

Stochastic Dynamics of Discrete Curves and Multi-Type Exclusion Processes

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This study deals with continuous limits of interacting one-dimensional diffusive systems, arising from stochastic distortions of discrete curves with various kinds of coding representations. These systems are essentially of a reaction-diffusion nature. In the non-reversible case, the invariant measure has in general a non Gibbs form. The corresponding steady-state regime is analyzed in detail, by using a tagged particle together with a state-graph cycle expansion of the probability currents. As a consequence, the constants appearing in Lotka–Volterra equations—which describe the fluid limits of stationary states—can be traced back directly at the discrete level to tagged particle cycles coefficients. Current fluctuations are also studied and the Lagrangian is obtained via an iterative scheme. The related Hamilton–Jacobi equation, which leads to the large deviation functional, is investigated and solved in the reversible case, just for the sake of checking.

KEY WORDS: exclusion process, Gibbs state, hydrodynamic limit, functional equation, current, Hamilton–Jacobi

1. INTRODUCTION

Interplay between discrete and continuous description is a recurrent question in statistical physics, which in some cases can be addressed quite rigorously via probabilistic methods. In the context of reaction-diffusion systems this amounts to studying fluid or hydrodynamic limits, and number of approaches have been proposed, in particular in the framework of exclusion processes, see Refs. 8, 23, 25, 30 and references therein. As far as the above limits are at stake, all these methods have in common to be limited to systems having stationary states given in closed product form, or at least to systems for which the invariant measure for finite N is explicitly known. For instance, ASEP with open boundary are described

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in terms of matrix product forms (really a sort of non-commutative product form), and the continuous limits can be understood by means of Brownian bridges.⁽⁹⁾ We propose to tackle these problems from a different view-point. The initial objects are discrete sample paths enduring stochastic deformations, and our primary concern is to understand the nature of the limit curves, when N goes to infinity: how do they evolve in time, and which limiting process do they represent as t goes to infinity: in other words, what are the equilibrium curves? Following Refs. 15 and 16, we give here some partial answers to these questions.

In Ref. 15 a specific model was considered, namely paths on the square lattice, and we could reformulate the problem in terms of coupled exclusion processes, to understand the thermodynamic equilibrium and a phase transition point above which curves reach a deterministic profile, solution of a nonlinear dynamical system which was solved explicitly by means of elliptic functions. Two extensions of this system were introduced in Ref. 16:

- one which comprises multi-type exclusion particle systems encountered in another context (see e.g. Refs. 13, 14), including the *ABC* model for which similar features occur;⁽⁷⁾
- a tri-coupled exclusion process to represent the stochastic dynamics of curves in the three-dimensional space.

With this extended formulation, we provided a set of general conditions for reversibility, by analyzing cycles in the state space and the corresponding invariant measure.

This paper focuses on non-Gibbs states and transient regimes. In another work in progress,⁽¹⁷⁾ we analyze the asymmetric simple exclusion process (ASEP) on a torus. Under suitable initial conditions, the usual sequence of empirical measures converges in probability to a deterministic measure, which is the unique weak solution of a Cauchy problem. The method presents some new features, and relies on the analysis of a family of parabolic differential operators, involving variational calculus. This approach let hope for a pretty large level of generalization, and we are working over its general conditions of validity.

Sections 3 and 4 are devoted to the stationary regime, for which, from Refs. 15 and 16, the limit curves are known to satisfy a differential system of Lotka–Volterra type which is the essence of the fluid limits in our context. Section 3 solves the steady state regime in the reversible case. A geometric interpretation of the free energy is provided (involving the algebraic area enclosed by the curve), as well as an urn model description for the underlying dynamical system, leading precisely to a Lotka–Volterra system.

Non-Gibbs states are considered in Sec. 4. In Ref. 16, necessary and sufficient conditions for reversibility were given, by identification of a family of independent cycles in the state graph, for which Kolmogorov's criteria have to be fulfilled. We pursue this analysis by showing that irreversibility occurs as a result

of particle currents attached to these cycles. A connection between recursion properties (originating matrix solutions) and particle cycles in the state-graph is found, with the introduction of loop currents by the analogy with electric circuits. These recursions at discrete level connect together invariant measures of systems of size N (the number of sites) and of size $N - 1$, and they involve coefficients which are given a concrete meaning. Indeed, by means of a functional approach, we map explicitly these structure coefficients onto special constants which intervene in the Lotka–Volterra systems describing the fluid limit, as $N \rightarrow \infty$.

In the last Sec. 5, we observe that local equilibrium takes place at a rapid time-scale, compared to the diffusion time which is the natural scale of the system. We extend the iterative scheme procedure initiated in Ref. 15 and developed in Ref. 16, which originally concerned only the steady-state regime. In fact, this scheme allow us to express in transient regime particle-currents in terms of deterministic particle densities: this is a mere consequence of a law of large numbers. At least when the diffusion scale is identical for all particle species, local correlations are found to be absent at the hydrodynamical scale. Finally, in the spirit of the study made in Ref. 4, we obtain the Lagrangian describing fluctuations of currents, and we analyze the related Hamilton–Jacobi equations.

2. MODEL DEFINITION

2.1. A Stochastic Clock Model

The system consists of an oriented path embedded in a bidimensional manifold, with N steps of equal size, each one being chosen among a discrete set of n possible orientations, drawn from the set of angles with some given origin $\{\frac{2k\pi}{n}, k = 0, \dots, n - 1\}$. The stochastic dynamics in force consists in displacing one single point at a time without breaking the path, while keeping all links within the set of admissible orientations. In this operation, two links are simultaneously displaced. This constrains quite strongly the possible dynamical rules, which are given in terms of *reactions* between consecutive links.

For any n , we can define

$$X^k X^l \xrightleftharpoons[\lambda_{lk}]{\lambda_{kl}} X^l X^k, \quad k \in [1, n], \quad k \neq l, \tag{2.1}$$

which in the sequel will be sometimes referred to as a local exchange process. It is necessary to discriminate between n odd and n even. Indeed, for $n = 2p$, there is another set of possible stochastic rules:

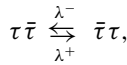
$$\left\{ \begin{array}{l} X^k X^l \xrightleftharpoons[\lambda_{lk}]{\lambda_{kl}} X^l X^k, \quad k = 1, \dots, n, \quad l \neq k + p, \\ X^k X^{k+p} \xrightleftharpoons[\delta^{k+1}]{\gamma^k} X^{k+1} X^{k+p+1}, \quad k = 1, \dots, n. \end{array} \right. \tag{2.2}$$

The distinction is simply due to the presence, for even n , of *folds* (two consecutive links with opposite directions), which may undergo different transition rules, leading to a richer dynamics. The parameters $\{\lambda_{kl}\}$ represent the exchange rates between two consecutive links, while the γ_k 's and δ_k 's correspond to the rotation of a fold to the right or to the left.

2.2. Examples

2.2.1. The Simple Exclusion Process

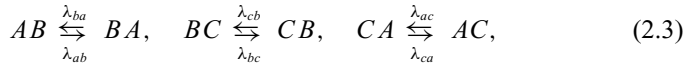
The first elementary and most studied example is the simple exclusion process, which after mapping particles onto links corresponds to a one-dimensional fluctuating interface. In that case, we simply have a binary alphabet. Letting $X^1 = \tau$ and $X^2 = \bar{\tau}$, the reactions rewrite



where λ^\pm is the transition rate for the jump of a particle to the right or to the left.

2.2.2. The Triangular Lattice and the ABC Model

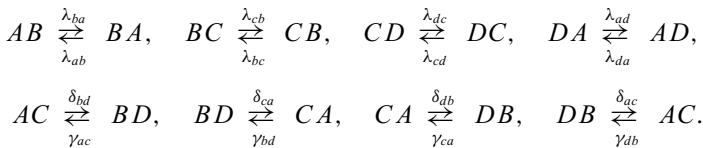
Here the evolution of the random walk is restricted to the triangular lattice. A link (or step) of the walk is either 1, $e^{2i\pi/3}$ or $e^{4i\pi/3}$, and quite naturally will be said to be of type A, B and C, respectively. This corresponds to the so-called *ABC model*, since there is a coding by a 3-letter alphabet. The set of *transitions* (or reactions) is given by



where the rates are arbitrary positive numbers. Also we impose *periodic boundary conditions* on the sample paths. This model was first introduced in Ref. 13 in the context of particles with exclusion, and, for some cases corresponding to reversibility, a Gibbs form has been found in Ref. 14.

2.2.3. A Coupled Exclusion Model in the Square Lattice

This model was introduced in Ref. 15 to analyze stochastic distortions of a walk in the square lattice. Assuming links are counterclockwise oriented, the following transitions can take place.



We studied a rotation invariant version of this model, namely when

$$\begin{cases} \lambda^+ \stackrel{\text{def}}{=} \lambda_{ab} = \lambda_{bc} = \lambda_{cd} = \lambda_{da}, \\ \lambda^- \stackrel{\text{def}}{=} \lambda_{ba} = \lambda_{cb} = \lambda_{dc} = \lambda_{ad}, \\ \gamma^+ \stackrel{\text{def}}{=} \gamma_{ac} = \gamma_{bd} = \gamma_{ca} = \gamma_{db}, \\ \gamma^- \stackrel{\text{def}}{=} \delta_{ac} = \delta_{bd} = \delta_{ca} = \delta_{db}. \end{cases} \tag{2.4}$$

Define the mapping $(A, B, C, D) \rightarrow (\tau^a, \tau^b) \in \{0, 1\}^2$, such that

$$\begin{cases} A \rightarrow (0, 0), \\ B \rightarrow (1, 0), \\ C \rightarrow (1, 1), \\ D \rightarrow (0, 1). \end{cases} \tag{2.5}$$

The dynamics can be formulated in terms of coupled exclusion processes. The evolution of the sample path is represented by a Markov process with state space the set of $2N$ -tuples of binary random variables $\{\tau_i^a\}$ and $\{\tau_i^b\}, i = 1, \dots, N$, taking the value 1 if a particle is present and 0 otherwise. The jump rates to the right (+) or to the left (-) are then given by

$$\begin{cases} \lambda_a^\pm(i) = \bar{\tau}_i^b \bar{\tau}_{i+1}^b \lambda^\mp + \tau_i^b \tau_{i+1}^b \lambda^\pm + \bar{\tau}_i^b \tau_{i+1}^b \gamma^\mp + \tau_i^b \bar{\tau}_{i+1}^b \gamma^\pm, \\ \lambda_b^\pm(i) = \bar{\tau}_i^a \bar{\tau}_{i+1}^a \lambda^\pm + \tau_i^a \tau_{i+1}^a \lambda^\mp + \bar{\tau}_i^a \tau_{i+1}^a \gamma^\pm + \tau_i^a \bar{\tau}_{i+1}^a \gamma^\mp. \end{cases} \tag{2.6}$$

Notably, one sees the jump rates of a given sequence are locally conditionally defined by the complementary sequence.

3. STATIONARY REGIME FOR REVERSIBLE SYSTEMS

In this section, we quote the main characteristics of the steady state distribution when the processes at stake are reversible.

3.1. The General Form of the Invariant Measure

Up to a slight abuse in the notation, we let $X_i^k \in \{0, 1\}$ denote the binary random variable representing the occupation of site i by a letter of type k . The state of the system is represented by the array $\eta \stackrel{\text{def}}{=} \{X_i^k, i = 1, \dots, N; k = 1, \dots, n\}$ of size $N \times n$. The invariant measure of the Markov process of interest is given by

$$\pi_\eta = \frac{1}{Z} \exp[-\mathcal{H}(\eta)], \tag{3.1}$$

where

$$H(\eta) = \frac{1}{N} \sum_{i < j} \sum_{k,l} \alpha_{kl}^{(N)} X_i^k X_j^l, \tag{3.2}$$

with $\alpha_{kl}^{(N)}$ and $\alpha_{lk}^{(N)}$ two N -dependent coefficients related by

$$\alpha_{kl}^{(N)} - \alpha_{lk}^{(N)} = N \log \frac{\lambda_{kl}}{\lambda_{lk}}, \tag{3.3}$$

provided that some *balance* conditions hold (see e.g. Ref. 22). For example, in the clock model (2.1), these conditions take the simple form

$$\sum_{k \neq l} \left(\alpha_{kl}^{(N)} - \alpha_{lk}^{(N)} \right) N_k = 0, \tag{3.4}$$

and they follow indeed directly from Kolmogorov’s criteria (applied to a particle crossing the system), which is tantamount to detailed balance equations.

3.1.1. An Example in the Square Lattice

To show a concrete exploitation of the form (3.1), we consider the square-lattice model introduced in Ref. 15. It does illustrate the rules (2.2). Instead of handling the problem directly with the natural set of four letters $\{A, B, C, D\}$, we found convenient to represent the degrees of freedom by pairs of binary components. In the symmetric version of the model defined by (2.4), when cycles are absent ($N_a = N_b = 1/2$ and $\gamma^+ = \gamma^-$), we could derive the invariant measure

$$\pi_\eta = \frac{1}{Z} \exp \left[\beta \sum_{i < j} \left(\tau_i^a \bar{\tau}_j^b - \tau_i^b \bar{\tau}_j^a \right) \right], \tag{3.5}$$

with $\eta = \{(\tau_i^a, \tau_i^b), i = 1, \dots, N\}$ with $\beta = \log \frac{\lambda^-}{\lambda^+}$. Let us see how this relates to the original formulation of the model in terms of the four letters A, B, C and D .

Proposition 3.1. *Under the reversibility conditions imposed on the transitions rates $\{\lambda_{kl}, \gamma^k, \delta^k, k = 1, \dots, 4, l = 1, \dots, 4\}$, the measure given by (3.1) and (3.2) reduces to*

$$\pi_\eta = \frac{1}{Z} \exp \left\{ \frac{\beta}{2} \sum_{i < j} \left[B_i A_j - A_i B_j + A_i D_j - D_i A_j + C_i B_j - B_i C_j + D_i C_j - C_i D_j \right] \right\}, \tag{3.6}$$

and is equivalent to (3.5).

The proof is not difficult, starting from (3.5). It can also be achieved by a direct argument, i.e. without using (3.5), from Theorem 3.2 of Ref. 16.

3.2. Free Energy

We consider again the *ABC* model as a typical example, and the extension to other models will be straightforward. Assume conditions (3.4) hold, so that the invariant measure is given by

$$\pi_\eta = \frac{1}{Z} \exp \left[\frac{1}{N} \sum_{i < j}^N \alpha_{ab}^{(N)} A_i B_j + \alpha_{bc}^{(N)} B_i C_j + \alpha_{ca}^{(N)} C_i A_j \right],$$

where the constants $\alpha_{ab}^{(N)}$, $\alpha_{bc}^{(N)}$ and $\alpha_{ca}^{(N)}$ take the values

$$\alpha_{ab}^{(N)} = N \log \frac{\lambda_{ab}}{\lambda_{ba}}, \quad \alpha_{bc}^{(N)} = N \log \frac{\lambda_{bc}}{\lambda_{cb}}, \quad \alpha_{ca}^{(N)} = N \log \frac{\lambda_{ca}}{\lambda_{ac}},$$

while $\alpha_{ba}^{(N)}$, $\alpha_{cb}^{(N)}$ and $\alpha_{ac}^{(N)}$ are set to zero, to be consistent with (3.3). The constraints (3.4) now become

$$\frac{N_A}{N_B} = \frac{\alpha_{bc}^{(N)}}{\alpha_{ca}^{(N)}}, \quad \frac{N_B}{N_C} = \frac{\alpha_{ca}^{(N)}}{\alpha_{ab}^{(N)}}, \quad \frac{N_C}{N_A} = \frac{\alpha_{ab}^{(N)}}{\alpha_{bc}^{(N)}}. \tag{3.7}$$

Following Ref. 7, we want to write a large deviation functional corresponding to the above Gibbs measure when $N \rightarrow \infty$. Set $x = \frac{i}{N}$, $J = \exp(2i\pi/3)$, and let $Z(x)$ denote the complex number given by

$$Z(x) = \frac{1}{N} \sum_{i=1}^{[xN]} \left(\frac{A_i}{\alpha} + J \frac{B_i}{\beta} + J^2 \frac{C_i}{\gamma} \right),$$

where we have introduced the parameters

$$\alpha \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \alpha_{bc}^{(N)}, \quad \beta \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \alpha_{ca}^{(N)}, \quad \gamma \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \alpha_{ab}^{(N)}.$$

The sequence $\eta = \{(A_i, B_i, C_i), i = 1, \dots, N\}$ is thus represented by a discrete path Γ in the complex plane, made of oriented links having only three possible directions

$$\{\theta = 0, \theta = 2\pi/3, \theta = 4\pi/3\},$$

depending on whether a particle A, B or C is present. The length of a link corresponding to A, B, or C is, respectively, $1/(N\alpha)$, $1/(N\beta)$ or $1/(N\gamma)$.

The equation of Γ is given by a function $Z := x \rightarrow Z(x), x \in \mathbb{C}$. Note that condition (3.7) ensures Γ is closed, that is

$$Z(1) = \frac{1}{\alpha + \beta + \gamma} (1 + J + J^2) = 0.$$

The area \mathcal{A} enclosed by Γ is given by

$$\mathcal{A} \stackrel{\text{def}}{=} \frac{1}{2i} \oint_{\Gamma} (\bar{z} dz - z d\bar{z}),$$

and, for large N , this coincide with

$$\mathcal{A} = \frac{\sqrt{3}}{N^2} \sum_{l < k} \frac{A_l}{\alpha} \left(\frac{B_k}{\beta} - \frac{C_k}{\gamma} \right) + \frac{B_l}{\beta} \left(\frac{C_k}{\gamma} - \frac{A_k}{\alpha} \right) + \frac{C_l}{\gamma} \left(\frac{A_k}{\alpha} - \frac{B_k}{\beta} \right) + o(1). \tag{3.8}$$

As a result,

$$\mathcal{H}(\{\eta\}) = \frac{N\alpha\beta\gamma}{2\sqrt{3}} \mathcal{A} + \frac{3N\alpha\beta\gamma}{(\alpha + \beta + \gamma)^2} + O(1).$$

The large deviation probability is easily obtained from the law of large numbers. It is given by

$$P_N(\rho_a, \rho_b, \rho_c) = \frac{1}{Z} \exp(-N\mathcal{F}(\rho_a, \rho_b, \rho_c)), \tag{3.9}$$

with the free energy

$$\mathcal{F}(\rho_a, \rho_b, \rho_c) = \frac{\alpha\beta\gamma}{2\sqrt{3}} \mathcal{A}(\rho_a, \rho_b, \rho_c) - \mathcal{S}(\rho_a, \rho_b, \rho_c), \tag{3.10}$$

where

$$\begin{aligned} \mathcal{A}(\rho_a, \rho_b, \rho_c) \stackrel{\text{def}}{=} & \sqrt{3} \int_0^1 dx \int_x^1 dy \frac{\rho_a(x)}{\alpha} \left(\frac{\rho_b(y)}{\beta} - \frac{\rho_c(y)}{\gamma} \right) \\ & + \frac{\rho_b(x)}{\beta} \left(\frac{\rho_c(y)}{\gamma} - \frac{\rho_a(y)}{\alpha} \right) + \frac{\rho_c(x)}{\gamma} \left(\frac{\rho_a(y)}{\alpha} - \frac{\rho_b(y)}{\beta} \right) \end{aligned}$$

and where the entropy term comes from a multinomial combinatorial factor $\frac{\eta!}{n_a!n_b!n_c!}$, namely the way of arranging a box of $n = [N dx]$ sites, with 3 species of identical particles having respective populations $n_i = \rho_i(x)Ndx, i \in \{a, b, c\}$ Stirling's formula for large N yields

$$\mathcal{S}(\rho_a, \rho_b, \rho_c) = - \int_0^1 dx [\rho_a(x) \log \rho_a(x) + \rho_b(x) \log \rho_b(x) + \rho_c(x) \log \rho_c(x)].$$

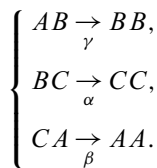
Stable and metastable deterministic profiles correspond to local minima of the free-energy. According to (3.10), an optimal profile is a compromise between a maximal entropy and a minimum of the enclosed algebraic area. Curves of maximal entropy are typically Brownian, and they have an area which scales like $1/N$; on the other hand, the opposite extreme configuration consisting of an equilateral triangle with negative orientation achieves the minimum algebraic area, but belongs to a class of profiles for which the entropy contribution is equal to zero (since $\rho \log \rho$ vanishes both for $\rho = 0$ and $\rho = 1$). Depending on the ratio $\alpha\beta\gamma/2\sqrt{3}$ of the two contributions, we obtain either Brownian (the degenerate point of the deterministic equations, see below) or deterministic profiles, both regimes being separated by a second order phase transition.

3.3. Lotka Volterra Systems

Under the scaling earlier defined, letting $N \rightarrow \infty$, we show on two examples that the limiting invariant measure is the solution of a non-linear differential system of Lotka–Volterra type.

3.3.1. Urn Model

Consider three species, denoted by $\{A, B, C\}$, and let $N_a^{(N)}(t)$, $N_b^{(N)}(t)$ and $N_c^{(N)}(t)$ be the corresponding time-dependent populations. The system is closed, $N_a + N_b + N_c = N$. At random times taken as exponential events, individuals do meet and population transfer take place at rates α, β, γ , associated with the reactions



This zero-range process is an urn-type model of Ehrenfest *Class*, as defined in Ref. 19, where individuals, rather than urns, are chosen at random. When N increases to infinity, we rather consider concentrations instead of integer numbers:

$$\rho_i(t) \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \frac{N_i^{(N)}(t)}{N},$$

for $i = a, b, c$. After a proper scaling limit, the dynamics of the model is described by the following Lotka–Volterra system

$$\begin{cases} \frac{\partial \rho_a}{\partial x} = \rho_a(\beta \rho_c - \gamma \rho_b), \\ \frac{\partial \rho_b}{\partial x} = \rho_b(\gamma \rho_a - \alpha \rho_c), \\ \frac{\partial \rho_c}{\partial x} = \rho_c(\alpha \rho_b - \beta \rho_a), \end{cases}$$

which, after replacing x by t and densities by concentrations, is nothing else but the differential system giving the invariant measure of the (A, B, C) model, in the fluid limit at thermodynamical equilibrium.⁽⁷⁾

3.3.2. The Square Lattice Model

From (3.6), one can write down the large deviation functional $\mathcal{F}(\rho_A, \rho_B, \rho_C, \rho_D)$ [as in (3.9)], together with the conditions ensuring an optimal profile. This leads again to a differential system of Lotka–Volterra class

$$\begin{aligned} \frac{\partial \rho_A}{\partial x} &= \eta \rho_A (\rho_B - \rho_D), & \frac{\partial \rho_B}{\partial x} &= \eta \rho_B (\rho_C - \rho_A), \\ \frac{\partial \rho_C}{\partial x} &= \eta \rho_C (\rho_D - \rho_B), & \frac{\partial \rho_D}{\partial x} &= \eta \rho_D (\rho_A - \rho_C), \end{aligned} \tag{3.11}$$

in which the last equation follows merely by summing up the three other ones. This system is structurally different from the one obtained in Ref. 15, which involved only two independent profiles (ρ_a, ρ_b) corresponding to deterministic densities for the particles τ_a and τ_b , while in the present case there are three (ρ_A, ρ_B, ρ_C) for example).

It is interesting to notice that, in both models, explicit level surfaces exist. Indeed, the above system satisfies $\rho_A \rho_B \rho_C \rho_D = cte$, in addition to constraint $\rho_A + \rho_B + \rho_C + \rho_D = 1$. On the other hand, $\rho_a(1 - \rho_a)\rho_b(1 - \rho_b)$ is the level surface of the former system encountered in Ref. 15. This can be explained by reversing the mapping (3.13), so that

$$\begin{aligned} A_i &= \bar{\tau}_i^a \bar{\tau}_i^b, & B_i &= \tau_i^a \tau_i^b, \\ C_i &= \tau_i^a \tau_i^b, & D_i &= \bar{\tau}_i^a \bar{\tau}_i^b. \end{aligned} \tag{3.12}$$

This indicates that the set of 4-tuples $\{\tau_i^a, \bar{\tau}_i^a, \tau_i^b, \bar{\tau}_i^b\}$ constitutes the elementary blocks of the system, and that letters A_i, B_i, C_i, D_i are composite variables encoding correlations of these building blocks. Therefore, in the continuous limit, we are left with two different descriptions of the same system, related in a non trivial manner. We propose now to explore more carefully this connection. In

particular, while the linear mapping

$$\begin{cases} \tau_i^a = B_i + C_i, & \bar{\tau}_i^a = A_i + D_i, \\ \tau_i^b = C_i + D_i, & \bar{\tau}_i^b = A_i + B_i, \end{cases} \tag{3.13}$$

still holds in the continuous limit, as a relation between expected values

$$\begin{cases} \rho_a = \rho_B + \rho_C, \\ \rho_b = \rho_C + \rho_D, \end{cases} \tag{3.14}$$

the non-linear equation (3.12) are instead expected to bring a different form, since they involve correlations.

Proposition 3.2. *The differential system given by*

$$\begin{cases} \frac{\partial}{\partial x} \left[\log \frac{\rho^a(x)}{1 - \rho^a(x)} \right] = 2\eta(2\rho_b(x) - 1), \\ \frac{\partial}{\partial x} \left[\log \frac{\rho^b(x)}{1 - \rho^b(x)} \right] = -2\eta(2\rho_a(x) - 1), \end{cases} \tag{3.15}$$

is related to (3.11) through the invertible functional mapping given by

$$\begin{cases} \rho_A = \bar{\rho}_a \bar{\rho}_b + K, & \rho_B = \rho_a \bar{\rho}_b - K, \\ \rho_C = \rho_a \rho_b + K, & \rho_D = \bar{\rho}_a \rho_b - K, \end{cases} \tag{3.16}$$

where K is a constant to be determined.

Proof: First, let $\{\rho_B, \rho_C, \rho_D\}$ be the set of independent variables in (3.11), and express them in terms of the new triple $\{\rho_a, \rho_b, \rho_c\}$ given by (3.14). This gives

$$\begin{aligned} \frac{\partial(\rho_a - \rho_C)}{\partial x} &= \eta(\rho_a - \rho_C)(\rho_a + \rho_b - 1), \\ \frac{\partial(\rho_b - \rho_C)}{\partial x} &= \eta(\rho_b - \rho_C)(1 - \rho_a + \rho_b), \\ \frac{\partial \rho_C}{\partial x} &= \eta \rho_C (\rho_b - \rho_a). \end{aligned} \tag{3.17}$$

Combining these equations yields

$$\begin{cases} \frac{\partial \rho_a}{\partial x} = \eta \rho_a (\rho_a + \rho_b - 1) + \eta \rho_C (1 - 2\rho_a), \\ \frac{\partial \rho_b}{\partial x} = \eta \rho_b (1 - \rho_a - \rho_b) + \eta \rho_C (2\rho_b - 1), \end{cases} \tag{3.18}$$

which in turn allows to express ρ_C as

$$\rho_C = \frac{1}{\rho_a - \rho_b} \left(\rho_a \frac{\partial \rho_b}{\partial x} + \rho_b \frac{\partial \rho_a}{\partial x} \right).$$

Instantiating this last value of ρ_C in (3.18) and in (3.17), we obtain (3.15), after immediate recombination, together with the relation

$$\frac{\partial \rho_C}{\partial x} = \frac{\partial(\rho_a \rho_b)}{\partial x}.$$

This last equation has its counterpart for ρ_A , ρ_B and ρ_D : after integration, we are left with four constants, which reduce to the one given in (3.16) only when compatibility with (3.14) is imposed. \square

4. NON-GIBBS STEADY STATE REGIME

We call non-Gibbs steady state regime, a regime for which the invariant measure is not described by means of a potential. This occurs when reversibility is broken, that is when there exists at least one cycle in the state graph for which the Kolmogorov criteria fails. A complete set of detailed balanced equations cannot be written in such a case, there exist at least two states η and η' , connected by a single particle jump, with rate $\lambda_{\eta\eta'}$ and $\lambda_{\eta'\eta}$ such that

$$\lambda_{\eta\eta'}\pi_\eta - \lambda_{\eta'\eta}\pi_{\eta'} = \phi \neq 0, \tag{4.1}$$

if π_η denotes the invariant measure. It is the second member of this equation we wish to study in this section. In the sequel we note \mathcal{S} the state space, \mathcal{G} the corresponding state graph, by assigning oriented edges between pair of nodes $(\alpha, \beta) \in \mathcal{S}^2$, when the rate $\lambda_{\alpha\beta}$ is non-zero, \mathcal{C} will denote a cycle in \mathcal{G} and we denote \mathcal{T} the set of spanning trees on \mathcal{G} .

4.1. The Tagged Particle Cycle

Cycles in the state graph for the n odd model are important in the analysis of reversibility, and they are the ones for which at least one particle performs a complete round-trip. For example if a given particle makes $N - 1$ successive jumps to the right, because of the circular geometry, the initial and final states are identical, up to a 1-step global shift to the left of the particles. As long as this particle is the only one in movement, the permutation order of the remaining other $N - 1$ particles is kept frozen. The corresponding subsequence $\eta^{(N-1)}$ will in the sequel denote these specific cycles. Let us examine this one particle model, by tagging a specific particle which is given a new label Y , and by following its motion conditionally on $\eta^* = \{X_i^k, i = 1, \dots, N, k \in \{1, \dots, n\}\}$, the

complementary frozen set of particles. This is equivalent to consider Y moving in the inter-sites $\{i + 1/2, i = 0, \dots, N - 1\}$ of the $N - 1$ frozen particles. The question is then to analyze the steady-state regime of a particle moving around a circular lattice in a random environment. To any allowed transition which is a jump of Y between sites $i - \frac{1}{2}$ and $i + \frac{1}{2}$, we let correspond the set of conditional transition rates given by

$$\begin{cases} \lambda_y^+(i) = \sum_{k=1}^n \lambda_{yk} X_i^k, \\ \lambda_y^-(i) = \sum_{k=1}^n \lambda_{ky} X_i^k. \end{cases}$$

Violation of condition (3.4) leads to

$$\det(\eta^*) \stackrel{\text{def}}{=} \prod_{i=0}^{N-1} \lambda_y^+(i) - \prod_{i=0}^{N-1} \lambda_y^-(i) \neq 0. \tag{4.2}$$

The coefficient $\det(\eta^*)$, attached to the cycle η^* , is exactly the determinant of the system of flux equations

$$\lambda_y^+(i)\pi_{i-\frac{1}{2}} - \lambda_y^-(i)\pi_{i+\frac{1}{2}} = \phi(\eta^*), \quad i = 0, \dots, N - 1, \tag{4.3}$$

giving the invariant measure $\pi_{i+\frac{1}{2}}$, which reads

$$\pi_{i+\frac{1}{2}} = \frac{1}{Z} \sum_{i=1}^N \exp \left\{ \sum_{m=1}^{n,N} \sum_{l+1 < j < i} X_j^m \log \lambda_{ym} + \sum_{i < j < l} X_j^m \log \lambda_{my} \right\},$$

$$i = 0, \dots, N - 1,$$

where Z is a normalization constant. A diagrammatic representation of each term in the summation (over l) is given in Fig. 1b. Each term is in fact a spanning tree on the reduced tagged-particle state-graph, weighted by the transitions rates and rooted at the considered point ($i + \frac{1}{2}$ for $\pi_{i+\frac{1}{2}}$). The constant Z is therefore the sum of all spanning-trees on the reduced tagged-particle state-graph. The probability current between site $i - \frac{1}{2}$ and site $i + \frac{1}{2}$ reads

$$\lambda_y^+(i)\pi_{i-\frac{1}{2}} - \lambda_y^-(i)\pi_{i+\frac{1}{2}} = \frac{1}{Z} \left[\exp \left(\sum_{m=1}^n N_m \log \lambda_{ym} \right) - \exp \left(\sum_{m=1}^n N_m \log \lambda_{my} \right) \right],$$

with N_m the number of particles of type m , a quantity independent of i . This shows that $\phi(\eta^*)$ is a quantity attached to the cycle η^* , which will be referred to as *cycle current* and reads

$$\phi(\eta^*) = \frac{1}{Z} \det(\eta^*). \tag{4.4}$$

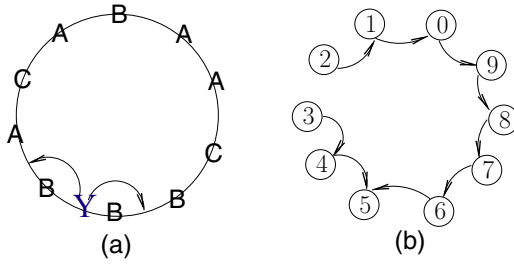


Fig. 1. (a) Relative motion of the tagged particle. (b) Corresponding state space and a spanning tree contribution to π_5 .

Depending on the sign of $\det(\eta^*)$, the diffusion of particle Y is biased in the right ($\det(\eta^*) > 0$) or in the left ($\det(\eta^*) < 0$) direction. Of course the reversible case is recovered when the determinant vanishes, which corresponds exactly to Kolmogorov’s criterion.

4.1.1. Case of Open Systems: Example of ASEP

Consider the well studied asymmetric simple exclusion process ASEP with open boundary conditions, defined by α the rate of particle entering to the left side and β the rate at which particles exit from the right side. The generalization to open systems of our definition of the tagged particle cycle (TPC) is depicted in Fig. 2a. We adopt the convention for the cycle orientation that particles move positively to the right and holes to the left. Assume we give a tag to one of the particles. Let it perform successive jumps until reaching the right side; when it leaves the system it is in fact transformed into a hole; We keep the tag attached to the hole which performs successive jumps in the opposite direction until it reaches the left side; again it transformed back into a particle which in turn performs jumps to the right until the reaching of the initial position, to conclude the cycle.

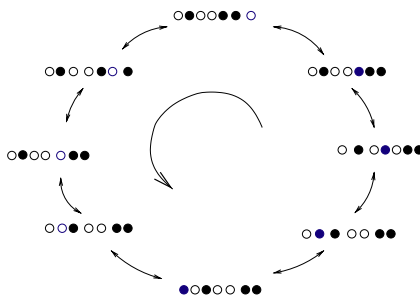


Fig. 2. Example of a tagged particle cycle in the state graph for ASEP with 7 particles and open boundary.

4.2. Combinatorial Formulas for Invariant Measure and Currents

We give here a combinatorial way of expressing the stationary measure on a connex finite state space \mathcal{S} of size \mathcal{N} , the number of states. Consider a continuous-time irreducible Markov chain, with transition rates $\lambda_{\alpha\beta}$ between states α and β , and define the corresponding state graph \mathcal{G} based on \mathcal{S} by assigning oriented edges between pair of nodes (α, β) , for any non-zero corresponding rate $\lambda_{\alpha\beta}$.

Proposition 4.1. *The invariant measure π_α is given by*

$$\pi_\alpha = \frac{\sum_{t \in \mathcal{T}_\alpha} w(t)}{\sum_{t \in \mathcal{T}} w(t)} \tag{4.5}$$

where \mathcal{T} is the set of spanning tree over \mathcal{G} , \mathcal{T}_α is the set of spanning tree over \mathcal{G} rooted in α , and $w(t)$ the weight of a tree t given by

$$w(t) = \prod_{(\alpha, \beta) \in t} \lambda_{\alpha, \beta}.$$

Proof: This is nothing else but the well known *Markov-chain tree theorem*. For a probabilistic proof, see Ref. 1 and references therein. A purely algebraic proof consists in rewriting the solution of the steady-state equation

$$\pi_\alpha G_{\alpha\beta} = 0, \quad \forall \beta \in \mathcal{S},$$

where G is the generator, and $G_{\alpha\beta} = -\left(\sum_\gamma \lambda_{\alpha\gamma}\right) \delta_{\alpha\beta} + \lambda_{\alpha\beta}$, using the Cramer relation. Indeed, since

$$\sum_{\beta=1}^{\mathcal{N}} G_{\alpha\beta} = 0,$$

the set of steady-state equations is of rank $\mathcal{N} - 1$ and π_α can be written as the ratio of two determinants, namely the cofactor $\tilde{G}_{\alpha\mathcal{N}}$ of $G_{\alpha\mathcal{N}}$ and the determinant $|\tilde{G}|$ of the matrix obtained from G by replacing $G_{\beta\mathcal{N}}$ by 1 for all $\beta = 1, \dots, \mathcal{N}$. Since G has a structure of an admittance-matrix, the expansions of $\tilde{G}_{\alpha\beta}$ and $|\tilde{G}|$ are tantamount to summing over spanning trees, so that

$$\tilde{G}_{\alpha\mathcal{N}} = \sum_{t \in \mathcal{T}_\alpha} w(t), \quad |\tilde{G}| = \sum_{t \in \mathcal{T}} w(t),$$

which yields formula (4.5). □

From this observation, we deduce a way to express the probability currents at steady-state, which generalizes formulas (4.3) and (4.4). First call $\det(C)$ a

coefficient attached to each cycle C ,

$$\det(C) \stackrel{\text{def}}{=} \prod_{(\gamma, \delta) \in C} \lambda_{\gamma\delta} - \prod_{(\gamma, \delta) \in C} \lambda_{\delta\gamma},$$

generalizing (4.2) and where the orientation of C is prescribed by the orientation of (α, β) and the product over the set $(\gamma, \delta) \in C$, is understood according to this orientation. Let $C_{\alpha\beta}$ the set of cycles in \mathcal{G} containing the oriented edge (α, β) . Let \mathcal{T}_C a set of subgraph of \mathcal{G} , s.t. when C is glued into a single node α_C , \mathcal{T}_C represents the set of spanning trees rooted in α_C .

Lemma 4.2. *The steady state current between states $(\alpha, \beta) \in \mathcal{S}^2$ is given by*

$$\lambda_{\alpha\beta}\pi_\alpha - \lambda_{\beta\alpha}\pi_\beta = \sum_{C \in C_{\alpha\beta}} \frac{\sum_{t \in \mathcal{T}_C} w(t)}{\sum_{t \in \mathcal{T}} w(t)} \det(C). \tag{4.6}$$

Proof: When π_α is multiplied by $\lambda_{\alpha\beta}$, each spanning tree contribution is transformed by drawing an oriented edge between α and β . Since the spanning tree contains by construction of π_α a path going from β to α , the added edges contributes to the forming of a cycle which contains α and β . If each oriented edge in this cycle have a reversed counterpart, then in $\lambda_{\beta\alpha}\pi_\beta$ there is to be found a corresponding term with the same edges but with reversed orientation in the cycle (see Fig. 3). In any case, $\det(C)$ factors out of an ensemble of contributions which consist in drawing trees spanning all the subgraph \mathcal{G} with endpoints on C , divided by the global normalization constant $\sum_{t \in \mathcal{T}} w(t)$. This complete the justification of formula (4.6). □

Note that $\sum_{t \in \mathcal{T}_C} w(t)$ in (4.6) represents the unnormalized invariant measure of α_C on the reduced graph \mathcal{G}/C . This indicates that (4.6) bears recursive properties which could be used for asymptotic limits when the size of the system tends to infinity. Let us call C a reversible [resp. non-reversible] cycle if $\det(C) = 0$ [resp. $\det(C) \neq 0$]. In the loop expansion of the currents provided by (4.6), only non-reversible cycles do contribute. For particle system, this distinction is embedded into a topological classification of cycles with respect to their corresponding determinant value $\det(C)$.

4.2.1. Connection with the Matrix Ansatz for ASEP

For the ASEP model, a simple algorithm has been discovered⁽¹⁰⁾ to obtain the steady-state probabilities of each individual state with the help of a matrix ansatz. In this representation, a given sequence $\eta = 1010 \dots 00$ is represented by a product of matrices D (for 1) and E (for 0), and the corresponding probability

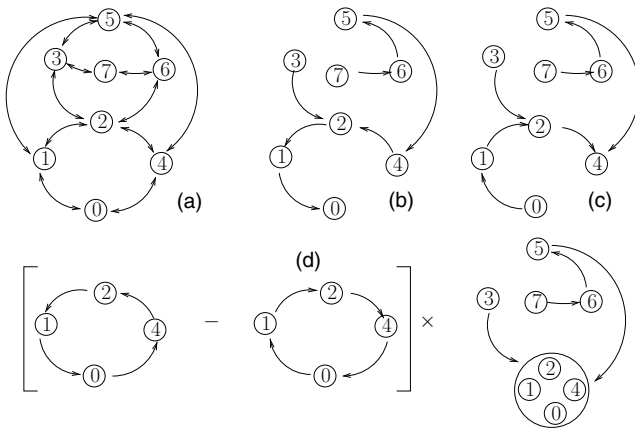


Fig. 3. (a) State-graph with $N = 8$ states. Arrows indicates possible transitions. (b) A contribution to π_0 . (c) A contribution to π_4 . (d) A combined contribution to J_{14} .

measure is obtained by taking the trace

$$\pi_\eta = \frac{1}{Z} \text{Tr}(WDEDE \dots EE),$$

where W is an additional matrix which takes into account the boundary property. A sufficient condition for this to be the invariant measure is that D, E, W satisfy

$$\begin{aligned} \lambda_{10}DE - \lambda_{01}ED &= D + E \\ DW &= \frac{1}{\beta}W \\ WE &= \frac{1}{\alpha}W. \end{aligned} \tag{4.7}$$

If $\lambda_{01} = 0$, the process is totally asymmetric (TASEP), particles can jump only to the right. Consider the system with only 3 sites, which graph is depicted in Fig. 4. Using these rules we find e.g. that

$$\pi_{000} = \frac{1}{Z}\alpha^3 \tag{4.8}$$

$$\pi_{100} = \frac{1}{Z} \left(\left(\frac{1}{\alpha} + \frac{1}{\beta} \right) \frac{1}{\lambda^2} + \frac{1}{\alpha^2\lambda} \right). \tag{4.9}$$

Comparison with the spanning tree expansion is done by counting deletions. A spanning tree is obtained from the complete graph by the deleting of a certain number of edges, and each deletion is accounted for by dividing with respect to

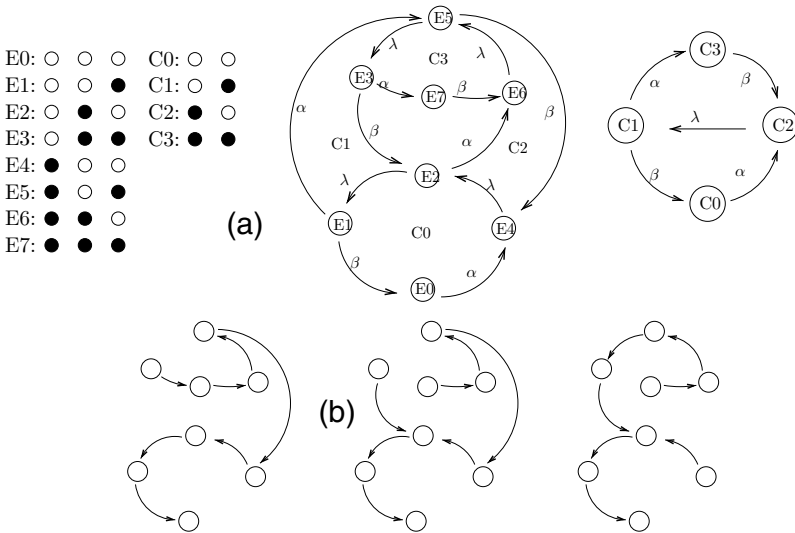


Fig. 4. (a) Graph of the state space for a TASEP with three particles and the dual graph corresponding to the possible cycles. (b) Spanning tree contributions to π_{000} .

the corresponding transition rate. The set of spanning trees contributing to π_{000} is given in Fig. 4b. The brut result (without normalization is):

$$\pi_{000} \propto \left(\frac{1}{\alpha\beta} + \frac{1}{\alpha\beta} + \frac{1}{\beta\lambda} \right) \alpha^3 \tag{4.10}$$

$$\pi_{100} \propto \left(\frac{1}{\alpha\beta} + \frac{1}{\alpha\beta} + \frac{1}{\beta\lambda} \right) \left(\left(\frac{1}{\alpha} + \frac{1}{\beta} \right) \frac{1}{\lambda^2} + \frac{1}{\alpha^2\lambda} \right). \tag{4.11}$$

The factor $\left(\frac{1}{\alpha\beta} + \frac{1}{\alpha\beta} + \frac{1}{\beta\lambda} \right)$ shows up for each state, and disappears after normalization. Nevertheless, it induces in this simple example a factor of 3 in the enumeration of terms, by comparison with the matrix ansatz. An underlying symmetry of the state graph is at the origin of this combinatorial factor. Indeed for the ASEP system, the steady-state probability current between two sequences η and η' separated by a single jump between site i and $i + 1$ reads,

$$\lambda_{10}\pi_{\eta}^{(N)} - \lambda_{10}\pi_{\eta'}^{(N)} = \pi_{\eta_i^*}^{(N-1)} + \pi_{\eta_{i+1}^*}^{(N-1)}, \tag{4.12}$$

as a consequence of (4.7), with the subsequence η_i^* [resp. η_{i+1}^*] of η obtained by deleting bit i [resp. $i + 1$]. We have not been able yet to fill the gap between (4.6) and (4.12). We believe that the combinatorial arrangement which occur is due to a hierarchical structure of the state-graph, revealed with the help of the tagged particle. The complete analysis of (4.6) is the subject of another work in progress. Beforehand, in the next sections, we simply propose a possible general form for

the detailed current Eq. (4.1), which leads (see Sec. 4.4) to the correct form of the Lotka–Volterra equations describing the fluid limits at steady state.

4.3. Cycle Currents

We interpret relation (4.12) in terms of *cycle currents*. A transition taking place between two particles of different types, say $AB \rightarrow BA$, can be viewed either as a particle A travelling to the right or, conversely, as a particle B travelling to the left. In this exchange two joint TPC are involved. In the state-graph, each TPC defines a face, which we will identify with a subsequence η^* , obtained from η by removing the tagged particle. Accordingly, we attach a set of variables $\{\phi(\eta^*)\} \in \mathbb{R}$ to each TPC face, while currents between states are variables attached to the edges of the graph. Conservation of probability currents at a given node is automatically fulfilled, provided that if one write (assuming a transition between site i and $i + 1$, see Fig. 5),

$$\lambda_{ab}\pi_\eta - \lambda_{ba}\pi_{\eta'} = \phi_a(\eta_i^*) - \phi_b(\eta_{i+1}^*), \tag{4.13}$$

which is tantamount to changing current variables into cycle variables.

The right-hand side members in (4.7) and (4.12) is reminiscent of the second member of (4.13). In fact we have

$$\begin{aligned} \phi_a(\eta_i^*) &= \text{Tr}(W\eta_i^*) \\ \phi_b(\eta_{i+1}^*) &= -\text{Tr}(W\eta_{i+1}^*). \end{aligned}$$

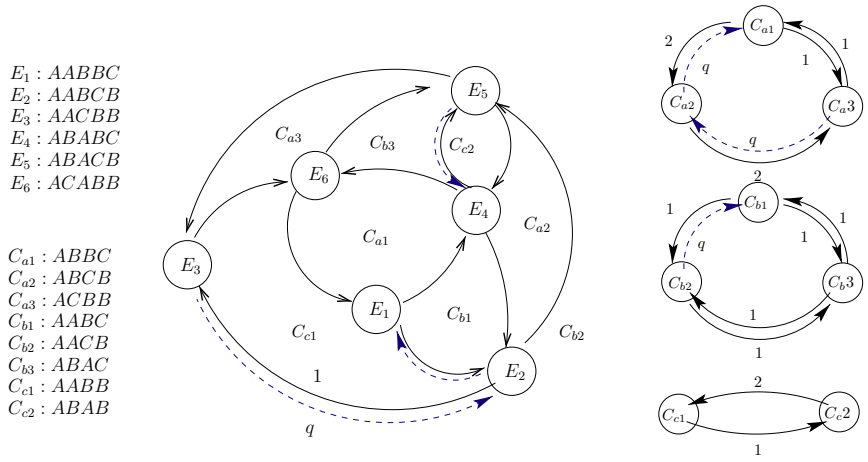


Fig. 5. Graph of the state space for an asymmetric ABC model with five particles, (A, A, B, B, C) and the dual graph corresponding to the possible cycles.

With each edge of the state-graph, we associate such an extended detailed balance equation. Then, eliminating all ϕ 's from this set of equations leads to the invariant measure equation. Consider the example given in Fig. 5. The transition rules are

$$AB \xrightarrow{1} BA \quad AC \xrightarrow{1} CA \quad BC \xrightleftharpoons[q]{1} CB.$$

The various weights corresponding to each sequence and subsequence associated with cycles are given in the following table, for $q = 0$ and $q = 1$. Note that one should expect $\pi_{c1} = \frac{1}{3}$ and $\pi_{c2} = \frac{2}{3}$ from the subgraph of Fig. 5. The correction results from the different degeneracy w.r.t. circular permutation symmetry (4 for C_1 and 2 for C_2).

	π_1	π_2	π_3	π_4	π_5	π_6	π_{a1}	π_{a2}	π_{a3}	π_{b1}	π_{b2}	π_{b3}	π_{c1}	π_{c2}	C_a	C_b	C_c
$q = 0$	$\frac{1}{10}$	$\frac{1}{10}$	$\frac{3}{10}$	$\frac{1}{10}$	$\frac{2}{5}$	$\frac{2}{5}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{5}$	0	$-\frac{1}{5}$
$q = 1$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{32}{105}$	$-\frac{41}{210}$	$-\frac{41}{315}$

In this two cases one has the decomposition of the dual variables ϕ of relation (4.13) according to

$$\phi_x(\eta^*) = C_x \pi_{\eta^*} \quad \text{with } x \in \{a, b, c\} \tag{4.14}$$

with the value of the structure coefficient also given in the table. For example we have

$$\pi_1 - q\pi_2 = C_b\pi_{b1} - C_c\pi_{c1}.$$

This decomposition is however not valid for arbitrary q . A certain number of compatibility constraint have to be imposed on the ϕ ', because the TPC do not constitute a complete bases of cycles in the state graph. When considering the complete system (4.13) of detailed currents, we have at hand m equations, m being the number of edges of the state-graph, and $n + \nu_{\text{tpc}}$ unknowns, where n is the number of nodes and ν_{tpc} the number of TPC. In matrix form, this reads

$$M\Pi = \Phi \tag{4.15}$$

where

- M is a $m \times n$ matrix;
- Π a column vector of size n , with the elements the invariant probability measure;
- Φ is a column vector of size m , where each component l is the algebraic contribution of the (two in general) TPC having the edge corresponding to l in common.

To fix the sign conventions, we agree that orientations of cycles are given by the natural orientation of the system, i.e. each particle travels positively from left to right. An exception is made for the simple exclusion system, since in this case holes travel positively to the left and there is only one type of TPC.

$$\begin{aligned} \lambda_{10}\pi_\eta - \lambda_{01}\pi_{\eta'} &= \phi(\eta_i^*) + \phi(\eta_{i+1}^*) && \text{for ASEP,} \\ \lambda_{ab}\pi_\eta - \lambda_{ba}\pi_{\eta'} &= \phi_a(\eta_i^*) - \phi_b(\eta_{i+1}^*) && \text{for multi-type systems,} \end{aligned}$$

(with $(i, i + 1)$ the sites involved in the transition). From basic graph theory (see Ref. 3), the quantity giving the number of independent cycles in an arbitrary graph \mathcal{G} is called the *cyclomatic number*

$$v(\mathcal{G}) = m - n + p,$$

where n, m and p are respectively the number of nodes, edges and components. In our cases, the system is irreducible, so $p = 1$. Since m is the number of equations and $n + v_{\text{tpc}}$ the number of unknown, the system is over-determined by a quantity

$$m - (n + v_{\text{tpc}}) = v - v_{\text{tpc}} - 1.$$

This over-determination is understood as follows. To each line of the matrix M corresponds a transition between two states, so that a given cycle in the state-graph corresponds to some combination of lines of M (namely the successive transitions taking part in the cycle), and the resulting sub-matrix is a square matrix of size the number of states visited by the cycle. The corresponding determinant vanishes for all trivial cycles. Hence the number of independent equations is $m - v + v_{\text{tpc}}$, which is equal to the number of unknown minus 1, the remaining degree of freedom being related to the global normalization condition. However, a certain number of compatibility conditions have to be imposed on the ϕ 's in order to eliminate safely all dependent equations of our system (4.15). These conditions are somehow related to the basic recurrence scheme which is at the origin of matrix-solutions obtained in the context of ASEP, but also for multi-type particle systems.⁽²⁾ Let us see how the specific form (4.14) encountered precedingly do combine with these compatibility conditions.

Lemma 4.3. *The form*

$$\phi_a^{(N)}(\eta^*) = C_a^{(N)} \pi_{\eta^*}^{(N-1)}, \tag{4.16}$$

of the cycle currents fulfills the compatibility condition imposed by trivial cycles if and only if

$$C_a^{(N)} C_b^{(N-1)} = C_b^{(N)} C_a^{(N-1)} \quad \forall a, b \in \{1, \dots, n\}.$$

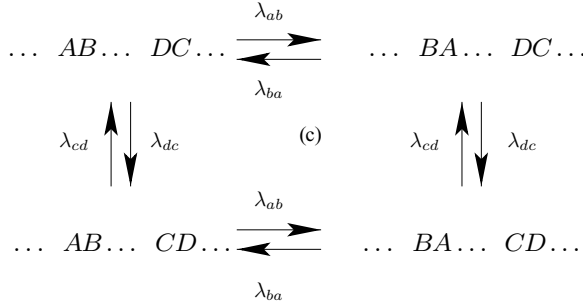


Fig. 6. Example of a reversible cycle.

Proof: Instead of proving this for an arbitrary trivial cycle, we do it for the one depicted in Fig. 6, the completion of the general case follows by recurrence, since any trivial cycle can be constructed as a combination of cycle of this type. To fix some notation, let η^1, η^2, η^3 and η^4 be the states visited by the cycle, with i the position of A and j the position of C in η_1 , so that

$$\begin{aligned}
 \eta^1 &= \dots AB \dots CD \dots & \eta_i^{1*} &= \dots B \dots CD \dots & \eta_{i+1}^{1*} &= \dots A \dots CD \dots \\
 \eta^2 &= \dots BA \dots CD \dots & \eta_j^{2*} &= \dots BA \dots D \dots & \eta_{j+1}^{2*} &= \dots BA \dots C \dots \\
 \eta^3 &= \dots BA \dots DC \dots & \eta_i^{3*} &= \dots A \dots DC \dots & \eta_{i+1}^{3*} &= \dots B \dots DC \dots \\
 \eta^4 &= \dots AB \dots DC \dots & \eta_j^{4*} &= \dots AB \dots C \dots & \eta_{j+1}^{4*} &= \dots AB \dots D \dots
 \end{aligned}$$

The sub-system of (4.15) corresponding to this cycle reads

$$\lambda_{ab}\pi_{\eta^1} = \lambda_{ba}\pi_{\eta^2} = \phi_a [\eta_i^{1*}] - \phi_b [\eta_{i+1}^{1*}], \tag{a}$$

$$\lambda_{cd}\pi_{\eta^2} - \lambda_{dc}\pi_{\eta^3} = \phi_c [\eta_j^{2*}] - \phi_d [\eta_{j+1}^{2*}], \tag{b}$$

$$\lambda_{ba}\pi_{\eta^3} - \lambda_{ab}\pi_{\eta^4} = \phi_b [\eta_i^{3*}] - \phi_a [\eta_{i+1}^{3*}], \tag{c}$$

$$\lambda_{dc}\pi_{\eta^4} - \lambda_{cd}\pi_{\eta^1} = \phi_d [\eta_j^{4*}] - \phi_c [\eta_{j+1}^{4*}]. \tag{d}$$

As already noted, these equations are not independent. Hence the combination $\lambda_{cd}(a) + \lambda_{ba}(b) + \lambda_{dc}(c) + \lambda_{ab}(d)$ eliminates one equation, but with the resulting constraint on the ϕ 's:

$$\begin{aligned}
 &\lambda_{cd}\phi_a [\eta_i^{1*}] - \lambda_{dc}\phi_a [\eta_{i+1}^{3*}] + \lambda_{dc}\phi_b [\eta_i^{3*}] - \lambda_{cd}\phi_b [\eta_{i+1}^{1*}] \\
 &+ \lambda_{ba}\phi_c [\eta_j^{2*}] - \lambda_{ab}\phi_c [\eta_{j+1}^{4*}] + \lambda_{ab}\phi_d [\eta_j^{4*}] - \lambda_{ba}\phi_d [\eta_{j+1}^{2*}] = 0. \tag{4.17}
 \end{aligned}$$

η_i^{1*} and η_{i+1}^{3*} are in correspondence through the transition $CD \rightarrow DC$ at site $j, j + 1$, as well as η_j^{2*} and η_{j+1}^{4*} with respect to the transition $AB \rightarrow BA$ at site

$i, i + 1 \dots$. From the hypothesis of the lemma, (4.17) rewrites

$$C_a^{(N)} \left(C_c^{(N-1)} \pi_{\eta_{i,j}^{1**}}^{(N-2)} - C_d^{(N-1)} \pi_{\eta_{i,j+1}^{1**}}^{(N-2)} \right) + C_b^{(N)} \left(C_d^{(N-1)} \pi_{\eta_{i,j}^{(3**)}}^{(N-2)} - C_c^{(N-1)} \pi_{\eta_{i,j+1}^{(3**)}}^{(N-2)} \right) + C_c^{(N)} \left(C_b^{(N-1)} \pi_{\eta_{i,j}^{2**}}^{(N-2)} - C_a^{(N-1)} \pi_{\eta_{i+1,j}^{2**}}^{(N-2)} \right) + C_d^{(N)} \left(C_a^{(N-1)} \pi_{\eta_{i,j}^{4**}}^{(N-2)} - C_b^{(N-1)} \pi_{\eta_{i+1,j}^{4**}}^{(N-2)} \right) = 0,$$

where $\eta_{i,j}^{1**}$ is the sequence obtained from η^1 by suppressing letters at site i and j . The elimination of letters in sequences is a commutative process, therefore this last equality holds because of the following identities:

$$\eta_{i,j}^{1**} = \eta_{i+1,j}^{2**}, \quad \eta_{i,j}^{3**} = \eta_{i+1,j}^{4**}, \quad \eta_{i,j}^{2**} = \eta_{i,j+1}^{3**}, \quad \eta_{i,j}^{4**} = \eta_{i,j+1}^{1**}. \quad \square$$

The complete study to establishing the range of validity of the recurrence relation (4.13) altogether with (4.16) is the object of another work in progress. We expect that in general this relation to be valid only asymptotically for large N , which could be proved possibly by selecting the dominant terms in the expansion (4.6).

4.4. Fluid Limits

In this section we examine how the microscopic coefficients $C_k^{(N)}$, whenever (4.16) holds, can be transposed at macroscopic level and how they are related to important coefficients showing up in the Lotka–Volterra equations of the fluid limit. Using the preliminary study,⁽¹⁷⁾ where a new functional method was introduced to handle the hydrodynamic limit of a simple exclusion process, we consider hereafter the n -type case.

4.4.1. Functional Approach

Let $\phi_k, k = 1, \dots, n$ a set of arbitrary functions in $C^2[0, 1]$, $\mathbf{G}^{(N)} \stackrel{\text{def}}{=} \mathbb{Z}/N\mathbb{Z}$ the discrete torus (circle). For $i \in \mathbf{G}^{(N)}$, $X_i^k(t)$ is a binary random variable and, at time t , the presence of a particle of type k at site i is equivalent to $X_i^k(t) = 1$. The exclusion constraint reads

$$\sum_{k=1}^n X_i^k(t) = 1, \quad \forall i \in \mathbf{G}.$$

The whole trajectory is represented by $\eta^{(N)}(t) \stackrel{\text{def}}{=} \{X_i^k(t), i \in \mathbf{G}^{(N)}, k = 1, \dots, n\}$ which is a Markov process. $\Omega^{(N)}$ will denote its generator and $\mathcal{F}_t^{(N)} = \sigma(\eta^{(N)}(s), s \leq t)$ is the associated natural filtration.

Define the real-valued positive measure

$$Z_t^{(N)}[\phi] \stackrel{\text{def}}{=} \exp \left[\frac{1}{N} \sum_{k=1, i \in \mathbf{G}^{(N)}}^n \phi_k \left(\frac{i}{N} \right) X_i^k \right],$$

where ϕ denotes the set $\{\phi_k, k = 1, \dots, n\}$. In Ref. 17 the convergence of this measure was analyzed for $n = 2$. A functional integral operator was used to characterize limit points of this measure, these were shown to be indeed the unique weak solution of a partial differential equation of Cauchy type.

In what follows, we will be interested in the quantities

$$\begin{cases} f_t^{(N)}(\phi) \stackrel{\text{def}}{=} [\mathbb{E}(Z_t^{(N)}[\phi])], \\ g_t^{(N)}(\phi) \stackrel{\text{def}}{=} \log [\mathbb{E}(Z_t^{(N)}[\phi])], \end{cases}$$

respectively the moment and cumulant generating function. The idea of using $Z_t^{(N)}[\phi]$ is that the generator, when applied to $Z_t^{(N)}$, can be expressed as a differential operator with respect to the arbitrary functions ϕ . Indeed, we have

$$\Omega^{(N)}[Z_t^{(N)}] = L_t^{(N)} Z_t^{(N)},$$

with

$$L_t^{(N)} = N^2 \sum_{k \neq l, i \in \mathbf{G}^{(N)}} \tilde{\lambda}_{kl} \frac{\partial^2}{\partial \phi_k \left(\frac{i}{N} \right) \partial \phi_l \left(\frac{i+1}{N} \right)},$$

after having set.

$$\begin{cases} \Delta \psi_{kl} \left(\frac{i}{N} \right) \stackrel{\text{def}}{=} \phi_k \left(\frac{i+1}{N} \right) - \phi_k \left(\frac{i}{N} \right) + \phi_k \left(\frac{i}{N} \right) - \phi_l \left(\frac{i+1}{N} \right), \\ \tilde{\lambda}_{kl}(i, N) \stackrel{\text{def}}{=} 2\lambda_{kl}(N) e^{\frac{\Delta \psi_{kl} \left(\frac{i}{N} \right)}{2N}} \sinh \left(\frac{\Delta \psi_{kl} \left(\frac{i}{N} \right)}{2N} \right). \end{cases}$$

We introduce now the key quantities for hydrodynamic scalings, by assuming an asymptotic expansion of the form

$$\lambda_{kl}(N) = D \left(N^2 + \frac{\alpha_{kl}}{2} N \right) + \mathcal{O}(1), \quad \forall k, l \ k \neq l,$$

where $\alpha_{kl} = -\alpha_{lk}$ are real constants. Here the system is assumed to be *equidiffusive*, which means there exists a constant D such that, for all pairs (k, l) ,

$$\lim_{N \rightarrow \infty} \frac{\lambda_{kl}(N)}{N^2} = D.$$

From now on we will omit the argument of $\lambda_{kl}(N)$ and retain the initial notation λ_{kl} . The coefficients α_{kl} express the asymmetry between types k and l .

Now one can write

$$\frac{\partial f_t^{(N)}}{\partial t} = N^2 \sum_{k \neq l, i \in \mathbf{G}^{(N)}} \tilde{\lambda}_{kl}(i, N) \frac{\partial^2 f_t^{(N)}}{\partial \phi_k \left(\frac{i}{N}\right) \partial \phi_l \left(\frac{i+1}{N}\right)}. \tag{4.18}$$

To rearrange the sum in (4.18), in order to select dominant terms in the expansion with respect to $1/N$, we make use of the exclusion property, which is formally equivalent to

$$\sum_{k=l}^n \frac{\partial}{\partial \phi_k \left(\frac{i}{N}\right)} = \frac{1}{N}.$$

Since we are on the circle $i \in \mathbf{G}^{(N)}$, Abel’s summation formula does not produce any boundary term, so that, skipping details, (4.18) can be rewritten as

$$\begin{aligned} \frac{\partial f_t^{(N)}}{\partial t} = & DN^2 \sum_{k=1, i \in \mathbf{G}^{(N)}}^n \left[\phi_k \left(\frac{i+1}{N}\right) - \phi_k \left(\frac{i}{N}\right) \right] \left[\frac{\partial f_t^{(N)}}{\partial \phi_k \left(\frac{i}{N}\right)} - \frac{\partial f_t^{(N)}}{\partial \phi_k \left(\frac{i+1}{N}\right)} \right. \\ & \left. + \frac{1}{2} \sum_{l \neq k} \alpha_{kl} \left(\frac{\partial^2 f_t^{(N)}}{\partial \phi_k \left(\frac{i}{N}\right) \partial \phi_l \left(\frac{i+1}{N}\right)} + \frac{\partial^2 f_t^{(N)}}{\partial \phi_l \left(\frac{i+1}{N}\right) \partial \phi_k \left(\frac{i}{N}\right)} \right) \right] + \mathcal{O}(N^{-1}). \end{aligned} \tag{4.19}$$

It is worth remarking that operators like $\frac{\partial}{\partial \phi_k \left(\frac{i}{N}\right)}$ and $\phi_k \left(\frac{i+1}{N}\right) - \phi_k \left(\frac{i}{N}\right)$ produce a scale factor $1/N$, while $\frac{\partial}{\partial \phi_k \left(\frac{i}{N}\right)} - \frac{\partial}{\partial \phi_k \left(\frac{i+1}{N}\right)}$ and $\frac{\partial}{\partial \phi_k \left(\frac{i+1}{N}\right) \partial \phi_l \left(\frac{i}{N}\right)}$ scale as $1/N^2$: this explains the selection of dominant terms in the above expansion.

Let $N \rightarrow \infty$ and assume the convergence of the sequence $f_0^{(N)}$. Then, from the tightness of the process, together with a zeste of variational and complex variable calculus, as in Ref. 17, we claim [the proof is omitted] $f_t^{(N)}$ also converges, in a *good tempered* functional space, and its limit f_t satisfies the functional integral equation

$$\frac{\partial f_t}{\partial t} = D \int_0^1 dx \sum_{k=1}^n \phi_k(x) \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} \frac{\partial f_t}{\partial \phi_k(x)} - \sum_{l \neq k} \alpha_{kl} \left(\frac{\partial^2 f_t}{\partial \phi_k(x) \partial \phi_l(x)} \right) \right].$$

Similarly, the cumulant characteristic function is a solution of

$$\begin{aligned} \frac{\partial g_t}{\partial t} = & D \int_0^1 dx \sum_{k=1}^n \phi_k(x) \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} \frac{\partial g_t}{\partial \phi_k(x)} \right. \\ & \left. - \sum_{l \neq k} \alpha_{kl} \left(\frac{\partial g_t}{\partial \phi_k(x)} \frac{\partial g_t}{\partial \phi_l(x)} - \frac{\partial^2 g_t}{\partial \phi_k(x) \partial \phi_l(x)} \right) \right]. \end{aligned} \tag{4.20}$$

Assume at time 0 the given initial profile $\rho_k(x, 0)$ to be twice differentiable with respect to x . Then (4.20) is given by

$$g_t(\phi) = \int_0^1 dx \sum_{k=1}^n \rho_k(x, t) \phi_k(x),$$

where $\rho_k(x, t)$ satisfy the hydrodynamic system of coupled Burger's equations

$$\frac{\partial \rho_k}{\partial t} = D \left[\frac{\partial^2 \rho_k}{\partial x^2} + \frac{\partial}{\partial x} \left(\sum_{l \neq k} \alpha_{lk} \rho_k \rho_l \right) \right], \quad k = 1, \dots, n$$

with a set of given initial conditions $\rho_k(x, 0), k = 1, \dots, n$.

Remark. It is important to note that, without differentiability conditions for the initial profiles $\rho_k(x, 0)$, one can only assert the existence of *weak solutions* (in the sense of Schwartz's distributions) of Burger's system.

4.4.2. Functional Equation at Steady-State

Theorem 4.4. Consider a particle system of size N , with rules 2.1, with n types of particles and periodic boundary conditions. Assume the detailed current equations holds, for any pair of particle types k and l ,

$$\lambda_{kl}^{(N)} \pi_\eta - \lambda_{lk}^{(N)} \pi_{\eta'} = C_k^{(N)} \pi_{\eta_i^*}^{(N-1)} - C_l^{(N)} \pi_{\eta_{i+1}^*}^{(N-1)}, \quad k, l = 1, \dots, n. \quad (4.21)$$

Then the limit functional $f_\infty[\phi] = \lim_{N \rightarrow \infty} f_\infty^{(N)}[\phi]$, where

$$f_\infty^{(n)}[\phi] = \sum_{\{\eta\}} \pi_\eta \exp \left(\frac{1}{N} \sum_{k=1, i=1}^{n, N} X_i^k \phi_k \left(\frac{i}{N} \right) \right),$$

satisfies the equation

$$\frac{\partial}{\partial x} \frac{\partial f_\infty}{\partial \phi_k(x)} + \sum_{l \neq k} \alpha_{kl} \frac{\partial^2 f_\infty}{\partial \phi_k(x) \partial \phi_l(x)} = c_k f_\infty - v \frac{\partial f_\infty}{\partial \phi_k(x)}, \quad (4.22)$$

under the fundamental scaling

$$\lim_{N \rightarrow \infty} \log \frac{\lambda_{kl}^{(N)}}{\lambda_{lk}^{(N)}} = \alpha_{kl} \quad \text{and} \quad \forall l \neq k, \quad \lim_{N \rightarrow \infty} \frac{N^2 C_k^{(N)}}{\lambda_{kl}^{(N)}} = \lim_{N \rightarrow \infty} \frac{C_k^{(N)}}{D} = c_k,$$

with

$$v \stackrel{\text{def}}{=} \sum_{l=1}^n c_k.$$

Proof: We use the notation of Sec. 4.4. In order to extract additional information at steady state, we refine our preceding variational analysis by defining the functional

$$T^{(N)}(\{\phi, \partial_x \phi\}) = \frac{N^2}{2} \left[\sum_{k=1, i=1}^{n, N} \tilde{\lambda}_{kl}^{(N)} \frac{\partial^2}{\partial \phi_l \left(\frac{i}{N}\right) \partial \phi_k \left(\frac{i+1}{N}\right)} + \tilde{\lambda}_{lk}^{(N)} \frac{\partial^2}{\partial \phi_k \left(\frac{i+1}{N}\right) \partial \phi_l \left(\frac{i}{N}\right)} \right] f_\infty^{(N)}, \tag{4.23}$$

which corresponds to the second member of Eq. (4.18) at steady state, and where it is understood that the sets $\{\phi\} \stackrel{\text{def}}{=} \{\phi(\frac{i}{N}), i = 1, \dots, N\}$ and $\{\partial \phi\} \stackrel{\text{def}}{=} \{\frac{\partial \phi}{\partial x}(\frac{i}{N}), i = 1, \dots, N\}$ are taken as independant parameters. This functional can be written in two different manners. Recalling the definitions

$$\Delta \psi_{kl}(i) \stackrel{\text{def}}{=} \phi_k(i + 1) - \phi_k(i) - \phi_l(i + 1) + \phi_l(i) \stackrel{\text{def}}{=} \Delta \psi_k(i) - \Delta \psi_l(i),$$

Eq. (4.23) may be rewritten in the form

$$T^{(N)}(\{\phi, \partial_x \phi\}) = ND \sum_{k=1, i=1}^{n, N} \partial_x \phi_k \left(\frac{i}{N}\right) \left[\frac{\partial f_\infty^{(N)}}{\partial \phi_k \left(\frac{i}{N}\right)} - \frac{\partial f_\infty^{(N)}}{\partial \phi_k \left(\frac{i+1}{N}\right)} + \sum_{l \neq k} \frac{\alpha_{kl}}{2} \left(\frac{\partial^2 f_\infty^{(N)}}{\partial \phi_k \left(\frac{i}{N}\right) \partial \phi_l \left(\frac{i+1}{N}\right)} + \frac{\partial^2 f_\infty^{(N)}}{\partial \phi_k \left(\frac{i+1}{N}\right) \partial \phi_l \left(\frac{i}{N}\right)} \right) \right] + \mathcal{O}\left(\frac{1}{N}\right). \tag{4.24}$$

On the other hand, combining the sums in (4.23) yields

$$T^{(N)}(\{\phi, \partial_x \phi\}) = N^2 \sum_{k, l=1, i=1}^{n, N} \sum_{\{\eta\}} e^{\frac{1}{N} \vec{\phi} \cdot \vec{\eta} + \frac{1}{2N} \Delta \psi_{kl}(i)} \sinh \frac{\Delta \psi_{kl}(i)}{2N} \times X_i^k X_{i+1}^l \left[\lambda_{kl}^{(N)} \pi_\eta^{(N)} - \lambda_{lk}^{(N)} \pi_{T_i \eta}^{(N)} \right], \tag{4.25}$$

where η is a given configuration, $T_i \eta$ being the one obtained from η by exchanging i and $i + 1$, and the shorthand notation

$$\vec{\phi}, \vec{\eta} = \sum_{k=1, i=1}^{n, N} X_i^k \phi_k \left(\frac{i}{N}\right).$$

From the assumptions in the statement of the proposition, we can rewrite (4.25) as

$$T^{(N)}(\{\phi, \partial_x \phi\}) = N^2 \sum_{k,l=1,i=1}^{n,N} \sum_{\{\eta\}} e^{\frac{1}{N}\bar{\phi} \cdot \bar{\eta} + \frac{1}{2N} \Delta \psi_{kl}(i)} \sinh \frac{\Delta \psi_{kl}(i)}{2N} \times X_i^k X_{i+1}^l \left[C_k^{(N)} \pi_{\eta_i^*}^{(N-1)} - C_l^{(N)} \pi_{\eta_{i+1}^*}^{(N-1)} \right], \quad (4.26)$$

where η_i^* is the sequence obtained from η by removing the site i . We also have

$$\sum_{\{\eta\}} X_i^k \pi_{\eta_i^*} e^{\frac{1}{N}\bar{\phi} \cdot \bar{\eta}} = f_\infty^{(N-1)}[\phi_i^*] e^{\frac{1}{N} \phi_k(\frac{i}{N})},$$

where $f_\infty^{(N-1)}[\phi_i^*]$ means that $f_\infty^{(N-1)}$ is considered as a function of the $n(N-1)$ variables $\{\phi_k(\frac{i}{N}), k = 1, \dots, n; j = 1, \dots, N, j \neq i\}$. Using all these ingredients, expanding (4.26) in powers of $\frac{1}{N}$ and keeping the dominant terms, we get

$$T^{(N)}(\{\phi, \partial_x \phi\}) = \frac{N^2}{2} \sum_{k,l=1,i=1}^{n,N} \Delta \psi_{kl}(i) \left[C_k^{(N)} \frac{\partial f_\infty^{(N-1)}}{\partial \phi_l(\frac{i+1}{N})} - C_l^{(N)} \frac{\partial f_\infty^{(N-1)}}{\partial \phi_k(\frac{i}{N})} \right] + \mathcal{O}\left(\frac{1}{N}\right). \quad (4.27)$$

Now, rearranging the summation, using the exclusion property

$$\sum_{l=1}^n \frac{\partial}{\partial \phi_l(\frac{i}{N})} = \frac{1}{N},$$

comparing (4.24) and (4.27), we finally obtain

$$\begin{aligned} & N^2 \sum_{k=1,i=1}^{n,N} \partial_x \phi_k \left(\frac{i}{N}\right) \left[\frac{\partial f_\infty^{(N)}}{\partial \phi_k(\frac{i}{N})} - \frac{\partial f_\infty^{(N)}}{\partial \phi_k(\frac{i+1}{N})} \right. \\ & \quad \left. + \frac{\alpha^{kl}}{2} \left(\frac{\partial^2 f_\infty^{(N)}}{\partial \phi_k(\frac{i}{N}) \partial \phi_l(\frac{i+1}{N})} + \frac{\partial^2 f_\infty^{(N)}}{\partial \phi_k(\frac{i+1}{N}) \partial \phi_l(\frac{i}{N})} \right) \right] \\ & = N^2 \sum_{k,i=1}^{n,N} \partial_x \phi_k \left(\frac{i}{N}\right) \left[\frac{C_k^{(N)}}{D} f_\infty^{(N-1)} - \sum_{l=1}^n \frac{C_l^{(N)}}{D} \frac{\partial f_\infty^{(N-1)}}{\partial \phi_k(\frac{i}{N})} \right] + \mathcal{O}\left(\frac{1}{N}\right). \end{aligned}$$

As the last equality holds for any $\partial_x \phi_k$, letting $N \rightarrow \infty$ implies easily (4.22), which was to be proved. \square

4.4.3. Lotka–Volterra Systems and Out-of-Equilibrium Stationary States

Here we will make the link between the structure coefficients of the current Eqs. (4.21) and the fluid limit description of stationary states. A solution is sought of the form

$$f_\infty(\phi) = \exp \left(\int_0^1 dx \sum_{k=1}^N \rho_k^\infty(x) \phi_k(x) \right),$$

which, instantiated into (4.22), yields gives the following equations for the ρ_k^∞ 's.

$$\frac{\partial \rho_k^\infty}{\partial x} - \rho_k^\infty \sum_{l \neq k} \alpha^{kl} \rho_l^\infty = c_k - v \rho_k^\infty, \quad k = 1, \dots, n.$$

The interpretation of this system is now quite obvious: it is exactly a particular stationary solution of the system formed by the coupled Burger's equations

$$\frac{\partial \rho_k}{\partial t} = \frac{\partial^2 \rho_k}{\partial x^2} - \frac{\partial}{\partial x} \left(\rho_k \sum_{l \neq k} \alpha^{kl} \rho_l \right), \quad k = 1, \dots, n,$$

where the functions ρ_k are sought in the class

$$\rho_k(x, t) \stackrel{\text{def}}{=} \rho_k^\infty(x - vt),$$

the variable $(x - vt)$ being taken [modulo 1]. Hence, there is a frame rotating at velocity v , in which ρ_k^∞ is periodic. Moreover, in this frame, the stationary currents do not vanish and have constant values

$$J_k(x) = \frac{\partial \rho_k^\infty}{\partial x} + \rho_k^\infty \left(v - \sum_{l \neq k} \alpha^{kl} \rho_l^\infty \right) = c_k.$$

Therefore, while the macroscopic constants $\{c_k, k = 1, \dots, n\}$ are in principle determined from the periodic boundary conditions constraints and from the fixed average values of each particle species, they can also be directly derived from the microscopic model.

5. TRANSIENT REGIME AND FLUCTUATIONS

The goal of this section is twofold: first, establish relationships between currents and particle densities at the deterministic level by means of the law of large numbers; secondly, compute the stochastic corrections to these relationships for large but finite systems by using central limit theorems and large deviations.

5.1. Time-Scale for Local Equilibrium

In keeping with our approach, we discuss the question of local equilibrium⁽³⁰⁾ by means of the following functional

$$Y_t^{(N)} \stackrel{\text{def}}{=} \exp \left[\frac{1}{N} \sum_{k,l=1,i=1}^{n,N} \phi_{kl} \left(\frac{i}{N} \right) X_i^k X_{i+1}^l \right].$$

Without entering into cumbersome technical details, let us just notice that the explicit computation of $L_t^{(N)} Y_t^{(N)}$ shows that $L_t^{(N)} Y_t^{(N)}$ scales like $\mathcal{O}(N)$ instead of $\mathcal{O}(1)$ as $L_t^{(N)} Y_t^{(N)}$. This fact can be interpreted as follows. The empirical measure

$$\mu_t^{(N)} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{k,l=1,i=1}^{n,N} \phi_{kl} \left(\frac{i}{N} \right) X_i^k X_{i+1}^l$$

is a convolution of the distribution of interfaces between particle domains with a set of arbitrary functions. To any given particle density distribution, drawn from the set of local hydrodynamic densities, there corresponds an arrangement of these interfaces which somehow characterizes the local correlations between particles. At steady-state, at least in the reversible case, it is easy to show that these correlations vanish. Moreover this scaling tells us that correlations vanish at a time-scale *faster* than the diffusion scale, by a factor of N . Therefore, even in transient regime, we expect correlations to be negligible for the family of diffusive processes under study. A more formal proof of this fact is postponed to the completion of the functional approach initiated in Ref. 17.

5.2. Hydrodynamical Currents

In our preceding studies, we devised a scheme to obtain a fluid limit at steady state, first for the reversible square-lattice model in Ref. 15, and also for the non-reversible ABC model.⁽¹⁶⁾ Here we generalize this procedure to transient n -type particle systems, resting upon the hydrodynamic hypothesis, which will be precisely stated. The principle of the method is to reverse the relationship between particle and current variables in a suitable manner, in order to apply a law of large numbers.

5.2.1. Diffusion Models

The system corresponds to rules (2.1). For any particle-type k , the rescaled discrete current reads

$$J_k^{(N)} \left(\frac{i}{N} \right) \stackrel{\text{def}}{=} \lambda_k^+(i+1) X_i^k - \lambda_k^-(i) X_{i+1}^k, \quad i = 1, \dots, N, \quad (5.1)$$

with

$$\begin{cases} \lambda_k^+(i) \stackrel{\text{def}}{=} \sum_{l \neq k} \frac{\lambda_{kl}}{N} X_i^l + \Gamma_k X_i^k, \\ \lambda_k^-(i) \stackrel{\text{def}}{=} \sum_{l \neq k} \frac{\lambda_{lk}}{N} X_i^l + \Gamma_k X_i^k, \end{cases}$$

where arbitrary constants Γ_k have been introduced (they not modify the value of J_k) to ensure that the λ_k^\pm 's never vanish. To be consistent with other scalings, Γ_k is assumed to scale like N . Our hypothesis is that J_k has a limiting distribution, $J_k(x)$, such that, for any integrable complex-valued function α ,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N \alpha\left(\frac{i}{N}\right) J_k^{(N)}\left(\frac{i}{N}\right) = \int_0^1 \alpha(x) J_k(x) dx. \tag{5.2}$$

In addition, the system will be said *equidiffusive*, if there exists a single diffusion constant D , such that, for all pair of species (k, l) ,

$$\lim_{N \rightarrow \infty} \frac{\lambda_{kl}(N)}{N^2} = D \quad [\text{equidiffusion}].$$

To simplify the notation, consider equation for $k = 1$, writing $J_a \stackrel{\text{def}}{=} J_1$ and replacing X_i^1 by A_i . Then solving (5.1) as a linear system yields

$$A_{i+1} = \frac{\lambda_a^+(i+1)A_i - J_a^{(N)}\left(\frac{i}{N}\right)}{\lambda_a^-(i)}.$$

This relationship between A_i and A_{i+1} can be iterated, by means of a 2×2 matrix products. Indeed, introducing the pair of numbers (u_i, v_i) such that $A_i = \frac{u_i}{v_i}$, the recursion becomes

$$\begin{bmatrix} u_{i+1} \\ v_{i+1} \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{\lambda_a^+(i+1)}{\lambda_a^-(i)}} & -\frac{J_a^{(N)}\left(\frac{i}{N}\right)}{\sqrt{\lambda_a^+(i+1)\lambda_a^-(i)}} \\ 0 & \sqrt{\frac{\lambda_a^-(i)}{\lambda_a^+(i+1)}} \end{bmatrix} \begin{bmatrix} u_i \\ v_i \end{bmatrix} \stackrel{\text{def}}{=} M_i \begin{bmatrix} u_i \\ v_i \end{bmatrix},$$

where for convenience we divided everything by the common factor $\sqrt{\lambda_a^-(i)\lambda_a^+(i+1)}$. Let us define the matrices (p being a positive integer)

$$G^0\left(\frac{i+p}{N}, \frac{i}{N}\right) \stackrel{\text{def}}{=} \prod_{j=i}^{i+p} \begin{bmatrix} \sqrt{\frac{\lambda_a^+(j+1)}{\lambda_a^-(j)}} & 0 \\ 0 & \sqrt{\frac{\lambda_a^-(j)}{\lambda_a^+(j+1)}} \end{bmatrix},$$

$$G^0\left(\frac{i+p}{N}, \frac{i}{N}\right) \stackrel{\text{def}}{=} \prod_{j=i}^{i+p} M_j,$$

$$\Sigma\left(\frac{i}{N}\right) \stackrel{\text{def}}{=} \begin{bmatrix} 0 & -\frac{J_a^{(N)}\left(\frac{i}{N}\right)}{\sqrt{\lambda_a^+(i+1)\lambda_a^-(i)}} \\ 0 & 0 \end{bmatrix},$$

(explicit references to the species (a) and the size N is omitted here, to lighten the notations). Because of the upper triangular structure of Σ , we may simply express G as

$$G\left(\frac{i+p}{N}, \frac{i}{N}\right) = G^0\left(\frac{i+p}{N}, \frac{i}{N}\right) + \sum_{j=0}^p G^0\left(\frac{i+p}{N}, \frac{i+j+1}{N}\right) \times \Sigma\left(\frac{i+j}{N}\right) G^0\left(\frac{i+j-1}{N}, \frac{i}{N}\right).$$

To handle this equation in the continuous limit, we need an additional transformation. Define

$$L_i = \begin{bmatrix} \sqrt{\frac{\Gamma_a}{\lambda_a^+(i)}} & 0 \\ 0 & \sqrt{\frac{\lambda_a^+(i)}{\Gamma_a}} \end{bmatrix}, \quad R_i = \begin{bmatrix} \sqrt{\frac{\lambda_a^-(i)}{\Gamma_a}} & 0 \\ 0 & \sqrt{\frac{\lambda_a^-(i)}{\Gamma_a}} \end{bmatrix},$$

together with

$$\begin{cases} \tilde{G}\left(\frac{i+p}{N}, \frac{i}{N}\right) = L_{i+p+1} G\left(\frac{i+p}{N}, \frac{i}{N}\right) R_i \\ \tilde{G}^0\left(\frac{i+p}{N}, \frac{i}{N}\right) = L_{i+p+1} G^0\left(\frac{i+p}{N}, \frac{i}{N}\right) R_i \end{cases} \tag{5.3}$$

Then \tilde{G} , \tilde{G}^0 and $\tilde{\Sigma}$ verify the same relation,

$$\tilde{G}\left(\frac{i+p}{N}, \frac{i}{N}\right) = \tilde{G}^0\left(\frac{i+p}{N}, \frac{i}{N}\right) + \sum_{j=0}^p \tilde{G}^0\left(\frac{i+p}{N}, \frac{i+j+1}{N}\right) \times \tilde{\Sigma}\left(\frac{i+j}{N}\right) \tilde{G}^0\left(\frac{i+j}{N}, \frac{i+1}{N}\right), \tag{5.4}$$

but

$$\tilde{\Sigma} \left(\frac{i}{N} \right) = \begin{bmatrix} 0 & -\frac{\Gamma_a J_a^{(N)}(\frac{i}{N})}{\lambda_a^+(i+1)\lambda_a^-(i)} \\ 0 & 0 \end{bmatrix}.$$

Noting that $A_{i+p+1}\Gamma_a/\lambda_a^+(i+p+1) = A_{i+p+1}$ and $A_i\Gamma_a/\lambda_a^-(i) = A_i$, the iteration between i and $i+p$ gives

$$A_{i+p+1} = \frac{\tilde{G}_{11} \left(\frac{i+p}{N}, \frac{i}{N} \right) A_i + \tilde{G}_{12} \left(\frac{i+p}{N}, \frac{i}{N} \right)}{\tilde{G}_{22} \left(\frac{i+p}{N}, \frac{i}{N} \right)}. \tag{5.5}$$

We can now take advantage of the law of large numbers in Eq. (5.4). First of all, for N large, and fixing $x = i/N$ and $y = p/N$, letting $\sigma = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ we have,

$$\begin{aligned} \tilde{G}^0 \left(\frac{i+p}{N}, \frac{i}{N} \right) &= \exp \left(\frac{\sigma}{2} \sum_{j=i+1, k=2}^{i+p+1} \log \frac{\lambda_{ak}}{\lambda_{ka}} X_k^k \right) \\ &= \exp \left(\frac{\sigma}{2} \int_x^{x+y} du \sum_{k=2}^n \alpha^{ak} \rho_k(u) + o(1) \right), \end{aligned}$$

from the hydrodynamic hypothesis. To proceed further, we have to distinguish between two situations.

[The equidiffusion case] Recalling that Γ_a is a free parameter which scales like N , it is convenient in the *equidiffusion* case to impose the limit

$$\lim_{N \rightarrow \infty} \frac{\Gamma_a(N)}{N} = D.$$

Then, expanding $\tilde{\Sigma}(i/N)$ with respect to $1/N$ yields

$$\tilde{\Sigma} \left(\frac{i}{N} \right) = \begin{bmatrix} 0 & -\frac{J_a^{(N)}(\frac{i}{N})}{ND} \\ 0 & 0 \end{bmatrix} + \mathcal{O}(N^{-2}),$$

and the limit

$$\mathcal{G}(x+y, x) \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \tilde{G} \left(\frac{i+p}{N}, \frac{i}{N} \right).$$

is provided by Eq. (5.4). Hence

$$\mathcal{G}(x + y, x) = \mathcal{G}^0(x + y, x) + \int_x^{x+y} du \mathcal{G}^0(x + y, x + u) \Xi(x + u) \mathcal{G}^0(x + u, x), \tag{5.6}$$

with

$$\mathcal{G}^0(y, x) = \exp\left(\frac{\sigma}{2} \int_x^y du \sum_{k=2}^n \alpha_{ak} \rho_k(u)\right), \quad \text{and} \quad \Xi(x) = \begin{bmatrix} 0 & -\frac{J_a^{(N)}(x)}{D} \\ 0 & 0 \end{bmatrix}, \tag{5.7}$$

still by virtue of the hydrodynamic hypothesis (5.2). Now it is possible to close the equations between densities and currents. Using again the hydrodynamic hypothesis with the fact that \mathcal{G} is a smooth deterministic operator, (5.5) leads to

$$\rho_a(x + y) = \frac{\mathcal{G}_{11}(x + y, x) \rho_a(x) + \mathcal{G}_{12}(x + y, x)}{\mathcal{G}_{22}(x + y, x)}.$$

Differentiating this last relation w.r.t. y , then taking into account (5.6) and (5.7), we obtain the final deterministic expression for the current

$$J_a(x) = D \left(-\frac{\partial \rho_a}{\partial x} + \sum_{k=2}^n \alpha_{ak} \rho_k \rho_a \right), \tag{5.8}$$

which, combined with the continuity equation

$$\frac{\partial \rho_a}{\partial t} + \frac{\partial J_a}{\partial x} = 0,$$

leads again to a Burger’s hydrodynamic equation.

[The hetero-diffusion case] Here, the limit (5.4) is a bit more tricky. In fact, the expansion of $\tilde{\Sigma}$ involves correlations between currents and densities which already appear in the leading terms, and we expect an effective diffusion constant of the form

$$D_a(\rho) = D \exp\left(\sum_{k=2}^n \beta^{ak} \rho_k\right),$$

with

$$\begin{cases} D \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \frac{1}{N^2} \exp\left(\frac{1}{n-1} \sum_{k=2}^n \log \lambda_{ak}(N)\right), \\ \beta^{ak} \stackrel{\text{def}}{=} \lim_{N \rightarrow \infty} \log\left(\frac{\lambda_{ak}}{N^2 D}\right). \end{cases}$$

We pursue no further the study of this case, which presumably could be handled with block-estimates techniques (see Ref. 30).

5.2.2. Diffusion with Reaction

Here we treat the square-lattice model, a special case of (2.2), where reactions take place, in addition to diffusion. The procedure follows the lines of the preceding subsection. Using the mapping (2.5), the model is formulated in terms of two coupled exclusion processes, and the current equations corresponding to both species have the form

$$J_a^{(N)}\left(\frac{i}{N}\right) = \lambda_a^+(i)\tau_i^a \bar{\tau}_{i+1}^a - \lambda_a^-(i)\bar{\tau}_i^a \tau_{i+1}^a,$$

$$J_b^{(N)}\left(\frac{i}{N}\right) = \lambda_b^+(i)\tau_i^b \bar{\tau}_{i+1}^b - \lambda_b^-(i)\bar{\tau}_i^b \tau_{i+1}^b,$$

with the rates given by (2.6), and we restrict the present analysis to the symmetric case (see relations (2.4)). Reversing for example the equation for J_a leads to the homographic relationship

$$\tau_{i+1}^a = \frac{\lambda_a^+(i)\tau_i^a - J_a^{(N)}\left(\frac{i}{N}\right)}{(\lambda_a^+(i) - \lambda_a^-(i))\tau_i^a + \lambda_a^-(i)},$$

which again can be iterated by means of a 2×2 matrix product, after defining u_i^a and v_i^a s.t. $\tau_i^a = u_i^a/v_i^a, \forall i \in \{1, \dots, N\}$. Define

$$\lambda(N) \stackrel{\text{def}}{=} \frac{\lambda^+(N) + \lambda^-(N)}{2}, \quad \mu(N) \stackrel{\text{def}}{=} \frac{\lambda^+(N) - \lambda^-(N)}{2},$$

and

$$\gamma(N) \stackrel{\text{def}}{=} \frac{\gamma^+(N) + \gamma^-(N)}{2}.$$

Then the proper scalings for large N are given by

$$\lim_{N \rightarrow \infty} \frac{\lambda(N)}{N^2} = D, \quad \lim_{N \rightarrow \infty} \frac{\gamma(N)}{N^2} = \Gamma, \quad \lim_{N \rightarrow \infty} \frac{\mu(N)}{N} = \eta.$$

Letting now

$$\Sigma\left(\frac{i}{N}\right) = \begin{bmatrix} 0 & -\frac{J_a^{(N)}\left(\frac{i}{N}\right)}{\sqrt{\lambda_a^+(i)\lambda_a^-(i)}} \\ \sqrt{\frac{\lambda_a^+(i)}{\lambda_a^-(i)}} - \sqrt{\frac{\lambda_a^-(i)}{\lambda_a^+(i)}} & 0 \end{bmatrix},$$

G cannot be given explicitly: it is instead solution of the following combinatorial self-consistent equation

$$G\left(\frac{i+p}{N}, \frac{i}{N}\right) = G_0\left(\frac{i+p}{N}, \frac{i}{N}\right) + \sum_{j=0}^p G_0\left(\frac{i+p}{N}, \frac{i+j}{N}\right) \times \Sigma\left(\frac{i+j}{N}, \frac{i+1}{N}\right). \tag{5.9}$$

The iteration now reads,

$$\begin{bmatrix} u_{i+p+1} \\ v_{i+p+1} \end{bmatrix} = G\left(\frac{i+p}{N}, \frac{i}{N}\right) \begin{bmatrix} u_i \\ v_i \end{bmatrix}.$$

For the same reason as before, the limit \mathcal{G} of G when $N \rightarrow \infty$ does satisfy

$$\mathcal{G}(x+y, x) = \mathcal{G}^0(x+y, x) + \int_x^{x+y} du \mathcal{G}^0(x+y, x+u) \Sigma(x+u) \mathcal{G}(x+u, x), \tag{5.10}$$

with

$$\mathcal{G}^0(y, x) = \exp\left(\eta\sigma \int_x^y (2\rho_b(u) - 1) du\right),$$

by just applying the law of large numbers in the formal expansion of G with respect to Σ . We leave aside the question concerning existence and analytic properties of a solution of (5.10). We must again discriminate between two situations.

[Case $\gamma = \lambda$]

$$\Sigma(x) = \begin{bmatrix} \eta(2\rho_b - 1) & -\frac{J_a(x)}{D} \\ 2\eta(2\rho_b - 1) & \eta(1 - 2\rho_b) \end{bmatrix},$$

which leads to the following differential system

$$\begin{aligned} \frac{\partial u^a}{\partial x} &= \eta(2\rho_b - 1)u^a - \frac{1}{D} J_a(x)v^a, \\ \frac{\partial v^a}{\partial x} &= 2\eta(2\rho_a - 1)u^a + \eta(1 - 2\rho_b)v^a, \end{aligned}$$

after making use of the law of large numbers and the hydrodynamic hypothesis. Combining these last two equations to express $\rho'_a = (u'_a v_a - v'_a u_a)/v_a^2$ leads to the relation

$$J_a(x) = -D \left(\frac{\partial \rho_a}{\partial x} + 2\eta\rho_a(1 - \rho_a)(1 - 2\rho_b) \right).$$

[Case $\gamma \neq \lambda$] Like in the *hetero-diffusion* case of the last section, the effective diffusion constant $D_a(\rho)$ involves correlations between τ_i^b and τ_{i+1}^b and $J_a(i/N)$ in the leading order term, and we expect a behavior of the form⁽¹⁵⁾

$$D_a(\rho_b) = D \exp \left[2\rho_b(1 - \rho_b) \log \frac{\gamma}{\lambda} \right],$$

as a result of a multiplicative process. This could be obtained through renormalization techniques applied directly to equation (5.9).

To conclude this section, we see that, for $\gamma = \lambda$, the differential system expressing, at steady state, the deterministic limit of the square lattice model with periodic boundary conditions finally reads, setting $v_{a,b} = 2p_{a,b} - 1$,

$$\begin{cases} \frac{\partial v_a}{\partial x} = \eta(1 - v_a^2)v_b + v v_a + \varphi^a, \\ \frac{\partial v_b}{\partial x} = -\eta(1 - v_b^2)v_a + v v_b + \varphi^b, \end{cases} \tag{5.11}$$

where v is a possibly finite drift velocity and $\varphi^a = \varphi(\bar{v}_a, \bar{v}_b)$ and $\varphi^b(\bar{v}_a, \bar{v}_b)$ are two constant currents in the translating frame. These currents have to be determined in a self-consistent manner, after fixing the average densities \bar{v}_a and \bar{v}_b and the periodic boundary conditions. For $v = 0$, the system (5.11) is Hamiltonian with

$$H = \frac{\eta}{2} [v_a^2 v_b^2 - v_a^2 - v_b^2] + \varphi_b v_a - \varphi_a v_b. \tag{5.12}$$

Indeed, it is easy to observe that (5.11) can be rewritten as

$$\frac{\partial v_a}{\partial x} = -\frac{\partial H}{\partial v_b}, \quad \frac{\partial v_b}{\partial x} = \frac{\partial H}{\partial v_a}.$$

The degenerate fixed point $v_{a,b}(x) = \bar{v}_{a,b}$ is always a trivial solution and corresponds to the relations

$$\varphi_a = \eta(\bar{v}_a^2 - 1)\bar{v}_b, \quad \varphi_b = \eta(1 - \bar{v}_b^2)\bar{v}_a.$$

5.3. Microscopic Currents

5.3.1. Particle Currents

An important feature of our particle systems is that the number of particles is locally conserved. This property is reflected as $N \rightarrow \infty$ by a continuity equation, which relates local variations of particle density to inhomogeneous currents. In a discretized framework, conservation of particles is expressed according to the following

Proposition 5.1. Let $\{J_i^k(t, \epsilon)\}_{i=1, \dots, N}$ be stochastic variables corresponding to the fluxes of particles of type $k \in \{1, \dots, n\}$ between site i and $i + 1$, such that

$$J_i^k(t, \epsilon) \stackrel{\text{def}}{=} \frac{1}{\epsilon} \sum_{l \neq k} (X_i^k(t)X_{i+1}^l(t)X_i^l(t + \epsilon)X_{i+1}^k(t + \epsilon) - X_i^l(t)X_{i+1}^k(t)X_i^k(t + \epsilon)X_{i+1}^l(t + \epsilon))$$

with $\epsilon > 0$. By definition $J_i^k(t, \epsilon)$ are ternary variables in $\{-\frac{1}{\epsilon}, 0, +\frac{1}{\epsilon}\}$. The following identify, equivalent to particle conservation,

$$\lim_{\epsilon \rightarrow 0} \frac{X_i^k(t + \epsilon) - X_i^k(t)}{\epsilon} + J_{i+1}^k(t, \epsilon) - J_i^k(t, \epsilon) = 0 \quad a.s., \tag{5.13}$$

holds for all $i \in \{1, \dots, N\}$, $\forall t \in \mathbb{R}^+$. In addition, letting $\eta^{(N)}(t)$ denote the sequence $\{X_i^k(t)\}$, $i = 1, \dots, N$; $k = 1, \dots, n\}$ then the variables $\{J_i^k(t, \epsilon)\}$, $i = 1, \dots, N$; $k = 1, \dots, n\}$, have a joint conditional Laplace transform given by

$$\begin{aligned} h_{t,\epsilon}^{(N)}(\phi) &\stackrel{\text{def}}{=} \mathbf{E}_t \left(\exp \left(\frac{1}{N} \sum_{\substack{k < l \\ i=1}}^{n,N} \phi_k \left(\frac{i}{N} \right) \epsilon J_i^k(t, \epsilon) \right) \middle| \eta(t) \right) \\ &= \mathbf{E}_t \left[\exp \left(\epsilon \sum_{\substack{k \neq l \\ i=1}}^{n,N} \lambda_{kl} X_i^k X_{i+1}^l \left(e^{\frac{1}{N} \psi_{kl}(\frac{i}{N})} - 1 \right) + \lambda_{lk} X_i^l X_{i+1}^k \left(e^{-\frac{1}{N} \psi_{kl}(\frac{i}{N})} - 1 \right) \right) \right] \\ &\quad + o(\epsilon), \end{aligned} \tag{5.14}$$

where ϕ_k , $k = 1, \dots, n$ is a set of \mathbf{C}^∞ bounded functions, and $\psi_{kl} = \phi_k - \phi_l$.

Proof: The points are mere consequences of the Markovian feature of the process and of its generator. In particular, (5.13) results from the fact that, almost surely, at most one jump takes place in the timeinterval ϵ , when $\epsilon \rightarrow 0$, since all events are due to independent Poisson processes. In addition, on the time interval $[t, t + \epsilon]$, the occurrence of a particle exchange between sites i and $i + 1$, corresponding to $\epsilon J_i^k(t, \epsilon) = 1$ is only conditioned by the presence of a pair (k, l) at $(i, i + 1)$, with a transition rate given by $\lambda_{kl} X_i^k X_{i+1}^l$. Therefore

$$h_{t,\epsilon}^{(N)}(\phi) = \mathbb{E}_t \left(\prod_{\substack{k \neq l \\ i=1}}^{n,N} \left[1 + \epsilon \lambda_{kl} X_i^k X_{i+1}^l \left(e^{\frac{1}{N} \psi_{kl}(\frac{i}{N})} - 1 \right) \right] \right),$$

which, after a first order expansion with respect to ϵ , leads to (5.14). □

5.3.2. An Iterative Numerical Scheme

Given a sample path $\eta^{(N)}(t)$ at time t , we may generate a current sequence $\{J_i^k(t, \epsilon)\}$ according to the local product form encountered earlier. In turn, once the set $\{J_i^k(t, \epsilon)\}$ is known, the sequence $\eta(t + \epsilon)$ is almost surely determined, as $\epsilon \rightarrow 0$, by the identity (5.13), expressing conservation law of particles. We therefore have at hand an explicit stochastic numerical scheme to generate the sequence $\eta(t)$ step by step.

Proposition 5.2. *For any $\epsilon > 0$, $N \in \mathbb{N}$, the iterative scheme given by*

$$Q_{n+1}(\eta) = \sum_{\eta'} P_\epsilon(\eta|\eta') Q_n(\eta),$$

where $P_\epsilon(\eta|\eta')$ is defined according to (5.13) and (5.14), converges when $\epsilon \rightarrow 0$ to the original probability measure $P_{t=ne}(\eta)$ corresponds to the original process.

Proof: There is only one thing to show: $\forall T > 0$, the probability p_ϵ that $\exists t \in [0, T]$, such that two adjacent transitions occur within the same time-interval $[t, t + \epsilon]$, tends to 0 when $\epsilon \rightarrow 0$. This is warranted by the fact that the total number of transitions for $t < T$ is almost certainly finite. Indeed, we have

$$p_\epsilon \leq 1 - \left(1 - \left(\max_{kl} \lambda_{kl}\right)^2 \epsilon^2\right)^{\frac{NT}{\epsilon}} \xrightarrow{\epsilon \rightarrow 0} 0.$$

For the hydrodynamic limit the rates λ_{kl} scale like N^2 for large N . Thus, it will be convenient to take a single limit $\epsilon \stackrel{\text{def}}{=} \epsilon(N) \rightarrow 0$ as $N \rightarrow \infty$, since the condition for the scheme to be meaningful writes

$$N\epsilon(N)(\max_{kl} \lambda_{kl})^2 = o(1),$$

so that we get a scaling of $\epsilon(N) = o(N^{-5})$ to meet our needs. This will allow us, in the sequel, to make use of the approximation

$$\sum_{i=1}^N \alpha_i^k \left(X_i^k(t + \epsilon) - X_i^k(t) - \sum_l (J_{i-1}^k - J_i^k)\epsilon \right) = o(\epsilon),$$

for any set of bounded complex numbers $\{\alpha_i^k\}$. □

5.3.3. Central Limit Theorem for Currents

We are in position to exploit the λ conditional product form (5.14) to perform a mapping, in the spirit of Lemma 4.1 of Ref. 15, allowing to obtain a dynamical description of the system, in terms of some external free random process. To this

end we assume, as a basic point, the hydrodynamic limit holds and we rest on the following lemma.

Lemma 5.1. *Suppose the existence of a set of density functions ρ_k , such that*

$$\begin{aligned} & \mathbb{E} \left[\exp \left(\frac{1}{N} \sum_{\substack{k=1 \\ i=1}}^{n,N} X_i^k \phi_k \left(\frac{i}{N} \right) \right) \right] \\ &= \exp \left(\sum_{\substack{k=1 \\ i=1}}^{n,N} \log \left[1 + \rho_k \left(\frac{i}{N} \right) \left(e^{\phi_k(\frac{i}{N})} - 1 \right) \right] + o(N^{-2}) \right), \end{aligned}$$

for any given bounded complex function ϕ_k , and let $\phi = \sup_{\substack{k \in \{1, \dots, n\} \\ x \in [0,1]}} (\phi_k(x))$. Then

$$\begin{aligned} & \mathbb{E} \left[\exp \left(\frac{1}{N} \sum_{\substack{k < l \\ i=1}}^N \phi_k \left(\frac{i}{N} \right) \phi_l \left(\frac{i}{N} \right) X_i^k X_i^l \right) \right] \\ &= \exp \left(\frac{1}{N} \sum_{\substack{k < l \\ i=1}}^N \phi_k \left(\frac{i}{N} \right) \phi_l \left(\frac{i}{N} \right) \rho_k \left(\frac{i}{N} \right) \rho_l \left(\frac{i}{N} \right) + o \left(\frac{\phi}{N} \right) \right). \end{aligned}$$

From this we deduce the following identity

$$\begin{aligned} h_{t,\epsilon}^{(N)}(\phi) = \exp & \left[\epsilon \sum_{\substack{k < l \\ i=1}}^{n,N} \lambda_{kl} \rho^k \left(\frac{i}{N} \right) \rho^l \left(\frac{i+1}{N} \right) \left(e^{\frac{1}{N} \psi_{kl}(\frac{i}{N})} - 1 \right) \right. \\ & \left. + \lambda_{lk} \rho^l \left(\frac{i}{N} \right) \rho^k \left(\frac{i+1}{N} \right) \left(e^{-\frac{1}{N} \psi_{kl}(\frac{i}{N})} - 1 \right) + o(\epsilon) \right], \end{aligned} \tag{5.15}$$

which leads to recover (in our specific context) a formulation of the general result of Ref. 4 concerning fluctuation laws of currents for diffusive systems.

Keeping up to quadratic terms w.r.t. to functions ϕ 's its argument, $h_{t,\epsilon}^{(N)}(\phi)$ reads,

$$\begin{aligned} h_{t,\epsilon}^{(N)}(\phi) = \exp & \left(\epsilon \sum_{\substack{k=1 \\ i=1}}^{n,N} \phi_k \left(\frac{i}{N} \right) \mathcal{J}^k \left(\rho \left(\frac{i}{N} \right) \right) \right. \\ & \left. + \frac{D\epsilon}{N^2} \sum_{k,l=1}^n \phi_k \left(\frac{i}{N} \right) \mathcal{Q}_{kl} \left(\frac{i}{N} \right) \phi_l \left(\frac{i}{N} \right) + o \left(\frac{\phi^2}{N^2} \right) \right), \end{aligned} \tag{5.16}$$

where \mathcal{J}^k are deterministic currents expressed, in terms of densities, by

$$\mathcal{J}^k(\{\rho_l, l = 1, \dots, n\}) \stackrel{\text{def}}{=} -D \left(\frac{\partial \rho_k}{\partial x} + \sum_{l \neq k} \alpha_{kl} \rho_k \rho_l \right),$$

and Q is a $n \times n$ symmetric matrix

$$\begin{cases} Q_{ij} = -\rho_i \rho_j, & i \neq j, \\ Q_{ii} = \rho_i(1 - \rho_i). \end{cases}$$

Q is of rank $n - 1$, because due to the exclusion constraint, currents are not independants,

$$\sum_{k=1}^n J_i^k(t, \epsilon) = 0, \quad \forall i \in \{1, \dots, N\}.$$

Let M the reduced matrix obtained from Q by deleting last row and last column. Its determinant is $\prod_{k=1}^n \rho_k$, so that it M invertible if none of the ρ_k vanishes, with

$$\begin{cases} M_{ij}^{-1} = \frac{1}{\rho_i} + \frac{1}{\rho_n}, & i \neq j, \\ M_{ii}^{-1} = \frac{1}{\rho_n}, \end{cases} \tag{5.17}$$

after having taken into account the exclusion condition $\sum_{n=1}^n \rho_k = 1$. Since every line k or column k sums to $\rho_k \rho_n > 0$, all the eigenvalues are strictly positive, and hence $M(\rho)$ owns a real square-root matrix $M^{1/2}(\rho)$.

Proposition 5.4. *Let $\phi_k, k = 1, \dots, n - 1$ denote a set of C^∞ bounded functions of the real variable $x \in [0, 1]$, $\{w_i^k, k = 1, \dots, n - 1\}$ a set of independent identically distributed Bernoulli random variables with parameters $1/2$, taking at time t values in $\{-1/2, 1/2\}$. Then there exists a probability space, such that*

$$\begin{aligned} \frac{1}{N} \sum_{k=1}^{n,N} \phi_k \left(\frac{i}{N} \right) J_i^k \epsilon &= \frac{1}{N} \sum_{k=1}^{n-1,N} \psi_{kn} \left(\frac{i}{N} \right) \left[\mathcal{J}^k \left(\rho \left(\frac{i}{N} \right) \right) \epsilon \right. \\ &\quad \left. + \sqrt{2D\epsilon} \sum_{l=1}^{n-1} M_{kl}^{\frac{1}{2}} \left(\rho \left(\frac{i}{N} \right) \right) \omega_i^l \right] + \mathcal{O}(N^{-2}), \text{ a.s.} \end{aligned} \tag{5.18}$$

The lines of arguments bare some features in common with the ones proposed in Ref. 15 (to study fluctuations at steady state). Recall, by law of large numbers, that correlations are negligible and do not affect the expression of the deterministic

currents (5.8). This justifies the mapping (5.18). On the other hand, the calculation of coefficients $M_{ij}^{\frac{1}{2}}$ is done by comparing $h_{t,\epsilon}^{(N)}$ in (5.16) with

$$\begin{aligned} & \mathbb{E} \left[\exp \left(\frac{1}{N} \sum_{\substack{k=1 \\ i=1}}^{n-1, N} \psi_{kn} \left(\frac{i}{N} \right) \sqrt{2D\epsilon} M_{kl}^{\frac{1}{2}} \left(\frac{i}{N} \right) \omega_i^l \right) \right] \\ &= \exp \left(\frac{D\epsilon}{N^2} \sum_{kl}^n \phi_k \left(\frac{i}{N} \right) Q_{kl} \left(\frac{i}{N} \right) \phi_l \left(\frac{i}{N} \right) + o(\epsilon) \right), \end{aligned}$$

because $M^{\frac{1}{2}}$ is symmetric and

$$\sum_{kl}^{n-1} \psi_{kn} \left(\frac{i}{N} \right) M_{kl} \psi_{ln} \left(\frac{i}{N} \right) = \sum_{kl}^n \phi_k \left(\frac{i}{N} \right) Q_{kl} \left(\frac{i}{N} \right) \phi_l.$$

Setting, for $k = 1, \dots, n - 1$,

$$Y_k^{(N)}(x, t) \stackrel{\text{def}}{=} \frac{1}{\sqrt{N}} \sum_{i=1}^{[xN]} w_i^k,$$

one sees that the space-time white noise processes

$$\bar{W}^k(x, t) = \lim_{N \rightarrow \infty} \frac{dY_k^{(N)}}{dx}(x, t)$$

describes all current fluctuations in the continuous limit.

5.4. Macroscopic Fluctuations

Two main quantities will be explored in this section: the Lagrangian and the large deviation functional.

5.4.1. The Lagrangian

The preceding section provides us with all coefficients required to achieve an informal derivation of the Lagrangian⁽⁴⁾ describing the current fluctuations. Given the empirical measure

$$\rho_k^{(N)}(x, t) \stackrel{\text{def}}{=} \frac{1}{N} \sum_{i=1}^n X_i^k(t) \delta \left(x - \frac{i}{N} \right),$$

and assuming the system admits a hydrodynamical description in terms of a density field $\rho_k(x, t)$, the statement in Ref. 4 says that there is a large deviation principle for the stationary measure. In other words, the probability that the measure $\rho_k^{(N)}$

deviates from the hydrodynamic density profile ρ_k is exponentially small and given by

$$P\{\rho^{(N)}(t) \simeq \hat{\rho}(t), t \in [t_1, t_2]\} \simeq e^{-NI_{[t_1, t_2]}(\hat{\rho})},$$

where

$$I_{[t_1, t_2]}(\hat{\rho}) = \int_{t_1}^{t_2} \mathcal{L}(\hat{\rho}(t), \partial_t \hat{\rho}(t)) dt.$$

Here the deviation from hydrodynamic solutions is due to current fluctuations.

Writing $\nabla^{-1} \stackrel{\text{def}}{=} \int_0^x$ the quantity $\nabla^{-1} \frac{\partial \hat{\rho}_k^{(N)}}{\partial t} + \mathcal{J}^k(\hat{\rho})$, represents the fluctuations of the current J^k . Reversing the relationship between current fluctuations and white noise process leads formally to

$$W^l(x, t) \simeq \sqrt{\frac{\epsilon}{2DN}} \sum_{k=1}^{n-1} M_{lk}^{-\frac{1}{2}} \left(\nabla^{-1} \frac{\partial \hat{\rho}_k}{\partial t} + \mathcal{J}_k(\hat{\rho}) \right), \quad l = 1, \dots, n-1. \tag{5.19}$$

Then, replacing (5.19) in the joint distribution of $\{W^k(x, t); x \in [0, 1], k = 1, \dots, n-1\}$ we obtain

$$\begin{aligned} \mathcal{L}(\hat{\rho}(t), \partial_t \hat{\rho}(t)) dt &= \frac{1}{2} \int_0^1 dx dt \sum_{k=1}^{n-1} (W^k(x, t))^2 \\ &= \frac{1}{4D} \int_0^1 dx dt \sum_{k=1}^{n-1} \left(\sum_{l=1}^{n-1} M_{lk}^{-\frac{1}{2}} \nabla^{-1} \frac{\partial \hat{\rho}_k}{\partial t} + J_k(\hat{\rho}) \right)^2, \end{aligned} \tag{5.20}$$

where ϵ has been identified with dt and dx with $1/N$. Then, the symmetry of $M^{-1/2}$, the form (5.17) of M^{-1} and the exclusion constraint

$$\sum_{k=0}^n \nabla^{-1} \frac{\partial \hat{\rho}_k}{\partial t} + \mathcal{J}^k(\hat{\rho}) = 0,$$

lead to the final compact form

$$\mathcal{L}(\hat{\rho}, \partial_t \hat{\rho}) = \frac{1}{4D} \int_0^1 dx \sum_{k=1}^n \frac{\left(\nabla^{-1} \frac{\partial \hat{\rho}_k}{\partial t} + \mathcal{J}^k(\hat{\rho}) \right)^2}{\hat{\rho}_k}.$$

5.4.2. Hamilton–Jacobi Equation and Large Deviation Functional

Here we proceed as in Ref. 4. Let π_k , the conjugate variable of ρ_k ,

$$\pi_k(x, t) \stackrel{\text{def}}{=} \frac{\partial \mathcal{L}(\rho, \partial_t \rho)}{\partial \partial_t \rho_k(x, t)}.$$

The Hamiltonian is then given by

$$\mathcal{H}(\{\rho_k, \pi_k\}) \stackrel{\text{def}}{=} \int_0^1 dx \sum_{k=1}^n \pi_k(x, t) \partial_t \rho_k(x, t) - \mathcal{L}.$$

Algebraic manipulations lead to the expression

$$\mathcal{H}(\{\rho_k, \pi_k\}) \stackrel{\text{def}}{=} \int_0^1 dx [\partial_x \pi_k \mathcal{J}_k(\rho) + D\rho_k (\partial_x \pi_k)^2].$$

Then the large deviation functional \mathcal{F} , satisfying

$$P(\rho^{(N)} \simeq \rho) \simeq e^{-N\mathcal{F}(\rho)},$$

might be derived as in Ref. 4, from the following regular variational principle

$$\mathcal{F}(\rho) = \inf_{\hat{\rho}} I_{[-\infty, 0]}(\hat{\rho}),$$

where the minimum is taken over all trajectories $\hat{\rho}$ connecting the stationary deterministic equilibrium profiles $\hat{\rho}_k$ to ρ . This means that \mathcal{F} and the action functional I must satisfy the related Hamilton–Jacobi equation

$$\mathcal{H}\left(\left\{\rho_k, \frac{\partial \mathcal{F}}{\partial \rho_k}\right\}\right) = 0.$$

In addition, one can check the relation

$$\mathcal{F} = \mathcal{U} - \mathcal{S},$$

where

$$\begin{cases} \mathcal{U} = \int_0^1 ds \int_0^x \sum_{k \neq l} \alpha_{kl} \rho_k(x) \rho_l(y) dy, \\ \mathcal{S} = - \int_0^1 dx \sum_{k=1}^n \rho_k \log \rho_k, \end{cases}$$

a form already encountered in the reversible case, see Eq. (3.10). Indeed, when the process is reversible, \mathcal{U} is translation invariant (i.e. independent of the initial integration point, here set to zero), and so

$$\partial_x \frac{\partial \mathcal{F}}{\partial \rho_k(x)} = - \frac{\mathcal{J}_k}{D\rho_k}.$$

This approach could be used to analyze the non-reversible case.

6. CONCLUDING REMARKS

In this report, we strove to put forward some techniques and methods allowing to tackle the problem of mapping discrete models to continuous equations. Even in

the context of a very specific case, that is stochastic distortions of discrete curves, some intricate questions (hereafter quoted) remain still unanswered.

- The determination of the invariant measure in the general case, at the discrete level: this would generalize the totally asymmetric case.^(18,27)
- The analysis of Hamilton–Jacobi equations to obtain a kind of continuous counterpart of the invariant measures, namely large deviation functionals.

With regard to hydrodynamic limits, a puzzling issue arises when particle-species diffuse at various speeds, in what we called the heterodiffusive case. For many one-dimensional models, it is well known that a single slow particle may considerably modify the macroscopic behavior of the system (see e.g. Ref. 26). For the time being, our approach is restricted to diffusive one-dimensional systems. Yet, other scalings (like Euler), as well as processes in higher dimension, are definitely worth being studied. In particular, it might be tempting to deal with more realistic exclusion processes, like those encountered in the field of traffic modelling. Besides, the analysis of irreversible invariant states in terms of cycles in a state-graph might well be extended to study ASEP on closed networks.

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