ldots, w_k \) with holding times (up to time \( t \)) given by \( \tau_0, \tau_1, \ldots, \tau_k \) we have

\[ dP(\{x_s\}_{s=0}^{t}, t) = A(\{x_s\}_{s=0}^{t}, t) B(\{x_s\}_{s=0}^{t}, t) \]

where

\[ A(\{x_s\}_{s=0}^{t}, t) = k-1 \prod_{i=0}^{k-1} p(w_i, w_{i+1}), \quad B(\{x_s\}_{s=0}^{t}, t) = \left[ \prod_{i=0}^{k-1} \psi(w_i) \right] \psi(w_k) (\tau_k, \infty). \]

Note that \( B(\{x_s\}_{s=0}^{t}, t) = B(\Gamma(\{x_s\}_{s=0}^{t}, t)) \). On the other hand, we have

\[ \frac{A(\{x_s\}_{s=0}^{t}, t)}{A(\Gamma(\{x_s\}_{s=0}^{t}, t))} = \prod_{i: 0 \leq i < k} \frac{p(w_i, w_{i+1})}{p(w_{i+1}, w_i)}. \]

where the product in the r.h.s. is among the edges \( (w_i, w_{i+1}) \) which are not edges of \( C_t \), neither when reversing orientation. To conclude, it remains to check that

\[ \sum_{i: 0 \leq i < k} \ln \frac{p(w_i, w_{i+1})}{p(w_{i+1}, w_i)} = \sum_{i=2}^{m} a_i(t) A(C_i). \]  \quad (B.2)

To this aim, for each unoriented edge not in \( C_t \), fix a canonical orientation and call \( E \) the family of such canonically oriented edges. Then we have

\[ \sum_{i: 0 \leq i < k} \ln \frac{p(w_i, w_{i+1})}{p(w_{i+1}, w_i)} = \sum_{(x, y) \in E} N_{x,y}(C_i) \ln \frac{p(x, y)}{p(y, x)}. \]

On the other hand, since \( C_t = \sum_{i=1}^{m} a_i(t) C_i \) and since \( N_{x,y}(C_i) = 0 \) for any \( (x, y) \in E \), we have

\[ \sum_{(x, y) \in E} N_{x,y}(C_i) \ln \frac{p(x, y)}{p(y, x)} = \sum_{i=2}^{m} a_i(t) \sum_{(x, y) \in E} N_{x,y}(C_i) \ln \frac{p(x, y)}{p(y, x)}. \]

To get (B.2) it is enough to observe that \( \sum_{(x, y) \in E} N_{x,y}(C_t) \ln \frac{p(x, y)}{p(y, x)} = A(C_t) \). This concludes the proof of our claim (B.1).

Calling \( \hat{a}_i(t) \) the generalised time-integrated currents associated to the path \( \Gamma(Y_s)_{s=0}^{t} \) and the same cycle basis \( C_1, C_2, \ldots, C_m \) (use the same definition of \( a(t) \) referred now to the transformed path), it holds \( a_1(t) = \hat{a}_1(t), \ a_i(t) = -\hat{a}_i(t) \) for all \( i = 2, 3, \ldots, m \). Combining these identities with (B.1) we get

https://doi.org/10.1088/1742-5468/aa6731
Fluctuation theorems for discrete kinetic models of molecular motors

\[ e^{-tI(\vartheta_1, \vartheta_2, \ldots, \vartheta_n)} \approx P\left( \frac{a_1(t)}{t} \sim \vartheta_1, \frac{a_2(t)}{t} \sim \vartheta_2, \ldots, \frac{a_m(t)}{t} \sim \vartheta_m \right) \]
\[ \approx Q\left( \frac{a_1(t)}{t} \sim \vartheta_1, \frac{a_2(t)}{t} \sim \vartheta_2, \ldots, \frac{a_m(t)}{t} \sim \vartheta_m \right) e^{\sum_{i=2}^{m} \vartheta_i A(C_i) + O(1)} \]
\[ = P\left( \frac{a_1(t)}{t} \sim \vartheta_1, \frac{a_2(t)}{t} \sim -\vartheta_2, \ldots, \frac{a_m(t)}{t} \sim -\vartheta_m \right) e^{\sum_{i=2}^{m} \vartheta_i A(C_i) + O(1)} \]
\[ = e^{-tI(\vartheta_1, -\vartheta_2, \ldots, -\vartheta_n) + t\sum_{i=2}^{m} \vartheta_i A(C_i) + O(1)} \]

From the above approximations, we trivially derive (14), thus concluding the proof of theorem 3.

Appendix C. Proof of proposition 2.2

Due to the discussion just after proposition 2.2, it is enough to exhibit an invertible matrix \( U \) satisfying (26). If \( N = 2 \) it is enough to take \( U = \begin{pmatrix} 1 & 0 \\ 0 & \xi_1 \end{pmatrix} \) and one can check (26) by direct computations.

Remark C.1. In the case \( N = 2 \) one can write explicitly the maximal eigenvalue \( \Lambda(\lambda) \) and check directly (25). Indeed, it holds

\[ \Lambda(\lambda) = -\frac{r(0) + r(1)}{2} + \frac{1}{2} \sqrt{[r(0) - r(1)]^2 + 4(\xi_1^+ + \xi_1^-)(\xi_0^+ + \xi_0^- e^{-\lambda})}. \]

Recalling the definition of the matrix \( A \) in (21) and that \( \Delta = \ln \frac{\xi_0^+ \xi_1^+ \cdots \xi_{N-1}^+}{\xi_0^- \xi_1^- \cdots \xi_{N-1}^-} \) we get

\[ A(-\Delta - \lambda)_{i,j} = \begin{cases} 
- r(i) & \text{if } i = j, \\
\xi_j^+ & \text{if } 0 < i \leq N - 1, \ j = i - 1, \\
\xi_j^- & \text{if } 0 \leq i < N - 1, \ j = i + 1, \\
\frac{\xi_0^+ \xi_1^+ \cdots \xi_{N-1}^+ e^\lambda}{\xi_1^+ \xi_2^+ \cdots \xi_{N-1}^-} & \text{if } i = N - 1, j = 0, \\
\frac{\xi_0^- \xi_1^- \cdots \xi_{N-1}^-}{\xi_0^+ \xi_1^+ \cdots \xi_{N-2}^+} e^{-\lambda} & \text{if } i = 0, j = N - 1, \\
0 & \text{otherwise.}
\end{cases} \]
Hence,

\[
\mathcal{A}^T(-\Delta - \lambda)_{i,j} = \begin{cases} 
-r(i) & \text{if } i = j, \\
\xi_{j-1}^+ & \text{if } 0 < j \leq N - 1, \ j = i + 1, \\
\xi_{j+1}^+ & \text{if } 0 \leq j < N - 1, \ j = i - 1, \\
\frac{\xi_0^+ \xi_1^+ \cdots \xi_{j-1}^+ e^{\lambda}}{\xi_0^+ \xi_1^+ \cdots \xi_{N-1}^+} & \text{if } j = N - 1, \ i = 0, \\
\frac{\xi_0^+ \xi_1^+ \cdots \xi_{j-1}^- e^{-\lambda}}{\xi_0^+ \xi_1^+ \cdots \xi_{N-2}^+} & \text{if } j = 0, \ i = N - 1, \\
0 & \text{otherwise.}
\end{cases}
\]

For example, for \( N = 3 \) we have

\[
\mathcal{A}(-\Delta - \lambda) = \begin{pmatrix} 
-r(0) & \xi_1^- & \xi_2^- e^{-(\Delta + \lambda)} \\
\xi_0^+ & -r(1) & \xi_2^- \\
\xi_0 e^{\Delta + \lambda} & \xi_1^+ & -r(2)
\end{pmatrix}, \quad \mathcal{A}^T(-\Delta - \lambda) = \begin{pmatrix} 
-r(0) & \xi_0^+ & \xi_0 e^{\Delta + \lambda} \\
\xi_1^- & -r(1) & \xi_1^+ \\
\xi_2^- e^{-(\Delta + \lambda)} & \xi_2^- & -r(2)
\end{pmatrix}.
\]

Take the diagonal matrix \( U = (U_{i,j})_{0 \leq i,j \leq N-1} \) such that \( U_{i,j} = \delta_{i,j} c(i) \) and \( c(0) = 1, \ c(i) = \frac{\xi_0^+ \xi_1^+ \cdots \xi_{i-1}^+}{\xi_0^+ \xi_1^+ \cdots \xi_{i}^+} \) for \( 1 \leq i \leq N - 1 \). Then trivially \( U^{-1}_{i,j} = \delta_{i,j} c(i)^{-1} \) and \( [U^{-1} \mathcal{A}(\lambda) U]_{i,j} = \mathcal{A}(\lambda)_{i,j} c(j)/c(i) \).

Let us check that the identity \( U^{-1} \mathcal{A}(\lambda) U = \mathcal{A}^T(-\Delta - \lambda) \) holds for each entry. We have that \( [U^{-1} \mathcal{A}(\lambda) U]_{i,j} = 0 \) if we are not in the case \( j = i - 1, \ i, \ i + 1 \) (with the convention that \( 0 - 1 = N - 1 \) and \( (N - 1) + 1 = 0 \)). Note that the same holds for \( \mathcal{A}^T(-\Delta - \lambda) \). Moreover, we have \( [U^{-1} \mathcal{A}(\lambda) U]_{i,i} = \mathcal{A}(\lambda)_{i,i} = -r(i) = \mathcal{A}^T(-\Delta - \lambda)_{i,i} \). Take now \( 0 < i, j \leq N - 1 \). Then

\[
[U^{-1} \mathcal{A}(\lambda) U]_{i,j-1} = \mathcal{A}(\lambda)_{i,j-1} \frac{c(i-1)}{c(i)} = \mathcal{A}(\lambda)_{i,j-1} \frac{\xi_i^-}{\xi_{i-1}^+} = \xi_{i-1}^+ \frac{\xi_i^-}{\xi_{i-1}^+} = \xi_i^- = \mathcal{A}^T(-\Delta - \lambda)_{i,i-1},
\]

\[
[U^{-1} \mathcal{A}(\lambda) U]_{j-1,j} = \mathcal{A}(\lambda)_{j-1,j} \frac{c(j)}{c(j-1)} = \mathcal{A}(\lambda)_{j-1,j} \frac{\xi_{j-1}^-}{\xi_j^+} = \xi_j^+ \frac{\xi_{j-1}^-}{\xi_j^+} = \xi_{j-1}^- = \mathcal{A}^T(-\Delta - \lambda)_{j-1,j}.
\]

Finally,

\[
[U^{-1} \mathcal{A}(\lambda) U]_{N-1,0} = \mathcal{A}(\lambda)_{N-1,0} \frac{c(0)}{c(N-1)} = \xi_{N-1}^- \frac{\xi_0^+ \xi_1^+ \cdots \xi_{N-1}^-}{\xi_0^+ \xi_1^+ \cdots \xi_{N-2}^+} = \mathcal{A}^T(-\Delta - \lambda)_{N-1,0},
\]

\[
[U^{-1} \mathcal{A}(\lambda) U]_{0,N-1} = \mathcal{A}(\lambda)_{0,N-1} \frac{c(N-1)}{c(0)} = \xi_{N-1}^+ \xi_1^+ \cdots \xi_{N-2}^+ e^{\lambda} \frac{\xi_0^+ \xi_1^+ \cdots \xi_{N-1}^+}{\xi_0^+ \xi_1^+ \cdots \xi_{N-2}^+} = \mathcal{A}^T(-\Delta - \lambda)_{0,N-1},
\]

thus concluding the proof of proposition 2.2.
Appendix D. Technical comments

In this appendix we explain how to deal with small fundamental cells in the proof of theorem 3. Let $G = (V, E)$ be a $(\nu, \sigma)$-minimal graph, and let $(z_0, ..., z_n)$ be the unique self-avoiding path from $\nu$ to $\sigma$ in $G$. In this section we explain how to deal with the cases $n = 1, 2$ in the proof of theorem 3, and in particular in the construction of the graph $\hat{G}$ introduced in section 4. We treat the case $n = 1$ in detail, $n = 2$ being analogous (note that in the case $n = 2$ the problem with $\hat{G}$ would be related with the presence of multiple edges between $\nu$ and $\sigma$).

When $n = 1$, the linear path $(z_0, ..., z_n)$ reduces to the single edge $(\nu, \sigma)$, and the definition of the graph $\hat{G}$ is not well posed. It is therefore useful to enlarge the fundamental cell as follows: let $\hat{G}$ be the finite graph obtained by gluing 3 copies of $G$ so that the vertex $\sigma$ of the first (respectively second) copy is identified with the vertex $\nu$ of the second (respectively third) one. Call $\hat{\nu}$ (resp. $\hat{\sigma}$) the vertex $\nu$ (resp. $\sigma$) of the first (resp. third) copy, as represented in figure D1. It is easy to see that if $G$ is $(\nu, \sigma)$-minimal, then $\hat{G}$ is $(\hat{\nu}, \hat{\sigma})$-minimal. It follows that we can regard $\hat{G}$ as a new fundamental cell, that we use to build a quasi-1d graph $\hat{\hat{G}}$.

Let $X_t, \hat{X}_t$ denote the skeleton processes associated to the CTRW $X_t$ considered as a process on $G, \hat{G}$ respectively. Then we have

$$|2X_t^* - \hat{X}_t| \leq 2$$

for all $t \geq 0$, from which we deduce that the processes $2X_t^*$ and $\hat{X}_t^*$ have the same asymptotic properties. In particular, if $\hat{X}_t^*/t$ satisfied a LDP with rate function $I(\vartheta)$, then

$$\mathbb{P}\left(\frac{X_t^*}{t} \approx \vartheta\right) \approx \mathbb{P}\left(\frac{\hat{X}_t^*}{t} \approx 2\vartheta\right) \approx e^{-tI(2\vartheta)},$$

i.e. $X_t^*/t$ satisfies itself a LDP with rate function $I(2\vartheta)$. The study of the large fluctuations and GC symmetry of the process $X_t^*$ can therefore be reduced to the one of the process $\hat{X}_t^*$, with the advantage that the latter is associated to a larger fundamental graph $\hat{G}$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figureD1.png}
\caption{Examples of small fundamental cells $G$ and associated graph $\hat{G}$. For $n = 1$ (up), $\hat{G}$ is obtained by gluing 3 copies of $G$. For $n = 2$ (down), it suffices to glue 2 copies of $G$.}
\end{figure}

https://doi.org/10.1088/1742-5468/aa6731
References

[1] Andrieux D and Gaspard P 2006 Fluctuation theorems and the nonequilibrium thermodynamics of molecular motor Phys. Rev. E 74 011906
[2] Andrieux D and Gaspard P 2007 Fluctuation theorem for currents and Schnakenberg network theory J. Stat. Phys. 127 107–31
[3] Andrieux D and Gaspard P 2007 Network and thermodynamic conditions for a single macroscopic current fluctuation theorem C. R. Phys. 8 579–90
[4] Andrieux D and Gaspard P 2008 The fluctuation theorem for currents in semi-Markov processes J. Stat. Mech. 11 P11007
[5] Asmussen S 2003 Applied Probability and Queues (Application of Mathematics vol 51) 2nd edn (New York: Springer) (https://doi.org/10.1007/b97236)
[6] Bertini L, Faggionato A and Gabrielli D 2015 Flows, currents, and cycles for Markov chains: large deviation asymptotics Stoch. Process. Appl. 125 2786–819
[7] Chetrite R and Gawędzki K 2008 Fluctuation relations for diffusion processes Commun. Math. Phys. 282 469–518
[8] Dagdug L and Berezhkovskii A M 2009 Drift and diffusion in periodic potentials: upstream and downstream step times are distributed identically J. Chem. Phys. 131 056101
[9] Das R K and Kolomeisky A B 2009 Dynamic properties of molecular motors in the divided-pathway model Phys. Chem. Chem. Phys. 11 4815–20
[10] Evans D and Searles D 2002 The fluctuation theorem Adv. Phys. 51 1529–85
[11] Faggionato A 2017 Fluctuation theorems for currents in semi-Markov processes (in preparation)
[12] Faggionato A and Di Pietro D 2011 Gallavotti–Cohen-type symmetry related to cycle decompositions for Markov chains and biochemical applications J. Stat. Phys. 143 11–32
[13] Faggionato A and Silvestri V 2014 Discrete kinetic models for molecular motors: asymptotic velocity and gaussian fluctuations J. Stat. Phys. 157 1062–96
[14] Faggionato A and Silvestri V 2017 Random walks on quasi one dimensional lattices: large deviations and fluctuation theorems Ann. Inst. Henri Poincaré 53 46–78
[15] Gallavotti G and Cohen E G D 1995 Dynamical ensembles in nonequilibrium statistical mechanics Phys. Rev. Lett. 74 2694–7
[16] Firman K and Youell J 2013 Molecular Motors in Bionanotechnology (Boca Raton, LA: CRC Press)
[17] Fisher M E and Kolomeisky A B 1999 The force exerted by a molecular motor Proc. Natl Acad. Sci. USA 96 6597–602
[18] Fisher M E and Kolomeisky A B 1999 Molecular motors and the force they exert Physica A 274 241–66
[19] den Hollander F 2000 Large Deviations (Fields Institute Monographs vol 14) (Providence, RI: American Mathematical Society) (https://doi.org/10.1090/fm/014)
[20] Howard J 2001 Mechanics of Motor Proteins and the Cytoskeleton (Sunderland, MA: Sinauer Associates)
[21] Jülicher F, Ajdari A and Prost J 1997 Modeling molecular motors Rev. Mod. Phys. 69 1269–81
[22] Kolomeisky A B 2001 Exact results for parallel-chain kinetic models of biological transport J. Chem. Phys. 115 7523
[23] Kolomeisky A B 2013 Motor proteins and molecular motors: how to operate machines at the nanoscale J. Phys.: Condens. Matter 25 463101
[24] Kolomeisky A B and Fisher M E 2000 Extended kinetic models with waiting-time distributions: exact results J. Chem. Phys. 113 10867–77
[25] Kolomeisky A B and Fisher M E 2000 Periodic sequential kinetic models with jumping, branching and deaths Physica A 279 1–20
[26] Kolomeisky A B and Fisher M E 2007 Molecular motors: a theorist perspective Annu. Rev. Phys. Chem. 58 675–95
[27] Kurchan J 1998 Fluctuation theorem for stochastic dynamics J. Phys. A.: Math. Gen. 31 3719–29
[28] Lacoste D, Lau A W C and Mallick K 2008 Fluctuation theorem and large deviation function for a solvable model of a molecular motor Phys. Rev. E 78 011915
[29] Lacoste D and Mallick K 2011 Fluctuation relations for molecular motors Biological Physics. Poincaré Seminar 2009 (Progress in Mathematical Physics vol 60) ed B Duplantier and V Rivoal (Basel: Verlag) (https://doi.org/10.1007/978-3-0346-0428-4)
[30] Lacoste D and Mallick K 2009 Fluctuation theorem for the flashing ratchet model of molecular motors Phys. Rev. E 80 021923
[31] Lau A W C, Lacoste D and Mallick K 2007 Non-equilibrium fluctuations and mechanochemical couplings of a molecular motor Phys. Rev. Lett. 99 158102

https://doi.org/10.1088/1742-5468/aa6731
[32] Montroll E W and Weiss G H 1965 Random walks on lattices. II J. Math. Phys. 6 167–81
[33] Lebowitz J L and Spohn H 1999 A Gallavotti–Cohen-type symmetry in the large deviation functional for stochastic dynamics J. Stat. Phys. 95 333–65
[34] Reimann P 2002 Brownian motors: noisy transport far from equilibrium Phys. Rep. 361 57265
[35] Ritort F 2006 Single-molecule experiments in biological physics: methods and applications J. Phys.: Condens. Matter 18 R531–83
[36] Schnakenberg J 1976 Network theory of microscopic and macroscopic behavior of master equation systems Rev. Mod. Phys. 48 571–85
[37] Seifert U 2012 Stochastic thermodynamics, fluctuation theorems, and molecular machines Rep. Prog. Phys. 75 126001
[38] Sevick E M, Prabhakar R, Williams S R and Searles D J 2008 Fluctuations theorems Annu. Rev. Phys. Chem. 59 603–33
[39] Tausky O and Zassenhaus H 1959 On the similarity transformation between a matrix and its transpose Pac. J. Math. 9 893–6
[40] Tsygankov D and Fisher M E 2008 Kinetic models for mechanoenzymes: structural aspects under large loads J. Chem. Phys. 128 015102
[41] Wang H and Qian H 2007 On detailed balance and reversibility of semi-Markov processes and single-molecule enzyme kinetics J. Math. Phys. 48 013303