Generalized Poisson-Kac processes and hydrodynamic modeling of systems of interacting particles I - Theory

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Abstract

This article analyzes the formulation of space-time continuous hyperbolic hydrodynamic models for systems of interacting particles moving on a lattice, by connecting their local stochastic lattice dynamics to the formulation of an associated (space-time continuous) Generalized Poisson-Kac process possessing the same local transition rules. The hyperbolic hydrodynamic limit follows naturally from the statistical description of the latter in terms of the system of its partial probability density functions. Several cases are treated, with particular attention to: (i) models of interacting particles satisfying an exclusion principle, and (ii) models defined by a given interparticle interaction potential. In both cases, the hydrodynamic models may display singularities, dynamic phase-transitions and bifurcations (as regards the flux/concentration-gradient constitutive equations), whenever the Kac limit of the model (infinite propagation velocity limit) is considered.

1 Introduction

The study of systems of interacting particles represents a central issue in the thermodynamics of irreversible processes and in transport theory since the seminal work by Boltzmann on the kinetic theory of dilute gases [1][2].

In many cases the analysis of this problem can be simplified by considering particle motion on a discrete lattice. In this way, local particle dynamics is expressed as a system of transition probabilities for particle hopping between the nearest neighboring sites of the lattice. For the setting of this class of problems the reader is referred to [3][4][5][6].

In lattice problems, interactions depend either on sterical and quantum effects, or by the explicit representation of the interaction potential. Sterical and quantum effect imply some form of exclusion principle, whenever no more that a single particle or at most a finite number of particles with different values of the some internal degree of freedom (spin) can be simultaneously present at the same lattice site. Interaction potentials, be them short or long-ranged, influences the hopping transition matrix in a continuous way.
One of the central issues in the physical understanding of these particle systems is the description of their collective statistical properties, i.e., the transition from the local probabilistic lattice dynamics at the level of the single lattice site to a continuous space-time evolution for the associated concentration field (probability density function), accounting for the collective motion of a statistical particle ensemble.

The transition from the lattice motion to the continuous and collective description of particle dynamics, which is the key problem in statistical physics, involves essentially two different and conceptually separate steps: (i) the collective description of the interaction amongst particles in the form of constitutive equations for the probability density flux, expressed as generic nonlinear functional of the particle concentration field, of its spatial gradient and, in principle of its spatial derivatives of any order, and (ii) the continuum limit of a lattice particle problem, the time evolution of which is defined at discrete time instants, in the form of a physical system defined in a continuous space-time.

The first problem is in general extremely difficult and its solution often requires suitable physical approximations on the representation of particle interactions in terms of functionals involving the particle probability density function (one-particle density). The classical example of this type of approximation is the stosszahlansatz in the Boltzmannian description, in which the effects of the binary collisions are treated (invoking the hypothesis of molecular chaos) as loss and gain terms in the evolution equation for the one-particle distribution function and can be assumed proportional to the product of the two one-particle distribution functions \( f(q, v, t), f(q', v', t) \) performing a collisional event with velocities \( v \) and \( v' \). A similar approximation characterizes the kinetic theory of other systems such e.g. a gas of electrons (plasma), where a self-consistent continuous approximation for the electric field is adopted in the Vlasov equation \([2]\).

An example of the latter problem (transition from a lattice to a continuum description) is the statistical formulation in a space-time continuum of lattice random walk for system of independent particles, i.e., in the absence of exclusion principles or potential contributions \([7]\). The technical issue in this case in the transformation of the discrete Markov process describing the evolution for the probability density function of particles evolving onto the lattice (characterized by a discrete spacing \( \delta \) between nearest neighbouring sites) at discrete times (corresponding to a physical time interval \( \tau \) between subsequent events), into a continuous group (or semigroup) of transformations parametrized with respect to the physical time \( t \in \mathbb{R}^+ \) acting on the probability density functions \( p(x, t) \), continuously parametrized with respect to the space coordinate \( x \in \mathbb{R} \).

The latter problem involves the so called hydrodynamic limit, defined for lattice spacing \( \delta \) and characteristic time \( \tau \) tending to zero, assuming a suitable scaling ansatz between the two characteristic space-time parameters, expressed in the form of a limit behavior

\[
\lim_{\tau \to 0} \frac{\delta^\alpha(\tau)}{\tau} = \text{constant} \tag{1}
\]

where \( \alpha > 0 \) is some characteristic exponent defining the scaling ansatz. For a thorough discussion on the mathematical physical aspects of the setting and formulation of the hydrodynamic limit for lattice particle dynamics and on the functional form of the resulting
hydrodynamic models for prototypical interacting particle systems, the reader is referred to the classical monographs on this topic [8, 9].

In principle, different choices of the scaling assumption (1) provide different hydrodynamic models as analyzed in [7], and briefly reviewed in Section 2. Some choices of the scaling ansatz (1), and specifically the diffusive scaling corresponding to \( \alpha = 2 \) destroy some fundamental physical properties associated with lattice propagation, and forces the hydrodynamic formulation of the statistical properties of the system to be described by parabolic models (first-order in time, second-order in space derivatives) that, by nature, violates fundamental physical conditions (finite propagation velocity, deriving from the Minkowskian metrics of the space-time).

The latter hydrodynamic approach (leading to parabolic models) is fully rigorous from the mathematical point of view. Nevertheless, it superimposes and intermingles two qualitative different physical properties: (i) the existence of long-term (emerging) statistical features in a lattice particle systems, with (ii) the formulation of a continuous space-time description of its statistical evolution, defined technically from the operation of letting \( \delta, \tau \to 0 \) with the constraint imposed by the scaling assumption.

From the physical point of view, the assessment of a continuous limit is in principle independent of the finite/infinitesimal values of \( \delta \) and \( \tau \). More precisely, there are situations, in which the lattice description is an approximation of the continuous evolution of a particle system in which the values of the parameters \( \delta \) and \( \tau \) do possess a well defined physical meaning, and are not allowed to attain vanishing values. A typical situation of this sort is a dilute particle gas system, where, near equilibrium, \( \delta \) corresponds to the mean-free path \( \lambda(T, P) \sim T/P \) between two subsequent collisions depending on the temperature \( T \) and on the pressure \( P \), while the characteristic lattice time scale \( \tau \) is related to the root mean square speed \( v_{\text{rms}}(T) \sim T^{1/2} \) depending solely on temperature. A diffusive scaling ansatz (\( \alpha = 2 \)) would imply \( T^{3/2}/P = \text{constant} \), which violates the equilibrium gas law in dilute condition \( P/T = \text{constant} \) for fixed volume and particle number.

The analysis developed in [7] for the random walk of independent particles on a lattice suggests another possibility for deriving a space-time continuous statistical description of a system of particles on a lattice for any finite value of \( \delta \) and \( \tau \), respectful of the local lattice dynamics. The tool for achieving this program, at least for lattice dynamics of independent particles, is the connection of the original lattice equation of motion with an associated Generalized Poisson-Kac process possessing the same transition probabilities amongst local directions of motion, out which a space-time continuous statistical description of the original lattice process follows.

The scope of the present work is to develop a similar program for systems of interacting particles, which is a much more challenging task as the local dynamic rules for particle motion depend on the state of the whole particle ensemble. These collective effects can be formally treated by invoking a molecular chaos assumption similar to the Boltzmannian “stosszahlansatz” (see Section 4).

Once the statistical description of systems of interacting particles has been embedded in the theory of GPK processes new physical phenomenologies can be unveiled, associated with: (i) the Kac limit of the resulting hyperbolic hydrodynamic description whenever the characteristic propagation velocity is hypothesized to diverge (this occurs for particle...
systems subjected to exclusion principles); (ii) a new class of dynamic phase transitions can occur in the presence of interparticle potentials, related to multiplicity and bifurcations in the constitutive equations for the concentration flux in terms of the concentration gradient.

Throughout this article the theory is developed for systems of interacting particles in one-dimensional spatial problems, in order to simplify the notation and highlight in the simple possible way the new and rich phenomenology that can occur. The numerical investigation of the main qualitative phenomenologies highlighted in this article is addressed in [10].

The article is organized as follows. Starting from a brief conceptual summary of the result presented in [7], section 2 reviews the formalism of Generalized Poisson-Kac processes, and its application to achieve a hyperbolic continuous statistical description of interacting particle systems. Section 3 analyzes the construction of the corresponding GPK processes for systems of particles satisfying an exclusion principle. The analysis is limited to the case of a tagged particle in a mean field characterized by a given (and fixed) particle concentration. Section 4 extends the analysis to the nonlinear case. The class of models considered corresponds to exclusion models where the exclusion principle is satisfied probabilistically. This concept is introduced in this Section and thoroughly explained. The resulting nonlinear hyperbolic hydrodynamic models display very interesting and singular features in the Kac limit. Finally section 5 develops the formalism of hyperbolic hydrodynamic models in the presence of interaction potentials.

2 Stochastic processes with finite propagation velocity and hydrodynamic behavior

In a recent work [7], Giona analyzed a very simple example of lattice particle dynamics: the random walk of independent particles on a one-dimensional lattice in the case of asymmetric transitions amongst the two nearest neighboring sites (Asymmetric Lattice Random Walk, ALRW) and its continuous statistical description. The discrete lattice dynamics is characterized by the lattice spacing $\delta$ between nearest neighboring sites and by the constant hopping time $\tau$ between two subsequent events.

The starting observations motivating this revisitation of ALRW are:

- the definition of a space-time continuous process associated with ALRW does not require the limit for $\delta$ and $\tau$ tending to zero. This is because a time-continuous formulation of the process requires solely the local interpolation of particle trajectories between subsequent time instants $t_n = n \tau$, and $t_{n+1} = (n+1) \tau$ and subsequent positions $x_n, x_{n+1}$, and eventually the assumption of some level of uncertainty in the initial particle position $x_0$.

- The long-term emergent statistical properties of the process are well defined for any (finite and non-vanishing) values of $\delta$ and $\tau$. Consequently, a space-time continuous hydrodynamic model for this process should be defined independently of any lattice limit $\delta, \tau \to 0$, and of any scaling ansatz connecting $\delta$ and $\tau$ in this limit.

- In a smooth, time-continuous, formulation of the process, the ratio $b_0 = \delta/\tau$, corresponding to the local propagation velocity, should be constant and bounded.
A time-continuous hydrodynamic model, subjected to the above mentioned constraint on the local propagation velocity, should be able to describe the whole process dynamics, from the early stages, at which particles perform a ballistic motion, to the long-term dispersive features, corresponding to a linear Einsteinian scaling of the mean square displacement, for any value of $\delta$ and $\tau$.

It has been shown in [7] that the formulation of such a “smooth” hydrodynamic model is possible and it is grounded on the formulation of a space-time continuous stochastic process, analogous to ALRW, belonging to the class of Generalized Poisson-Kac processes [11, 12, 13, 14]. Here the diction “smooth” has been used to indicate that the local propagation velocity is bounded, contrarily to the classical limit formulation grounded on a diffusive scaling assumption $\delta^2/\tau = \text{constant}$, leading to a stochastic description based on almost nowhere differentiable Wiener processes. In the next paragraph, the basic concept of GPK theory are reviewed.

2.1 Generalized Poisson-Kac processes

The introduction of Generalized Poisson-Kac processes (GPK for short) stems originally from two main physical reasons: (i) to generalize the class of stochastic models proposed by Marc Kac in one-dimensional spatial systems [15], possessing finite propagation velocity and driven by a simple Poisson process, to any spatial dimension and to any number of stochastic states (including the limit towards a continuum of states); (ii) the setting of stochastically consistent transport models of hyperbolic nature suitable for describing physical transport processes possessing finite propagation velocity. Here, “stochastically consistent” means that there exists a stochastic process admitting these models as its statistical description. This issue is closely connected to the fact, that while the original one-dimensional model considered by Kac provides a stochastic interpretation for the one-dimensional Cattaneo equation $\partial_t p(x, t) + \tau_c \partial^2_t p(x, t) = D \partial_x^2 p(x, t)$, there are no stochastic processes in $\mathbb{R}^n$ with $n \geq 2$ admitting the higher dimensional Cattaneo model $\partial_t p(x, t) + \tau_c \partial^2_t p(x, t) = D \nabla^2 p(x, t)$ as the evolution equation for their probability density function $p(x, t)$. This property follows also from the observation that the Green function for the Cattaneo hyperbolic transport model in $\mathbb{R}^n$, $n \geq 2$ does not present positivity and attains negative values [17] (which is deprecable in a probabilistic context). The definition of GPK processes is closely connected with the class of higher-dimensional stochastic models studied by Kolesnik [18, 19, 20].

A GPK process in $\mathbb{R}^n$ is defined by a finite number $N$ of stochastic states, by a family of $N$ constant velocity vectors $\{b_h\}_{h=1}^N$, $b_h \in \mathbb{R}^n$, by a vector of transition rates $\Lambda = (\lambda_1, \ldots, \lambda_N)$, $\lambda_h > 0$, $h = 1, \ldots, N$, and by a $N \times N$ transition probability matrix $A = (A_{h,k})_{h,k=1}^N$, $A_{h,k} \geq 0$, $\sum_{h=1}^N A_{h,k} = 1$, $\forall k = 1, \ldots, N$. The generator of stochasticity is a finite $N$-state Poisson process $\chi_N(t; \Lambda, A)$ attaining $N$ distinct values $\chi_N = 1, \ldots, N$, and such that the probabilities $\hat{P}_h(t) = \text{Prob}[\chi_N(t) = h]$, $h = 1, \ldots, N$ satisfy the Markov
chain dynamics
\[
\frac{d\hat{P}_h(t)}{dt} = -\lambda_h \hat{P}_h(t) + \sum_{k=1}^{N} A_{h,k} \lambda_k \hat{P}_k(t)
\]  
(2)

From the above setting it follows that a GPK process \(X(t)\) in \(\mathbb{R}^n\) is defined by the stochastic differential equation
\[
dx(t) = b_{\chi_N(t;\mathbf{A},\mathbf{A})} \, dt
\]  
(3)

This means that according to the transition mechanism of state recombination specified by the \(N\)-state finite Poisson process \(\chi_N(t;\mathbf{A},\mathbf{A})\), defined by \(\mathbf{A}\) and \(\mathbf{A}\), the velocity vector defining eq. (2) switches amongst the \(N\) possible realizations \(b_1, \ldots, b_N\).

Since \(\max_{h=1,\ldots,N} |b_h| \leq B\) is bounded, the process possesses finite propagation velocity and the trajectory \(x(t)\) of each realization of a GPK process is with probability 1 an almost everywhere smooth function of time consisting of smooth line segments. It is therefore differentiable at all the time instant, but at the transition points, where \(\chi_N(t;\mathbf{A},\mathbf{A})\) switches from one state to another, still possessing well defined left and right derivatives at the transition points (Lipschitz continuity).

The statistical description of a GPK process involves \(N\) partial probability density functions \(p_h(x, t), \, h = 1, \ldots, N\),
\[
p_h(x, t) \, dx = \text{Prob} [X(t) \in (x, x + dx), \ \chi_N(t) = h]
\]  
(4)

where \(x = (x_1, \ldots, x_N)\), \(X(t) = (X_1(t), \ldots, X_N(t))\), \(dx = \prod_{h=1}^{N} dx_h\) is the measure element, and \(X(t) \in (x, x + dx)\) means that for each \(X_h(t)\), \(X_h(t) \in (x_h, x_h + dx_h)\), \(h = 1, \ldots, N\). The partial probability densities satisfy the system of first-order differential equations
\[
\frac{\partial p_h(x, t)}{\partial t} = -b_h \cdot \nabla p_h(x, t) - \lambda_h p_h(x, t) + \sum_{k=1}^{N} A_{h,k} \lambda_k p_k(x, t)
\]  
(5)

Eq. (5) represents the complete statistical description of a GPK process: it plays the same role of the classical parabolic Fokker-Planck equation for Langevin models driven by Wiener noise. The difference with the latter case is that, for GPK processes, a system of \(N\) partial probability densities, accounting also for the local state of the stochastic perturbation should be defined, owing to the non strictly Markovian structure of the process. The overall probability density function of the process is \(p(x, t) = \sum_{h=1}^{N} p_h(x, t)\), and satisfies the conservation equation
\[
\frac{\partial p(x, t)}{\partial t} = -\nabla \cdot J_p(x, t)
\]  
(6)

where the probability density flux \(J_p(x, t)\) is expressed by
\[
J_p(x, t) = \sum_{h=1}^{N} b_h p_h(x, t)
\]  
(7)

and the constitutive equation for \(J_p(x, t)\), follows from the definition (7) and from the balance equations (5).
Depending on the structural properties of the GPK, i.e., on \( \{b_h\}_{h=1}^{N} \) \( \Lambda \) and \( A \), a variety of different stochastic models can be constructed and the reader is referred to [12] for a structural characterization of these processes. Consider below the simple case where all the stochastic velocity vectors possess the same modulus \( b_0 \), i.e., \( b_h = b_0 e_h, \ h = 1, \ldots, N \), where \( e_h \) are unit vectors and all the transition rates are equal i.e., \( \lambda_h = \lambda_0, \ h = 1, \ldots, N \). Under this conditions, it is natural to formulate the Kac limit of a GPK process, i.e., the asymptotics of the GPK process in the case \( b_0, \lambda_0 \to \infty \), keeping fixed the ratio \[
\frac{b_0^2}{2\lambda_0} = D_{\text{nom}} \tag{8}\]
where \( D_{\text{nom}} \) is referred to as the “nominal diffusivity” of the GPK process. The Kac limit corresponds to the limit behavior of a GPK process in the case its propagation velocity diverges and the same does the transition rate, under the scaling hypothesis [8]. Under this conditions, and assuming reasonable no-bias constraints on the system of velocity vectors \( \{e_h\}_{h=1}^{N} \) (see [12] for details), the balance equations [13] for the partial probability density functions \( p_h(x, t) \) collapse into a single parabolic equation for the overall probability density \( p(x, t) \)
\[
\frac{\partial p(x, t)}{\partial t} = \nabla \cdot (D \nabla p(x, t)) \tag{9}\]
where \( D = (D_{h,k})_{h,k=1}^{N} \) is the effective diffusivity tensor. If the system possesses enough symmetries, \( D \) is isotropic, i.e., \( D = D_0 I \), and the Kac limit of the process is characterized by the single overall probability density function \( p(x, t) \), solution of the diffusion equation
\[
\frac{\partial p(x, t)}{\partial t} = D_0 \nabla^2 p(x, t) \tag{10}\]
where \( D_0 \) is the scalar effective diffusivity, depending linearly on \( D_{\text{nom}} \), i.e. \( D_0 = D_{\text{nom}} \kappa \), where \( \kappa \sim O(1) \).

In the case of ALRW (\( n = 1 \)), the number of states is \( N = 2 \), corresponding to the movements towards the two (left and right) neighboring sites of any lattice site. Correspondingly, the velocity vectors are expressed by \( b_1 = b_0, \ b_2 = -b_0 \), where \( b_0 = \delta/\tau \). As regards the transition probabilities, if \( r_1 \) and \( r_2 \) are probabilities of moving to the right/left site respectively, letting \( r = r_1 - r_2 \), it follows that the transition probability matrix is given by
\[
A = \left( \begin{array}{cc} \frac{1+r}{2r} & \frac{1+r}{2r} \\ \frac{1-r}{2r} & \frac{1-r}{2r} \end{array} \right) \tag{11}\]
The GPK process associated with the ALRW dynamics on the real line is thus expressed by
\[
dx(t) = b_{\chi x(t; \lambda_0 I, A)} \ dt \tag{12}\]
where the transition rate vector \( \Lambda = \lambda_0 I \) is isotropic and characterized by the value \( \lambda_0 \). The expression for \( \lambda_0 \) in terms of the lattice parameters can be obtained from the long-term linear scaling of the mean square displacement in the simplest case of symmetric motion (\( r = 0 \)) for which \( \lambda_0 = 2/\tau \) follows.
Lattice Particle Dynamics

Construction of the associated GPK process

Statistical description of the GPK process via hyperbolic balance eq. for \( \{p_h(x, t)\} \)

Kac limit (classical hydrodynamic limit) for \( p(x, t) \) at \( b_0 \to \infty \) (parabolic equation)

Figure 1: Program towards the hyperbolic formulation of continuous hydrodynamic models of interacting particle systems.

The system of hyperbolic first-order equation for the partial probability densities \( p_1(x, t) \), \( p_2(x, t) \) represents a continuous hydrodynamic model for the statistical properties of ALRW, and the classical hydrodynamic limit (see e.g. [21]) can be regarded as the Kac limit of this hyperbolic model.

The latter observation provides a novel way of interpreting the classical parabolic hydrodynamic limit of lattice particle dynamics: not as the limit for space-time discretized characteristic scales (\( \delta \) and \( \tau \)) tending to zero (as eq. (12) is already defined in a space-time continuum \( (x, t) \in \mathbb{R} \times \mathbb{R}^+ \)), but as the limit for the characteristic propagation velocity of the process \( b_0 \) tending to infinity, assuming also that the transition rate would diverge \( \lambda_0 \to \infty \). In the latter (Kac) limit, the scaling relation (5) is essential in ensuring the existence of this limit. For further details see [7].

2.2 The program

From the analysis developed above, it follows a conceptual program towards the construction of continuous hydrodynamic models of systems of interacting particles. This program is reviewed schematically in figure [1] and follows the same approach applied in [7] to ALRW.

The central issue is the association with a local lattice dynamics of its corresponding continuous GPK process, possessing the same transition probability structure of the original lattice model. Once this step is performed, the derivation of the different forms of
continuous hydrodynamic models follows directly from GPK theory. In the remainder of this article, this program is outlined and developed for prototypical models of interacting particle systems.

3 Model systems and mean field analysis of tagged particle diffusion

In this Section we consider typical random walk models with exclusion, meaning that at each lattice site no more than one particle or a finite number of them, possessing different characteristic properties (spin), can be present simultaneously.

For several prototypical models we first derive the mean-field behavior of a tagged particle i.e., the properties of the particle diffusive motion by assuming that the average particle concentration is given. Subsequently, we provide the formalization of the same process within the GPK formalism.

Throughout this Section, we consider one-dimensional spatial models.

3.1 Fermionic random walk with exclusion

This model has been addressed by Colangeli et al. [22] and represents, in the absence of other interactions, a form of Kawasaki model [23]. Particles behave as fermions, and the direction of the velocity \( \pm 1 \), corresponds to their spin. At each lattice site, at most two particles can be simultaneously present with opposite spins (i.e., opposite velocity directions).

The dynamic of the exclusion interaction is as follows:

1. first, a velocity switch is considered, meaning that if solely a particle is present at a given site it switches its direction with probability \( \frac{1}{2} \); 

2. the next step is the advective step: particles at a given site move towards the nearest neighboring sites consistently with their velocity directions, i.e., with the values of their spins, and compatibly with the exclusion principle. For instance, a particle at site \( k \) possessing velocity \( +1 \) moves towards \( k + 1 \) provided that the arrival site does not contain already a particle with positive velocity.

As stated at the beginning of this Section, consider the self-diffusion dynamics of a tagged particle, assuming that the average fraction of positively and negatively oriented particles is equal to \( \pi \in [0,1] \).

The random walk model of a tagged particle following the recipe stated above, (which is a mean-field approximation), can be described by considering at time \( n \) both the particle position \( x_n \) and its spin variable \( s_n \).

The dynamics for the spin variable is given by:

\[
s_{n+1} = \xi_{n+1} s_n
\]
starting at time $n = 0$ from $s_0 = \{0, 1\}$, where $\xi_n$ are uncorrelated random variables attaining values $\pm 1$, according to the probabilistic scheme

$$
\xi_{n+1} = \begin{cases} 
1 & \text{Prob } (1 + \pi)/2 \\
-1 & \text{Prob } (1 - \pi)/2
\end{cases}
$$

For instance $\text{Prob}[\xi_{n+1} = -1] = (1 - \pi)/2$, corresponding to the probability of a velocity switching, equals the probability that a switching event occurs (which is 1/2) times the probability that the arrival site does not contain already a particle with opposite velocity (which equals $1 - \pi$). Observe that the random variables $\xi_n, n = 1, 2, \ldots$ are uncorrelated with each other, i.e.,

$$
\langle \xi_h \xi_k \rangle = \begin{cases} 
\langle \xi_h^2 \rangle & k = h \\
\langle \xi_h \rangle \langle \xi_k \rangle & k \neq h
\end{cases}
$$

As regards the initial condition $s_0$, one has

$$
s_0 = \begin{cases} 
1 & \text{Prob } 1/2 \\
-1 & \text{Prob } 1/2
\end{cases}
$$

so that $\langle s_0 \rangle = 0$.

The dynamics of particle position $x_n$ is then expressed by

$$
x_{n+1} = x_n + s_{n+1} \eta_{n+1}
$$

where $\eta_{n+1}$ are random variables attaining values 0, 1 according to the rule

$$
\eta_{n+1} = \begin{cases} 
0 & \text{Prob } \pi \\
1 & \text{Prob } (1 - \pi)
\end{cases}
$$

For instance, $\text{Prob}[\eta_{n+1} = 0]$ corresponds to the probability that the arrival site contains already a particle with the same spin, and therefore equals $\pi$. Also the variables $\eta_h$ are uncorrelated with each other,

$$
\langle \eta_h \eta_k \rangle = \begin{cases} 
\langle \eta_h^2 \rangle & k = h \\
\langle \eta_h \rangle \langle \eta_k \rangle & k \neq h
\end{cases}
$$

and independent of the $\xi_k$-variables, $\langle \eta_h \xi_k \rangle = \langle \eta_h \rangle \langle \xi_k \rangle$. Setting $x_0 = 0$, it follows from eqs. (13) and (17) that

$$
x_n = \sum_{h=1}^{n} s_h \eta_h
$$

for $n \geq 1$, where

$$
s_h = s_0 \prod_{k=1}^{h} \xi_k
$$

It follows that

$$
\langle s_n \rangle = 0, \quad \langle s_h s_k \rangle = \langle s_0 \rangle \langle s_{|k-h|} \rangle
$$
and therefore
\[ \langle x_n \rangle = 0, \quad \langle x_n^2 \rangle = \sum_{h=1}^{n} \sum_{k=1}^{n} \langle s_h s_k \rangle \langle \eta_h \eta_k \rangle \] (23)

Since
\[ \langle \eta_h \eta_k \rangle = \begin{cases} 1 - \pi & k = h \\ (1 - \pi)^2 & k \neq h \end{cases} \] (24)

and
\[ \langle s_0^2 \rangle = 1 \]
\[ \langle s_0 s_m \rangle = \prod_{k=1}^{m} \langle \xi_k \rangle = \pi^m, \quad m \geq 1 \] (25)

the expression for the mean square displacement \( \langle x_n^2 \rangle \) can be explicited in the form
\[ \langle x_n^2 \rangle = \sum_{h=1}^{n} (1 - \pi) + 2 \sum_{h=1}^{n} \sum_{k=1}^{h-1} \pi^h (1 - \pi)^2 \]
\[ = (1 - \pi) n + 2 (1 - \pi)^2 \sum_{h=1}^{n} \pi^h \sum_{k=1}^{h-1} \pi^{-k} \] (26)

Since \( \sum_{h=1}^{m} \alpha^h = (\alpha - \alpha^{m+1})/(1 - \alpha) \), for any real \( \alpha \), it follows that
\[ \sum_{h=1}^{n} \pi^h \sum_{k=1}^{h-1} \pi^{-k} = \sum_{h=1}^{n} \pi^h \frac{1/\pi - 1/\pi^h}{1 - 1/\pi} \]
\[ = -\frac{\pi}{1 - \pi} \left( \frac{1}{\pi} \sum_{h=1}^{n} \pi^h - n \right) \] (27)

For any \( \pi \in [0, 1) \), \( \sum_{h=1}^{n} \pi^h \) converges to \( 1/(1 - \pi) \) and consequently,
\[ \langle x_n^2 \rangle = (1 - \pi) n + \frac{2 (1 - \pi)^2 \pi}{1 - \pi} n + \mathcal{O}(1) \]
\[ = (1 - \pi) (1 + 2 \pi) n + \mathcal{O}(1) \] (28)

Eq. (28) indicates that the effective self-diffusion coefficient \( D_{sd}(\pi) \) for this random walk scheme in the mean-field approximation equals
\[ D_{sd}(\pi) = \frac{(1 - \pi) (1 + 2 \pi)}{2} \] (29)

The interesting feature of this result is that \( D_{sd}(\pi) \) displays a non monotonic behavior as a function of \( \pi \): for small \( \pi \), \( D_{sd}(\pi) \) increases above the value \( D_{sd}(0) = 1/2 \), while for \( \pi \to 1 \), \( D_{sd}(\pi) \to 0 \). This phenomenon is depicted in figures 2 and 3. Figure 2 shows the mean square displacement \( \sigma_x^2(n) = \langle x_n^2 \rangle \) vs time \( n \) obtained for stochastic simulations of
Figure 2: Mean square displacement $\sigma_x^2(n)$ vs $n$ for the fermionic random walk model with exclusion described in the main text, deriving from the stochastic simulation of eqs. (13) and (17). Line (a) refers to $\pi = 0$, line (b) to $\pi = 0.2$, line (c) to $\pi = 0.6$, line (d) to $\pi = 0.8$.

Figure 3: Self-diffusion coefficient for the fermionic random walk model with exclusion. Solid line corresponds to the graph of eq. (29), symbols (●) refer to the results of random walk simulations depicted in figure 2.
Table 1: Correspondence between the four states of the GPK models and particle velocity and spin.

| State | Velocity | Spin |
|-------|----------|------|
| 1     | $b_0$    | +    |
| 2     | $-b_0$   | -    |
| 3     | 0        | +    |
| 4     | 0        | -    |

eqs. 13, 17, using an ensemble of $10^5$ particles, while figure $\mathcal{K}$ compares the values of the self-diffusivity obtained from the simulations against the theoretical prediction (29).

Next, consider the same process in the framework of the theory of GPK processes, still assuming a mean-field approximation. While there are only two different spin states $\pm 1$ as regards the lattice model, there are four different velocity/spin states in its GPK counterpart: namely the two states $\pm b_0$ in which particles possess spin states $\pm 1$, and an effective velocity $\pm b_0$, and the two “ghost states” $O(\pm)$, at which the velocity is vanishing while the value of the spin state is $\pm 1$. Let us label these four states with $i = 1, \ldots, 4$ Let $\lambda_0$ be a uniform transition rate. The stochastic GPK model is thus given by

$$dx(t) = b_\chi_4(t; \lambda_0, \mathbf{A}) \, dt$$

where the stochastic velocity vector $\mathbf{b} = (b_i)_{i=1}^4$ corresponds to the second row of table 1.

$$\mathbf{b} = \begin{pmatrix} b_0 \\ -b_0 \\ 0 \\ 0 \end{pmatrix}$$

$\chi_4(t; \lambda_0, \mathbf{A})$ is a 4-state finite Poisson process characterized by a uniform transition rate $\lambda_0$ and by the transition probability matrix $\mathbf{A}$ given by

$$A = \begin{pmatrix} \pi(1-\pi) & (1-\pi)^2 & \pi(1-\pi) & (1-\pi)^2 \\ (1-\pi)^2 & \pi(1-\pi) & (1-\pi)^2 & \pi(1-\pi) \\ \pi^2 & \pi(1-\pi) & \pi^2 & \pi(1-\pi) \\ \pi(1-\pi) & \pi^2 & \pi(1-\pi) & \pi^2 \end{pmatrix}$$

Let us clarify the structure of the transition probability matrix. Consider as initial state, the state “1”. The transition from this state to state “2”, corresponding to a moving particle with opposite velocity, can occur solely if the initial site does not contain any other particle, and this happens in the mean-field approximation with probability $1-\pi$ and the nearest neighbouring site can be reached without violating the exclusion principle, which occurs with probability $1-\pi$. The probability $A_{2,1}$ is therefore equal to $A_{2,1} = (1-\pi)^2$. The transition from state “1” to state “3”, corresponding to a rest particle with the same spin, can occur solely if the initial site contains a particle with oppositive spin, and the nearest neighboring site is occupied by a particle with the same spin. Both these events occur
with probability $\pi$, and are independent of each other, so that $A_{3,1} = \pi^2$. The transition from state “1” to state “4” corresponding to a rest particle with opposite spin, can occur solely if the initial state does not contain any other particle (occurring with probability $1 - \pi$), and the nearest neighbouring site is occupied by a particle possessing the same spin (occurring with probability $\pi$), so that $A_{4,1} = \pi(1 - \pi)$. As regards $A_{1,1}$, its expression follows from the probabilistic closure condition $A_{1,1} = 1 - A_{2,1} - A_{3,1} - A_{4,1}$. An analogous derivation can be applied to determine all the other entries of the matrix $A$.

The statistical description of the process (30) involves four partial probability density functions $p_1(x,t), p_2(x,t), p_3(x,t), p_4(x,t)$ associated with the four states of $\chi_4(t; \lambda_0, A)$, fulfilling the balance equations

$$\frac{\partial p_i(x,t)}{\partial t} = -b_i \frac{\partial p_i(x,t)}{\partial x} - \lambda_0 p_i(x,t) + \lambda_0 \sum_{j=1}^{4} A_{i,j} p_j(x,t)$$

(33)

and the overall probability density function is obviously $p(x,t) = \sum_{i=1}^{4} p_i(x,t)$. Let us define the two probabilistic 2-vectors $p_b(x,t), p_0(x,t)$ as

$$p_b = \left( \begin{array}{c} p_1 \\ p_2 \end{array} \right), \quad p_0 = \left( \begin{array}{c} p_3 \\ p_4 \end{array} \right)$$

(34)

$p_b$ is the vector of the partial probability density associated with moving states, i.e., with states corresponding to an effective particle motion, while $p_0$ groups together the partial probabilities pertaining to the rest states. With this notation, the balance equations for the partial probability waves can be compactly expressed as

$$\frac{\partial p_b}{\partial t} = -b_0 L_x [p_b] - \lambda_0 p_b + \lambda_0 A_1 p_b + \lambda_0 A_0 p_0$$

$$\frac{\partial p_0}{\partial t} = -\lambda_0 p_0 + \lambda_0 A_2 p_b + \lambda_0 A_2 p_0$$

(35)

where $L_x$ is the advection operator

$$L_x = \left( \begin{array}{cc} \partial/\partial x & 0 \\ 0 & -\partial/\partial x \end{array} \right)$$

(36)

and the two $2 \times 2$ matrices $A_1, A_2$ read

$$A_1 = \left( \begin{array}{cc} \pi(1-\pi) & (1-\pi)^2 \\ (1-\pi)^2 & \pi(1-\pi) \end{array} \right), \quad A_2 = \left( \begin{array}{cc} \pi^2 & \pi(1-\pi) \\ \pi(1-\pi) & \pi^2 \end{array} \right)$$

(37)

The balance equation for the overall probability density $p(x,t)$ follows from (33) by summing over the states (i.e., over the index $i$),

$$\frac{\partial p(x,t)}{\partial t} = - \frac{\partial J_p(x,t)}{\partial x}$$

(38)

where $J_p(x,t) = b_0[p_1(x,t) - p_2(x,t)]$. 

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Next, consider the Kac limit of this model, corresponding to \( b_0, \lambda_0 \to \infty \) keeping fixed the ratio \( b_0^2/2\lambda_0 = D_0 \) to a fixed nominal diffusivity \( D_0 \). Letting \( \lambda_0 \to \infty \), the second equation (35) provides the ration between \( p_0 \) and \( p_b \),

\[
(I - A_2) p_0 = A_2 p_b
\]

i.e., \( p_0 = (I - A_2)^{-1} A_2 p_b \). Indicating with \( p_b(x, t) = p_1(x, t) + p_2(x, t) \) and \( p_0(x, t) = p_3(x, t) + p_4(x, t) \), from eq. (39), and from the identity \( p(x, t) = p_b(x, t) + p_0(x, t) \) one obtain the relation between \( p(x, t) \), \( p_b(x, t) \) and \( p_0(x, t) \), namely

\[
p_0(x, t) = \frac{\pi}{1 - \pi} p_b(x, t), \quad p_b(x, t) = (1 - \pi) p(x, t)
\]

that, substituted into the first equation (35), yields a balance equation involving solely the partial probability density associated with moving particles

\[
\frac{\partial p_b}{\partial t} = -b_0 L_x[p_b] - \lambda_0 [I - A_1 - A_1 (I - A_2)^{-1} A_2] p_b
\]

\[
= -b_0 L_x[p_b] - \lambda_0 \Lambda_{eff}(\pi) p_b
\]

After some elementary algebra, the matrix \( \Lambda_{eff}(\pi) \) takes the form

\[
\Lambda_{eff}(\pi) = \begin{pmatrix} \ell(\pi) & -\ell(\pi) \\ -\ell(\pi) & \ell(\pi) \end{pmatrix}, \quad \ell(\pi) = \frac{1}{1 + 2\pi}
\]

With respect to the partial probability densities associated with moving states \((p_1, p_2)\), the statistical description of the process reduces to a classical Poisson-Kac model

\[
\frac{\partial p_1}{\partial t} = -b_0 \frac{\partial p_1}{\partial x} - \lambda_0 \ell(\pi) [p_1 - p_2]
\]

\[
\frac{\partial p_2}{\partial t} = b_0 \frac{\partial p_2}{\partial x} + \lambda_0 \ell(\pi) [p_1 - p_2]
\]

the Kac limit of which provides the expression for probability flux \( J_d(x, t) \) entering the balance equation (38)

\[
J_d(x, t) = -\frac{b_0}{2\lambda_0} \frac{1}{\ell(\pi)} \frac{\partial p_b(x, t)}{\partial x} = -b_0 \frac{1 - \pi}{\ell(\pi)} \frac{\partial p(x, t)}{\partial x}
\]

\[
= -D_0(1 - \pi) (1 + 2\pi) \frac{\partial p(x, t)}{\partial x}
\]

Setting the nominal diffusivity \( D_0 = 1/2 \), one obtains from eq. (43) the expression for the mean-field self-diffusivity (29) derived from the original stochastic model. Several observations deserve some attention:

- in the derivation of eq. (43) we have first considered the limit for \( \lambda_0 \to \infty \) in the second equation (35) for the probability densities \( p_0(x, t) \) for the non-moving particles, and the result obtained is then substituted back in the first equation (35) for \( p_b(x, t) \), deriving the self-diffusion from the Kac limit of this equation. We have
use this, more physically oriented, approach to obtain $D_{sd}(\pi)$ in order to derive eq. (43) corresponding to the quasi steady-state approximation for the dynamics of the partial probability density functions associated with non-moving particles. If one perform simultaneously the Kac limit, (i.e., $\lambda_0, b_0 \to \infty$, keeping fixed the nominal diffusivity $D_0 = b_0^2/2\lambda_0$) one still obtains eq. (43).

• The analysis of the above problem involving interacting particles through an exclusion principle indicates that, once the microdynamics of the interacting particles has been specified (in the present case within the mean-field approximation), it is rather straightforward to define and derive the corresponding stochastic GPK model, in the present case eq. (30), specified by the number $N$ of GPK states, by the stochastic velocities $b_i$ of each state $i = 1, \ldots, N$, by the transition rate vector $\Lambda$ and by the transition probability matrix $A$.

• Observe that the number of states in the GPK model may be different, and in general greater than the number of spin states of the original system. In the present case, the number of different spin configurations is 2, while $N = 4$. This is because two additional states are required to discriminate between moving and non-moving particles in order to account for the exclusion principle;

• As discussed with the aid of the present case study, it is fairly easy to derive the structure of $\Lambda$ and $A$ and their dependence on the partial probability density functions (in the presence case on the concentration $\pi$, since the simpler case of a mean-field approximation is considered) from the rules of particle interaction. The analysis developed in this Section is limited to the mean-field case. The general problem is treated in the next Section.

• Given the stochastic GPK model (in the present case eq. (30)), the hydrodynamic limit of this model follows directly from GPK theory, in the present case eq. (33). Out of it, the Kac-limit of the latter, provides the classical parabolic transport model. Therefore, and this represents a very powerful by-product of GPK theory, there are several classes of hydrodynamic limits of the same interacting particle systems, depending, once $D_0$ is fixed, on the characteristic time scales of the stochastic process, i.e., essentially on the value of $\lambda$. In some cases, due to the presence of particle interactions, while the hyperbolic hydrodynamic limit exists, the Kac limit of the corresponding model could not exist.

3.2 Simple exclusion random walk

Let us consider another classical exclusion random walk without spin. In this model, particles on a lattice move towards the nearest neighbouring site (with equal probability towards the left or right neighboring site) solely if no other particle is simultaneously occupying it.

In the mean-field approximation, indicating with $\pi$ particle concentration, the random walk model takes the form

$$x_{n+1} = x_n + r_{n+1} \eta_{n+1}$$

(44)
where the random variables \( r_{n+1}, \eta_{n+1} \) are specified by

\[
\begin{align*}
  r_{n+1} &= \begin{cases} 
    -1 & \text{Prob } 1/2 \\
    1 & \text{Prob } 1/2
  \end{cases}, \\
  \eta_{n+1} &= \begin{cases} 
    0 & \text{Prob } (1 - \pi) \\
    1 & \text{Prob } \pi
  \end{cases}
\end{align*}
\]

(45)

where \( r_h \) and \( \eta_k \) are uncorrelated with each other, \( \langle r_h \rangle = 0, \langle r_h r_k \rangle = \delta_{h,k} \) and \( \eta_h \) satisfy eq. (19). Consequently, starting from \( x_0 = 0 \),

\[
x_n = \sum_{h=1}^{n} r_h \eta_h
\]

(46)

, and \( \langle x_n \rangle = 0 \) while for the mean square displacement

\[
\langle x_n^2 \rangle = \sum_{h=1}^{n} \sum_{k=1}^{n} \langle r_h r_k \rangle \langle \eta_h \eta_k \rangle = \sum_{h=1}^{n} \langle \eta_h^2 \rangle = (1 - \pi) n
\]

(47)

Thus, for the self diffusion coefficient of a tagged particle one obtains, in the mean-field approximation,

\[
D_{sd}(\pi) = \frac{1 - \pi}{2}
\]

(48)

Next, consider the GPK modeling. The GPK version of the process involves three states: state “1” corresponding to particles moving forward along the \( x \)-axis, state “2” to particles moving backward, and state “3” corresponding to resting particles, that do not perform any motion due to the exclusion principle. Indicating with \( b_0 \) and \( \lambda_0 \) the characteristic velocity and transition rate of the GPK process, it follows that

\[
b = \begin{pmatrix} b_0 \\ -b_0 \\ 0 \end{pmatrix}, \quad A = \lambda_0 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}
\]

(49)

and the stochastic GPK version of the model is formally analogous to eq. (30), namely

\[
dx(t) = b_\chi_3(t;\lambda_0 A) \, dt
\]

(50)

where the transition probability matrix \( A \) depends on the mean-field concentration \( \pi \) and is given by

\[
A = \begin{pmatrix} 
  \frac{1 - \pi}{\pi} & \frac{1 - \pi}{\pi} & \frac{1 - \pi}{\pi} \\
  \frac{1 - \pi}{\pi} & \frac{1 - \pi}{\pi} & \frac{1 - \pi}{\pi} \\
  \frac{1 - \pi}{\pi} & \frac{1 - \pi}{\pi} & \frac{1 - \pi}{\pi}
\end{pmatrix}
\]

(51)

The statistical description of eq. (50) involves three partial probability densities \( p_1(x,t), p_2(x,t) \) and \( p_3(x,t) \), where the latter corresponds to the density of resting particles. The overall probability density is \( p(x,t) = \sum_{i=1}^{3} p_i(x,t) \), and indicate with \( p_h(x,t) = p_1(x,t) + p_2(x,t) \) the probability density function of the moving particles. The balance equations for
the partial densities, accounting for eqs. (49) and (51) are

\[
\begin{align*}
\frac{\partial p_1(x,t)}{\partial t} &= -b_0 \frac{\partial p_1(x,t)}{\partial x} - \lambda_0 p_1(x,t) + \lambda_0 a(\pi) p(x,t) \\
\frac{\partial p_2(x,t)}{\partial t} &= b_0 \frac{\partial p_2(x,t)}{\partial x} - \lambda_0 p_2(x,t) + \lambda_0 a(\pi) p(x,t) \\
\frac{\partial p_3(x,t)}{\partial t} &= -\lambda_0 p_3(x,t) + \lambda_0 \pi p(x,t)
\end{align*}
\]

where \( a(\pi) = (1 - \pi)/2 \), from which one obtains that the conservation equation for the overall density is still expressed by eq. (38) with \( J_d(x,t) = b_0 \left[ p_1(x,t) - p_2(x,t) \right] \). As regards the probability flux \( J_d(x,t) \), from the first two equations (52) one obtains

\[
\frac{\partial J_d(x,t)}{\partial t} = -b_0^2 \frac{\partial p_0(x,t)}{\partial x} - \lambda_0 J_d(x,t)
\]

In the Kac limit, eq. (53) provides

\[
J_d(x,t) = -2 D_0 \frac{\partial p_0(x,t)}{\partial x}
\]

where, as usual, \( D_0 = b_0^2/2\lambda_0 \) corresponds to the nominal diffusivity of the GPK scheme. In the Kac limit, from the third equation (52) one obtains \( p_3(x,t) = \pi p(x,t) \), thus

\[
p_0(x,t) = (1 - \pi) p(x,t)
\]

which inserted into eq. (54) provides

\[
J_d(x,t) = -2 D_0 (1 - \pi) \frac{\partial p(x,t)}{\partial x}
\]

which implies for the self-diffusion \( D_{sd}(\pi) = 2 D_0 (1 - \pi) \) that coincides with eq. (48), by setting the nominal diffusivity equal to \( D_0 = 1/4 \).

### 3.3 TASEP model

To conclude, let us consider another simple and paradigmatic example, namely the Totally Asymmetric Simple Exclusion Process (TASEP) on the real line. In this model, particles move solely in the forward direction satisfying an exclusion principle, corresponding to one particle per site, at most. The mean field dynamics of TASEP, letting \( \pi \) be the mean-field particle concentration, is described by the dynamics

\[
x_{n+1} = x_n + \xi_{n+1}
\]

where the random variables \( \xi_h \) are uncorrelated with each other and described statistically by

\[
\xi_{n+1} = \begin{cases} 
0 & \text{Prob } \pi \\
1 & \text{Prob } 1 - \pi
\end{cases}
\]


Consequently,
\[ \langle \xi_h \xi_k \rangle = \begin{cases} 1 - \pi & h = k \\ (1 - \pi)^2 & h \neq k \end{cases} \] \hspace{1cm} (59)

If \( x_0 = 0 \), the integral representation of the dynamics is \( x_n = \sum_{h=1}^{n} \xi_h \), thus
\[ \langle x_n \rangle = \sum_{h=1}^{n} \langle \xi_h \rangle = (1 - \pi) n \] \hspace{1cm} (60)

and
\[ \langle x_n^2 \rangle = \sum_{h=1}^{n} \sum_{k=1}^{n} \langle \xi_h \xi_k \rangle = (1 - \pi)^2 n^2 + \pi (1 - \pi) n \] \hspace{1cm} (61)

The mean square displacement attains the expression \( \sigma_x^2(n) = \langle x_n^2 \rangle - \langle x_n \rangle^2 = \pi (1 - \pi) n \), thus the mean-field self-diffusion coefficient is given by
\[ D_{sd}(\pi) = \frac{\pi (1 - \pi)}{2} \] \hspace{1cm} (62)

It vanished both for \( \pi = 0 \) (infinite dilution) and for \( \pi = 1 \) corresponding to total exclusion. In both cases the dynamics is strictly (and trivially) deterministic.

Let us analyze the GPK formulation of TASEP. It implies the occurrence of two state: state “1” which is the mobile state, and state “2” which is the stationary (non-moving) state. Correspondingly, \( b_1 = b_0 \), and \( b_2 = 0 \). The transition rates are uniform and equal to \( \lambda_0 \). As regards the transition probability matrix, TASEP dynamics indicates the following dependence on the mean field concentration \( \pi \)
\[ A = \begin{pmatrix} 1 - \pi & 1 - \pi \\ \pi & \pi \end{pmatrix} \] \hspace{1cm} (63)

The process is described stastically by the two partial probability density functions satisfying the hyperbolic equations
\[ \frac{\partial p_1(x, t)}{\partial t} = -b_0 \frac{\partial p_1(x, t)}{\partial x} - \lambda_0 \pi p_1(x, t) + \lambda_0 (1 - \pi) p_2(x, t) \]
\[ \frac{\partial p_0(x, t)}{\partial t} = \lambda_0 \pi p_1(x, t) - \lambda_0 (1 - \pi) p_2(x, t) \] \hspace{1cm} (64)

In the limit \( \lambda_0 \to \infty \), \( \lambda_0^{-1} \partial p_2/\partial t = 0 \), thus the second equation \hspace{0.5cm} (64) provides
\[ p_2(x, t) = \frac{\pi}{1 - \pi} p_1(x, t) \], \hspace{0.5cm} p_1(x, t) = (1 - \pi) p(x, t) \] \hspace{1cm} (65)

where \( p(x, t) = p_1(x, t) + p_2(x, t) \) is the overall concentration, the dynamics of which is given by
\[ \frac{\partial p(x, t)}{\partial t} = -b_0 \frac{\partial p_1(x, t)}{\partial x} \] \hspace{1cm} (66)
Inserting in it the expression (65), obtained for \( \lambda_0 \to \infty \), one finally arrive to the hyperbolic model for \( p(x, t) \)

\[
\frac{\partial p(x, t)}{\partial t} = -b_0 (1 - \pi) \frac{\partial p(x, t)}{\partial x}
\]  

(67)

providing an effective mean velocity \( v_{\text{eff}} \) equal to

\[
v_{\text{eff}} = b_0 (1 - \pi)
\]  

(68)

Observe that eqs. (67)-(68) does not correspond to any Kac limit, but solely to the limit of infinitely fast recombination kinetics \( (\lambda_0 \to \infty) \).

In order to extract from the GPK process defined statistically by eq. (64) the value for the effective diffusivity and to perform a Kac limit of the process, let us consider TASEP dynamics in the inertial frame moving with the effective velocity \( v_{\text{eff}} \). Let \( x' \) be the position coordinate in this moving reference system

\[
x' = x - b_0 (1 - \pi) t
\]  

(69)

In the moving system, let \( p'_1(x', t), p'_2(x', t) \) the two partial probability densities characterized by the velocities

\[
b'_1 = b_0 - b_0 (1 - \pi) = b_0 \pi, \quad b'_2 = -b_0 (1 - \pi)
\]  

(70)

which satisfy the balance equations

\[
\begin{align*}
\frac{\partial p'_1(x', t)}{\partial t} & = -b_0 \pi \frac{\partial p'_1(x', t)}{\partial x'} - \lambda_0 \left[ \pi p'_1(x', t) - (1 - \pi) p'_2(x', t) \right] \\
\frac{\partial p'_2(x', t)}{\partial t} & = b_0 (1 - \pi) \frac{\partial p'_2(x', t)}{\partial x'} + \lambda_0 \left[ \pi p'_1(x', t) - (1 - \pi) p'_2(x', t) \right]
\end{align*}
\]  

(71)

The stochastic GPK process

\[
dx'(t) = b_{\chi_2(t; \lambda_1, A(\pi))} \, dt
\]  

(72)

associated with the statistical description (71), where \( b_i, i = 1, 2 \), are given by eq. (69), and the transition probability matrix \( A(\pi) \) by eq. (63) will be referred to as the zero-bias TASEP model. The balance equation for the overall probability density \( p(x', t) = p'_1(x', t) + p'_2(x', t) \) is obviously given by

\[
\frac{\partial p(x', t)}{\partial t} = -\frac{\partial J'_d(x', t)}{\partial x'}
\]  

(73)

where \( J_d = b_0 (\pi p'_1 - (1 - \pi) p'_2) \), the evolution of which is given by

\[
\frac{\partial J'_d(x', t)}{\partial t} = -b_0^2 \frac{\partial}{\partial x'} \left[ \pi^2 p'_1(x', t) + (1 - \pi)^2 p'_2(x', t) \right] - \lambda_0 J'_d(x', t)
\]  

(74)
From the definition of $p'$ and $J_p'$ in terms of $p'_1$, $p'_2$ the inverse relations follow

$$
p'_1 = (1 - \pi) p' + \frac{J_p}{b_0}, \quad p'_2 = \pi p' - \frac{J_p}{b_0}
$$

(75)

Therefore, in the Kac limit, $b_0$, $\lambda_0 \to \infty$ it follows that

$$
J'_p = -2 D_0 \frac{\partial}{\partial x'} \left[ \pi^2 p'_1 + (1 - \pi)^2 p'_2 \right] \bigg|_{p'_1 = (1 - \pi) p', \ p'_2 = \pi p'}
$$

(76)

and therefore the effective self-diffusion coefficient is given by $D_{sd}(\pi) = 2 D_0 \pi (1 - \pi)$, consistently with the expression (62) deriving from the lattice representation of TASEP, by choosing $D_0 = 1/4$ for the nominal diffusivity.

4 Dynamic nonlinear models

In the previous Section we have considered exclusively the mean-field approximation corresponding to the motion of tagged particles in the mean-field characterized by a fixed concentration. The mean-field approximation has been introduced essentially in order: (i) to connect a generic physical model of interacting particles, with its corresponding GPK process, (ii) to show how the latter can be easily built up from lattice dynamics, and (iii) to show the existence of several hydrodynamic limits.

In considering the dynamics of an interacting particle system, it is rather clear that the mean field approximation is insufficient to provide a correct description of its evolution for the simple reason that the average concentration $\pi$ (introduced in the mean-field modeling) cannot be regarded as constant as it is a function of both time and space coordinates.

From the analysis developed in the previous section, the mean-field GPK model of a system of interacting particles is defined by

$$
dx(t) = b_{\chi_N(t; \mathbf{A}(\pi), \mathbf{A}(\pi))}(\pi) \, dt
$$

(77)

where the parameters defining the process, namely the stochastic velocities $b_i(\pi)$ characteristic of the $i$-th state, $i = 1, \ldots, N$, the transition rate vector $\mathbf{A}(\pi)$ and the transition probability matrix $\mathbf{A}(\pi)$, depend in general on the mean-field concentration $\pi$. Observe that eq. (77) implicitly assume that no external biasing fields are present, as for the cases treated in Section 3 (the TASEP model considered in paragraph 3.3 is obviously characterized by an internal drift, but the GPK model of the process refers to its description in a reference system moving at the effective velocity of the process). If an external velocity field $v(x)$ is present, it can be included into eq. (77) by adding to as a drift $v(x(t)) \, dt$ in the equation for $dx(t)$.

In order to consider the proper dynamics of a system of particles, the mean-field formulation (77) should be replaced by a nonlinear stochastic dynamics of the form

$$
dx(t) = \tilde{b}_{\chi_N(t; \tilde{\mathbf{A}}(\mathbf{p}(x(t), t)), \tilde{\mathbf{A}}(\mathbf{p}(x,t))})(\mathbf{p}(x, t)) \, dt
$$

(78)
where \( \hat{b}_i, \hat{A} = (\hat{\lambda}_1, \ldots, \hat{\lambda}_N) \) and \( \hat{\Lambda} \) depend on the entire system of partial probability densities \( p_i(x, t), i = 1, \ldots, N \) characterizing the process, i.e., on the vector-valued probability density \( p(x, t) = (p_1(x,t), \ldots, p_N(x, t)) \). The explicit expression for \( \hat{b}_i, \hat{\Lambda} \) and \( \hat{A} \), can be derived from the mechanics of particle interaction, similarly to what developed in Section 3 for the mean-field case. Moreover, a self-consistency condition should be fulfilled, namely that if all the \( p_i \) equal \( \pi/N \) that these quantities should coincide with the corresponding mean-field counterparts, i.e.,

\[
\hat{b}_i(p) = \begin{cases} 
 b_i(\pi), & i = 1, \ldots, N \end{cases} \quad (79)
\]

and analogous for the remaining quantities. Since a slightly different normalization has been adopted in the case of the fermionic model addressed in paragraph 3.1 where \( \pi \) is the mean-field concentration associated to a given spin-value (either +1 or −1) the consistency condition (79) still applies to this case with \( p_h = 2\pi/N \), since the spin states are two.

Henceforth, for simplifying the notation, we will indicate the “hatted” quantity, say \( \hat{b}_i \), solely with the bare letters and superscript, e.g. \( b_i \).

Equation (78) is a nonlinear stochastic model, in which particle stochastic motion depends on the collective state of the system at any time \( t \). It should be interpreted a la McKean [24, 25] and leads to nonlinear balance equations for the partial probability densities [14] which can be explicitized as

\[
\frac{\partial p_i(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left( b_i(p(x,t)) p_i(x,t) \right) - \lambda_i(p(x,t)) + \sum_{j=1}^{N} A_{i,j}(p(x,t)) \lambda_j(p(x,t)) p_j(x,t) \quad (80)
\]

Below, we analyze the systems addressed in Section 3 in order to extract their proper dynamic characterization and to derive the Kac limit of eq. (80), proceeding in the reverse order, namely from the simpler (TASEP) to the most elaborate fermionic model addressed in paragraph 3.1

### 4.1 TASEP in the moving reference frame

Consider again the TASEP model in the moving reference frame addressed in paragraph 3.3 eqs. (70)-(72), dropping the prime superscript \( (t) \) for notational simplicity. In the TASEP model, the mean-field concentration \( \pi \) corresponds, in a fully dynamic description of the process to \( p(x, t) = p_1(x, t) + p_2(x, t) \). Consequently the stochastic velocity vector of the two-state GPK process are given by

\[
b_1 = b_0 p(x,t), \quad b_2 = -b_0[1 - p(x,t)] \quad (81)
\]

the transition rates are uniform, i.e, \( \Lambda = (\lambda_0, \lambda_0) \), and the transition probability matrix \( A(p) \) takes the form

\[
A(p) = \begin{pmatrix} 1 - p & 1 - p \\ p & p \end{pmatrix} \quad (82)
\]
Therefore, the balance equations for the partial probability densities (partial concentrations) are given by

\[
\frac{\partial p_1}{\partial t} = -b_0 \frac{\partial (p_1 p_1)}{\partial x} - \lambda_0 [p_1 p_1 - (1 - p) p_2] \\
\frac{\partial p_2}{\partial t} = b_0 \frac{\partial [(1 - p) p_1]}{\partial x} + \lambda_0 [p_1 p_1 - (1 - p) p_2]
\] (83)

Eq. (83) already represents a hydrodynamic limit of the zero-bias TASEP model, characterized by a finite value of the characteristic transition rate \(\lambda_0\) and by the diffusivity \(D_0\), as \(b_0\) is related to \(\lambda_0\) and \(D_0\) by the relation \(b_0 = \sqrt{2 D_0 \lambda_0}\). Summing together the two equations in (83) the dynamics of the overall probability density follows

\[
\frac{\partial p}{\partial t} = - \frac{\partial}{\partial x} [b_0 (p_1 p_1 - (1 - p) p_2)] = - \frac{\partial}{\partial x} [b_0 (p_2 - p_2^2)]
\] (84)

Therefore, the probability flux \(J_p\) is given by \(J_p = b_0 (p_2^2 - p_2)\). Taking its time derivative

\[
\frac{\partial J_p}{\partial t} = b_0 \left( 2 p \frac{\partial p}{\partial t} - \frac{\partial p_2}{\partial t} \right) = -2 b_0 p \frac{\partial J_p}{\partial x} - b_0^2 \frac{\partial [(1 - p) p_2]}{\partial x} - \lambda_0 b_0 J_p
\] (85)

which, in the Kac limit, takes the form

\[
J_p = -2 D_0 \frac{\partial [(1 - p) p_2]}{\partial x}
\] (86)

The first eq. (83) can be rewritten as

\[
\frac{1}{\lambda_0} \frac{\partial p_1}{\partial t} = - \frac{2 D_0}{b_0} \frac{\partial (p_1 p_1)}{\partial x} - [p_1 p_1 - (1 - p) p_2]
\] (87)

which implies in the Kac limit

\[
P_1 = \frac{1 - p}{p} p_2
\] (88)

thus \(p = (1 + (1 - p)/p) p_2\), leading to

\[
P_2 = p^2
\] (89)

Substituting this result into eq. (83), the probability flux becomes \(J_p = -2 D_0 \frac{\partial [p^2 (1 - p)]}{\partial x}\), and correspondingly the Kac limit of the dynamic TASEP model (in the zero-bias case) provides the nonlinear diffusion equation

\[
\frac{\partial p}{\partial t} = 2 D_0 \frac{\partial^2 [p^2 (1 - p)]}{\partial x^2}
\] (90)
4.2 Simple exclusion random walk

The dynamic analysis of the simple exclusion random walk, that in mean-field approximation has been analyzed in paragraph 3.2, is conceptually identical to the previous case, and is completely resolved by identifying the mean-field effective concentration $\pi$ entering the transition probability matrix $A$ eq. (63) with the overall probability density $p = p_1 + p_2 + p_3$. Thus, the statistical characterization of the process is characterized by hyperbolic system

$$\frac{\partial p_1}{\partial t} = -b_0 \frac{\partial p_1}{\partial x} - \lambda_0 p_1 + \lambda_0 a(p) p$$
$$\frac{\partial p_2}{\partial t} = b_0 \frac{\partial p_2}{\partial x} - \lambda_0 p_2 + \lambda_0 a(p) p$$
$$\frac{\partial p_3}{\partial t} = -\lambda_0 p_3 + \lambda_0 p^2$$

(91)

The overall balance for $p(x,t)$ is still expressed by eq. (38), the probability flux $J_p(x,t)$ is a solution of eq. (53) where $p_b = p_1 + p_2$. From the third equation (91), in the limit for $\lambda_0 \to \infty$, $p_3 = p_2$, thus $p = p_b + p_3 = p_b + p_2 + p_4 \Rightarrow p_3 = (1 - p)$ (92)

Consequently, from eqs. (53), (92) follows that $J_p = -2 D_0 \partial [p(1 - p)]/\partial x$, and the Kac limit for the simple exclusion process attains the form

$$\frac{\partial p}{\partial t} = 2 D_0 \frac{\partial^2 [p(1 - p)]}{\partial x^2}$$

(93)

4.3 Fermionic random walk with exclusion

The dynamic characterization of the fermionic process described in paragraph 3.1 is slightly more difficult than the cases so far considered due to the existence of two spin states. The concentrations of particles possessing spin $+1$ and $-1$ are given by

$$p_+ = p_1 + p_3 , \quad p_- = p_2 + p_4$$

(94)

respectively, and both these quantities equal $\pi$ in the mean-field approximation.

By considering carefully the exclusion rules characterizing this process, the dynamic representation of the transition probability matrix of the associated GPK model is given by

$$A(p) = \begin{pmatrix}
    p_- (1 - p_+) & (1 - p_+) & p_- (1 - p_+) & (1 - p_+)^2 \\
    (1 - p_-)^2 & p_+ (1 - p_-) & (1 - p_-)^2 & p_+ (1 - p_-) \\
    p_+ p_- & p_+ (1 - p_+) & p_+ p_- & p_+ (1 - p_+) \\
    p_- (1 - p_-) & p_+ p_- & p_+ (1 - p_-) & p_+ p_- 
\end{pmatrix}$$

(95)

while $b = (b_0, -b_0, 0, 0)$ and $\Lambda = \lambda_0 (1, 1, 1, 1)$. From the expression of the quantities describing the GPK process, the balance equations for the partial densities can be straightforwardly derived. The Kac limit of this model can be obtained following the same approach applied in paragraph 3.1 for the mean-field analysis, and is not repeated here. One obtains for $p_b = p_1 + p_2$

$$p_b = \left(1 - \frac{p}{2}\right) p$$

(96)
Table 2: Functional form of the function $W(p)$ entering eq. (99) for the Kac limit of the random walk models satisfying an exclusion principle considered in the main text. “RW” stands for “Random Walk”.

| Model                                      | Function $W(p)$             |
|--------------------------------------------|-----------------------------|
| TASEP with no bias                         | $p^2 (1 - p)$               |
| Simple exclusion RW                        | $p (1 - p)$                 |
| Fermionic RW with exclusion                | $p (1 - p^2/3)$             |

and for the probability flux

$$J_d = -D_0 (1 + p) \frac{\partial p_0}{\partial x} = -D_0 (1 + p) \frac{\partial}{\partial x} \left[ \left(1 - \frac{p}{2}\right) p \right]$$  \hspace{1cm} (97)

Consequently the balance equation for the $p(x, t)$ in the Kac limit reads

$$\frac{\partial p}{\partial t} = D_0 \frac{\partial}{\partial x} \left[ (1 + p) \frac{\partial}{\partial x} \left(p - \frac{p^2}{2}\right) \right]$$  \hspace{1cm} (98)

Observe that this result is consistent with the mean-field analysis, as the mean-field concentration $\pi$ corresponds to $p/2$.

4.4 General observations

From the analysis developed above it follows that the Kac limit of the exclusion processes analyzed leads to nonlinear diffusion equations of the form

$$\frac{\partial p(x, t)}{\partial t} = \frac{\partial^2 W(p(x, t))}{\partial x^2}$$  \hspace{1cm} (99)

where $W(p)$ is a function of the overall concentration $p(x, t)$ and depends on the specific model considered, as reviewed in table 2

In all these models, for physically admissible values of $p$, the function $W(p)$ displays a non-monotonic behavior (see figure 11), corresponding to the occurrence of a local negative effective diffusivity $D_{\text{eff}}(p) = dW(p)/dp < 0$. This phenomenon, that is exclusively a consequence of the assessment of some form of exclusion dynamics, generates instabilities, the full characterization of which is addressed in [10] both in a thermodynamic perspective and via numerical experiments. The study of these phenomena permits to highlight clearly the meaning of the different hydrodynamic limits and the role of correlations in these paradigmatic examples of simple particle interaction.
Figure 4: Graph of the characteristic function $W(p)$ defined by eq. (99) in the Kac limit for the different model of random walk with exclusion treated in the main text. Panel (a): curve (a) refers to TASEP; curve (b) to the simple exclusion model. Panel (b) refers to the fermionic transport model.
5 Inclusion of potentials

The inclusion of potentials within the GPK formalism of interacting particle systems is relatively straightforward. The presence of a potential contribution in particle motion, expressed as a functional of the concentration field, modifies the transition probabilities \[^{22}\]. The same effect occurs for the GPK model associated with a system of interacting particles.

In order to analyze this phenomenology consider the simplest GPK process, namely the classical Poisson-Kac process on the real line defined by the classical Kac’s equation

\[
dx(t) = b_0 (-1)^{\chi(t; \lambda_0)} \, dt,
\]

where \(\chi(t; \lambda_0)\) is a usual Poisson process with transition rate \(\lambda_0\), the statistical characterization of which involves the two partial probability density functions \(p_+(x, t), p_-(x, t)\) \[^{15, 12}\]. Furthermore, assume that the nominal diffusivity is fixed and equal to \(b_0^2/2\lambda_0 = D_0\).

Consider a generic potential \(f\), that in the GPK formalism can be regarded as a functional of \(p_\pm(x, t)\), eventually depending on both space \(x\) and time \(t\) explicitly,

\[
f[p_+, p_-; x, t, b_0] = C(b_0) F[p_+, p_-; x, t, b_0] \tag{100}
\]

For reasons that it will be soon clear, we assume that the potential depends explicitly on the basic parameter of the Poisson-Kac process, i.e., on \(b_0\) as indicated in the functional dependence \[^{100}\], as \(\lambda_0\) is constrained by the actual value of the diffusivity \(D_0\). In eq. \(^{100}\) we have added a prefactor \(C(b_0)\), apparently in a redundant way as \(F\) depends on \(b_0\), for reasons that are related to the assessment of the hydrodynamic limit as developed below.

In the presence of a potential, the transition probabilities are no longer constants and equal to each other, but are explicit functions of the potential. Specifically,

\[
\begin{align*}
\text{Prob}[\chi(t) = 1 | \chi(t^-) = -1] & \sim (1 + f) \\
\text{Prob}[\chi(t) = -1 | \chi(t^-) = 1] & \sim (1 - f)
\end{align*} \tag{101}
\]

where \(t^- = \lim_{\varepsilon \to 0} t - \varepsilon, \varepsilon > 0\). The presence of a potential exerts its action exclusively on the functional form of the transition probability matrix, that becomes, through \(f[p_+, p_-; x, t, b_0]\), a functional of the partial probability densities,

\[
A[p_+, p_-] = \begin{pmatrix}
1 + f[p_+, p_-] & 1 + f[p_+, p_-] \\
1 - f[p_+, p_-] & 1 - f[p_+, p_-]
\end{pmatrix} \tag{102}
\]

where, for short, \(f[p_+, p_-] = f[p_+, p_-; x, t, b_0]\), and \(f \in [-1, 1]\). Correspondingly, the original Poisson-Kac process in the presence of potentials admits the GPK representation

\[
dx(t) = b_0 \chi_2(t; \lambda_0 1; A[p_+, p_-]) \, dt \tag{103}
\]

corresponding to a 2-state nonlinear GPK dynamics characterized by \(b = (b_0, -b_0)\), \(A = \lambda_0 (1, 1)\), and by the transition probability matrix expressed by eq. \(^{102}\). The statistical
description of eq. (103) involves the two partial densities \( p_\pm(x, t) \) satisfying the nonlinear evolution equations

\[
\begin{align*}
\frac{\partial p_+(x, t)}{\partial t} &= -b_0 \frac{\partial p_+(x, t)}{\partial x} - \frac{\lambda_0}{2} \left[ (1 - f[p_+, p_-]) p_+(x, t) - (1 + f[p_+, p_-]) p_-(x, t) \right] \\
\frac{\partial p_-(x, t)}{\partial t} &= b_0 \frac{\partial p_-(x, t)}{\partial x} + \frac{\lambda_0}{2} \left[ (1 - f[p_+, p_-]) p_+(x, t) - (1 + f[p_+, p_-]) p_-(x, t) \right]
\end{align*}
\]

(104)

The analysis of the Kac limit of this process is particularly interesting as it reveals novel features of this hydrodynamic limit in the presence of potential interactions and it discloses the eventual occurrence of new physical phenomena associated with the emergence of phase-transitions, and field-bifurcation phenomena. Letting \( p = p_+ + p_- \), the balance equation for the overall concentration coincides with eq. (38), where \( J_p(x, t) = b_0 [p_+(x, t) - p_-(x, t)] \) is a solution of the equation

\[
\frac{\partial J_p}{\partial t} = -b_0^2 \frac{\partial J_p}{\partial x} - \frac{\lambda_0}{b_0} \left[ J_p - f J_p \right]
\]

(105)

In order to obtain a proper Kac limit in the presence of potential interactions it is not sufficient to consider \( b_0, \lambda_0 \to \infty \), keeping fixed the nominal diffusivity \( D_0 \), as the quantity \( b_0 f \) enters in the constitutive equation for the flux and its asymptotic properties are essential in the assessment of the limit. As regards this quantity, set

\[
b_0 f[p_+, p_-; x, t, b_0] = b_0 C(b_0) F[p_+, p_-; x, t; b_0]
\]

(106)

substitute for \( p_\pm \) their expressions in terms of \( p \) and \( J_p \), and consider the limit

\[
\lim_{b_0 \to \infty} b_0 C(b_0) F \left[ \frac{1}{2} \left( p + \frac{J_p}{b_0} \right) , \frac{1}{2} \left( p - \frac{J_p}{b_0} \right) , x, t, b_0 \right] = F^*[p, J_p, x, t]
\]

(107)

Assume that \( C(b_0) \) is given by a physical model and its functional dependence on \( b_0 \) is fixed. In this case it can be always assumed \( C = 1 \), since the functional dependence on \( b_0 \) is contained in the functional form of \( F \).

Three situations can occur, as regards the limit functional \( F^*[p, J_p, x, t] \):

1. the limit \( F^* \) given by eq. (107) exists and defines a smooth non trivial functional \( F^* \) of \( p \) and \( J_p \);
2. the limit \( F^* \) is uniformly vanishing and consequently the effect of the potential is negligible in the Kac limit;
3. the limit (107) is diverging at some point, \( F^* \) does not exists, and the Kac limit of the process cannot be defined.

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The latter case is further addressed subsequently. To begin with, consider the first possibility, which is obviously the most interesting one for physical reasons. Eq. (105) can be rewritten as

$$\frac{1}{\lambda_0} \frac{\partial J_p}{\partial t} = -2D_0 \frac{\partial p}{\partial x} - J_p + b_0 f p \quad (108)$$

that, in the Kac limit, becomes

$$J_p = F^*[p, J_p; x, t] p - 2D_0 \frac{\partial p}{\partial x} \quad (109)$$

that formally corresponds to a constitutive equation for the flux expressed by the superposition of a "convective flux $F^* p$ and a diffusive flux $-2D_0 \partial p/\partial x$.

The latter interpretation is correct if and only if $F^*$ depends solely on the overall concentration $p$, and not on $J_p$, i.e., $F^*[p; x, t]$. Substituting eq. (109) in this case into the balance equation (38), a nonlinear advection-diffusion equation for $p$ is obtained

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left[ F^*[p; x, t] p(x, t) \right] + 2D_0 \frac{\partial^2 p(x, t)}{\partial x^2} \quad (110)$$

This equation can display non-local features, depending on the nature of the functional $F^*[p; x, t]$ that in general may depend on the whole spatial concentration profile, and not only on the local value $p(x, t)$ at $(x, t)$.

But there is another case, namely that $F^*[p, J_p; x, t]$ would depend explicitly on the flux $J_p$. The structure of the implicit flux constitutive equation opens up a wealth of potentially interesting physical and mathematical issues, depending whether eq. (109) can be explicited or not, and on the nature of the resulting explicit expression of the flux $J_p$ in terms of $p$ and $-\partial p/\partial x$. Below, we discuss qualitatively some typical cases, leaving a thorough investigation of this subject to forthcoming works.

To begin with consider the case where eq. (109) can be explicited with respect to $J_p$, i.e., there exists a functional $K[p, -2D_0 \partial p/\partial x; x, t]$, such that

$$J_p(x, t) = K \left[ p, -2D_0 \frac{\partial p}{\partial x}; x, t \right] \quad (111)$$

fulfilling the functional equation

$$K \left[ p, -2D_0 \frac{\partial p}{\partial x}; x, t \right] = F^* \left[ p, K \left[ p, -2D_0 \frac{\partial p}{\partial x}; x, t \right]; x, t \right] - 2D_0 \frac{\partial p(x, t)}{\partial x} \quad (112)$$

so that the resulting balance equation for $p(x, t)$ becomes

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} \left\{ K \left[ p, -2D_0 \frac{\partial p}{\partial x}; x, t \right] \right\} \quad (113)$$

It is easy to observe that the constitutive equation (113) is no longer Fickian, i.e., the probability flux is no longer, in general, proportional to the probability gradient. Moreover, for a suitable choice of the functional $f$, it may occur locally, i.e., at some $x$ and $t$ that

$$J_p(x, t) \frac{\partial p(x, t)}{\partial x} \geq 0 \quad (114)$$
i.e., that the flux $J_p$ is oriented towards the direction of increasing probability gradients (uphill diffusion). This situation is analyzed, via some numerical examples, in [10].

The other situation occurs in the case eq. (109) cannot be explicited with respect to $J_p$, leading to a multivalued expression for the flux as a function of the concentration gradient. In this case, multiple branches of the flux-concentration gradient constitutive equation can occur, determining new physical phenomena. In order to provide a first qualitative understanding of this class of problem, assume for simplicity that the functional $F^*$ reduces to a local function solely of $J_p(x,t)$, i.e.,

$$F^* [J_p; p, x, t] = f^*(J_p(x,t)).$$

The functional form of $f^*(J_p)$ cannot be completely arbitrary, as the original functional $f$ admits a probability interpretation and consequently is should be bounded by $|f| \leq 1$. This prevents, for example, the physical occurrence of a global relation of the form $f^*(J_p) = c J_p^2$, where $c$ is a constant, as it would imply for sufficiently large $b_0$.

$$f[p_+, p_-; x, t] \simeq \frac{c J_p^2}{b_0} = c b_0 (p_+ - p_-)^2$$

that attains arbitrarily large values for large $b_0$ and generic $(p_+ - p_-)$.

It is therefore reasonable, from the above observation, that in a physical model the function $f^*(J_p)$ should diverge as most linearly with $J_p$, i.e.,

$$f^*(J_p) = J_p h(J_p)$$

where $h(J_p)$ is a bounded function of $J_p$, such that $|h(J_p)(p_+ - p_-)| \leq 1$. For instance a model of the form

$$f^*(J_p) = c J_p e^{-\beta J_p^2}$$

where $c$ and $\beta$ are positive constants, satisfies this condition. Setting $z = -2 D_0 \frac{\partial p}{\partial x}$, the flux constitutive equation attains in this case the expression

$$\Phi(J_p; p, z) = -J_p + c p J_p e^{-\beta J_p^2} + z = 0$$

Figure 5 depicts the behavior of the function $\Phi(J_p; p, z)$ vs $J_p$ at $z = 1$ for different values of $p$ (henceforth, we set $c = \beta = 1$ a.u.), showing that there exists a critical value $p_c$ of $p$ above which the constitutive equation displays three difference branches, associated with the solution of eq. (118).

The analysis of this problem is essentially a classical bifurcation problem of equilibria. Figure 5 panel (a) depicts the constitutive equation, i.e., the graph of $J_p$ vs $z = -2 D_0 \partial p/\partial x$ at $p = 3$, indicating the occurrence of two saddle-node bifurcations, generating the transition from a sigle to a three-fold structure. The stability of the constitutive branches, follows directly from the observation that for large $b_0$,

$$\frac{1}{\lambda_0} \frac{\partial J_p}{\partial t} \simeq \Phi(J_p, p, z)$$

indicating that a constitutive branch is stable provied that $\partial \Phi(J_p; p, z)/\partial J_p < 0$, and unstable in the opposite case.
A similar bifurcation diagram depicting $J_p$ vs $p$ at a fixed value of $z$ is shown in panel (b) of figure 6. It follows from the graphs depicted in figure 6 (a) that, along the stable constitutive branches, the flux $J_p$ is a monotonically increasing function of $z$, as expected from thermo-dynamic consistency, i.e., $\partial J_p / \partial z > 0$, and the oppositive holds for the unstable branches.

Nevertheless, it can be observed that, for small absolute values of $z$, the product $J_p z$ can be negative, even for the stable constitutive branches, indicating the possibility of local uphill diffusion phenomena. This result is clearly shown in the graph depicted in figure 7.

To sum up, it has been shown via a very simple example, that system of interacting particles may give rise, in the Kac limit, to implicit constitutive equations, producing multiple constitutive branches. The bifurcations associated with the explicit representation of the constitutive equation for the flux as a function of the concentration gradient may give rise to new classes of non-equilibrium phase transitions, the physical and mathematical characterization of which is still to be developed, and it will be approached in forthcoming works.

## 6 Concluding remarks

This article has introduced the formal setting of hyperbolic transport models for systems of interacting particles by considering either lattice dynamics subjected to simple exclusion principles or the presence of interaction potentials. The latter phenomenology involves, in a hyperbolic continuous setting, solely the functional dependence of the transition probability matrix on the partial probability density functions.
Figure 6: Panel (a) Constitutive branches of the flux/concentration gradient constitutive equation ($J_p$ vs $z$) for the model system eqs. (116)-(118) at $p = 3$. Panel (b) $J_p$ vs $p$ at $z = -1$ for the same problem. The labels "s" and "u" indicate respectively the stable and unstable branches.
Figure 7: Function $z J_p(z; p)$ vs $z$, where $J_p(z; p)$ are the solution of eq. (118) for the data depicted in figure 6 panel (a).

For further applications, the hyperbolic formalism in the presence of interaction potentials deserves particular attention, as the resulting hydrodynamic models may display a wealth of non trivial dynamic phenomena. These phenomena are intrinsically associated with the hyperbolic nature of the model implying bifurcations and multiplicity of flux/concentration-gradient constitutive equations. This is particularly evident in the Kac limit of these models, where, depending on the interaction potentials, a multiplicity of constitutive equations may appear. The phenomenology associated with these dynamic instabilities is analysed in [10].

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