# Chapter 2
# Iterative Measurement-Feedback Procedure for Large Deviation Statistics

## 2.1 Introduction

In the last two decades, large deviation functions in time-series statistics have gathered attention in the field of nonequilibrium physics. The beginning is the discovery of the fluctuation theorem, which is the symmetry property of the large deviation function of the time-averaged entropy production rate [1–6]. After that, several results for the large deviation functions have followed, such as an additivity principle for driven diffusive systems [7–12], generalised Onsager–Machlup approach [13, 14], dynamical phase transitions of kinetically constrained models [15–17], a Lyapunov function for non-equilibrium steady states without relying on entropy production [18], exact results for the current statistics of lattice gas models [17, 19].

Also, with these developments, there were some studies that focused on the thermodynamic structure in time-series statistics [20–26]. Especially in these analysis, a technique to map a biased ensemble to another steady state ensemble has been utilised. This mapping is well defined in mathematical sense, however, in order to construct this mapping, we need pre-information for generating a special external force added. That requires to solve eigenvalue problems of a matrix in a large dimension: the degrees of freedom of the system, which is demanding in computational point of view. For overcoming this difficulty, we proposed a variational principle constituted of observable quantities to determine that external force [24–26]. Since the variational parameter of this variational principle was an external field of the system, it offers a simple method for determining that external force without solving any mathematical largest eigenvalue problems. However, there is still a problem for large size systems, because the domain of the variational functional increases exponentially as the system size becomes larger in general.

Here in this chapter, we propose a new computational method for large deviation statistics. This exploits a property in time-series statistics, which is *an additive property of the rareeventness with a special measurement and feedback*.: By iterating a procedure constituted of measurements and feedbacks, we gradually renormalise



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the system, and let the obtained modified systems attain the rare-event property. We stress that this method is constituted of measurements and feedbacks. Thus, it can be implemented in real experiment in principle. Furthermore, by combining it with an idea of *effective description of exponential family*, we show a good numerical performance of the method. Indeed, as a demonstration, we apply this method to many-body systems, and obtain some non-trivial features of the rare fluctuations in those systems.

The construction of this chapter is as follows. In Sect. 2.2, we show some preliminaries. In Sect. 2.2.1–2.2.4, we give the definition of the model and some basics of a large deviation principle. Then, in Sect. 2.2.5, we show and prove a mapping method from a biased ensemble to the steady state dynamics, which is the key formula to construct the phenomenological structure in time-series statistics. In Sect. 2.3, we explain our computational method. From Sect. 2.3.1–2.3.3, we explain the idea behind the method, and in Sect. 2.3.4, we show explicitly the procedure of the method. Section 2.4 is devoted to the application of the method to non-equilibrium many-body lattice gas models. In particular, in Sect. 2.4.1, we introduce an effective description of the exponential family, and in the following subsections, with the effective description, we analyse these many-body systems. Finally, in Sect. 2.5, we make a conclusion of this chapter. This chapter is based on the paper published in [27].

## 2.2 Preliminary

### *2.2.1 Model*

The state space $\Omega$ is a finite set. On $\Omega$, we consider continuous time Markov processes. For $\boldsymbol{n}, \boldsymbol{n}' \in \Omega$, we define a transition rate $w(\boldsymbol{n} \to \boldsymbol{n}')$ as an irreducible matrix that satisfies $w(\boldsymbol{n} \to \boldsymbol{n}) = 0$ and $w(\boldsymbol{n} \to \boldsymbol{n}') \neq 0$ if $w(\boldsymbol{n}' \to \boldsymbol{n}) \neq 0$. The escape rate is defined as

$$\lambda(\boldsymbol{n}) \equiv \sum_{\boldsymbol{n}' \in \Omega} w(\boldsymbol{n} \to \boldsymbol{n}'). \tag{2.1}$$

We start with an initial distribution function $P_0(\boldsymbol{n})$. Then, the distribution function of $\boldsymbol{n}$ at time $t$, $P(\boldsymbol{n}) \equiv \left\langle \delta_{\boldsymbol{n}(t),\boldsymbol{n}} \right\rangle$, is determined from the following Master equation [28]:

$$\frac{\partial}{\partial t} P(\boldsymbol{n}, t) = \sum_{\boldsymbol{n}} P(\boldsymbol{n}) w(\boldsymbol{n} \to \boldsymbol{n}') - \delta_{\boldsymbol{n},\boldsymbol{n}'} \lambda(\boldsymbol{n}). \tag{2.2}$$

We denote the history of states during a time interval $t$ by $\omega$, which is specified by the total number of transitions $n$, a collection of transition times $(t_i)_{i=1}^{n}$, and a sequence of states $(\boldsymbol{n}_i)_{i=0}^{n}$, where $\boldsymbol{n}_i = \boldsymbol{n}(t)$ for $t_i \leq t \leq t_{i+1}$ with $t_0 \equiv 0$, $t_{n+1} \equiv t$. See Fig. 2.1 for the schematic diagram explaining this definition. We denote the path probability density with an initial condition $\boldsymbol{n}_0$ by $P(\omega|\boldsymbol{n}_0)$. It becomes

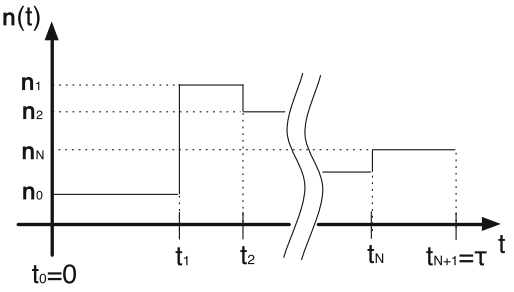


**Fig. 2.1** The schematic diagram to explain the definition of the history of states, $\omega$

$$P(\omega|\boldsymbol{n}_0) = e^{-\lambda(\boldsymbol{n}_0)t_1} \prod_{i=1}^{N} \left[ w(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i) e^{-\lambda(\boldsymbol{n}_i)(t_{i+1}-t_i)} \right] \tag{2.3}$$

or equivalently,

$$P(\omega|\boldsymbol{n}_0) = e^{-\int_0^t d\tilde{t}\lambda(\boldsymbol{n}(\tilde{t}))} \prod_{i=1}^{N} \left[ w(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i) \right] \tag{2.4}$$

For the sake of completeness, we show a simple derivation of the path probability in Appendix A.1.

### *2.2.2 Cumulant Generating Function*

For each transition $\boldsymbol{n}_i \to \boldsymbol{n}_{i+1}$, we define a quantity $\alpha(\boldsymbol{n}_i \to \boldsymbol{n}_{i+1})$. Then, we consider the corresponding time-averaged value $A(\omega)$, which is defined as

$$A(\omega) = \frac{1}{\tau} \sum_{i=0}^{n-1} \alpha(\boldsymbol{n}_i \to \boldsymbol{n}_{i+1}). \tag{2.5}$$

Since the system is Markovian, $A(\omega)$ has a large deviation principle in the limit of $\tau \to \infty$. That is, with a probability density for $A(\omega)$, $p(A)$, shows the following asymptotic form:

$$p(A) \sim e^{-\tau I(A)}, \tag{2.6}$$

where $I(A)$ is a large deviation function. We note that the expected value or typical value of $A(\omega)$, $\langle A(\omega) \rangle$ is determined by a variational principle

$$\langle A(\omega) \rangle = \underset{A}{\text{Argmin}} \left[ I(A) \right]. \tag{2.7}$$

Here, we introduce a scaled cumulant generating function defined by

$$G(h) \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \log \left\langle e^{h\tau A(\omega)} \right\rangle, \tag{2.8}$$

where $h$ is called a biasing parameter. It resembles the definition of the Helmholtz free energy in equilibrium statistical mechanics, so that this function is called a dynamical free energy. Similar to equilibrium thermodynamics, the large deviation function $I(A)$ and the cumulant generating function is connected through Legendre transformation:

$$I(A) = \max_h [hA - G(h)], \tag{2.9}$$

or

$$G(h) = \max_A [hA - I(A)]. \tag{2.10}$$

We should mention that we are now considering the case that $I(A)$ is a concave function. Otherwise, this relationship can be broken. See Ref. [29] for the explanation of the example.

### 2.2.3 Biased Ensemble

In the analysis of a large deviation principle, a class of modified pass probability measure called *an exponential family* or *a biased ensemble*, $P(\omega; h)$, is often studied. With a parameter $h$ representing how much the system is biased, $P(\omega; h)$ is defined as

$$P(\omega; h) = \frac{1}{Z(\tau, h)} P(\omega) e^{h\tau A(\omega)}, \tag{2.11}$$

where $Z(\tau, h)$ is the normalisation constant defined by $Z(\tau, h) = \left\langle e^{h\tau A(\omega)} \right\rangle$. In this biased ensemble, rare trajectories characterised by the large deviation principle of $A(\omega)$ has a large (or small) probability compared with the one in the original ensemble. Indeed, by denoting the probability density of $A(\omega)$ in the biased ensemble by $p(A; h)$, we obtain

$$p(A; h) = \frac{1}{Z(\tau, h)} p(A) e^{h\tau A} \sim \frac{1}{Z(\tau, h)} e^{-\tau(I(A) - hA)}. \tag{2.12}$$

for large $\tau$, where we used the large deviation principle of $A(\omega)$. We first notice that the large deviation function of $A(\omega)$ in the biased ensemble is given as $I(A) - hA$. Then, the following result directly yields: the expected value (or typical value) of $A$ in the biased ensemble is determined by the variational principle

$$\frac{\left\langle A(\omega)e^{h\tau A(\omega)}\right\rangle}{Z(\tau,h)} = \underset{A}{\mathrm{Argmin}}\left[I(A) - hA\right]. \tag{2.13}$$

The typical value is thus deviated from $\langle A(\omega)\rangle$. Furthermore it is connected to the cumulant generating function through

$$\frac{\partial G(h)}{\partial h} = \lim_{\tau\to\infty}\frac{\left\langle A(\omega)e^{h\tau A}\right\rangle}{Z(\tau,h)}. \tag{2.14}$$

Therefore, due to the equivalence between $G(h)$ and $I(A)$, we find a relation connecting the expected value in the biased ensemble with the large deviation function:

$$I(A) = \max_{h}\left[hA - \int_0^h d\tilde{h}\lim_{\tau\to\infty}\frac{\left\langle A(\omega)e^{\tilde{h}\tau A(\omega)}\right\rangle}{Z(\tau,\tilde{h})}\right]. \tag{2.15}$$

### 2.2.4 *Revisit of the Phenomenological Structure for the Large Deviation Principle in Equilibrium Statistical Mechanics*

Here, let us revisit the phenomenological structure for the large deviation principle in equilibrium statistical mechanics with a viewpoint of biased ensemble. The biased ensemble (2.11) reminds us of the canonical distribution function (given in (1.6)). We here show that this similarity leads to the key of the phenomenological structure for the large deviation principle in equilibrium statistical physics.

In the system considered in the introduction 1.2, we define the biased ensemble $p(\Gamma;h)$ by

$$p(\Gamma;h) = \frac{1}{Z(h)}p(\Gamma)e^{hH(\Gamma)}. \tag{2.16}$$

Then, we obtain the distribution function of $U$ in the biased ensemble as

$$p(U;h) = \frac{1}{Z(h)}\Omega(U)e^{-(\beta-h)U} \sim \frac{1}{\tilde{Z}(h)}e^{N[s(u)-(\beta-h)u]}. \tag{2.17}$$

Because no $\beta$ dependence appears here in the first term $s(u)$ of this exponential function, this equation indicates that the biased ensemble is the equilibrium distribution function of the system with temperature $\beta-h$. Thus the biasing parameter $h$ is renormalised as the temperature of the system in another equilibrium system. The same structure, namely the correspondence between biasing parameters and equilibrium intensive parameters, is true not only for the energy density discussed here, but also for the density of general thermodynamic extensive quantities.

This is the key for the phenomenological structure in equilibrium statistical mechanics. Indeed, from this relation, we can connect the large deviation function

$I(U)$ with the expected value of $U$ in another equilibrium system, which has a new temperature $\beta' = \beta - h$. Indeed, by denoting this expected value by $\langle U \rangle_{\beta'=\beta-\tilde{h}}$ and using the corresponding equation to (2.15) in equilibrium statistical mechanics, we have

$$I(U) = \max_h \left[ hU - \int_0^h d\tilde{h} \, \langle U \rangle_{\beta'=\beta-\tilde{h}} \right]. \tag{2.18}$$

In short, the key to the phenomenological structure for the large deviation principle is the physical correspondence of the biased ensemble. Because the biased ensemble corresponds to another equilibrium system, we can construct a large deviation function from expected values.

### 2.2.5 Steady Dynamics Corresponding to Biased Ensemble

The phenomenological structure for the large deviation principle in equilibrium statistical mechanics is clarified in the previous subsection, where we found what we need to construct the same structure in time-series statistics: It is the construction of a physical system corresponding to the biased ensemble (2.11) in time-series statistics. Now, in order to achieve this construction, we follow the following strategy:

1. We define a new transition rate

$$w^h(\boldsymbol{n} \to \boldsymbol{n}') \equiv w(\boldsymbol{n} \to \boldsymbol{n}') f^h(\boldsymbol{n} \to \boldsymbol{n}') \tag{2.19}$$

with an unknown function $f^h(\boldsymbol{n} \to \boldsymbol{n}')$ that depends on $h$. Then, the new path probability $P^h(\omega|\boldsymbol{n}_0)$ is given as

$$P^h(\omega|\boldsymbol{n}_0) = e^{-\int_0^t d\tilde{t} \lambda^h(\boldsymbol{n}(\tilde{t}))} \prod_{i=1}^N \left[ w(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i) \right] \prod_{i=1}^N \left[ f^h(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i) \right], \tag{2.20}$$

where we defined $\lambda^h(\boldsymbol{n}) \equiv \sum_{\boldsymbol{n}'} w^h(\boldsymbol{n} \to \boldsymbol{n}')$.

2. We consider the ratio between this new path probability density and the biased path probability density $P(\omega; h|\boldsymbol{n}_0)$,

$$\frac{P^h(\omega|\boldsymbol{n}_0)}{P(\omega; h|\boldsymbol{n}_0)} = e^{-\int_0^t d\tilde{t} \left[ \lambda^h(\boldsymbol{n}(\tilde{t})) - \lambda(\boldsymbol{n}(\tilde{t})) \right]} \prod_{i=1}^N \left[ f^h(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i) e^{-h\alpha(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i)} \right] Z(t, h). \tag{2.21}$$

Then, we determine $f^h(\boldsymbol{n} \to \boldsymbol{n}')$ so as to make the right-hand side of (2.21) a constant. This construction leads to the conclusion that the new system characterised by $w^h(\boldsymbol{n} \to \boldsymbol{n}')$ has the same path probability density as the one in this modified dynamics. In the following part, we show how to determine $f^h(\boldsymbol{n} \to \boldsymbol{n}')$.

3. First, we look at the product part ($\prod[\cdots]$). For obtaining a benefit from this product structure, we set

$$f^h(\boldsymbol{n} \to \boldsymbol{n}') = e^{h\alpha(\boldsymbol{n}\to\boldsymbol{n}')}\frac{\phi(\boldsymbol{n}')}{\phi(\boldsymbol{n})} \tag{2.22}$$

with an unknown function $\phi(\boldsymbol{n})$. In the product from $i = 1$ to $i = N$, a ratio in this right-hand side will be canceled each other in total. Indeed, the total product becomes

$$\prod_{i=1}^{N}\left[f^h(\boldsymbol{n}_{i-1} \to \boldsymbol{n}_i)e^{-h\alpha(\boldsymbol{n}_{i-1}\to\boldsymbol{n}_i)}\right] = \frac{\phi(\boldsymbol{n}_N)}{\phi(\boldsymbol{n}_0)}. \tag{2.23}$$

Since this right-hand side is small compared with the other parts in large $\tau$ limit, we can neglect it in (2.21).
Second, we determine the unknown function $\phi(\boldsymbol{n})$ so as to make the first exponential part in (2.21) a constant. For this purpose, we set a condition to $\phi(\boldsymbol{n})$ as

$$\lambda^h(\boldsymbol{n}) - \lambda(\boldsymbol{n}) = \text{const.} \equiv K, \tag{2.24}$$

which indeed ensures that that first exponential part a constant $e^{-tK}$. This equation can be rewritten as an eigenvalue problem of an irreducible matrix

$$L^h_{\boldsymbol{n}',\boldsymbol{n}} = w(\boldsymbol{n} \to \boldsymbol{n}')e^{h\alpha(\boldsymbol{n}\to\boldsymbol{n}')} - \delta_{\boldsymbol{n},\boldsymbol{n}'}\lambda(\boldsymbol{n}). \tag{2.25}$$

Indeed, we rewrite (2.24) as

$$\sum_{\boldsymbol{n}'} w(\boldsymbol{n} \to \boldsymbol{n}')e^{h\alpha(\boldsymbol{n}\to\boldsymbol{n}')}\phi(\boldsymbol{n}') - \lambda(\boldsymbol{n})\phi(\boldsymbol{n}) = K\phi(\boldsymbol{n}), \tag{2.26}$$

which is equivalent to

$$\sum_{\boldsymbol{n}'} \phi(\boldsymbol{n}')L^h_{\boldsymbol{n}',\boldsymbol{n}} = K\phi(\boldsymbol{n}). \tag{2.27}$$

Here, we remember that we need to impose a condition that the eigenfunction $\phi(\boldsymbol{n})$ is a positive vector, because the transition matrix $w^h(\boldsymbol{n} \to \boldsymbol{n}')$ can not take a negative value. We thus find that the $K$ is the largest eigenvalue of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ due to Perron-Frobenius theory [30]. Also, we note that the largest eigenvalue $K$ and the corresponding left-eigenvector $\phi(\boldsymbol{n})$ surely exist and are unique, due to this theory.

Therefore, by choosing $\phi(\boldsymbol{n})$ as the left-eigenvector of the largest eigenvalue of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$, we will reach the desired result.

Many formulas similar to this have been derived [20–26]. Exactly the same form as this result was reported in the paper by Jack and Sollich in [23]. For

Langevin systems, the corresponding formulas were also derived independently by us [24, 25] and Chetrite, Touchette [20, 21]. Mathematically, the formula is regarded as the generalisation of Doob's $h$-transform. See Ref. [21] for the details of the explanation.

We mention that the corresponding system is characterised by a variational principle [24–26]. With a variational functional $\tilde{V}(\boldsymbol{n})$, we introduce a variational transition rate $\tilde{w}_h^{\tilde{V}}(\boldsymbol{n} \to \boldsymbol{n}')$ as

$$\tilde{w}_h^{\tilde{V}}(\boldsymbol{n} \to \boldsymbol{n}') = w(\boldsymbol{n} \to \boldsymbol{n}') e^{h\alpha(\boldsymbol{n} \to \boldsymbol{n}') - (1/2)\tilde{V}(\boldsymbol{n}') + (1/2)\tilde{V}(\boldsymbol{n})}. \tag{2.28}$$

Also, we denote the expected value in the stationary state generated by $\langle\, \rangle_h^{\tilde{V}}$, and the escape rate in the system $\tilde{w}_h^{\tilde{V}}(\boldsymbol{n} \to \boldsymbol{n}')$ by $\tilde{\lambda}_h^{\tilde{V}}$. Then, that variational principle is written as

$$w^h(\boldsymbol{n} \to \boldsymbol{n}') = \operatorname*{Argmax}_{\tilde{V}} \left\langle \tilde{\lambda}^{\tilde{V}} - \lambda \right\rangle_h^{\tilde{V}} \tag{2.29}$$

and the maximum value gives the cumulant generating function itself

$$G(h) = \max_{\tilde{V}} \left\langle \tilde{\lambda}^{\tilde{V}} - \lambda \right\rangle_h^{\tilde{V}}. \tag{2.30}$$

This variational principle was studied by us with a motivation to construct the corresponding steady state from *observable quantities of the system* [25]. Indeed, if we apply it to Langevin equation, the escape rate is replaced by an entropy production rate and the variational potential corresponds to the real potential added to the Brownian particle. The mathematical origin of the variational principle is different from the thermodynamic one. Rather, that variational principle is related to Donsker–Varadhan formula for empirical measure [31]. See Appendix A.2 for the derivation of the variational principle from Donsker–Varadhan formula. Furthermore, when the system satisfies detailed balance condition, the variational principle can be connected to the one in quantum mechanics. This is explained in the Chap. 3, where we apply the variational principle to a kinetically constrained model for deriving a scaling function around the phase transition.

Here, we also mention that there is the case that the derivation above is not correct, where the boundary term $\phi(\boldsymbol{n}_N)/\phi(\boldsymbol{n}_0)$ in (2.23) can not be neglected. This problem is one of the origin of the extended fluctuation theorem of heat dissipation, reported by van Zon and Cohen [32, 33]. In Chap. 4, we discussed this connection explicitly.

As a corollary of this formulation, we obtain an equivalence between the largest eigenvalue $K$ and the cumulant generating function $G(h)$:

$$K = G(h). \tag{2.31}$$

Indeed, by using (2.23) and (2.24) in (2.21), we have

$$P^h(\omega|\boldsymbol{n}_0) = P(\omega; h|\boldsymbol{n}_0)e^{-Kt}\frac{\phi(\boldsymbol{n}_N)}{\phi(\boldsymbol{n}_0)}Z(t,h) \tag{2.32}$$

By taking the sum with respect to $\omega$ and considering only the dominant term in large $t$ limit, we obtain

$$K = \lim_{t\to\infty}\frac{1}{t}\log Z(t,h), \tag{2.33}$$

which is (2.31). The cumulant generating function is obtained from the largest eigenvalue problem of $L^h_{\boldsymbol{n},\boldsymbol{n}'}$, and then the result is connected to the large deviate function through Legendre transformation (2.9). Because it is easier to deal with the largest eigenvalue problem than the large deviation principle itself, this structure has been used in many situation for mathematically rigorous analysis in large deviation theory [34]. Furthermore, the relation has been used for analysing non equilibrium systems. The example includes the fluctuation theorem by Lebowitz and Spohn [5], where they found a symmetry property in cumulant generating function of entropy production rate due to the fluctuation theorem.

## 2.3 Main Result

In the previous subsection, we finally understood how we could create the corresponding system to the biased ensemble, where we needed to solve the largest eigenvalue problem of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$. For many body systems, however, it is demanding and almost impossible to solve the corresponding largest eigenvalue problem because the number of the degrees of the freedom in these systems increases exponentially with the system size. Here in order to overcome this difficulty, we propose a method to obtain the corresponding system with measurements and feedbacks.

### *2.3.1 Measurement Formula of $\phi(\boldsymbol{n})$ in Monte-Carlo Simulations*

Because the direct diagonalisation of the largest eigenvalue of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ is hopeless, we rely on Monte-Carlo simulations instead. First, we show a method to obtain $\phi(\boldsymbol{n})$ from Monte-Carlo simulations.

First, we define $\tilde{\psi}(\boldsymbol{n}, t|\boldsymbol{n}_0)$ obtained from the following initial condition and evolution equation:

$$\tilde{\psi}(\boldsymbol{n}, 0|\boldsymbol{n}_0) = \delta_{\boldsymbol{n},\boldsymbol{n}_0} \tag{2.34}$$

$$\frac{\partial\tilde{\psi}(\boldsymbol{n}, t|\boldsymbol{n}_0)}{\partial t} = \sum_{\boldsymbol{n}'}\tilde{\psi}(\boldsymbol{n}', 0|\boldsymbol{n}_0)L^h_{\boldsymbol{n},\boldsymbol{n}'}. \tag{2.35}$$

Then, $\tilde{\psi}(\boldsymbol{n}, t|\boldsymbol{n}_0)$ equals to $\left\langle \delta_{\boldsymbol{n}(t),\boldsymbol{n}} e^{htA(\omega)} \right\rangle_{\boldsymbol{n}_0}$, where $\langle\ \rangle_{\boldsymbol{n}_0}$ is the expected value with respect to the Monte-Carlo simulation with an initial condition $\boldsymbol{n}(0) = \boldsymbol{n}_0$:

$$\tilde{\psi}(\boldsymbol{n}, t|\boldsymbol{n}_0) = \left\langle \delta_{\boldsymbol{n}(t),\boldsymbol{n}} e^{htA(\omega)} \right\rangle_{\boldsymbol{n}_0}. \tag{2.36}$$

The way to prove this is to show that $\left\langle \delta_{\boldsymbol{n}(t),\boldsymbol{n}} e^{htA(\omega)} \right\rangle_{\boldsymbol{n}_0}$ also satisfies (2.34) and (2.35). This is done in Appendix A.3. Next, since $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ is irreducible, the large time behaviour of $\tilde{\psi}(\boldsymbol{n}, t|\boldsymbol{n}_0)$ is

$$\tilde{\psi}(\boldsymbol{n}, t|\boldsymbol{n}_0) \sim \phi(\boldsymbol{n}_0)\psi(\boldsymbol{n})e^{tK}. \tag{2.37}$$

with a definition of $\psi(\boldsymbol{n})$ as the right-largest eigenvector of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$. Thus, by combining (2.36) with (2.37), we arrive at

$$\phi(\boldsymbol{n}) \propto \left\langle e^{htA(\omega)} \right\rangle_{\boldsymbol{n}} \tag{2.38}$$

for large $t$. This is a basic result that directly came from the largest eigenvalue analysis. Thanks to (2.38), we can reach $\phi(\boldsymbol{n})$ just by using a Monte Carlo simulation in principle, however, we will face a difficulty with this formula soon, which is explained next.

### 2.3.2 Rare Events Required for Measurement of $\left\langle e^{hTA(\omega)} \right\rangle_{\boldsymbol{n}}$

Even though we obtain (2.38), it is easy to show that the dominant contribution of the ensemble to obtain $\left\langle e^{htA(\omega)} \right\rangle_{\boldsymbol{n}}$ is rare, which is characterised by a large deviation principle. With the large deviation principle $p(A) \sim e^{-tI(A)}$, we can show that the dominant path takes a value of $A(\omega)$ close to

$$A^*(h) \equiv \underset{A}{\mathrm{Argmin}}\,[I(A) - hA]. \tag{2.39}$$

Then, the probability taking $A^*(h)$ is exponentially small:

$$p(A^*) \sim e^{-tI(A^*(h))} \tag{2.40}$$

with $I(A^*(h)) \neq 0$. This means that we need the rare events characterised by a large deviation principle, in order to obtain the information of the large deviation principle itself. We thus conclude that the direct application of (2.38) is not useful. We need some ideas to overcome this difficulty.

### 2.3.3 Renormalisation of Rare-Eventness via Measurements and Feedbacks

Now, we explain the key idea of our method. It is composed of two parts: Firstly, we consider small values of $h$ in (2.40), more precisely, sufficiently small so that it satisfies

$$t_a I(A^*(h)) = O(1), \tag{2.41}$$

where $t_a$ is the correlation time of $\alpha(\boldsymbol{n} \to \boldsymbol{n}')$. Then, we can easily say that the dominant contribution to obtain $\left\langle e^{htA(\omega)} \right\rangle_{\boldsymbol{n}}$ is not rare, which is, in other words, $\left\langle e^{htA(\omega)} \right\rangle_{\boldsymbol{n}}$ is measurable for sufficiently small $h$. Secondly, the exponentially biased measure $P(\omega; h|\boldsymbol{n}_0)$ has a renormalisable structure with respect to the biasing with exponential function. That is,

$$P(\omega; h + h'|\boldsymbol{n}_0) \propto P(\omega; h|\boldsymbol{n}_0) e^{h'tA(\omega)}. \tag{2.42}$$

These two ideas lead to a method of the rare event sampling method. First, for sufficiently small $h$, we measure $\left\langle e^{htA(\omega)} \right\rangle_{\boldsymbol{n}}$. Then, by using the obtained result, we modify the transition rate to create the (probability preserving) system corresponding to the biased measure $P(\omega; h|\boldsymbol{n}_0)$. Then, again in the new system, we measure $\left\langle e^{htA(\omega)} \right\rangle_{\boldsymbol{n}}$ for sufficiently small $h$. Thanks to the property (2.42), the obtained result will lead to the next system corresponding to the biased ensemble $P(\omega; 2h|\boldsymbol{n}_0)$. In this method, just with measuring $e^{htA(\omega)}$, we could reach the biased ensemble $P(\omega; 2h|\boldsymbol{n}_0)$. This is the important property in the rare events of the large deviation principle in time-series statistics. This property can be phrased as follows: *Rare events characterised by the large deviation principle of time-averaged quantity is additive in a sense of measurement. The rare-eventness can be renormalised during the measurements through a feedback (or a modification) to the system.* See Fig. 2.2 for the schematic diagram of this structure.

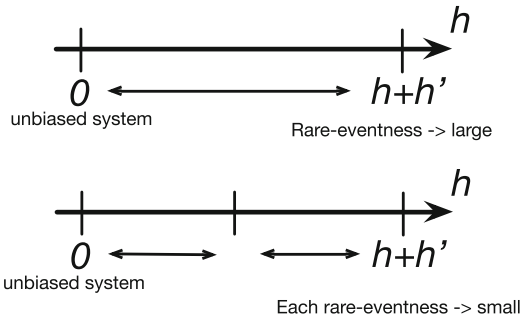


**Fig. 2.2** The schematic diagram for renormalisability of rare-eventness

### 2.3.4 Rare-Event Sampling Method Constituted of an Iterative Measurement-and-Feedback Procedure

By using the property explained above, we propose a method for rare-events sampling method constituted of an iterative measurement-and-feedback procedure.

First we set a measurement time $t$ to be much larger than the correlation time of $\alpha(\boldsymbol{n} \to \boldsymbol{n}')$, $t_\alpha$. Then, we define a small increment $\delta h$ from the condition (2.41), or more precisely,

$$t_a \delta h^2 \sigma = O(1), \tag{2.43}$$

where $\sigma$ is a scaled variance of $A(\omega)$ defined as

$$\sigma = \lim_{t\to\infty} t \left\langle A(\omega)^2 - (\langle A(\omega)\rangle)^2 \right\rangle. \tag{2.44}$$

With this $\delta h$, the procedure is defined as follows:

1. For the first step, we measure $\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}}$ as a function of $\boldsymbol{n}$ in the original system. Here, we remind us that the measurement is not hard because of the condition (2.43).
2. Then, depending on the value of $\left\langle e^{\tau\delta h A(\tau)} \right\rangle_{\boldsymbol{n}}$, we modify the transition rate to

$$w^{\delta h}(\boldsymbol{n} \to \boldsymbol{n}') = w(\boldsymbol{n} \to \boldsymbol{n}') e^{\delta h \alpha(\boldsymbol{n}\to\boldsymbol{n}')} \frac{\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}'}}{\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}}}. \tag{2.45}$$

3. Next, in the created modified system, we measure the expected value of the same quantity $e^{\tau\delta h A(\omega)}$. We denote the obtained expected value by $\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}}^{\delta h}$.
4. Again, we define the second modified transition rate as

$$w^{2\delta h}(\boldsymbol{n} \to \boldsymbol{n}') = w^{\delta h}(\boldsymbol{n} \to \boldsymbol{n}') e^{\delta h \alpha(\boldsymbol{n}\to\boldsymbol{n}')} \frac{\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}'}^{\delta h}}{\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}}^{\delta h}}. \tag{2.46}$$

5. We iterate this procedure for many times. Then, we obtain a set of transition rates

$$w^{l\delta h}(\boldsymbol{n} \to \boldsymbol{n}') = w(\boldsymbol{n} \to \boldsymbol{n}') e^{l\delta h \alpha(\boldsymbol{n}\to\boldsymbol{n}')} \prod_{k=0}^{l-1} \frac{\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}'}^{k\delta h}}{\left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}}^{k\delta h}} \tag{2.47}$$

   with $l = 0, 1, 2, \ldots$.
6. Our computational method is based on the following formula. We denote by $\langle f \rangle^h$ the expected value of time-extensive quantities $f(\omega)$ in the system with the modified transition rate $w^h$ ($h = 0, \delta h, 2\delta h, \ldots$). Then, $\langle f \rangle^h$ equal to the expected values by biased ensemble $P(\omega; h)$. That is,

$$\langle f(\omega)\rangle^h \simeq \frac{\left\langle f(\omega)e^{h\tau A(\omega)}\right\rangle}{\left\langle e^{h\tau A(\omega)}\right\rangle}. \tag{2.48}$$

Here and hereafter in this chapter, $\simeq$ represents the asymptotic equality when $\tau \gg \tau_\alpha$.

7. From the formula, we obtain the expected value of any quantity in biased ensemble. For example, for the large deviation function of $A(\omega)$, by combining (2.48) with (2.15), we reaches a formula

$$I(A) = \max_h \left[ hA - \sum_{k=0}^{N-1} \langle f(\omega)\rangle^{\tilde{h}}\, \delta h \right] + O(\delta h^2) \tag{2.49}$$

with $h = N\delta h$. We write this formula as

$$I(A) = \max_h \left[ hA - \int_0^h d\tilde{h}\, \langle f(\omega)\rangle^{\tilde{h}} \right], \tag{2.50}$$

which shows the correspondence to the formula (2.18) in equilibrium statistical mechanics.

We showed the basic strategy to derive (2.48) in the previous subsection. For a mathematically rigorous derivation, see Appendix A.4.

## 2.4 Applications

As a demonstration, we apply our method to non-equilibrium many-body lattice gas models. The first example is an asymmetric simple exclusion process (ASEP) with non equilibrium open boundary conditions, and the second one is Fredrickson–Andersen (FA) model, which is one of kinetically constrained models.

### *2.4.1 Effective Descriptions of Exponential Family*

Before going to the demonstration, we here introduce a strategy to approach many body systems. That is, *effective descriptions of the exponential family*.

The rare trajectories most contributing to $G(h)$ are generated by the modified transition rate $w^h(\boldsymbol{n} \to \boldsymbol{n}')$ in (2.47). Then, the modification rate $\prod_{k=0}^{l-1} \left\langle e^{\tau\delta h A(\omega)}\right\rangle_{\boldsymbol{n}}^{k\delta h}$ in (2.47) is a function of the configuration of the system. Thus, it may be difficult to apply the method to many-body systems, because the degree of the freedom in them exponentially increases and the computation time for obtaining $w^h(\boldsymbol{n} \to \boldsymbol{n}')$ does as well.

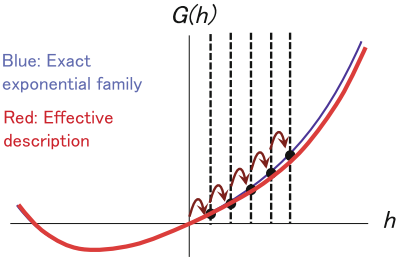


**Fig. 2.3** Schematic picture explaining the effective description of exponential family

However, we expect that there are many physical examples that allow us to use the *effective description of the exponential family*. It is to introduce an effective transition rate with $K$ unknown parameters for each value of $h$, where these unknown parameters are determined by employing (2.47). We then assume that these effective descriptions describe very well the statistical property of the rare trajectories. See Fig. 2.3 for the explanation of this effective description. The system that we are going to analyse in this section has indeed these effective descriptions.

## 2.4.2 Asymmetric Simple Exclusion Process (ASEP)

### Definition of the Model

Let us consider a one dimensional lattice of size $L$ with open boundary conditions. Each site accommodates one particle at most. The configuration of the particles is denoted by $\boldsymbol{n} \equiv (n_i)_{i=1}^{L}$, where $n_i$ takes a value of 1 (occupied) or 0 (empty). The transition rate $w(\boldsymbol{n} \to \boldsymbol{n}')$ is defined as follows: For a configuration $\boldsymbol{n} = (n_1, n_2, n_3, \ldots, n_i, n_{i+1}, \ldots, n_L)$, we define an exchange operator $F_{i,i+1}$ as

$$F_{i,i+1}\boldsymbol{n} = (n_1, n_2, n_3, \ldots, n_{i+1}, n_i, \ldots, n_L). \tag{2.51}$$

Also we define a removing, or filling operator $F_1$ and $F_L$ for the boundaries as

$$F_1 = (1 - n_1, n_2, n_3, \ldots, n_i, n_{i+1}, \ldots, n_L) \tag{2.52}$$

and

$$F_L = (n_1, n_2, n_3, \ldots, n_i, n_{i+1}, \ldots, 1 - n_L). \tag{2.53}$$

Then, by using these operators, we define $w(\boldsymbol{n} \to \boldsymbol{n}')$ as

$$w(\boldsymbol{n} \to F_{i,i+1}\boldsymbol{n}) = \delta_{n_i,0}\delta_{n_{i+1},1}q + \delta_{n_i,1}\delta_{n_{i+1},0}, \tag{2.54}$$

$$w(\boldsymbol{n} \to F_1\boldsymbol{n}) = \delta_{n_1,0}\alpha + \delta_{n_1,1}\gamma, \tag{2.55}$$

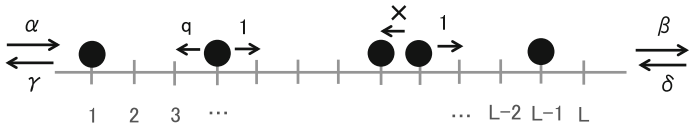


**Fig. 2.4** Schematic picture representing the definition of ASEP

$$w(\boldsymbol{n} \to F_L \boldsymbol{n}) = \delta_{n_L,0}\delta + \delta_{n_L,1}\beta, \tag{2.56}$$

and

$$w(\boldsymbol{n} \to \boldsymbol{n}') = 0 \tag{2.57}$$

for any other transition that cannot be expressed by using the operators $F_{i,i+1}$, $F_1$, and $F_L$. Equation (2.54) means that a particle moves to the left empty site with a rate $q$ and to the right empty site with a rate 1, when the target site is not occupied. Equation (2.55) and (2.56) represents the injection and the remove of a particle: A particle is injected into the boundary site $i = 1$ ($i = L$) with a rate $\alpha$ ($\delta$) and the particle at the boundary site $i = 1$ ($i = L$) is removed with a rate $\gamma$ ($\beta$). See Fig. 2.4 for the schematic picture to explain these transitions. This model is called ASEP and has been studied as a cornerstone of non-equilibrium physics. See the introduction of Ref. [17] and also Ref. [35] for the review.

In this model, we study the fluctuation of time-averaged bulk current. We first define an instantaneous current at $i$th site as $j_i(\boldsymbol{n} \to \boldsymbol{n}') = \pm 1$, which takes the value 1 (or $-1$) when a particle moves from $i$ to $i+1$ ($i+1$ to $i$). By using this instantaneous current, we then define the bulk current as

$$\alpha(\boldsymbol{n} \to \boldsymbol{n}') = \frac{1}{L-1}\sum_{i=1}^{L-1} j_i(\boldsymbol{n} \to \boldsymbol{n}'). \tag{2.58}$$

The time-averaged bulk current $A(\omega)$ is defined as the time-averaged quantity of this $\alpha(\boldsymbol{n} \to \boldsymbol{n}')$. See Sect. 2.2.2 for the definition or $A(\omega)$.

**Numerical Check of Our Formulation**

We first verify our formulation numerically. On one hand, we evaluate

$$\prod_{k=0}^{l-1} \left\langle e^{\tau\delta h A(\omega)} \right\rangle_{\boldsymbol{n}}^{k\delta h} \tag{2.59}$$

for a integer $l$, which is the modification factor appeared in (2.47). On the other hand, with a Monte Carlo simulation, we evaluate the left-eigenvector $\phi(\boldsymbol{n})$ corresponding to the largest eigenvalue of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ defined in (2.25). According to our formulation, (2.59) is proportional to $\phi(\boldsymbol{n})$, which can be seen by comparing (2.22) with (2.47). See Fig. 2.5 for the examples of the obtained results.

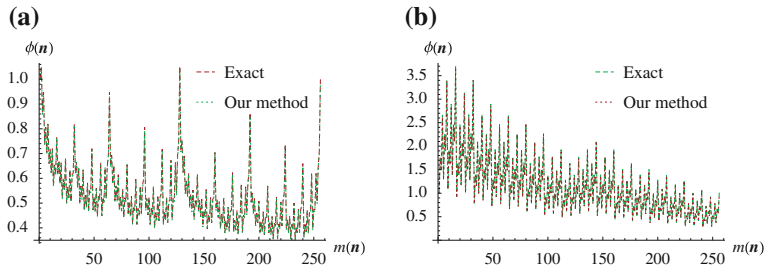


**Fig. 2.5** Numerical check of our formulation for the open boundary ASEP. We set $q = 0.5$, $L = 8$, $\alpha = 0.8$, $\beta = 0.8$, $\gamma = 0.2$, and $\delta = 0.2$. We perform our computational method on Monte Carlo simulations with setting $l = 100$ and 300 with $\delta h = -0.02$. The obtained $\prod_{k=0}^{l-1} \langle e^{\tau \delta h A(\omega)} \rangle_{\boldsymbol{n}}^{k\delta h}$ are plotted on **a** (for $l = 100$) and **b** (for $l = 300$) labeled as our method. In the figure, the $x$ axis represents $m(\boldsymbol{n}) = \sum_{i=0}^{L-1} n_{L-i} 2^i$, which is the decimal value of the binary number $\boldsymbol{n}$. On the same figures, we also plot $\phi(\boldsymbol{n})$ that is the left eigenvector corresponding to the largest eigenvalue of $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ defined in (2.25) for $h = -2$ and $h = -6$ (Exact). In these two figures, we can see the coincidence very well between $\prod_{k=0}^{l-1} \langle e^{\tau \delta h A(\omega)} \rangle_{\boldsymbol{n}}^{k\delta h}$ and $\phi(\boldsymbol{n})$. Reprinted with permission from Ref. [27]. Copyright 2014 by American Physical Society

### The Effective Description

Next, we study an effective description of the exponential family. First, we define an effective transition rate $w^h_{\text{eff}}(\boldsymbol{n} \to \boldsymbol{n}')$ with $L+1$ unknown parameters $(\psi_{h,i})_{i=0}^{L}$ as

$$w^h_{\text{eff}}(\boldsymbol{n} \to F_{i,i+1}\boldsymbol{n}) \equiv w(\boldsymbol{n} \to F_{i,i+1}\boldsymbol{n}) e^{(n_i - n_{i+1})h/(L-1)} \left( \frac{\psi_{h,i+1}}{\psi_{h,i}} \right)^{n_i - n_{i+1}}. \quad (2.60)$$

For the left and right boundary transitions, we also define

$$w^h_{\text{eff}}(\boldsymbol{n} \to F_1\boldsymbol{n}) \equiv w(\boldsymbol{n} \to F_1\boldsymbol{n})(\psi_{h,1}/\psi_{h,0})^{1-2n_1} \quad (2.61)$$

and

$$w^h_{\text{eff}}(\boldsymbol{n} \to F_L\boldsymbol{n}) \equiv w(\boldsymbol{n} \to F_L\boldsymbol{n})(\psi_{h,L}/\psi_{h,0})^{1-2n_L}. \quad (2.62)$$

Here, we note that this new transition rate corresponds to an ASEP that has a spatially varying transition rate as shown in Fig. 2.6. Furthermore, in a sense of local detailed balance condition [1], the effective transition rate represents the system, where a one-body external potential is applied.

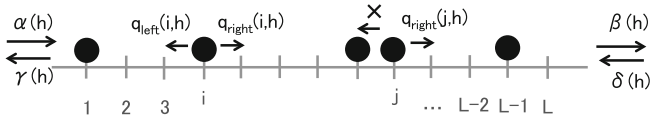


**Fig. 2.6** An example of an effective description for ASEP. In this figure, each transition rate is given as follows: $q_{\text{left}}(i,h) = qe^{-h/(L-1)}\psi_{h,i-1}/\psi_{h,i}$, $q_{\text{right}}(i,h) = qe^{h/(L-1)}\psi_{h,i+1}/\psi_{h,i}$, $\alpha(h) = \alpha\psi_{h,1}/\psi_{h,0}$, $\gamma(h) = \gamma\psi_{h,0}/\psi_{h,1}$, $\beta(h) = \beta\psi_{h,0}/\psi_{h,L}$ and $\delta(h) = \delta\psi_{h,L}/\psi_{h,0}$

We determine the values of the parameters $(\psi_{h,i})_{i=0}^{L}$ from our computational method as follows:

1. For $l = 0$ ($h = 0$), we have $\psi_{h,i} = 1$ for $i = 0, \ldots, L$.
2. For given $(\psi_{l\delta h,i})_{i=0}^{L}$, we determine the next $(\psi_{(l+1)\delta h,i})_{i=0}^{L}$ from the following procedure: We measure $\left\langle e^{\tau\delta h A(\omega)}\right\rangle_{\boldsymbol{n}}^{l\delta h}$ for $L+1$ different configurations $\boldsymbol{n} = \boldsymbol{n}_j$ ($j = 0, 1, 2, \ldots, L$). Especially, here, we choose $(\boldsymbol{n}_j)_i = \delta_{ij}$ as the simplest choice.
3. Next, by applying (2.47) to the effective transition rate (2.60), we obtain

$$\psi_{(l+1)\delta h,i} = \psi_{l\delta h,i} \left\langle e^{\tau\delta h A(\omega)}\right\rangle_{\boldsymbol{n}_i}^{l\delta h} \tag{2.63}$$

   for $i = 0, \ldots, L$. Thus, we obtain the next parameters $(\psi_{(l+1)\delta h,i})_{i=0}^{L}$ from $(\psi_{l\delta h,i})_{i=0}^{L}$.
4. By iterating this procedure, we obtain the effective description of the exponential family.

Now, we apply our computational method to Monte-Carlo simulations. We calculated $G(h)$, then plot it in Fig. 2.7. On the same figure, for the comparison, we also plot the largest eigenvalue of $L^{h}_{\boldsymbol{n},\boldsymbol{n}'}$, $K$, because it is equal to $G(h)$ as shown in (2.31). For further comparison, we also plot the truncated cumulant expansions up to the second order: $G_2(h) = hg_1 + h^2 g_2$ and the fourth order: $G_4(h) = hg_1 + h^2 g_2 + h^3 g_3 + h^4 g_4$, where the coefficients $g_i$ are defined as $(1/i!)\partial^i G(h)/\partial h^i|_{h=0}$. These coefficients are calculated from the exact formula in Refs. [17, 19]. Even though one can see a small deviation between our result (red dotted line) and the exact result (green dashed line) around $h = -7$, the accuracy of our one is considerably better than the one for the truncated cumulant expansions (blue and yellow solid lines). We thus claim that *rare fluctuations of the ASEP in a sense of the large deviation of the current*

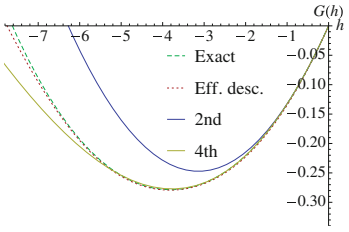


**Fig. 2.7** $G(h)$ in the open boundary ASEP obtained from our effective description. We set $q = 0.5$, $L = 8$, $\alpha = 0.8$, $\beta = 0.8$, $\gamma = 0.2$, and $\delta = 0.2$. Following the procedure for the effective description described in the text, we perform Monte Carlo simulations with fixed $\delta h = -0.02$. The result is labeled as Eff. desc. For comparison, we also plot the largest eigenvalue of $L^{h}_{\boldsymbol{n},\boldsymbol{n}'}$ (Exact), the truncated cumulant expansions up to the second order: $G_2(h) = hg_1 + h^2 g_2$ (2nd) and the fourth order: $G_4(h) = hg_1 + h^2 g_2 + h^3 g_3 + h^4 g_4$ (4th), where the coefficients $g_i$ are defined as $(1/i!)\partial^i G(h)/\partial h^i|_{h=0}$. These coefficients are calculated from the exact formula in Refs. [17, 19]. Reprinted with permission from Ref. [27]. Copyright 2014 by American Physical Society

*with this parameter set are well described by the effective transition rate* (2.60).We expect that there are some mathematical formulas related to this observation.For this, we mention a variational principle determining the large deviation function of the current in lattice gas models in thermodynamic limit (infinite size limit), which was proposed in [7, 8]. In the paper, Bodineau and Derrida derived the formula from a phenomenology called *an additivity principle.* If we restrict ourselves to the system of SSEP or (WASEP), this variational principle, on the other side, can be derived from the general variational principle given as (2.30). In the derivation, we assume the effective transition rate in thermodynamic limit [36]. We need further investigation for clarifying the applicability of this effective-description approach upon general lattice gas models.

### *2.4.3 Fredrickson–Andersen (FA) Model*

#### Definition of the Model

Next, we consider a Fredrickson–Andersen (FA) model [37, 38]. This is an example of kinetically constrained models (KCMs), which has been studied for understanding the glassy features from the dynamical aspect of the system. We define an occupation variable $n_i = 1$ or 0 on each site of a one-dimensional lattice. The size of the lattice is $L$, and the boundary condition is periodic. For a configuration $\boldsymbol{n} = (n_1, \ldots, n_L)$, we define a flipping operator $C_i$ as

$$C_i \boldsymbol{n} = (n_1, \ldots, 1 - n_i, \ldots, n_L). \tag{2.64}$$

Then, from a configuration $\boldsymbol{n}$ to $C_i \boldsymbol{n}$, we define the corresponding transition rate as

$$w(\boldsymbol{n} \to C_i \boldsymbol{n}) = [(1 - c)n_i + c(1 - n_i)] f_i(\boldsymbol{n}), \tag{2.65}$$

with the definition of $f_i(\boldsymbol{n})$ as

$$f_i(\boldsymbol{n}) \equiv n_{i-1} + n_{i+1}. \tag{2.66}$$

See Fig. 2.8 for the schematic picture explaining the definition of this FA model. The transition rate is a product of two parts. The one is a part without any interaction $[(1-c)n_i + c(1-n_i)]$, and the other one is a part for the kinetically constraint $f_i(\boldsymbol{n})$. Only the first part takes responsibility for the stationary state. Indeed, if we consider the detailed balance condition, $f_i(\boldsymbol{n})$ is canceled out. Then the stationary probability $p(\boldsymbol{n})$ is just determined from this non interacting part $[(1 - c)n_i + c(1 - n_i)]$, which leads to

$$p(\boldsymbol{n}) = \prod_{i=1}^{L} [cn_i + (1 - c)(1 - n_i)]. \tag{2.67}$$

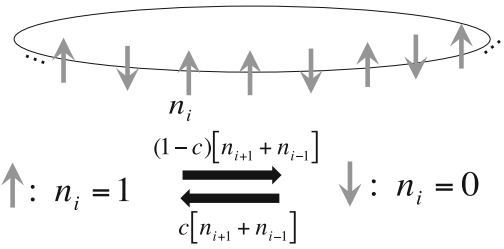


**Fig. 2.8** Schematic picture explaining FA model

The second part $f_i(\boldsymbol{n})$ actually represents a kinetic constraint. For example, we look at the configuration, where $i$th site is surrounded by unoccupied site. In this case, the flipping is indeed blocked due to $f_i(\boldsymbol{n})$. Although the stationary state is trivial, the system shows the same features as the one in glassy systems, due to this kinetic constraint. See Ref. [15, 39] for this review. Recently, for studying these features, the approach using a large deviation principle gathered attention. In 2007, Garrahan, Jack, Lecomte, Pitard, van Duijvendijk and van Wijland considered a dynamical activity defined as

$$\alpha(\boldsymbol{n} \to \boldsymbol{n}') = 1, \tag{2.68}$$

which represents how often the state of the system changes. Then, in several KCMs, they numerically calculated the cumulant generating function of this time-averaged activity, and found the singularity in it in $L \to \infty$ [15, 16, 40]. This represents a dynamical phase transition of the system, which is believed to be related to dynamical heterogeneities. After the finding, the finite size effect of the singularity has been studied by Bodineau, Lecomte and Toninelli [41, 42]. Since the system that we can simulate is always finite, the study to extract the property of dynamical phase transition from finite-size systems is important. In this section, we approach to this problem with our formulation, especially, by looking at the effective description of the system.

**The Effective Description**

First, we define the effective transition rate as

$$w^h_{\mathrm{eff}}(\boldsymbol{n} \to C_i\boldsymbol{n}) \equiv w(\boldsymbol{n} \to C_i\boldsymbol{n}) e^h [C^h((n_{i\pm j})^r_{j=1})]^{1-2n_i}, \tag{2.69}$$

where $r$ is a truncating number of the interaction range and the function $C^h((n_{i\pm j})^r_{j=1})$ is an unknown function of local variables. See Fig. 2.9 for the schematic picture explaining this effective transition rate. This is defined for investigating how much the long-rang interactions can affect the dynamical phase transition. The transition rate becomes more accurate as $r$ increases up to $r \simeq L/2$. For fixed $r$, like the application to ASEP in the previous subsection, we determine the function $C^h((n_{i\pm j})^r_{j=1})$ as follows:

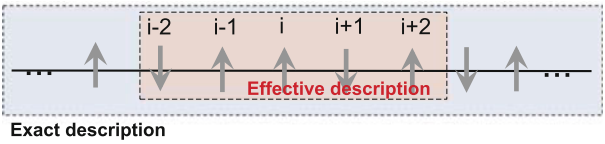


**Fig. 2.9** Schematic picture explaining an example of the effective description in FA model

1. For $l = 0$ ($h = 0$), we have $C^h((n_{i\pm j})_{j=1}^r) = 1$.
2. For given $C^{l\delta h}((n_{i\pm j})_{j=1}^r)$, we determine the next $C^{(l+1)\delta h}((n_{i\pm j})_{j=1}^r)$ with the following procedure: We measure $\left\langle e^{\tau\delta h A(\omega)}\right\rangle_{\boldsymbol{n}}^{l\delta h}$ for $2^{2r+1}$ different configurations $\boldsymbol{n} = \boldsymbol{n}_j$ ($j = 1, 2, \ldots, 2^{2r+1}$). Here, we choose $\boldsymbol{n}_j = (0, n_2, \ldots, n_{r+1}, 0, \ldots, 0, n_{L-r+1}, \ldots n_L)$ with $n_i = 1$ or 0 ($i = 2, \ldots, r+1, L-r+1 \ldots, L$) and $\boldsymbol{n}_j = (1, n_2, \ldots, n_{r+1}, 0, \ldots, 0, n_{L-r+1}, \ldots n_L)$ with $n_i = 1$ or 0 ($i = 2, \ldots, r+1, L-r+1 \ldots, L$). Because the system has translational invariance, we can regard the site $i = 1$ as the centre of the system without loss of generality.
3. Next, by applying (2.47) to the effective transition rate (2.60), we obtain

$$C^{(l+1)\delta h}((n_{1\pm j})_{j=1}^r) = C^{l\delta h}((n_{1\pm j})_{j=1}^r)\frac{\left\langle e^{\tau\delta h A(\omega)}\right\rangle_{C_1\boldsymbol{n}}^{l\delta h}}{\left\langle e^{\tau\delta h A(\omega)}\right\rangle_{\boldsymbol{n}}^{l\delta h}} \tag{2.70}$$

   for $i = 1, \ldots, 2^{2r+1}$. Thus, we obtain the next parameters $C^{(l+1)\delta h}((n_{1\pm j})_{j=1}^r)$ from $C^{l\delta h}((n_{1\pm j})_{j=1}^r)$.
4. By iterating this procedure, we obtain the effective description of the exponential family.

First, we check the validity of our formulation by launching Monte Carlo simulations for small system sizes. We diagonalise the matrix $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ defined in (2.25), then we calculate

$$\phi(C_1\boldsymbol{n})/\phi(\boldsymbol{n}) \tag{2.71}$$

with $\boldsymbol{n} = (0, n_2, \ldots, n_{r+1}, 0, \ldots, 0, n_{L-r+1}, \ldots n_L)$, which corresponds to $C^h((n_{1\pm j})_{j=1}^r)$ in our formulation. The examples of this result are shown in Fig. 2.10a.

Next, we investigate the long-range nature of the dynamical phase transition. We fix relatively large values of $L$, where the direct diagonalization of the matrix $L^h_{\boldsymbol{n}',\boldsymbol{n}}$ is too demanding. Then, we launch the Monte Carlo simulations and obtain $G(h)$ for several values of $r$. On the other hand, we apply the population dynamics method to the same system, which is a numerical technique to calculate large deviation functions [43, 44]. We plot all the obtained results in Fig. 2.10b. In the figure, we can see that the curves obtained $r = 3, 4$ shows the convergence, especially for the region $h < 0$. Since this part $h < 0$ takes responsibility for the dynamical phase transition explained above [41, 42], this result suggests that the long-range interactions for the modified transition rate is not relevant to it. We mention that the long-range nature of

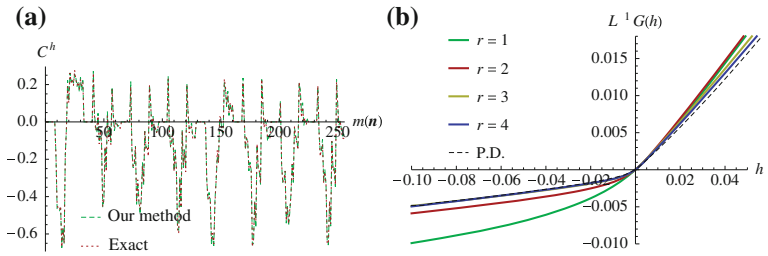


**Fig. 2.10** Statistical properties of an activity for the FA model with $c = 0.3$. **a** We set $L = 10, r = 4$, $l = 40$ and $\delta h = -0.0025$, then we perform our formulation. We plot obtained $C^{l\delta h}((n_{1+j})_{j=1}^{r})$ (Our method), where the $x$ axis represents $m(\boldsymbol{n}) = \sum_{i=0}^{r-1} n_{L-i}2^i + \sum_{i=r}^{2r-1} n_{2r+1-i}2^i$. On the same figure, we also plot $\phi(C_1\boldsymbol{n})/\phi(\boldsymbol{n})$ with $\boldsymbol{n} = (0, n_2, \ldots, n_{r+1}, 0, \ldots, 0, n_{L-r+1}, \ldots n_L)$ obtained from the left eigenvector corresponding to the largest eigenvalue of $L^h_{\boldsymbol{n},\boldsymbol{n}'}$ for $L = 10$ with $h = -0.1$ (Exact). **b** We set $L = 30$ and $\delta h = -0.0025$, and we perform our formulation for several $r$. The obtained $G(h)/L$ are plotted on the figure. At the same time, we also perform the population dynamics method [43, 44] for obtaining $G(h)/L$. The obtained result is plotted as a black dashed line (P. D.) in the figure. Reprinted with permission from Ref. [27]. Copyright 2014 by American Physical Society

the effective interactions has also been studied very recently in Ref. [45] for the East model. They solved analytically a variational principle that characterises modified systems (which is the same as the one that we explained in Sect. 2.2.5). Then, they focused on the part $h > 0$ and concluded that the long range interaction could not be negligible. This result is not contradictory to ours, because they focused on the different region of $h$, and also, they measured different quantities from ours. Indeed, in Fig. 2.10b for $h > 0$, we can see a small difference between results with effective interactions and the one with population dynamics.

In this system, for investigating the singular behaviour of $G(h)$ more precisely, a scaled biasing parameter $\tilde{h} \equiv hL$ has been introduced by Bodineau, Lecomte, and Toninelli [41, 42]. They proved that

$$\tilde{G}(\tilde{h}) = G(\tilde{h}/L) \tag{2.72}$$

is not an analytic function in the limit $L \to \infty$. However, the nature of the singularity, for example how the singularity arrises as the system size becomes larger, has not been understood yet. The problem was in the numerical study of it because the population dynamics method does not exhibit good convergence of $\tilde{G}(\tilde{h})$ for relatively large values of $L$ [41]. In Appendix A.5, we show that our method can also be applied for obtaining the reliable $L$ dependence of $\tilde{G}(\tilde{h})$ even in this situation.

## 2.5 Conclusion

In this chapter, we studied the phenomenological structure for the large deviation principle in time-series statistics. By using this structure, we proposed a rare-event sampling method composed of a measurement and feedback, which produced a set of transition rates that had the same statistical properties as those in the biased ensemble of large deviation statistics. For applying the method to spatially extended many-body systems, where the number of degrees of freedom increased exponentially, we also proposed a method to construct an effective description of the biased ensemble. The example of the effective description is as follows: For the case of ASEP, spatially varying one-body potentials instead of many-body potentials can be this effective description. For FA model, the finite-size effect of dynamical phase transition appearing in $G(h)$ is well described by the effective description without long-range interactions.

Here, we mention a future possibility related to this effective description. In order to get a good effective description, physical intuition and some efforts with trial-and-error are needed. But once after we get a good effective description, the computation time of large deviation statistics will be shortened very much. What we need to know now is the theory to determine such effective descriptions automatically if a system is given. For constructing this theory, we need many examples of effective descriptions in many systems. We start with a simple problem such as heat conduction, then increase the complexity of the problem gradually. One of the challenging goals to achieve is to find an effective description of fully-developed turbulence. (See Conclusion for the detail.) Since there is an important problem related to rare-events in turbulence, such a description, if it is found, will certainly promote the understanding of turbulence, especially from a viewpoint of rare-event sampling application to real experiments.

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