Waiting for rare entropic fluctuations

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Abstract – Nonequilibrium fluctuations of various stochastic variables, such as work and entropy production, have been widely discussed recently in the context of large deviations, cumulants and fluctuation relations. Typically one looks at the probability distributions for entropic fluctuations of various sizes to occur in a fixed time interval. An important and natural question is to ask for the time one has to wait to see fluctuations of a desired size. We address this question by studying the first-passage time distribution (FPTD). We derive the general basic equation to get the FPTD for entropic variables. Based on this, the FPTD on entropy production in a driven colloidal particle in the ring geometry is illustrated. A general asymptotic form of the FPTD and integral fluctuation relation symmetry in terms of the first passages are found.

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Introduction. – The past two decades have witnessed a significant development in nonequilibrium thermodynamics [1–4]. The fluctuation relations are remarkable discoveries which have quantitatively refined the concept of the second law [5–9] as applied to small systems. One of the central issues in nonequilibrium statistical physics has been in characterizing the universal nature of fluctuations of thermodynamic variables, such as heat and work that quantify the entropy generated in nonequilibrium processes. Usually, one measures these accumulated “entropic” variables, say \( A \), over a fixed time interval \( t \), and its fluctuations are characterized by a distribution \( P(A|t) \). Defining, for example, \( A = S \) as the stochastic total entropy, one can prove the detailed and integral type of fluctuation relation for any fixed time interval \( t \), in various Markov processes [9]. For large observation times, one finds the large deviation form \( P(S|t) \sim e^{th(S/t)} \) [10], where \( h(s) \) is the large deviation function (LDF). For physical quantities related to entropy production, it is well known that the LDF shows the fluctuation relation symmetry [11,12]. This symmetry is not only mathematically beautiful but also physically important since it reproduces linear response results and also gives nontrivial relationships for nonlinear responses [13–15]. Large deviations have been crucial towards constructing the thermodynamic structure of the nonequilibrium steady state [16–18].

The distribution function \( P(A|t) \) gives us the probability of observing a fluctuation of size \( A \) in some fixed observation time window \( t \). An interesting question is: how long would one have to wait to see a fluctuation of a specified size? This is precisely the question of the first-passage problem for the stochastic variable \( A \). Surprisingly, not much is known on this. One expects the time evolution of the relevant stochastic variables to be a biased random walk in an extended configuration space, and it is of interest to study its temporal aspect. The main aim of this paper is to investigate this aspect. In particular, we consider the problem of the first-passage time distribution (FPTD) of \( A \), which is an experimentally measurable quantity. We define the FPTD of interest, \( F(t|A) \), as the probability that the entropic variable hits the value \( A \) for the first time between times \( t \) and \( t + dt \). Apart from proposing a general formalism, we address questions on the typical long-time functional form of the FPTD, its dependence on the sign of the entropy produced and possible fluctuation relations.

Let us begin by considering one of the simplest example of a nonequilibrium process, that of a colloidal particle moving on a ring (of length \( L \)) and driven by a constant force \( f \). The particle’s motion is described by the overdamped Langevin equation \( \dot{x} = f/\gamma + \sqrt{2D\eta(t)} \), where \( \gamma \) is the damping coefficient, \( D = k_B T/\gamma \) the diffusion constant, with \( T \) the ambient temperature, and \( \eta \) is...
Gaussian white noise with unit variance. In the steady state, the particle moves around the circle with an average speed \( f/\gamma \). The driving force does work on the particle at a rate \( I_1 = f^2/\gamma \) and this is dissipated as heat into the baths. This is thus the rate of entropy production. In a given realization of the process, the entropy produced in a time interval \( t \) is given by \( S = f x \), where \( x \) is the net displacement of the particle in time \( t \). We can equivalently think of \( x \) as the displacement of a diffusing particle moving on the open line, down a potential slope. The statistics of entropy can thus be obtained from those of \( x \). From the known results for biased diffusion, we get

\[
P(S|t) = e^{-(S-I_1 t)/2\gamma t} / \sqrt{2\pi\gamma t} \tag{1}
\]

at large times, where we have defined the cumulants \( I_n = \lim_{t \to \infty} \langle S^n \rangle / t \). Using this as a reference, we now examine the stochastic time evolution of entropic variables. We will discuss first the basic equation to get FPTD of general entropic variables and then explicit results for a specific example.

We now summarize some of the formalism of stochastic thermodynamics and show how it can be extended to study the problem of FPTD. Consider any physical system whose microscopic configuration is described by a discrete set of variables \( X \). We assume that its time evolution is described by a stochastic Markovian dynamics. This means that the probability \( P(X|t) \) that the system is in state \( X \) at time \( t \) evolves via a master equation \( \partial_t P(X|t) = WP(X|t) \), where \( W \) is a Markov transition rate matrix. One can extend the configuration space to also include the variable, \( A \), which could be the entropy \( S \) or, in general, any accumulated quantity like work, heat, etc. [12]. The joint distribution, \( P(X,A|t) \), will satisfy a modified equation with another linear operator \( W_A \),

\[
\partial_t P(X,A|t) = W_A P(X,A|t). \tag{2}
\]

Let us denote the solution for the initial condition \( X = Y, A = 0 \) at \( t = 0 \) by \( T_{X,Y}(A|t) \). The corresponding generating function \( T_{X,Y}(\xi|t) = \int dA e^{\xi A} T_{X,Y}(A|t) \) satisfies the equation

\[
\partial_t T_{X,Y}(\xi|t) = W_\xi T_{X,Y}(\xi|t), \tag{3}
\]

where \( W_\xi \) is obtainable from \( W_A \) (explicit constructions of \( W_\xi \) can be seen in [12,20,21]). The above equation has the long-time solution

\[
T_{X,Y}(\xi|t) \sim e^{\mu t} \phi(\xi) \chi(\xi), \tag{4}
\]

where \( \mu, \phi, \chi \) are, respectively, the largest eigenvalue of \( W_\xi \), and the corresponding right and left eigenvectors. Integrating this over \( Y \) chosen from a steady-state distribution, and over all final states \( X \), leads to the generating function \( \langle e^{\xi A} \rangle \). Thus, we see that \( \mu(\xi) \) is the cumulant generating function (CGF) for \( A \), connected to the LDF \( h(\xi)/(\xi) \) by a Legendre transform [10]. The \( n \)-th order of the cumulant is given by

\[
I_n = \langle A^n \rangle e/\tau = \partial^n \mu(\xi)/\partial \xi^n \big |_{\xi=0}. \tag{5}
\]

First passage in entropic variables. – For the Markov process in the extended phase space \( (X,A) \), we now consider the time for first passage through a specified value of \( A \), where we do not care about the configuration coordinates \( X \). Let us define \( F_{X,Y}(t|A) \) as the probability that the system starts from \( Y \) at time \( t = 0 \) with \( A = 0 \), and then first reaches \( A \) in the time interval \((t, t+dt)\) and with \( Y \) being the “entry point” (see fig. 1) at the time of this first-passage event (this need not be a first entry). Then we have the following general relation between \( F \) and the transition matrix \( T \):

\[
T_{X,Y}(A|t) = \sum_Z \int_0^t da T_{X,Z}(A=0|u)F_{Z,Y}(t-u|A), \tag{6}
\]

for \( t \neq 0 \). After Laplace transforming in time, the FPTD matrix is given by \( F_{X,Y}(s|A) = \sum_Z T_{X,Z}(A=0|s)F_{Z,Y}(A|s) \). Note that the set of points \( X \) forms a subset of the full set of configurations and so the matrices \( F_{X,Y}(s|A) \) and \( T_{X,Y}(A|s) \) are in general rectangular. The above equation relates the FPTD to the distribution in the extended state space and provides a general framework for the study of FPTD for entropic variables. This equation is our first main result. We now focus on a specific model and obtain explicit results on FPTD.

Model of driven particle. – We consider a well-established paradigmatic model of stochastic thermodynamics, namely a colloidal particle confined to moving on a ring, and driven by a constant force [1,22–24]. A schematic picture for this system is shown in fig. 2. The dynamics of the particle is given by the overdamped Langevin equation

\[
\gamma \dot{x} = -\partial_x U(x) + f + \eta(t), \tag{7}
\]
Where \( \eta(t) \) is the Gaussian noise satisfying \( \langle \eta(t)\eta(t') \rangle = 2\gamma \beta^{-1}\delta(t-t') \), \( \beta^{-1} \) is the bath temperature, and we impose the periodic boundary condition \( (x + L \equiv x) \). \( U(x) \) is a periodic potential and \( f (> 0) \) is a nonconservative force driving the system into a nonequilibrium state.

For the extensive variable \( A \), we consider two quantities, namely the winding number \( N \), and the entropy increase of the environment \( S \). As we will see, they are closely related. The winding number is defined as an integer variable which is initially set to zero and increases (decreases) by one whenever the particle makes a complete circuit in the direction of increasing (decreasing) \( x \). If, during a time interval \( t \), the particle makes a transition from site \( x \) to \( y \), and its winding number changes by \( N \), then the entropy increase in the bath is \( S = \beta[f(N + y - x) - U(y) + U(x)] \).

At large times, the entropy generated is thus proportional to the winding number. Note that due to the positive force \( f \), the particle on average moves in the positive direction and the average winding number increases with time. However, there is a finite probability to observe the particle moving in the opposite direction. The ratio of probabilities between positive and negative winding number at large times is quantitatively given by the fluctuation relation [1]. Let \( F_\text{SS}(t|N) \) be the FPTD for the particle starting at the position \( x \). Then, we define the steady-state FPTD:

\[
F(t|N) = \int dx F_\text{SS}(t|N) p_\text{SS}(x),
\]

where \( p_\text{SS} \) is the steady-state distribution.

As our second main result, we derive the typical structure of asymptotic behavior of the FPTD using eq. (6):

\[
F(t|N) = A(N) \exp[-\Gamma t - (3/2) \log t],
\]

where \( A(N) \) is a function of \( N \), which depends on the details of the system. For the biased diffusion (special case with \( U(x) = 0 \)) in eq. (1) we obtained \( \Gamma = I_1^3/(2I_2) \).

With this example in mind, it is convenient to express \( \Gamma \) as a series in \( I_1 \). We find

\[
\Gamma = \sum_{n=0}^{\infty} \frac{(-I_1)^{n+2}}{(n+2)!} g_n(\xi)|_{\xi=0}
\]

\[
= \frac{I_1^2}{2I_2} + \frac{I_4I_3^2}{6I_2^2} + \frac{(3I_3^2 - I_2I_4)I_1^4}{24I_2^4} + \cdots,
\]

where the function \( g_n(\xi) \) is connected to the cumulant generating function of the winding number as

\[
q_n(\xi) = \left( \frac{d^2 \mu(\xi)}{d\xi^2} \right)^{-1} \frac{d^n \mu(\xi)}{d\xi^n} \left( \frac{d^2 \mu(\xi)}{d\xi^2} \right)^{-1}.
\]

Note also the logarithmic term which is the same dependence as in eq. (1).

Here we discuss some physically important observations on these results, leaving the derivation of the above results at the end of the paper. The asymptotic temporal decay form depends neither on the sign nor on the amplitude of the winding number, though the actual probability of negative and positive winding numbers differ by exponential factors (in the entropy produced). Thus, intrinsically, even extremely rare events follow the same asymptotic form of FPTD as likely events. In the linear response regime with small first cumulant, the asymptotic behavior is well explained by the biased diffusion result \( F^{BD} \) in eq. (1) \((\Gamma = I_1^3/(2I_2)) \). In the far-from-equilibrium regime, however, a significant deviation from this picture reveals itself in the higher-order terms with nontrivial expressions. This deviation is more so in small systems, where the degree of nonequilibrium is easily increased. We demonstrate these important physical aspects with a numerical simulation of FPTD of the winding number \( N \) for a driven particle in a periodic potential (see fig. 3(a)). The initial state was sampled from the steady state. For events with a negative entropy production there is a finite probability of the event \textit{not occurring at all} in a given realization. Hence for negative \( N \), we plot the distribution, conditioned on the probability that it occurs. In short time scales, the FPTD is in general nonunimodal. However, the figure clearly shows that the asymptotic behavior is well described by the theory (10), irrespectively of the fixed values of \( N \). At finite times the logarithmic correction is important. The deviation from the biased diffusion result is also clear. In fact, the asymptotic form (10) widely holds. To demonstrate this, we show results for another model.
We consider the coupled oscillator system, exchanging heat with two heat reservoirs at temperatures $T_L,T_R$, whose dynamics is described by the overdamped Langevin equation

$$\gamma \dot{x}_1 = -kx + \eta_L(t), \quad \gamma \dot{x}_2 = kx + \eta_R(t),$$  \hspace{1cm} (11)

where $x_1,x_2$ are the positions of the first and second particles which are coupled via spring constant $k$, and $x = x_1 - x_2$. The noise terms $\eta_i$ satisfy the fluctuation dissipation relations $\langle \eta_i(t)\eta_j(t') \rangle = 2\delta_{ij}\gamma \delta(t-t')$. In this case we consider the heat transfer into the right bath in time $t$ and this is given by $Q = \int_0^t dt' kx(t')[kx(t') + \eta_R(t')]/\gamma$ and we are interested in the FPTD for transition from an initial state $(x,Q=0)$ to a state with $Q$ amount of heat transferred. See fig. 3(b), which shows that asymptotic behavior is again given by eq. (10).

**Integral fluctuation relation in terms of first passage.** – One can apply eq. (6) to derive nontrivial relations for the FPTD of $S$ in our driven-particle model. For fixed $S$, the entry site $\bar{y}$ depends on the initial site $x$. It is uniquely determined if $|S|$ is sufficiently large, while for small $|S|$, there can be at most two choices of $\bar{y}$, respectively on the two sides of $x$. As example, see the right figure in fig. 2 of a case where two $\bar{y}$ (denoted by $\bar{y}_\pm$) can be reached for a fixed negative $S$, starting from the site $x$.

To obtain the FPTD relations we first note the following exact relations for the mean residence time at a given lattice point for a given entropy production:

$$\int_0^\infty dt T_{y,x}(-S|t) = e^{-S}p_{x|y}^{SS}/J,$$

$$\int_0^\infty dt T_{x,y}(S|t) = p_x^{SS}/J,$$  \hspace{1cm} (12)

where $J$ is the steady-state current. In the first relation, it is assumed that the process $(x,0) \rightarrow (y,-S)$ is opposite to the direction of current, while in the second relation, $(y,0) \rightarrow (x,S)$ is in the direction of current. These are connected by the detailed fluctuation relation [25]. The proof of eq. (12) is lengthy and we will present it in the last section.

We now employ the usual definition of total entropy $S_{\text{tot}} = \ln(p_{x|y}^{SS}/p_x^{SS}) + S$ for the process $x \rightarrow \bar{y}$. Then, for fixed negative entropy $S < 0$, using (6) and (12) leads to the equality $\int_0^\infty dt \sum_x \exp(-S_{\text{tot}})F_{\bar{y}|x}(t|S) = 1$. Averaging over initial $x$ chosen from the steady state, $p_x^{SS}$, we obtain the integral type of fluctuation relation in terms of the first passage, which is our third main result,

$$\langle \langle e^{-S_{\text{tot}}} \rangle \rangle_S = 1,$$  \hspace{1cm} (13)

where the average $\langle \langle \ldots \rangle \rangle_S$ implies taking all possible first-passage paths producing the negative entropy $S$, and that start from the steady state. Numerical demonstrations of eqs. (12) and (13) are presented in fig. 4.

**Summary.** – We considered the FPTD of entropy production. We have proposed eq. (6) as the basic equation for the computation of FPTD. Using this framework for the paradigmatic nonequilibrium example of a driven particle in a periodic potential, we find several nontrivial properties, i.e., the asymptotic behavior of eq. (10) and the integral fluctuation relation in terms of first passages (13).

**Derivation of eq. (10).** – We discretize space into $L$ sites on the ring separated by a small spacing $a$, such that $x = ja$. The time evolution of the probability $P_j(t)$ that the particle is on the $j$-th site at time $t$ is given by the master equation

$$\dot{P}_j(t) = \sum_{j'=j \pm 1} W_{j,j'}P_{j'}(t) - \sum_{j' \neq j} W_{j,j'}P_j(t),$$  \hspace{1cm} (14)

where $W$ is the transition rate matrix and satisfies the local detailed balance condition $W_{j+1,j}/W_{j,j+1} = e^{-3(U_{j,j+1}-U_{j+1,j})}$. Here $U_j$ is the potential energy at the $j$-th site. We are interested in the average FPTD (8), given in the discretized space as $F(t|N) = \sum_i F_{ii}(t|N)p_i^{SS}$, where $p_i^{SS}$ is the steady-state distribution. We now use the general formalism (6) for FPTD. We note that for our present example, the observable is the winding number. The asymptotic behavior is determined by the function $F_{ii}(t|N)$ and hence we focus on this. To use eq. (6) for the first-passage of the winding number, we note that for a given initial starting point $i$, the entry point is also $i$. We recall that $T_{ji}(N|t)$ is the probability that, with initial position $i$, the particle is at site $j$ and has winding number $N$ at time $t$. Using eq. (6) and after taking an inverse Laplace transform we get the following basic equation on the FPTD for the winding number:

$$F_{ii}(t|N) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} ds e^{st} T_{ii}(N|s) T_{ii}(0|s).$$  \hspace{1cm} (15)

To obtain the function $T_{ii}(N|t)$, it is useful to define $T_{kk}(N|t)$, the probability of transition from the initial site $k$ to the site $l$ with $N$ as the number of transitions from $L \rightarrow 1$ (reverse transitions $1 \rightarrow L$ are counted with a negative sign). This quantity has a simple dynamics and

Fig. 4: (Color online) Numerical demonstration of eq. (12) and fluctuation-relation–like symmetry, eq. (13) (inset). The model and parameter set are as in fig. 3(a).
is useful to obtain $T_i(t)$, since one can easily check that $T_i(t) = T_i \exp(t)$. The dynamics is given by

$$\partial_t T_{k \ell}^\alpha(N|t) = W_{\ell \ell-1} T_{k \ell-1}^\alpha(N - \delta_{\ell,1} t) - W_{\ell+1} T_{k \ell}^\alpha(N|t) + W_{\ell+1} T_{k \ell+1}^\alpha(N + \delta_{\ell,L} t) + \partial_t \theta \delta_{N,0} \delta(t).$$

Through Fourier-Laplace transformation, it is straightforward to get the formal solution in the matrix form

$$T_{k \ell}(N|s) = \frac{1}{2\pi i} \int \frac{dz}{z} \frac{A(z, s)}{\det[s - W_z]}, \quad (16)$$

where the contour is the unit circle in the complex plane and the matrix $W_z$ is given by the matrix $W$ replacing the $(1, L)$ and $(L, 1)$ elements by $zW_{11}$ and $-1W_{L1}$, respectively, and $A(z, s)$ is the co-factor matrix of $s - W_z$.

One readily finds that the denominator gives the simple form

$$z \det[s - W_z] = \left( \prod_{k=1}^L W_{k+1, k} \right) [z - z_+(s)] [z - z_-(s)],$$

where two roots $z_{\pm}$ ($z_+ \geq 1 > z_-)$ are connected to each other by the fluctuation relation symmetry

$$z_+(s)z_-(s) = e^{-\beta f L a}.$$  \quad (17)

The complex value integration for (16) and manipulation with the fluctuation relation and (15) leads to the following expression for the FPTD:

$$F_{i_1}(t|N) = \frac{C_i(N)}{2\pi i} \int ds e^{-t[-s + b \xi(s)]}, \quad \text{(18)}$$

where $b = |N|/t$ and $\xi(s) = \log z_+(s)$. The constant value $C_i(N)$ depends on $i$ and $N$. For large $t$, we make a saddle point analysis. Let us define the function $g(s) = -s + b \xi(s)$. Solving the equation $-1 + b d\xi(s)/ds = 0$ gives the saddle point $s^*(b)$. The decay constant $\Gamma$ is thus given by $b(h(b))|_{b=0}$ where $h(b) = g(s^*(b))$. The logarithmic correction in eq. (10) comes from the fact $d^2 g(s)/ds^2|_{s=s^*} \sim 1/b^2$.

We now recall, from eq. (4), that the largest eigenvalue of $W_z$ gives the CGF, $\mu(\xi)$, for the variable $N$. By comparing the equation $\det[s - W_z] = 0$ around $s = 0$ and the CGF equation, one finds that the singular value $z_+(s)$ is connected to the CGF through the relation

$$s - \mu(\xi) = 0.$$ \quad (19)

Using this and the saddle point condition we find that the function $h(b)$ is in fact just the LDF, connected to the CGF through the Legendre transformation $h(b) = b \xi(s^*) - \mu(\xi)$. Finally, the Taylor expansion of $h(b)|_{b=0}$ around the value $b = 1$ leads to eq. (10).

**Derivation of the mean residence time (12).** - We first note that the steady-state distribution and current can be exactly solved,

$$p_j^{SS} = \left[ 1 + \frac{W_{jj-1}}{W_{jj-2}} + \frac{W_{jj-1}W_{jj-3} + \cdots}{W_{jj-2} - 1W_{jj-3} - 2} \right]^{\frac{L}{}} \frac{\prod_{k=1}^{L} W_{kk+1}}{W_{jj+1}} / \mathcal{Z}, \quad (20)$$

where we used the notation $W_{ij} = W_{i+j} + W_{i+j}$ and $\mathcal{Z}$ is the normalization factor.

We consider the joint probability $P_j(n, t)$ that the particle is at the position $j$ at time $t$ and $n$ transitions between the sites $L$ and $1$ occur until then. We are interested in finding the probability vector $\mathbf{P}(n, t) = \{P_1(n, t), P_2(n, t), \ldots, P_L(n, t)\}^T$. Then it is easy to see that this joint probability satisfies the following equation in the Laplace representation in time:

$$s \mathbf{P}(n, s) = \mathbf{W} \mathbf{P}(n - 1, s) + \mathbf{W}_0 \mathbf{P}(n + 1, s) + \delta_{n,0} \mathbf{P}_0.$$ \quad (22)

Here $\mathbf{W}_-$, $\mathbf{W}_+$ are $L \times L$ matrices whose only non-vanishing elements are $[\mathbf{W}_-]_{L1} = W_{1L}$, $[\mathbf{W}_+]_{L1} = W_{1L}$, and $W_0 = \mathbf{W} - \mathbf{W}_- - \mathbf{W}_+$. For $n \neq 0$, we try a solution of the form $\mathbf{P}(n, s) = Z^N \mathbf{v}$, where $\mathbf{v}$ is a constant vector. Plugging this into (22) for $n \neq 0$ gives the equation $[\mathbf{W} - \mathbf{W}_-] \mathbf{v} = 0$ for determining $z$ and $\mathbf{v}$. To find the solutions to this equation, we write it in the form

$$\left( \begin{array}{c} s + [W_{L1} + W_{21}] \mathbf{- z_+} \mathbf{U} \\ -z_- \mathbf{U} \end{array} \right) \left( \begin{array}{c} 1 \\ \mathbf{V}^+ \end{array} \right) = 0, \quad (23)$$

where $\mathbf{z}_+ = (W_{12}, 0, \ldots, zW_{1L}); \mathbf{z}_- = (W_{21}, 0, \ldots, z^{-1}W_{1L})^T, \mathbf{U} = s \mathbf{I}_{L-1} - \mathbf{W}_2^{2L}, \mathbf{V}^+ = (V_2, V_3, \ldots, V_L)^T$. Here the matrix $\mathbf{W}_2^{2L}$ denotes the $(L - 1) \times (L - 1)$ submatrix of $\mathbf{W}$ excluding the first row and column, while $\mathbf{I}_{L-1}$ is the unit matrix of dimension $(L - 1)$. We have set the first element $V_1$ to one. Then we get the following equations for $\mathbf{v}$ and $z$: $s + W_{L1} + W_{21} - W_{12} V_2 - zW_{1L} V_2 = 0, \mathbf{v} = \mathbf{U}^{-1} \mathbf{z}_-$. The second equation leads to the relation $V_2 = (U_{21} W_{12} + U_{L1}^{-1} z^{-1} W_{1L}) / W_{12}$, for $j = 1, \ldots, L - 1$. Since $\mathbf{U}$ does not depend on $z$, we see that $V_j$'s are linear functions of $z^{-1}$. Hence putting back $V_2, V_3$ into the first equation above, we get a quadratic equation for $z$. For the two solutions we get two corresponding explicit forms for the vectors $\mathbf{v}$. We denote the two solutions by $\{z_+(s), \mathbf{v}^+(s)\}$ and $\{z_-(s), \mathbf{v}^-(s)\}$. The equation for $z$ gives eq. (17).

Let us now look for a solution corresponding to the initial condition that the point starts from $i$ with $n = 0$. A possible solution of eq. (22) is

$$\mathbf{P}(n, s) = \begin{cases} A_+ z^n \mathbf{v}^+, & \text{for } n > 0, \\ A_- z^{-n} \mathbf{v}^-, & \text{for } n < 0, \\ \mathbf{v}^0, & \text{for } n = 0. \end{cases} \quad (24)$$

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The unknown constants $A_+ , A_-$ and $\mathbf{V}^0$ can fixed by requiring that our above solution satisfies eqs. (22) at the sites corresponding to $i$ and its two nearest neighbors. Clearly then the vector $\mathbf{V}^0$ must have the structure $\mathbf{V}^0 = (A_+ V^-_i , A_+ V^-_{i+1} , \cdots , A_+ V^-_{i-n} , A_0 , A_+ V^+_i , \cdots , A_+ V^+_n )$.

There are three constants $(A_-, A_+, A_0 )$ to be determined from the equations at the site $i$ and its neighbors. Let us assume, for the moment, that none of these three sites is a boundary site on the cell $(i.e., i-1 > 1 , i+1 < L)$. Then we get the following equations by looking at the $n = 0$ block, from which $A_+, A_-$ and $A_0$ are determined:

$$ W_{i-1} A_0 = [ s + W_{i-1} - W_{i-1} ] V^-_{i-1} A_+ - W_{i-1} V^-_{i-2} A_-, 1 = [ s + W_{i-1} + W_{i+1} ] A_0 - W_{i-1} V^-_{i-1} A_+ - W_{i+1} V^+_i A_+ ,$$

$$ W_{i+1} A_0 = [ s + W_{i+1} + W_{i+2} ] V^+_i A_+ - W_{i+1} V^+_i A_+ - W_{i+2} V^+_i A_+ .$$

(25)

(26)

(27)

Using the equation satisfied by $\mathbf{V}^\pm$ which is given from the block of $n \neq 0$, we find that the first and third equations yield $A_- = A_0 / V^-_i , A_+ = A_0 / V^+_i$. Plugging these into the middle equation, one gets

$$ A_0 = \left[ s + W_{i-1} + W_{i+1} - W_{i-1} V^-_{i-1} - W_{i+1} V^+_i \right]^{-1} .$$

(28)

For the case $s = 0$, eq. (23) has one solution with $z_+ = 1$ and this corresponds to the steady-state so we choose $\mathbf{V}^+ = \mathbf{p}^{SS}$. The other solution for $z_- = \prod_{k=1}^{L} W_{k+1} / W_{k+1}$ is given by

$$ \mathbf{V}^- = \left( \begin{array}{cccc} W_{21} & W_{22} W_{32} & \cdots & W_{21} W_{L-1} \cr W_{12} W_{23} & \cdots & \cdots & \cdots \cr \vdots & \vdots & \ddots & \cdots \cr W_{L-1} V^-_{L-1} \end{array} \right)^T ,$$

(29)

as can be easily verified. From (28) and the fact that $J = [ W_{i+1} V^+_i - W_{i+1} V^+_i ]$ we get

$$ A_0 = V^+_i / J , \quad A_- = V^-_i / J V^-_i , \quad A_+ = 1 / J .$$

(30)

From these we finally obtain, for the case $s = 0$, the following transition matrices for any states $j , i$ where $i$ is the one “down the hill” $(i.e. \text{current is in the direction } i \rightarrow j)$:

$$ T^P_{j=j} (n = 0 | s = 0) = \rho^{SS} / J .$$

(31)

We finally explain how to obtain the expression (12), using eq. (31). We note that the entropy produced in the thermal reservoir for the process $j \rightarrow i$ is given by $S = \beta [ U_j - U_i + f_a (i-j + L) ]$. This implies that the process $(j,n = 0) \rightarrow (j,n = 0)$ is equivalent to the process $(j,S = 0) \rightarrow (j',S = 0)$. Hence eq. (31) is equivalent to $T_{j_0} (S = 0 | s = 0) = \rho^{SS} / J$. Now consider the process $(j,S = 0) \rightarrow (i,S)$ whose direction is the same as that of the average current. This process eventually occurs with a probability one. Hence we have $T_{j_0} (S = 0 | s = 0) = T_{j_0} (S = 0 | s = 0) = \rho^{SS} / J$. In the backward process $(i,S = 0) \rightarrow (j,-S)$ which is opposite to the direction of the average current, the detailed fluctuation relation immediately gives $T_{j_0} (-S | s = 0) = e^{-\beta} \rho^{SS} / J$. These give the expression (12).

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