Stochastic foundations of undulatory transport phenomena: generalized Poisson–Kac processes—part III extensions and applications to kinetic theory and transport

Massimiliano Giona¹,², Antonio Brasiello² and Silvestro Crescitelli³

¹ Dipartimento di Ingegneria Chimica DICMA, Facoltà di Ingegneria, La Sapienza Università di Roma, via Eudossiana 18, 00184, Roma, Italy
² Dipartimento di Ingegneria Industriale, Università degli Studi di Salerno, via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy
³ Dipartimento di Ingegneria Chimica dei Materiali e della Produzione Industriale, Università degli Studi di Napoli ‘Federico II’, piazzale Tecchio 80, 80125 Napoli, Italy

E-mail: massimiliano.giona@uniroma1.it

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Abstract

This third part extends the theory of Generalized Poisson–Kac (GPK) processes to nonlinear stochastic models and to a continuum of states. Nonlinearity is treated in two ways: (i) as a dependence of the parameters (intensity of the stochastic velocity, transition rates) of the stochastic perturbation on the state variable, similarly to the case of nonlinear Langevin equations, and (ii) as the dependence of the stochastic microdynamic equations of motion on the statistical description of the process itself (nonlinear Fokker–Planck–Kac models). Several numerical and physical examples illustrate the theory. Gathering nonlinearity and a continuum of states, GPK theory provides a stochastic derivation of the nonlinear Boltzmann equation, furnishing a positive answer to the Kac’s program in kinetic theory. The transition from stochastic microdynamics to transport theory within the framework of the GPK paradigm is also addressed.

Keywords: transport theory, nonlinear Langevin equations, kinetic theory, stochastic processes, Kac’s program

(Some figures may appear in colour only in the online journal)
1. Introduction

This third and last part of the work on Generalized Poisson–Kac (GPK) processes and their physical applications extends the analysis developed in parts I and II [1, 2], developing the generalization of GPK theory to a broad spectrum of stochastic phenomenologies. With respect to the theory developed in [1, 2], two lines of attack characterize this extension: (i) the inclusion of nonlinearities, and (ii) the extension to a continuum of states.

Nonlinearities can be treated in two different ways. The first class of nonlinear models assumes that the state (position) variable $x$ can influence the basic parameters characterizing stochastic GPK perturbations. In the case of GPK perturbations, this reflects into the functional dependence of $b_\alpha$, $\lambda_\alpha$, and $A_{\alpha,\beta}$ on $x$. In the case of a position dependent system of stochastic velocities, i.e., $\{b_\alpha(x)\}_{\alpha=1}^N$, GPK models correspond to nonlinear Langevin equations [3, 4], since the latter provide the Kac limit (in the Stratonovich interpretation of the stochastic integral) for this class of systems. The functional dependence of the transition rates $\lambda_\alpha(x)$, or of the entries of the transition probability matrix $A_{\alpha,\beta}(x)$ on $x$, provides new phenomena, as it emerges from the analysis of their Kac limits.

The second way to include nonlinearities, analogous to the McKean approach to Langevin equations [5] leads to GPK microdynamic equations which depend on the statistical characterization of the process itself (in the present case, the system of partial probability density functions $\{p_\alpha(x,t)\}_{\alpha=1}^N$). This leads to the concept of nonlinear Fokker–Planck–Kac equation (this diction stems from the Langevin counterpart [6]), the dynamic properties of which can be extremely rich.

The extension from a discrete number $N$ of states to a continuum of stochastic states is fairly straightforward within the formalism developed in part I (see also the discussion in part I on the multidichotomistic approach). Moreover, the coupling of nonlinear effects with a continuum of stochastic states permits to derive the classical nonlinear Boltzmann equation of the kinetic theory of gases [7] within the GPK formalism. This result deserves particular attention as it shows, unambiguously, that the Boltzmann equation admits a fully stochastic explanation. In some sense, this result completes the original Kac’s program in kinetic theory [8–11], originated from the article [12] aimed at providing an extended Markov model for interpreting the celebrated Boltzmann equation of kinetic theory. For a discussion on extended Markov models see [13].

Finally, the article outlines the bridge between the stochastic description of particle microdynamics based on GPK equations, and transport theory of continuous media. This connection is developed with the aid of some classical problems. In developing a transport theory from GPK microdynamics the role of the primitive statistical formulation of GPK processes, based on the system of partial probability densities $\{p_\alpha(x,t)\}_{\alpha=1}^N$, clearly emerges (for a discussion see also section 2 in part I), and it is mapped into a corresponding system of partial concentrations/velocity fields. This part of the article is of primary interest in extended thermodynamic theories of irreversible processes [14–16], as it provides a novel way to develop these theories enforcing the assumption of finite propagation velocity for thermodynamic processes, and overcoming the intrinsic limitations of models based on the higher-dimensional Cattaneo equation (see part I for details).

The article is organized as follows. Section 2 reviews in a extremely succinct way the notation and the statistical characterization of Poisson–Kac and GPK processes. Section 3 develops the extensions of GPK models (nonlinearity, continuum of stochastic states), presenting for each class of models a physical example. Section 4 derives the connection
(equivalence) between a nonlinear GPK process admitting a continuum of stochastic states and the Boltzmann equation, discussing some implications of this result. Section 5 addresses the connection between GPK microdynamics and the associated transport formalism in continua by considering several problems ranging from dynamo theory [17, 18] to mass and momentum balances, including a brief description of chemical reactions.

2. Poisson–Kac and GPK processes

A Poisson–Kac process \( X(t) \) on the real line \( \mathbb{R} \), in the presence of a deterministic biasing field \( v(x) \), is defined by the evolution equation

\[
dx(t) = v(x(t)) \, dt + b \, (-1)^{\chi(t)} \, dt
\]

where \( b > 0 \) and \( \chi(t) \) is a Poisson process characterized by the transition rate \( \lambda > 0 \). Henceforth, we will indicate with \( X(t) \) the stochastic process at time \( t \) and with \( x(t) \) a realization of it.

Owing to its non Markovian character associated with the finite propagation velocity \( b \), its statistical description involves two partial probability density functions \( p^\pm(x, t) \), also referred to as partial probability waves, defined as \( p^\pm(x, t) \, dx = \text{Prob} \{ X(t) \in (x, x + dx) \}, \, (-1)^{\chi(t)} = \pm 1 \) and accounting for the actual state of the stochastic perturbation \( (-1)^{\chi(t)} \), that in the present case can attain solely two different values.

The partial probability densities satisfies the hyperbolic system of equations

\[
\partial_t p^\pm(x, t) = -\partial_x [(v(x) \pm b) \, p^\pm(x, t)] \mp \lambda (p^+(x, t) - p^-(x, t)).
\]

The overall probability density \( p(x, t) \), corresponding to the marginal density with respect to \( x \) is \( p(x, t) = p^+(x, t) + p^-(x, t) \).

Introducing the ‘diffusional’ probability flux \( J_d(x, t) = b \, (p^+(x, t) - p^-(x, t)) \), i.e. the flux associated solely with the stochastic perturbation, the partial densities can be expressed as \( p^\pm = (p + J_d/b)/2 \).

Generalized Poisson–Kac (GPK) processes have been introduced in order to extend this one-dimensional model in higher dimensions with the constraint that these model would possess an emergent Brownian behavior whenever the order of magnitude of the stochastic velocities and of the transition rates diverge. This is referred to as the Kac limit and it is thoroughly addressed in [1]. Essentially, a GPK process in \( \mathbb{R}^n \) is generated by a finite \( N \)-state Poisson process \( \chi_N(t) \) admitting \( N \) stochastic states \( \alpha = 1, \ldots, N \), and switching from the (initial) stochastic state \( \alpha \) to the (subsequent) state \( \beta \) according to the transition rate \( \lambda_{\alpha \beta} \) and to the transition probability matrix \( A_{\beta, \alpha} \), \( \alpha, \beta = 1, \ldots, N \), where \( A_{\beta, \alpha} \geq 0 \), \( \sum_{\beta=1}^N A_{\beta, \alpha} = 1 \). A constant velocity vector \( b_\alpha \in \mathbb{R}^n \) is associated with each stochastic state \( \alpha \), so that the evolution equation for a GPK process \( X(t) \) in the presence of a deterministic biasing field \( v(x) \) is expressed by

\[
dx(t) = v(x(t)) \, dt + b_\chi(x(t)) \, dt.
\]

Owing to the occurrence of \( N \) distinct states, the statistical description of a GPK process involves \( N \) partial probability density functions \( p_\alpha(x, t) \), where \( \alpha \) refers to the actual value of the stochastic state, satisfying the system of hyperbolic equations

\[
\partial_t p_\alpha(x, t) = -\nabla \cdot [(v(x) + b_\alpha) \, p_\alpha(x, t)] - \lambda_\alpha p_\alpha(x, t) + \sum_{\gamma=1}^N \lambda_\gamma A_{\alpha \gamma} p_\gamma(x, t)
\]

The overall (marginal) probability density function for \( X(t) \) is obviously \( p(x, t) = \sum_{\alpha=1}^N p_\alpha(x, t) \).
3. Generalizations

The theory of GPK processes can be generalized in several different directions that provide, from one hand, a valuable system of stochastic modeling tools of increasing complexity and, from the other hand, the possibility of interpreting a broader physical phenomenology. In the remainder of this section we introduce the various generalizations by considering first one-dimensional Poisson–Kac processes, and subsequently extending the theory to GPK processes.

3.1. Nonlinear GPK processes and Poisson fields

In order to define nonlinear GPK processes it is convenient to introduce the concept of Poisson fields. A Poisson field \( \chi(x,t) \), \( x \in \mathbb{R} \) is a Poisson process over the real line \( \mathbb{R} \) such that its transition rate \( \lambda \) depends on \( x \) and possibly on time \( t \). If \( \lambda = \lambda(x) \) the Poisson field is said to be stationary, while if \( \lambda(x,t) \) depends explicitly on time \( t \) is referred to as a non-stationary field.

Let \( \lambda_0 = \inf_{x \in \mathbb{R}} \lambda(x,t) > 0 \), and let \( b(x) \) be a positive real-valued function. A nonlinear GPK process is defined via the stochastic differential equation

\[
\frac{dx(t)}{dt} = v(x(t)) \, dt + b(x(t)) \left( -1 \right)^{\chi(x(t),t)} \, dt
\]

(3)

where \( v(x) \) is a deterministic bias. The presence of a position dependent stochastic velocity \( b(x) \), and the dependence on \( x \) of the transition rate defining the Poisson field \( \chi(x,t) \), makes this model conceptually similar to the nonlinear Langevin equations [3, 4].

We have assumed that \( b(x) \) does not depend explicitly on time \( t \). This condition can be easily removed, but the generalization to time-dependent \( b(x,t) \) involves more lengthy calculations of the Kac limit, the full development of which is left to the reader.

For the process associated with equation (3), the partial probability density functions \( p^\pm(x,t) \) fully characterize its statistical properties. These quantities satisfy the balance equations

\[
\partial_t p^\pm(x,t) = -\partial_x \left( v(x) p^\pm(x,t) \right) \mp \partial_x \left( b(x) p^\pm(x,t) \right) \mp \lambda(x,t) \left[ p^+(x,t) - p^-(x,t) \right]
\]

(4)

and the ‘diffusive’ probability flux is given by \( J_d(x,t) = b(x) \left[ p^+(x,t) - p^-(x,t) \right] \).

Let \( \hat{b}(x) = b(x)/b^{(c)} \), where \( b^{(c)} = \inf_{x \in \mathbb{R}} b(x) > 0 \). Set \( J_d(x,t) = \hat{b}(x) \phi(x,t) \) where \( \phi(x,t) = b^{(c)} \left[ p^+(x,t) - p^-(x,t) \right] \). In terms of normalized quantity \( \phi(x,t) \) the constitutive equation for the diffusive flux becomes

\[
\partial_t \phi(x,t) = -\partial_x \left( v(x) \phi(x,t) \right) - \left( \frac{b^{(c)}}{\lambda^{(c)}} \right)^2 \partial_x \left( \hat{b}(x) \phi(x,t) \right) - 2 \lambda(x,t) \phi(x,t)
\]

(5)

Let \( \hat{\lambda}(x,t) = \lambda(x,t)/\lambda^{(c)} \), where \( \lambda^{(c)} = \lambda_0 \). In the limit \( b^{(c)}, \lambda^{(c)} \rightarrow \infty \), \( D_{nom} = (b^{(c)})^2/2\lambda^{(c)} \) = constant the constitutive equation for \( \phi(x,t) \) becomes

\[
\phi(x,t) = -\frac{D_{nom}}{\hat{\lambda}(x,t)} \partial_x \left( \hat{b}(x) \phi(x,t) \right)
\]

(6)

that, substituted into the balance equation for \( p(x,t) = p^+(x,t) + p^-(x,t) \), provides

\[
\partial_t p(x,t) = -\partial_x \left( v(x) p(x,t) \right) + D_{nom} \partial_x \left[ \frac{\hat{b}(x)}{\hat{\lambda}(x,t)} \partial_x \left( \hat{b}(x) p(x,t) \right) \right]
\]

(7)
which represents the Kac limit for the nonlinear Poisson–Kac process considered. In terms of the original quantities $b(x)$ and $\lambda(x,t)$, the Kac limit can be expressed equivalently as

$$\partial_t p(x,t) = -\partial_x [v(x)p(x,t)] + \frac{1}{2} \partial_x \left[ \frac{b(x)}{\lambda(x,t)} \frac{\partial_b(x)}{\lambda(x,t)} p(x,t) \right] + \frac{1}{2} \partial_x \left[ \frac{b(x)}{\lambda(x,t)} \frac{b(x)}{\lambda(x,t)} \partial_x p(x,t) \right]$$  \hspace{1cm} (8)

Equation (8) corresponds to an advection-diffusion equation characterized by an effective velocity

$$v_{\text{eff}}(x,t) = v(x) - \frac{b(x)}{2\lambda(x,t)} \frac{\partial b(x)}{\lambda(x,t)}$$  \hspace{1cm} (9)

and by an effective diffusivity

$$D_{\text{eff}}(x,t) = \frac{b^2(x)}{2\lambda(x,t)}$$  \hspace{1cm} (10)

The above-derived Kac limit should be compared with the statistical description of a classical Langevin equation driven by Wiener fluctuations

$$\partial_x = v_S(x,t) \partial_t + \sqrt{2D_S(x,t) \circ dw(t)}$$  \hspace{1cm} (11)

where $dw(t)$ are the increments of a one-dimensional Wiener process in the time interval $(t,t+\Delta t)$, to be interpreted ‘a la Stratonovich’. In equation (11), ‘‘’ indicates the Stratonovich recipe for the stochastic integrals. The Fokker–Planck equation associated with equation (11) is given by

$$\partial_t p(x,t) = -\partial_x [v_S(x,t)p(x,t)] + \frac{1}{2} \partial_x \left[ p(x,t) \partial_x D_S(x,t) \right] + \partial_x \left[ D_S(x,t) \partial_x p(x,t) \right]$$  \hspace{1cm} (12)

The reason for the choice of the Stratonovich rather than the Ito calculus follows from the Wong–Zakai theorem [19, 20]: Poisson–Kac processes are stochastic dynamical systems excited by a.e. differentiable smooth perturbations, converging in the Kac limit to ordinary Brownian motion. According to the Wong–Zakai result, that in the present case corresponds to the Kac limit, these processes should converge in the Kac limit to the Stratonovich formulation of the Langevin equation (11), where $v_S(x,t)$ and $D_S(x,t)$ should coincide with $v_{\text{eff}}(x,t)$ and $D_{\text{eff}}(x,t)$, respectively. Below, we discuss this convergence that, in point of fact, is slightly more subtle than expected.

Two cases should be considered. Case (A): $\lambda(x,t)$ does not depend on $x$. It follows from the comparison of equations (8) and (12) that the Kac limit of equation (3) coincides with equation (11) provided that

$$v_S(x) = v(x), \quad D_S(x,t) = D_{\text{eff}}(x,t)$$  \hspace{1cm} (13)

and this can be viewed as a corollary of the Wong–Zakai theorem. In this case, the Poisson–Kac process is a stochastic mollification of the Langevin–Stratonovich equation (11). Case (B): $\lambda(x,t)$ depends explicitly on $x$. Also in this case

$$D_S(x,t) = D_{\text{eff}}(x,t)$$  \hspace{1cm} (14)

The equivalence between the convective contributions deriving from equations (9) and (12), enforcing equation (14), implies that

\[ J. \text{Phys. A: Math. Theor. 50 (2017) 335004} \]
\[ v_{\text{eff}}(x) = v(x) - \frac{b(x) \partial_b(x)}{2 \lambda(x,t)} = v_3(x,t) - \frac{1}{2} \partial_t D_3(x,t) \]

\[ = v_3(x,t) - \frac{1}{2} \partial_t \left( \frac{b^2(x)}{2 \lambda(x,t)} \right) \]

(15)

thus providing, after differentiation of the latter expression, the relation

\[ v_3(x,t) = v(x) - \frac{D_3(x,t)}{2} \partial_t \log \lambda(x,t) \]

(16)

which shows that the equivalent Stratonovich velocity field does not coincide with \( v(x) \) and depends on the spatial derivative of the transition rate \( \lambda(x,t) \). A physical justification of this phenomenon is addressed at the end of this paragraph.

Using the formal apparatus of GPK processes briefly reviewed in section 2, the generalization to nonlinear GPK processes in \( \mathbb{R}^n \) is straightforward. Define a \( N \)-state finite Poisson field \( \chi_N(x,t) \) a stochastic process parametrized with respect to \( x \in \mathbb{R}^n \), attaining \( N \) different possible states, such that the transition structure between the states is described by the time-continuous Markov chain

\[ \partial_t P^{(x)}_{\alpha}(x,t) = -\lambda_{\alpha}(x,t) P^{(x)}_{\alpha}(x,t) + \sum_{\gamma=1}^{N} K_{\alpha,\gamma}(x,t) P^{(x)}_{\gamma}(x,t) \]

(17)

\( \alpha = 1, \ldots, N \), where \( P^{(x)}_{\alpha}(x,t) \) is the probability of the occurrence of \( \chi_N(x,t) = \alpha \) at position \( x \) and time \( t \). In equation (17) \( \lambda_{\alpha}(x,t) = \sum_{\gamma=1}^{N} K_{\gamma,\alpha}(x,t) > 0 \), and \( K_{\alpha,\gamma}(x,t) \) are the entries of a symmetric transition matrix, \( K_{\alpha,\gamma}(x,t) = K_{\gamma,\alpha}(x,t) \), for any \( x \in \mathbb{R}^n, t \geq 0 \). Moreover, let us assume that

\[ A_{\alpha,\gamma}(x,t) = \frac{K_{\alpha,\gamma}(x,t)}{\lambda_{\gamma}(x,t)} \]

(18)

represents an irreducible left-stochastic matrix function for any \( x \in \mathbb{R}^n \) and \( t \geq 0 \). Given \( N \) vector valued functions \( b_1(x), \ldots, b_N(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n \), satisfying the zero-bias condition

\[ \sum_{\alpha=1}^{N} b_{\alpha}(x) = 0 \]

(19)

identically for \( x \in \mathbb{R}^n \), a nonlinear GPK process is described by the stochastic differential equation

\[ d\mathbf{x}(t) = v(\mathbf{x}(t)) \, dt + b_{\chi_N(x,t)}(x) \, dt \]

(20)

Its statistical characterization involves \( N \) partial probability density functions \( p_{\alpha}(x,t) \), \( \alpha = 1, \ldots, N \) satisfying the balance equations

\[ \partial_t p_{\alpha}(x,t) = -\nabla \cdot ( v(\mathbf{x}) p_{\alpha}(x,t) ) - \nabla \cdot ( b_{\alpha}(x) p_{\alpha}(x,t) ) - \lambda_{\alpha}(x,t) p_{\alpha}(x,t) + \sum_{\gamma=1}^{N} K_{\alpha,\gamma}(x,t) p_{\gamma}(x,t) \]

(21)

Using the representation in terms of \( \mathbf{A}(x,t) = (\lambda_1(x,t), \ldots, \lambda_N(x,t)) \) and \( \mathbf{A}(x,t) = (A_{\alpha,\beta}(x,t))_{\alpha,\beta=1}^{N} \), it is straightforward to construct a stochastic simulator of equation (21) analogous to that defined in section 4 of part I for linear GPK processes.
It is worth observing that there is a substantial difference between nonlinear Poisson–Kac/GPK process of the form (3) or (20) and the nonlinear Langevin equations driven by Wiener perturbations, such as equation (11). In the latter case, the \( x \)-dynamics does not influences the statistical properties of the stochastic Wiener forcing and implies solely a modulation of the intensity of the stochastic perturbation, that depends on \( x \), via the factor \( \sqrt{2D_S(x, t)} \) as in equation (11). Conversely, in the case of Poisson–Kac/GPK processes, there is a two-way coupling between the \( x \)-dynamics of the Poissonian perturbation, as the evolution of \( x(t) \) influences the statistics of the Poissonian field, whenever the transition rate \( \lambda(x, t) \) or the transition rate vector \( \Lambda(x, t) \) depend explicitly on \( x \) and \( x \), respectively.

This observation, physically explain the apparently ‘anomalous’ correspondence relation (16), as this model does not fall within the range of application of the Wong–Zakai theorem.

### 3.2. Continuous GPK processes

A further generalization of GPK theory is the extension to a continuous number of states. Such a continuous extension is not suitable within the framework of multi-dichotomic processes discussed in section 3 of part I, and this constitutes the main shortcoming of this class of models in the applications to statistical physical problems.

Next, consider the one-dimensional case. Let \( \Xi(t) \) be a time-continuous Markov process attaining a continuum of states belonging to a domain \( D \in \mathbb{R} \). Its statistical description involves the transition rate kernel \( K(\alpha, \beta) \), which is a positive symmetric kernel

\[
K(\alpha, \beta) = K(\beta, \alpha), \quad K(\alpha, \beta) \geq 0
\]  

(22)

Given \( K(\alpha, \beta) \), it is possible to introduce the transition rates \( \lambda(\alpha) \)

\[
\lambda(\alpha) = \int_D K(\beta, \alpha) \, d\beta > 0
\]  

(23)

and the transition probability kernel \( A(\alpha, \beta) \)

\[
A(\alpha, \beta) = \frac{K(\alpha, \beta)}{\lambda(\beta)}
\]  

(24)

The transition probability kernel \( A(\alpha, \beta) \) possesses the following properties: (i) normalization, i.e.

\[
\int_D A(\beta, \alpha) \, d\beta = 1
\]  

(25)

i.e. it is a left-stochastic kernel, and (ii) it is assumed that \( A(\alpha, \beta) \) is irreducible, meaning that solely the constant function \( 1_{\mathbb{D}} \in D \) is the left eigenfunction of \( A(\alpha, \beta) \), associated with the Frobenius eigenvalue 1. In other terms, the multiplicity of the Frobenius eigenvalue is 1.

Indicating with \( P^\Xi(\alpha, t) \, d\alpha = \text{Prob}[\Xi(t) \in (\alpha, \alpha + d\alpha)] \), \( \int_D P^\Xi(\alpha, t) \, d\alpha = 1 \) for any \( t \geq 0 \), the evolution of this probability density follows the Markovian character of the transition dynamics

\[
\partial_t p^\Xi(\alpha, t) = - \left( \int_D K(\beta, \alpha) \, d\beta \right) p^\Xi(\alpha, t) + \int_D K(\alpha, \beta) p^\Xi(\beta, t) \, d\beta
\]  

(26)
Let \( b(x, \alpha) : \mathbb{R} \times D \to \mathbb{R} \), the stochastic velocity function satisfying the zero-bias property
\[
\int_D b(x, \alpha) \, d\alpha = 0
\]
(27)
for any \( x \in \mathbb{R} \). Within this setting, it is possible to introduce the stochastic differential equation
\[
dx(t) = v(x) \, dt + b(x, \Xi(t)) \, dt
\]
(28)
which represents the microdynamic description of a one-dimensional Continuous GPK process (CGPK). The statistical description of a CGPK process involves the partial probability density functions \( p(x, t; \alpha) \) continuously parametrized with respect to the state variable \( \alpha \) of the stochastic forcing \( \Xi(t) \).
\[
p(x, t; \alpha) \, dx \, d\alpha = \text{Prob} \{ X(t) \in (x, x + dx), \Xi(t) \in (\alpha, \alpha + d\alpha) \}
\]
(29)
such that the overall probability density function for \( X(t) \) and its diffusive flux are respectively given by
\[
p(x, t) = \int_D p(x, t; \alpha) \, d\alpha, \quad J_d(x, t) = \int_D b(x, \alpha) \, p(x, t; \alpha) \, d\alpha
\]
(30)
In the continuous setting \( p(x, t; \alpha) \) represents the primitive statistical description of a CGPK process, and its evolution equation is expressed by
\[
\partial_t p(x, t; \alpha) = -\partial_x (v(x) \, p(x, t; \alpha)) - \partial_\alpha (b(x, \alpha) \, p(x, t; \alpha))
\]
(31)
\[
+ \int_D K(\alpha, \beta) \left[ p(x, t; \beta) - p(x, t; \alpha) \right] \, d\beta
\]
where the symmetry of the kernel \( K(\alpha, \beta) \) has been applied.

Assume for simplicity that \( b(x, \alpha) \) does not depend on \( x \), and that the stochastic velocity function \( b(\alpha) \) is a monotonic function of \( \alpha \). Under these conditions one can simply map the states of \( \Xi(t) \) using the transformation \( c = b(\alpha) \), thus defining the new stochastic process \( \Theta(t) \) defined as
\[
b(\Xi(t)) = \Theta(t) \quad \Xi(t) = b^{-1}(\Theta(t))
\]
(32)
Let \( C = b(D) \). In this way, the stochastic differential equation defining CGPK process attains the more compact expression
\[
dx(t) = v(x(t)) \, dt + \Theta(t) \, dt
\]
(33)
where \( \Theta(t) \in C \). Letting \( f(c) = b^{-1}(c) \) the inverse of \( b(\alpha) \), and define
\[
\bar{p}(x, t; c) = p(x, t; \alpha) \big|_{\alpha = f(c)} \frac{df(c)}{dc}
\]
(34)
\[
\bar{K}(c, c') = K(\alpha, \beta) \big|_{\alpha = f(c), \beta = f(c')} \frac{df(c)}{dc}
\]
(35)
the CGKP process, parametrized with respect to the values \( c \) attained by stochastic velocity \( b(\alpha) \), is described by the transformed probability density functions \( \bar{p}(x, t; c) \) associated with equation (33), that satisfy the balance equations
\[
\partial_t \bar{p}(x, t; c) = -\partial_x (v(x) \, \bar{p}(x, t; c)) - c \, \partial_c \bar{p}(x, t; c)
\]  
\[
+ \left( \int_C \bar{K}(c', c) \, dc' \right) \bar{p}(x, t; c) - \int_C \bar{K}(c, c') \, \bar{p}(x, t; c') \, dc'
\]
(36)
The transformation of the transition kernel \( (35) \) is such that the transition rates \( \bar{\lambda}(c) \) coincide with the corresponding ones expressed with respect to the parameter \( \alpha \), namely

\[
\bar{\lambda}(c) = \int_{c} K(c',c) \, dc' = \int_{D} K(\beta, f(c)) \, d\beta = \lambda(\alpha)|_{\alpha = f(c)}
\]  

(37)

while the transformed transition probability matrix kernel \( \bar{K}(c',c) \) is defined as

\[
\bar{K}(c',c) = \frac{K(c',c)}{\bar{\lambda}(c)} = A(\beta, \alpha)|_{\alpha = f(c), \beta = f(c')} \frac{df(c')}{dc'}
\]  

(38)

Observe that if \( K(\alpha, \beta) \) is symmetric, this is no longer true for \( \bar{K}(c, c') \) in the presence of a nonlinear expression of \( b(\alpha) \).

In the case \( b(\alpha) = \alpha \), and \( K(\alpha, \beta) \) symmetric, the analysis greatly simplifies, and equation \( (36) \) reduces to

\[
\partial_t \bar{p}(x, t; c) = -\partial_x \left( (c - b(x, t; c)) \bar{p}(x, t; c) \right) - c \partial_x \bar{p}(x, t; c)
\]  

+ \[
\int_{D} \bar{K}(c, c') \left[ \bar{p}(x, t; c') - \bar{p}(x, t; c) \right] \, dc'
\]

(39)

since \( C = D \). It can be recognized that equation \( (39) \) represents a one-dimensional linearized Boltzmann equation. The zero-bias condition \( (27) \) becomes

\[
\int_{B} c \, dc = 0
\]  

(40)

which indicates that the domain \( C \) must be the union of symmetric intervals with respect to \( c = 0 \). The simplest case is when it reduces to a single interval \( C = B = (-b(c), b(c)) \). The overall probability density function \( \bar{p}(x, t) = \int_{B} \bar{p}(x, t; c) \, dc \) satisfies the balance equation

\[
\partial_t \bar{p}(x, t) = -\partial_x \left( (c - b(x, t; c)) \bar{p}(x, t; c) \right) - \partial_x \bar{J}_d(x, t)
\]  

(41)

where the diffusive flux \( \bar{J}_d(x, t) \) fulfills the constitutive equation

\[
\partial_t \bar{J}_d(x, t) = -\partial_x \left( (c - b(x, t; c)) \bar{J}_d(x, t) \right) - \partial_x \int_{B} c \, \bar{p}(x, t; c) \, dc
\]  

- \[
\int_{B} c \, \bar{\lambda}(c) \, \bar{p}(x, t; c) \, dc + \int_{B} \int_{B} c \, \bar{K}(c, c') \, \bar{p}(x, t; c') \, dc' \, dc
\]

(42)

where \( \bar{\lambda}(c) = \int_{B} K(c', c) \, dc \).

The Kac limit can be ascertained in the continuous case using techniques and arguments analogous to those developed in part I. To give an example, assume \( B = (-b(c), b(c)) \), \( \bar{\lambda}(x) = \bar{\lambda} = \) constant, and that there exists a \( \delta < 1 \) such that

\[
\int_{B} c \, \bar{K}(c, c') \, dc = \delta \, c'
\]  

(43)

For \( b(c), \bar{\lambda} \to \infty \), keeping fixed the nominal diffusivity \( D_{nom} = (b(c))^2/2\bar{\lambda} \), the infinitely fast recombination implies the equi-partition amongst the partial probability waves,

\[
p(x, t; c) = \frac{p(x, t)}{2b(c)} + o\left( \bar{\lambda}^{-1} \right)
\]  

(44)
and the effective diffusivity can be obtained in closed form

\[ D_{\text{eff}} = \frac{1}{2(1-\delta)} \lambda b^{(c)} \int_B c^2 \, dc = \frac{2D_{\text{nom}}}{3(1-\delta)} \quad (45) \]

Other cases of interest are addressed in section 3.4.

3.3. Nonlinear FPK models

In section 3.1 we have indicated with the diction nonlinear GPK those processes in which, either the stochastic velocity vectors, or the transition rates/transit probability matrix, or both, depend on the state variable \( x \). There is another, significant, source of nonlinearity in stochastic models occurring whenever the statistical properties of the stochastic perturbation influence the dynamics of the stochastic process \( X(t) \) itself, so that the stochastic microdynamics depends on the collective behavior of \( X(t) \), i.e. on its probability density functions. This is the case of the nonlinear Fokker–Planck equation introduced by McKean for Langevin-Wiener stochastic models [5]. For review see [6]. In the case of Poisson–Kac and GPK model this means that the stochastic velocity vectors and the transition rates are functionals of the probability densities describing \( X(t) \), i.e. of the partial probability density functions \( \{ p_\alpha(x,t) \}_{\alpha=1}^N \). We refer to this situation as a Nonlinear Fokker–Planck–Kac model (NFPK).

The paradigm of Nonlinear FPK processes is represented by the one-dimensional Poisson–Kac model

\[ \frac{dx(t)}{dt} = v(x(t)) \, dt + b(-1) \chi \{ x \} d\lambda \quad (46) \]

where \( \chi \{ x \} \) is a Poisson field, the transition rate of which \( \lambda(x, \{ p^\pm(x(t),t) \}) \) is a positive functional of the partial probability waves associated with \( X(t) \). For example, it can depend linearly on \( p^\pm(x,t) \), such as

\[ \lambda(x, \{ p^\pm(x(t),t) \}) = \lambda_0(x) + \int_{\mathbb{R}} a^+(x) p^+(x,t) \, dx + \int_{\mathbb{R}} a^-(x) p^-(x,t) \, dx \quad (47) \]

where \( \lambda_0(x), a^+(x), a^-(x) \) are functions of \( x \), or can be a function of the partial moment hierarchy associated with \( p^\pm(x,t) \). For the NFPK process (46), the evolution equations for the partial probability waves become nonlinear, namely

\[ \partial_t p^\pm(x,t) = -\partial_x \left[ \left( v(x) \pm b \right) p^\pm(x,t) \right] + \lambda(x, \{ p^\pm(x(t),t) \}) \left[ p^+(x,t) - p^-(x,t) \right] \quad (48) \]

Alternatively, another class of NGPK processes can be defined in the case the advective contribution \( v(x, \{ p^\pm(x(t),t) \}) \) represents a functional of the partial probability waves. An example of this class of models is addressed in the next paragraph.

The generalization to GPK processes in \( \mathbb{R}^n \) is straightforward. We develop an example in the next section, combining all the extension discussed so far in order to address a physically relevant problem, namely the stochastic nature of the collisional Boltzmann equation.

3.4. Examples

In this paragraph we analyze three prototypical examples covering the range of generalization of GPK processes treated in the previous paragraphs.

To begin with, consider a one-dimensional Poisson–Kac process in \( \mathbb{R} \), defined by the stochastic differential equation
\[ \text{dx}(t) = b \left( -1 \right) \chi(x,t) \, dt \]  

where the Poisson field \( \chi(x,t) \) is characterized by the following transition-rate function
\[ \lambda(x) = \lambda_0 \left( 1 + |x| \right) \]  

Figure 1 depicts the behavior of the mean square displacement \( \sigma_x^2(t) \) versus \( t \), obtained from the stochastic simulation of equations (49) and (50), using \( N_p = 10^6 \) particles starting from \( x = 0 \) at \( D_{\text{nom}} = b^2 / 2 \lambda_0 = 1 \), for two different values of \( b \): \( b = 0.1 \) (line a) and \( b = 1 \) (line b).

In this problem \( \langle x(t) \rangle = 0 \), so that \( \sigma_x^2(t) = \langle x^2(t) \rangle \).

The mean square displacement \( \sigma_x^2(t) \) admits a crossover behavior,
\[ \sigma_x^2(t) \sim \begin{cases} t^2 & t < t^* \\ t^{2/3} & t \gg t^* \end{cases} \]  

where the crossover time \( t^* \) is about \( 10^4 \) at \( b = 0.1 \), and order of \( 10^3 \) at \( b = 1 \). At short timescales \( \sigma_x^2(t) \) grows quadratically with time \( t \), due to the finite propagation velocity (a.e. smoothness) characterizing Poisson–Kac and GPK processes. Asymptotically, i.e. for \( t \gg t^* \), the mean square displacement exhibits an anomalous scaling in time with an exponent equal to \( 2/3 \).

This result can be easily interpreted using elementary scaling analysis, as the transition rate expression (50) corresponds to a position dependent diffusion coefficient \( D_{\text{eff}} \sim 1 / |x| \). Consequently, \( \sigma_x^2(x) \sim L^2 \sim D_{\text{eff}}(L) t \sim t L \), and therefore \( L \sim t^{1/3} \), implying \( L^2 \sim \sigma_x^2(t) \sim t^{2/3} \).

This example admits another byproduct: in the framework of nonlinear GPK processes it is possible to generate anomalous diffusion scalings just by a suitable choice of the transition rate function \( \lambda(x) \) characterizing the Poissonian fields \( \chi(x,t) \) or \( \chi_N(x,t) \).

As a second example, consider a continuous GPK process in \( \mathbb{R}^2 \) corresponding to the dynamics, in the overdamped regime, (for which the velocity field \( \mathbf{v}(x) \) is proportional to the gradient of the potential, i.e. \( \mathbf{v}(x) = -\nabla U(x) / \eta \), where \( \eta \) is the friction factor), of a particle moving in the potential

\[ \text{Figure 1.} \ \sigma_x^2(t) \text{ versus } t \text{ for the nonlinear Poisson–Kac process associated with the state-dependent transition rate (50) at } D_{\text{nom}} = 1. \text{ Line (a) refers to } b = 0.1, \text{ line (b) to } b = 1. \text{ Lines (c) and (d) represent the scalings } \sigma_x^2(t) \sim t^2, \text{ and } \sigma_x^2(t) \sim t^{2/3}, \text{ respectively.} \]
\[ U(x) = U(x, y) = \frac{x^4}{4} - \frac{x^2}{2} + \frac{y^2}{2} = U_x(x) + U_y(y) \quad (52) \]

the contour plot of which is depicted in figure 2 panel (a). This expression corresponds to the superposition of a bistable potential \( U_z(x) \) along the x-coordinate, and of a harmonic potential in the y-coordinate. Assume a friction factor \( \eta = 1 \) a.u., and let \( \Xi(t) \) a continuous Markov process attaining values in \([0, 2\pi]\), characterized by a uniform transition rate \( \lambda \) and by a uniform transition kernel

\[ K(\alpha, \beta) = \frac{\lambda}{2\pi}, \quad \alpha, \beta \in [0, 2\pi) \quad (53) \]

Consider the Continuous GPDK process defined by the stochastic differential equation

\[ dx(t) = -\nabla_x U(x(t)) \, dt + b(\Xi(t)) \, dt \quad (54) \]

where the stochastic velocity function \( b(\alpha) \) is defined by

\[ b(\alpha) = b(\cos(\alpha), \sin(\alpha)) \quad \alpha \in [0, 2\pi) \quad (55) \]

For this problem, the balance equation for the partial probability waves \( p(x, t; \alpha) \) reads

\[ \partial_t p(x, t; \alpha) = \nabla_x \cdot (\nabla_x U(x) \, p(x, t; \alpha)) - b(\alpha) \cdot \nabla_x p(x, t; \alpha) \\
- \lambda p(x, t; \alpha) + \frac{\lambda}{2\pi} \int_0^{2\pi} p(x, t; \beta) \, d\beta \quad (56) \]

In this case, the diffusive flux is given by \( J_d(x, t) = \int_0^{2\pi} b(\alpha) \, p(x, t; \alpha) \, d\alpha \). For the dyadic tensor associated with \( b(\alpha) \) one has

\[ \int_0^{2\pi} b(\alpha) b(\alpha) \, d\alpha = \frac{b^2}{2} I \quad (57) \]

where \( I \) is the identity matrix, and consequently the Kac limit provides \( D_{\text{eff}} = D_{\text{nom}} = b^2 / 2\lambda \). The numerical simulation of this stochastic process, possessing a continuum of states \( \alpha \), is simple: (i) the intervals between two consecutive transitions \( \tau \) are distributed exponentially with probability density \( p_\tau(\tau) = \lambda e^{-\lambda \tau} \); (ii) whenever a transition occurs from a state \( \alpha \) to a new state, say \( \beta \), the determination of the new state \( \beta \) is chosen randomly from a uniform probability distribution in \([0, 2\pi]\).

Figures 2 panels (b)-(d) depict the contour plot of the stationary overall probability density functions \( p^* (x, y) \) for several values of \( D_{\text{eff}} \) and \( b \), obtained from stochastic simulations of equation (54) using an ensemble of 10^6 particles. The corresponding stationary marginal distributions \( p^*_x(x) = \int_R p^*(x, y) \, dy \) with respect to the x coordinate are depicted in figure 3 panel (a). At low values of \( D_{\text{eff}} \) and \( b \), panel (b) in figure 2 and curve (a) in figure 3, the stationary probability density concentrates in an external shell far away from the minima of the potential. This is a peculiar feature of undulatory transport models in the presence of conservative potentials, which may possess an invariant region \( \Omega \) such that \( (-\nabla_x U(x) + b(\alpha)) \cdot n_r(x) \big|_{\partial\Omega} \leq 0 \), where \( n_r(x) \) is the external normal unit vector at points \( x \in \partial\Omega \) (see also the discussion in part II on invariant regions).

As \( D_{\text{eff}} \) decreases, \( p^*(x, y) \) displays the typical bimodal shape characterizing bistable motion with diffusion, panel (d) in figure 2 and lines (b) and (d) in figure 3. As \( b \) increases, keeping constant the value of the effective diffusivity, the stationary density approaches the Boltzmannian distribution. An example is depicted in figure 2 panel (d) and it is clearly evident from figure 3 panel (b) that the marginal stationary distribution \( p^*_x(x) \), at \( D_{\text{eff}} = 0.1 \) and
\( b = 10 \), practically coincides with its Boltzmann-Kac limit \( p^*(x) = A e^{-U(x)/D_{\text{eff}}} \) (observe that \( \eta = 1 \)).

Finally, consider a Nonlinear FPK process expressed in the form of a Shimizu-Yamada model \[21\]. More precisely, consider the stochastic one-dimensional differential equation

\[
dx(t) = v(x(t), \{ p^\pm(x(t), t) \}) \, dt + b(-1)^{\chi(t)} \, dt
\]

where \( \chi(t) \) is a usual Poisson process possessing constant transition rate \( \lambda \), and the drift velocity depends on the partial probability densities as

\[
v(x, \{ p^\pm(x, t) \}) = -x + \varepsilon \left[ m_+^{(1)}(t) + m_-^{(1)}(t) \right] + v_f = -x + \varepsilon m^{(1)}(t) + v_f
\]

where \( m_{\pm}^{(1)}(t) = \int x p^\pm(x, t) \, dx \) are the partial first-order moments of the process, and \( \varepsilon, v_f \) two constant parameters. This model corresponds to the dynamics of a stochastic particle in a harmonic potential (in the overdamped regime), subjected to an external constant bias \( v_f \) and to an additional contribution proportional to the overall first-order moment \( m^{(1)}(t) \).

The balance equation for the partial waves attains the form

\[
\partial_t p^\pm(x, t) = \partial_x \left[ (x - \varepsilon m^{(1)}(t) - v_f \mp b) p^\pm(x, t) \right] \mp \lambda \left[ p^+(x, t) - p^-(x, t) \right]
\]

Figure 2. Panel (a): contour plot of the potential \( U(x, y) \) equation (52). Panels (b) to (d): contour plots of the stationary densities \( p^*(x, y) \) for the Continuous GPK process (54) at different values of the parameters. Panel (b): \( D_{\text{eff}} = 1, \ b = 1 \), panel (c): \( D_{\text{eff}} = 0.1, \ b = 1 \), panel (d): \( D_{\text{eff}} = 1, \ b = 10 \).
where \( m^{(1)}(t) = m_+^{(1)}(t) + m_-^{(1)}(t) \). As initial condition for the partial probability waves consider
\[
p^\pm(x, 0) = \frac{\delta(x)}{2}
\]  
(61)

Figure 4 panel (a) depicts the evolution of the overall density function \( p(x, t) \) in the case of a pure harmonic oscillator \( \varepsilon = v_f = 0 \) (linear case) at \( D_{\text{eff}} = 1, \lambda = 100 \), for which the density function becomes localized at \( x = 0 \) with a variance equal to \( D_{\text{eff}} \). Panel (b) refers to \( \varepsilon = 1, v_f = 10 \) i.e. to a truly Nonlinear FPK model.

In order to derive the salient qualitative properties of this model consider the first elements of the partial moment hierarchy. For the zero-th order moments, the symmetric initial condition (61) implies
\[
m_+^{(0)}(t) = m_-^{(0)}(t) = \frac{1}{2} \quad t \geq 0
\]  
(62)

The evolution equations for the first-order moments attain the form
\[
\partial_t m^{(1)}_\pm(t) = -m^{(1)}_\pm(t) + [m^{(1)}_+(t) + v_f \pm b] m^{(0)}_\pm(t) - \lambda \left[ m^{(1)}_+(t) - m^{(1)}_- (t) \right]
\]  
(63)
Summing the equations for $m_\pm^{(1)}(t)$ and accounting for equation (62) one obtains
\[ \partial_t m_\pm^{(1)}(t) = v_f t \] (64)
which implies
\[ m_\pm^{(1)}(t) = v_f t \] (65)
Therefore, the probability profile moves at constant speed $v_f$. As regards the partial second-order moments
\[ \partial_t m_\pm^{(2)}(t) = -2 m_\pm^{(2)}(t) + 2 \left[ m_\pm^{(1)}(t) + v_f \pm b \right] m_\pm^{(1)}(t) - \lambda \left[ m_\pm^{(2)}(t) - m_\pm^{(2)}(t) \right] \] (66)
From equations (62)–(66), the overall variance $\sigma^2(t) = m_+^{(2)}(t) + m_-^{(2)}(t) - \left[ m_+^{(1)}(t) + m_-^{(1)}(t) \right]^2$ fulfills the balance equation
\[ \partial_t \sigma^2(t) = -2 \sigma^2(t) + 2 b \left[ m_+^{(1)}(t) - m_-^{(1)}(t) \right] \] (67)
Taking the difference between the evolution equations of the first-order partial moments provides
\[ \partial_t \left[ m_+^{(1)}(t) - m_-^{(1)}(t) \right] = - \left[ m_+^{(1)}(t) - m_-^{(1)}(t) \right] + b - 2 \lambda \left[ m_+^{(1)}(t) - m_-^{(1)}(t) \right] \] (68)
Asymptotically, the difference between the partial first-order moments converges towards the value

$$m_{1,\infty}^{(1)} - m_{-\infty}^{(1)} = \frac{b}{2\lambda + 1}$$  \hspace{1cm} (69)$$

which implies that

$$\lim_{t \to \infty} \sigma^2(t) = \sigma^2_{\infty}$$

where

$$\sigma^2_{\infty} = \frac{b^2}{2\lambda + 1} = \frac{D_{\text{eff}}}{1+1/2\lambda}$$  \hspace{1cm} (70)$$

The variance of the overall probability density wave attains asymptotically a constant value equal to $\sigma^2_{\infty}$. The NFPK considered above describes the evolution of a soliton traveling with constant speed $v_f$ and possessing a constant variance $\sigma^2_{\infty}$ (as can be observed from the profiles in figure 4 panel (b)). Figure 5 depicts the comparison of numerical simulation results for $\sigma^2(t)$ and the asymptotic expression (70).

The shape of the propagating solitons depends significantly on the transition rate $\lambda$. For high values of $\lambda$, a nearly Gaussian soliton propagates as expected from the Kac limit, see figure 4 panel (b). However, for small values of $\lambda$, profiles completely different from the Gaussian one can occur. This phenomenon is depicted in figures 6 panels (a) and (b), corresponding to $\lambda = 1$ and $\lambda = 0.2$, respectively. The resulting probability density profiles $p^*(x)$ of the propagating solitons, depicted in this figure, are rescaled to unit zero-th order moment, i.e. $\int p^*(x) \, dx = 1$, and zero mean. As can be observed, a nearly rectangular-shaped soliton occurs for $\lambda = 1$ (panel (a)), while bimodal profiles characterize its shape for lower values of $\lambda$ (panel (b)).

4. The Boltzmann equation

Gathering together the generalizations of GPK process introduced in the previous section (nonlinearity and continuity of stochastic states), we arrive at a remarkable result. To get it, we need two ingredients: (i) a Continuous GPK process parametrized with respect to the stochastic velocity vector $b \in D \subseteq \mathbb{R}^n$, and described by means of the transition kernel.
\( K(b, b') \). Letting \( p(x, t; b) \) be the associated partial probability densities parametrized with respect to \( b \), and assuming for simplicity \( v(x) = 0 \), their evolution equation is given by

\[
\partial_t p(x, t; b) = -b \cdot \nabla_x p(x, t; b) - \int_{\mathcal{D}} K(b', b) \, db' \, p(x, t; b) + \int_{\mathcal{D}} K(b, b') \, p(x, t; b') \, db'
\]

\[ (71) \]

(ii) the further assumption that this Continuous GPK process is a Nonlinear FPK process, in which the transition kernel \( K(b, b'; [p]) \) is a linear homogeneous functional of the partial probability waves \( p(x, t; b) \), i.e.

\[
K(b, b'; [p]) = \int_{\mathcal{D}} \int_{\mathcal{D}} H(b, b''[b', b'']) \, p(x, t; b'') \, db'' \, db'''
\]

\[ (72) \]

where the kernel \( H(b, b''[b', b'']) \) fulfills the symmetry

\[
H(b, b''[b', b'']) = H(b', b''[b, b'''])
\]

\[ (73) \]

In the absence of a deterministic biasing field, the balance equation for the partial probability density \( p(x, t; b) \) associated with the above-defined Nonlinear CGPK process reads

\[
\partial_t p(x, t; b) = -b \cdot \nabla_x p(x, t; b) + \int_{\mathcal{D}} \int_{\mathcal{D}} H(b, b''[b', b'']) \, [p' \, p'' - p \, p'''] \, db' \, db'' \, db'''
\]

\[ (74) \]

where \( p = p(x, t, b) \), \( p' = p(x, t, b') \) and \( p'' = p(x, t, b'') \), \( p''' = p(x, t, b''') \).

Equation (74) corresponds to the nonlinear Boltzmann equation once the expression for the ‘collision’ kernel \( H(b, b''[b', b'']) \) has been defined consistently with the conservation laws (momentum and kinetic energy) associated with the elastic nature of the collisions [7], i.e.

\[
H(b, b''[b', b'']) = G(b, b''[b', b'']) \delta(b + b'' - b' - b'') \delta(|b|^2 + |b'|^2 - |b''|^2 - |b'''|^2)
\]

\[ (75) \]

where the kernel \( G(b, b''[b', b'']) \) accounts for the particle scattering cross section and possesses obvious symmetries.

In the GPK framework, the partial probability density waves \( p(x, t; b) \) correspond to the one-particle distribution function \( f(x, v, t) \) [7], once the particle velocity \( v \) is identified with the stochastic velocity vector \( b \) parametrizing the Continuous GPK process.
In equations (72)–(74) we assumed that $b$ is defined in the domain $D$, which can be either bounded, e.g. by the velocity of light in vacuo $c$, and in this case $D = \{ b \mid |b| \leq c \}$, or $D = \mathbb{R}^n$ as in the classical Boltzmann equation, where no constraints are posed on the maximum attainable velocity. In the CGPK model for the Boltzmann equation, the binary collisions amongst particles correspond to the ordinary recombination process amongst the partial probability waves.

Therefore, the theory of CGPK processes, including nonlinearity effects in the transition kernel, provides a simple, intuitive and fully stochastic route to the basic equation of kinetic theory. In some sense this result is surprising for its simplicity, and supports what is usually referred to as the Kac’s program in kinetic theory originated by the 1954-paper by Kac on the stochastic foundations of the kinetic theory [12], in which a simple one-dimensional Markovian toy-model is introduced to describe the relaxation properties of a rarefied particle gas. For further details on the Kac’s program, and on related recent advances, the reader is referred to [8–11].

While a thorough analysis of the implications of this result will be addressed in future communications, it is important to point out several observations of general nature:

• The Boltzmann H-theorem, namely the definition of the entropy function to prove dissipation

$$S_B(t) = -\int_{\mathbb{R}^n} \int_D p(x, t; b) \log p(x, t; b) \, db$$

(76)
corresponds, in the CGPK formalism to the Boltzmann–Shannon entropy introduced in part II in the discrete $N$-state case, and here generalized to a continuum of stochastic states. The entropy function (76) is based on the whole structure of the partial probability waves $p(x, t; b)$, and not on the overall density function $\int_D p(x, t; b) \, db$.

• The stochastic formulation permits to identify, from the transition kernel $K(b, b', [p])$, the transition rate function

$$\lambda(b; [p]) = \int_D \int_D \int_D H(b', b'''|b, b'') p(x, t; b'') \, db' \, db''' \, db''$$

(77)

and the transition probability kernel

$$A(b, b'; [p]) = \frac{1}{\lambda(b'; [p])} \int_D \int_D H(b, b'''|b', b'') p(x, t, b''') \, db'' \, db'''$$

(78)

which is a left-stochastic kernel. These quantities can be useful in the mathematical analysis of the model to assess the relaxation properties and the propagation of chaos—to quote an expression by Kac [12]—in the system.

• The quantities $\lambda(b; [p])$ and $A(b, b'; [p])$ define completely a stochastic simulator of the Nonlinear CGPK process associated with the Boltzmann equation, which can be viewed as a stochastic molecular simulator.

• The derivation of the nonlinear collisional Boltzmann equation from a simple stochastic model justifies, on stochastic grounds, the intrinsic irreversibility associated with the Boltzmann equation. In this framework, the irreversible behavior is not related with the underlying, possibly chaotic, conservative Hamiltonian dynamics associated with the collision process. This claim, is strongly related to the classical Zermelo’s objection on the purely mechanical interpretation of the Boltzmann equation based on the application of the Poincaré recurrence theorem, and the CGPK theory of the kinetic equation, outlined above, gives a simple answer to the Zermelo’s criticism. In equa-
tions (72)–(74), Hamiltonian conservative mechanics enters solely in order to specify the functional form of the kernel $H(b, b''|b', b'')$ in order to be consistent with the conservation requirements (as regards momentum and kinetic energy) dictated by the assumption of elastic collisions equation (75). The assumption of a rarefied particle-gas systems enters in the linearity of $K(b, b'; [p])$ with respect to the partial density waves $p(x, t; b)$. As the theory of CGPK processes concerns, the functional form of the Boltzmann equation resides exclusively on the Markovian character of the recombination mechanism amongst the partial probability waves.

- The above derivation opens up relevant issues in atomic physics associated with stochasticity and its physical meaning. The problem can be stated as follows: given the above derivation of the Boltzmann equation starting from a purely stochastic model, the stochastic nature of a particle gas system is solely a mathematical result following from CGPK theory or, rather it is a manifestation of more fundamental processes underlying relaxation and irreversibility in atomic and molecular systems? We believe that the second approach would prove to be correct, and further investigation would hopefully lead to new results on an old classical subject, in order to explain the dissipative behavior of an ensemble of identical gas molecules mutually interacting via binary collisions.

- As for the elastic Boltzmann equation, the kinetic equations for granular materials [24], for which the collisions are no longer elastic, and an inelastic restitution coefficient is introduced, can be treated on stochastic grounds using Nonlinear CGPK. Similarly, it would be possible to identify stochastic models for other kinetic equations (such as those of plasma physics) using CGPK processes. In this respect, solely the collisionless Vlasov equation [7] represents an exception in this stochastic paradigm. This is not surprising, as the Vlasov equation is an isentropic model that cannot be easily treated within a stochastic theory in which the entropy production occurs as a consequence of the recombination amongst the partial probability waves.

5. Transport equations from GPK processes

The equations for the partial probability waves represent the basic archetype of transport equations derived from GPK processes. Consistently with the principle of primitive variables, these equations are parametrized with respect to the state of the stochastic perturbation, expressed by the partial probability densities $p_\alpha(x, t)$. This represents a major difference with respect to transport equations derived starting from Langevin microdynamics driven by Wiener processes. In the latter case, due to the independence of the increments, the state of the stochastic perturbation is completely renormalized out of the associated Fokker–Planck equation. In this section, we analyze in some detail the functional structure of the transport equations deriving from GPK models. To begin with, we develop the transport equation from GPK dynamics associated with the evolution of the mean magnetic field in a solenoidal flow field (dynamo problem) [17, 18]. Subsequently, transport equations for matter and momentum density in a fluid continuum are derived starting from a GPK Ornstein–Uhlenbeck process. Finally, the theory is extended to chemical reaction kinetics.

5.1. Transport of magnetic field and the GPK dynamo problem

Let $v(x, t)$ be a solenoidal time-dependent velocity field in $\mathbb{R}^n$, and consider a GPK process $(n, N, A, A, \{b_\alpha\}_{\alpha=1}^N, v(x, t))$ admitting an isotropic Kac limit, characterized by the effective diffusivity $D_{\text{eff}}$. Let $B(x, t)$ be the magnetic field, and consider the transport of $B(x, t)$ due to
the advective action of the velocity field \( \mathbf{v}(x,t) \) in the case stochastic fluctuations are superimposed. This is the essence of the dynamo problem in the presence of diffusion admitting interesting astrophysical applications [25–27].

A stochastic microdynamic equation for this process, written in the form of a GPK process, can be expressed as

\[
\begin{align*}
\mathbf{dx}(t) &= \mathbf{v}(x(t)) \, dt + \mathbf{b}_{\chi}(t) \, dt \\
\mathbf{dB}(t) &= \mathbf{G}(x(t), t) \cdot \mathbf{B}(t) \, dt
\end{align*}
\]  

(79)

where \( \mathbf{G}(x(t), t) \cdot \mathbf{B}(t) = \nabla \mathbf{v}(x,t) \cdot \mathbf{B}(t) \) accounts for the stretching of the magnetic field induced by the velocity field \( \mathbf{v}(x(t), t) \), the \( h \)-entry of which is given by

\[
(G \cdot B)_h = (\nabla \mathbf{v} \cdot \mathbf{B})_h = \sum_{k=1}^{n} \frac{\partial v_h}{\partial x_k} B_k
\]  

(80)

Equation (79) represents the stochastic formulation of the magnetic dynamo problem under the assumption that the magnetic field does not influence the evolution of the flow field \( \mathbf{v}(x,t) \), corresponding to the one-way coupling approximation.

The statistical description of this GPK process involves the partial probability waves \( p_\alpha(x, B, t) \), that are solution of the system of hyperbolic equations

\[
\partial_t p_\alpha = -\nabla_x \cdot (v \, p_\alpha) - \nabla_x \cdot (\mathbf{b}_\alpha \, p_\alpha) - \nabla_B \cdot (G \cdot B \, p_\alpha) - \lambda_\alpha p_\alpha + \sum_{\gamma=1}^{N} \lambda_\gamma A_{\alpha \gamma} p_\gamma
\]  

(81)

where \( \nabla_x \) and \( \nabla_B \) are the nabla-operators with respect to the \( x \)- and \( B \)-variables, respectively.

The basic macroscopic observable in the dynamo problem is the mean magnetic field \( \langle B(x,t) \rangle \) defined as

\[
\langle B(x,t) \rangle = \int_{\mathbb{R}^n} B \, p(x,B,t) \, dB = \sum_{\alpha=1}^{N} \int_{\mathbb{R}^n} B \, p_\alpha(x,B,t) \, dB
\]  

(82)

and depending on the position \( x \) and time \( t \).

The parametrization with respect to the stochastic state \( \alpha \) suggests to introduce the auxiliary quantities

\[
\langle B_\alpha(x,t) \rangle = \int_{\mathbb{R}^n} B \, p_\alpha(x,B,t) \, dB
\]  

(83)

Obviously,

\[
\langle B(x,t) \rangle = \sum_{\alpha=1}^{N} \langle B_\alpha(x,t) \rangle
\]  

(84)

From equation (81), after some algebra, the evolution equation for \( \langle B_\alpha(x,t) \rangle \) can be derived. Componentwise, it reads

\[
\partial_t \langle B_{\alpha,h} \rangle = -v \cdot \nabla_x \langle B_{\alpha,h} \rangle + \sum_{k=1}^{n} \frac{\partial v_h}{\partial x_k} \langle B_{\alpha,k} \rangle - b_\alpha \cdot \nabla_x \langle B_{\alpha,h} \rangle
\]

\[
- \lambda_\alpha \langle B_{\alpha,h} \rangle + \sum_{\gamma=1}^{N} \lambda_\gamma A_{\alpha \gamma} \langle B_{\gamma,h} \rangle
\]  

(85)
where \( \langle \mathbf{B}_{\alpha,h} \rangle \) is the \( h \)-entry of \( \langle \mathbf{B}_{\alpha} \rangle \), \( h = 1, \ldots, n \).

In the Kac limit, this system of equations converges towards the solution of the parabolic equation

\[
\partial_t \langle \mathbf{B} \rangle = - \mathbf{v} \cdot \nabla_x \langle \mathbf{B} \rangle + \nabla_x \mathbf{v} \cdot \langle \mathbf{B} \rangle + D_{\text{eff}} \nabla^2 \langle \mathbf{B} \rangle
\]  

(86)

involving the overall magnetic field \( \langle \mathbf{B} \rangle \) defined by equation (84), which is the classical evolution equation for the dynamo problem in the presence of diffusion [17, 18].

The system of equation (85) represents the exact transport equation for the first-order partial moments \( \langle \mathbf{B}_{\alpha} \rangle \) within the framework of GPK theory. The derivation of these equations does not involve any constitutive assumption, and this is the reason why we have considered this problem as the first example of undulatory transport theory.

Maxwell equations dictate that the magnetic field should be solenoidal. From equation (85) it follows that

\[
\partial_t \nabla_x \cdot \langle \mathbf{B}_{\alpha} \rangle = -(\mathbf{v} + \mathbf{b}_{\alpha}) \cdot \nabla_x (\nabla_x \cdot \langle \mathbf{B}_{\alpha} \rangle) - \lambda_\alpha \nabla_x \cdot \langle \mathbf{B}_{\alpha} \rangle + \sum_{\gamma=1}^{N} \lambda_\gamma \mathbf{A}_{\alpha,\gamma} \nabla_x \cdot \langle \mathbf{B}_{\gamma} \rangle
\]

where the solenoidal nature of the velocity field \( \mathbf{v}(x,t) \) has been enforced. Equation (87) indicates that, if all the partial averages of \( \langle \mathbf{B}_{\alpha}(x,0) \rangle \), \( \alpha = 1, \ldots, N \) at time \( t = 0 \) are solenoidal, i.e. \( \nabla_x \cdot \langle \mathbf{B}(x,0) \rangle = 0 \), then the transport model (85) preserves this property, namely \( \nabla_x \cdot \langle \mathbf{B}_{\alpha}(x,t) \rangle = 0 \), and \textit{a fortiori}, \( \nabla_x \cdot \langle \mathbf{B}(x,t) \rangle = 0 \) for any time \( t > 0 \).

The classical theory of the dynamo problem in the presence of diffusion provides that, for two-dimensional spatial problems \( (x = (x_1, x_2) \in \mathbb{R}^2) \), the \( L^2 \)-norm of the magnetic field, solution of the parabolic equation (86), decays exponentially in time for generic smooth time-periodic velocity fields [17]. Conversely, a positive dynamo action, i.e. an exponential divergence with time of the \( L^2 \)-norm of the magnetic field may occur starting from \( n = 3 \).

It is easy to check that for \( n = 2 \), in the case the average magnetic field possesses zero mean, this property holds also for the GPK dynamo equation (87). This result, stems straightforwardly from the observation that the partial fields \( \langle \mathbf{B}_{\alpha}(x,t) \rangle = (\langle \mathbf{B}_{\alpha,1}(x,t) \rangle, \langle \mathbf{B}_{\alpha,2}(x,t) \rangle) \) can be expressed in terms of a family of (scalar) vector potentials \( \psi_{\alpha}(x,t) \)

\[
\langle \mathbf{B}_{\alpha,1}(x,t) \rangle = \frac{\partial \psi_{\alpha}(x,t)}{\partial x_2}, \quad \langle \mathbf{B}_{\alpha,1}(x,t) \rangle = -\frac{\partial \psi_{\alpha}(x,t)}{\partial x_1}
\]

(88)

\( \alpha = 1, \ldots, N \) which, in turn, are solutions of the associated advection-diffusion equations for a scalar field

\[
\partial_t \psi_{\alpha} = -\mathbf{v} \cdot \nabla_x \psi_{\alpha} - \mathbf{b}_{\alpha} \cdot \nabla_x \psi_{\alpha} - \lambda_\alpha \psi_{\alpha} + \sum_{\gamma=1}^{N} \lambda_\gamma \mathbf{A}_{\alpha,\gamma} \psi_{\gamma}
\]

(89)

As shown in part II, GPK advection-diffusion of a scalar field in the standard-map flow, the \( L^2 \)-norms of \( \psi_{\alpha}(x,t) \) decay exponentially to zero as a function of time.

Therefore, the effect of GPK perturbations is essentially to modify the decay exponent (in two-dimensional spatial problems) with respect to the Kac limit (as in the case of the chaotic advection-diffusion problem for a scalar field addressed in part II), but not the quality of stability. The three dimensional case is fully open for investigation, and there is the possibility that Poissonian perturbations could modify the stability properties of the diffusive dynamo problem, determining the occurrence of a positive dynamo action, also in those cases where the corresponding parabolic model (86) possesses all the eigenvalues with negative real part.
The comparison with the analysis developed by Arnold and Korkina [28] and by Galloway and Proctor [29] for the ABC flow would be an interesting benchmark of this hypothesis.

5.2. Mass and momentum transport

In this paragraph we consider the structure of mass and momentum transport equation in a moving continuum as it emerges from GPK theory. A moving continuum is nothing but an extremely useful macroscopic approximation of the granularity of matter at microscale, resulting from the averaging of the local stochastic motion.

According with the basic principles outlined in section 2 of part I (principle of stochastic reality), let us consider for the granular entities (be them particles, molecules, aggregates, clusters, etc), forming the continuous fluid phase, a GPK equation of motion of the form

\[ \dot{x}(t) = v(t) \, dt \]
\[ m \dot{v}(t) = f(x(t)) \, dt + b_{\alpha}(t) \, dt \]  

(90)

where \( x \in \mathbb{R}^n, v \in \mathbb{R}^n \). Equation (90) represents a Ornstein–Uhlenbeck process, in which all the microscopic ‘granules’ possess equal mass \( m \), in the presence of a force field \( f(x) \) and of stochastic fluctuations of Poisson–Kac nature, described by a \( N \)-state finite Poisson process modulating a system of \( N \) stochastic acceleration vectors \( b_\alpha, \alpha = 1, \ldots, N \).

Let \( p_\alpha(x,v,t), \alpha = 1, \ldots, N \), be the partial probability densities associated with equation (90), which satisfy the balance equations

\[ \partial_t p_\alpha = -\nabla_x \cdot (v p_\alpha) - \frac{1}{m} \nabla_v \cdot (f p_\alpha) - \frac{1}{m} b_\alpha \cdot \nabla_v p_\alpha - \lambda_\alpha p_\alpha + \sum_{\gamma=1}^{N} \lambda_{\alpha,\gamma} A_{\alpha,\gamma} p_\gamma \]

(91)

where, as above, \( \nabla_x \) and \( \nabla_v \) represent the nabla operators with respect to the \( x \)- and \( v \)-variables, respectively. As in the classical setting of the hydrodynamic limit from kinetic schemes, we are interested in the lower-order moments of the partial densities \( p_\alpha(x,v,t) \). In the present analysis we focus exclusively on the mass and momentum densities. A complete analysis involving energy density will be developed in a forthcoming work.

Let

\[ \rho_\alpha(x,t) = m \int_{\mathbb{R}^n} p_\alpha(x,v,t) \, dv \]

(92)

\[ \rho_\alpha(x,t) v_\alpha(x,t) = m \int_{\mathbb{R}^n} v p_\alpha(x,v,t) \, dv \]

(93)

\( \alpha = 1, \ldots, N \), be the partial mass \( \rho_\alpha \) and momentum \( \rho_\alpha v_\alpha \) densities, respectively. The overall mass \( \rho(x,t) \) and momentum \( \rho(x,t) v(x,t) \) densities are the sum with respect to \( \alpha \) of the corresponding partial quantities

\[ \rho(x,t) = \sum_{\alpha=1}^{N} \rho_\alpha(x,t), \quad \rho(x,t) v(x,t) = \sum_{\alpha=1}^{N} \rho_\alpha(x,t) v_\alpha(x,t) \]

(94)

From equation (91) it follows that \( \rho_\alpha(x,t) \) satisfy the system of partial continuity equations

\[ \partial_t \rho_\alpha = -\nabla_x \cdot ( \rho_\alpha v_\alpha ) - \lambda_\alpha \rho_\alpha + \sum_{\gamma=1}^{N} \lambda_{\alpha,\gamma} A_{\alpha,\gamma} \rho_\gamma \]

(95)
that, once summed over $\alpha$, provide the overall continuity equation
\begin{equation}
\partial_t \rho(x, t) = -\nabla_x \cdot (\rho(x, t) V(x, t)) \tag{96}
\end{equation}

Next, consider the partial momentum densities. Multiplying equation (91) by $m v$ and integrating over $v$ one obtains
\begin{equation}
\partial_t (\rho_\alpha V_\alpha) = -\nabla_x \cdot \left( \int_{\mathbb{R}^n} m v p_\alpha \, dv \right) + \frac{f}{m} \rho_\alpha + \frac{b_\alpha}{m} \rho_\alpha \\
- \lambda_\alpha (\rho_\alpha V_\alpha) + \sum_{\gamma=1}^N \lambda_\gamma A_{\alpha,\gamma} (\rho_\gamma V_\gamma) \tag{97}
\end{equation}

Let $T_\alpha(x, t)$ be the comprehensive partial stress tensor, corresponding to the dyadic second-order term
\begin{equation}
T_\alpha(x, t) = m \int_{\mathbb{R}^n} v v p_\alpha(x, v, t) \, dv \tag{98}
\end{equation}

$\alpha = 1, \ldots, N$, that includes also the inertial contribution. The comprehensive partial stress tensor can be dissected into a partial inertial contribution $\rho_\alpha V_\alpha V_\alpha$, and into a partial stress tensor (sensu stricto) $\hat{\tau}_\alpha$,
\begin{equation}
T_\alpha = \rho_\alpha V_\alpha V_\alpha + \hat{\tau}_\alpha \tag{99}
\end{equation}

which in turn can be developed, as in classical continuum mechanics [30], into a traceless stress tensor $\tau_\alpha$ and into a compressive isotropic pressure contribution $P_\alpha I$ ($I$ is the identity tensor)
\begin{equation}
\hat{\tau}_\alpha = \tau_\alpha + P_\alpha I \tag{100}
\end{equation}

$\alpha = 1, \ldots, N$, where $\text{Trace}(\tau) = 0$. Enforcing the above decompositions, one obtains the system of momentum balance equations
\begin{equation}
\partial_t (\rho_\alpha V_\alpha) = -\nabla_x \cdot (\rho_\alpha V_\alpha V_\alpha) - \nabla_x \cdot \tau_\alpha - \nabla_x P_\alpha + \frac{f}{m} \rho_\alpha \\
+ \frac{b_\alpha}{m} \rho_\alpha - \lambda_\alpha (\rho_\alpha V_\alpha) + \sum_{\gamma=1}^N \lambda_\gamma A_{\alpha,\gamma} (\rho_\gamma V_\gamma) \tag{101}
\end{equation}

$\alpha = 1, \ldots, N$, that represent the general setting of momentum transfer in the hydrodynamic limit of GPK theory for a single phase/single component moving continuum.

Summing equation (101) over $\alpha$, the balance equation for the overall momentum density is obtained
\begin{equation}
\partial_t (\rho V) = -\nabla_x \cdot \left( \sum_{\alpha=1}^N \rho_\alpha V_\alpha V_\alpha \right) - \nabla_x \cdot \tau - \nabla_x P + \frac{f}{m} \rho \\
+ \sum_{\alpha=1}^N \frac{\rho_\alpha b_\alpha}{m} \tag{102}
\end{equation}

where the overall stress tensor $\tau$ and pressure $P$ are simply the sum over $\alpha$ of the corresponding partial quantities
\begin{equation}
\tau = \sum_{\alpha=1}^N \tau_\alpha, \quad P = \sum_{\alpha=1}^N P_\alpha \tag{103}
\end{equation}
There are two main qualitative differences with respect to the classical hydrodynamic formulation of momentum transport:

- the inertial term does not reduce to \( \rho \mathbf{V} \mathbf{V} \), but contains explicit reference (memory) of all the partial inertial contributions expressed by the term \( \sum_{\alpha=1}^{N} \rho_{\alpha} \mathbf{V}_{\alpha} \mathbf{V}_{\alpha} \);
- there is an additional contribution expressed by the term \( \sum_{\alpha=1}^{N} \rho_{\alpha} \mathbf{b}_{\alpha} / m \) accounting for the nonuniformity effects of the stochastic acceleration terms amongst the partial structures of the fluid mixture. This term obviously vanishes in the Kac limit where, due to the fast recombination amongst the partial probability waves \( \rho_{\alpha} \simeq \rho / N \) and \( \sum_{\alpha=1}^{N} \rho_{\alpha} \mathbf{b}_{\alpha} / m \simeq 0 \), due to the zero-bias condition \( \sum_{\alpha=1}^{N} \mathbf{b}_{\alpha} = 0 \).

It follows from the above observations, that in the GPK theory of hydrodynamics one cannot reduce mass and momentum transport exclusively to the analysis of the overall fields \( \rho(x, t) \) and \( \mathbf{V}(x, t) \), but one is forced to solve simultaneously mass and momentum balance equations for the full system of partial fields \( \{ \rho_{\alpha}(x, t), \mathbf{V}_{\alpha}(x, t) \}_{\alpha=1}^{N} \).

Also for the GPK mass and momentum balance equations, the concept of Kac limit applies, and these equations should reduce for \( \mathbf{b}(c), \lambda(c) \to \infty \), keeping constant the nominal diffusivity, to the usual continuity and Navier-Stokes equations, upon a suitable assumption on the constitutive equations for \( \mathbf{\tau}_{\alpha}(x, t) \).

A discussion on the constitutive equations for the partial stress tensors \( \mathbf{\tau}_{\alpha}(x, t) \), as well as a comprehensive analysis of the GPK hydrodynamics and its qualitative differences with respect to the classical approach will be developed in a forthcoming article.

5.3. Chemical reactions

In this paragraph we briefly discuss the modeling of chemical reaction kinetics within the framework of GPK theory. Consider the simplest case of a bimolecular elementary isothermal chemical reaction

\[ A + B \to P \] (104)

in \( \mathbb{R}^n \), the rate of which, in the mean-field limit, is given by

\[ r(c_A, c_B) = k_r c_A c_B \] (105)

where \( c_A, c_B \) are the molar concentrations of the two reacting species, and \( k_r \) is the rate coefficient independent of the concentrations but possibly function of temperature. Assume that the reacting process evolves in a fluid continuum where the reacting molecules of the two species are subjected to a deterministic drift \( \mathbf{v}(x) \) and to stochastic fluctuations expressed by means of a GPK process.

Consider a GPK process possessing a finite number \( N \) of states. Let \( c_{A,\alpha}(x, t), c_{B,\beta}(x, t) \) be the partial (molar) concentrations of the two reacting species parametrized with respect to the stochastic state \( \alpha = 1, \ldots, N \). The overall molar concentrations are just the sum of the partial concentrations with respect to the stochastic index \( \alpha \)

\[ c_A(x, t) = \sum_{\alpha=1}^{N} c_{A,\alpha}(x, t), \quad c_B(x, t) = \sum_{\alpha=1}^{N} c_{B,\alpha}(x, t) \] (106)

Let \( (n, N, \Lambda, \mathbf{A}, \{ \mathbf{b}_{\alpha} \}_{\alpha=1}^{N}, \mathbf{v}(x)) \) be a GPK process admitting in the Kac limit an effective diffusivity \( D_{\text{eff}} \). Taking into account the presence of the deterministic velocity field \( \mathbf{v}(x) \), the GPK balance equations for the partial concentrations of the two reacting species can be expressed by
\[ \partial_t c_{A,\alpha} = -\nabla \cdot (\mathbf{v}_c c_{A,\alpha}) - \mathbf{b}_\alpha \cdot \nabla c_{A,\alpha} - k_r \left( \sum_{\gamma=1}^{N} c_{B,\gamma} \right) c_{A,\alpha} - \lambda_\alpha c_{A,\alpha} + \sum_{\gamma=1}^{N} \gamma_\alpha A_{\alpha,\gamma} c_{A,\gamma} \]

\[ \partial_t c_{B,\alpha} = -\nabla \cdot (\mathbf{v}_c c_{B,\alpha}) - \mathbf{b}_\alpha \cdot \nabla c_{B,\alpha} - k_r \left( \sum_{\gamma=1}^{N} c_{A,\gamma} \right) c_{B,\alpha} - \lambda_\alpha c_{B,\alpha} + \sum_{\gamma=1}^{N} \gamma_\alpha A_{\alpha,\gamma} c_{B,\gamma} \]

\[ \alpha = 1, \ldots, N. \] Observe that the way a chemical reaction can be introduced within the GPK balance equation is not unique. The two reacting contributions \( k_r \left( \sum_{\gamma=1}^{N} c_{B,\gamma} \right) c_{A,\alpha} \) and \( k_r \left( \sum_{\gamma=1}^{N} c_{A,\gamma} \right) c_{B,\alpha} \) entering the balance equations for \( c_{A,\alpha} \) and \( c_{B,\alpha} \), respectively correspond to the assumption that the reaction rate at the space-time point \((\mathbf{x}, t)\) depends exclusively on the actual overall concentrations of the two reacting species at \((\mathbf{x}, t)\). Other choices are also possible.

In the Kac limit, equations (107) converge towards the system of two parabolic equations for the overall concentrations \( c_A(\mathbf{x}, t) \) and \( c_B(\mathbf{x}, t) \),

\[ \partial_t c_h = -\nabla \cdot (\mathbf{v}_c c_h) + D_{\text{eff}} \nabla^2 c_h - k_r c_A c_B, \quad h = A, B \]  

(108)

In point of fact, the formal structure of Continuum GPK processes provides a natural way to account for the collision efficiency and its influence on the reaction rate, in an analogous way the reactive Boltzmann equation does [31]. This is by no means surprising, due to the equivalence between CGPK process in the presence of NFPK kernels and the non-reactive Boltzmann equation developed in section 4. Next, we consider briefly this class of models, in the absence of a deterministic velocity field \( \mathbf{v}(\mathbf{x}) = 0 \) (for simplifying the notation), assuming a linear model where both \( \mathbf{A} \) and \( \mathbf{A} \) do not depend on the partial density waves. The state of the stochastic perturbation is parametrized with respect to the stochastic velocity vector \( \mathbf{b} \), attaining values in \( \mathbb{D} \subseteq \mathbb{R}^d \), and the bimolecular reaction (104) is considered under isothermal conditions.

Consequently, the partial concentrations \( c_A(\mathbf{x}, t, \mathbf{b}) \), \( c_B(\mathbf{x}, t, \mathbf{b}) \) in this setting depend continuously on the stochastic velocity vector \( \mathbf{b} \). As regards the chemical kinetic contribution to the evolution of \( c_A(\mathbf{x}, t, \mathbf{b}) \), \( c_B(\mathbf{x}, t, \mathbf{b}) \), two reaction kernels \( R_s(\mathbf{b}, \mathbf{b}'; 1), R_b(\mathbf{b}, \mathbf{b}') \) are introduced, representing the fraction per unit time of colliding molecules of \( \mathbf{A} \) and \( \mathbf{B} \), respectively, possessing stochastic velocities \( \mathbf{b} \) and \( \mathbf{b}' \) which perform the reaction, i.e. that are able to overcome the reaction activation energy. Although not explicit, these kernels depend on temperature by an Arrhenius–Kramers factor \( \exp(-E_R/k_B T) \), where \( E_R \) is the reaction activation energy, \( k_B \) the Boltzmann constant, and \( T \) the absolute temperature. Stoichiometry dictates that \( R_A = R_B = R \) and, moreover the reaction kernel can be assumed, for simplicity, symmetric with respect to their argument, namely

\[ R(\mathbf{b}, \mathbf{b}') = R(\mathbf{b}', \mathbf{b}) \]

(109)

Taking into account the analysis developed in section 4, the balance equations for \( c_A(\mathbf{x}, t, \mathbf{b}), c_B(\mathbf{x}, t, \mathbf{b}) \) now read

\[ \partial_t c_A = -\mathbf{b} \cdot \nabla c_A - \int_D K(\mathbf{b}, \mathbf{b}') \left[ c_A - c'_A \right] d\mathbf{b}' - c_A \int_D R(\mathbf{b}, \mathbf{b}') c'_B d\mathbf{b}' \]

\[ \partial_t c_B = -\mathbf{b} \cdot \nabla c_B - \int_D K(\mathbf{b}, \mathbf{b}') \left[ c_B - c'_B \right] d\mathbf{b}' - c_B \int_D R(\mathbf{b}, \mathbf{b}') c'_A d\mathbf{b}' \]

(110)
where \( c_A = c_A(x, t; b) \), \( c_B = c_B(x, t; b) \), \( c'_A = c_A(x, t; b') \), \( c'_B = c_B(x, t; b') \), and \( K(b, b') \) is the transition kernel of the Continuous GPK process. Given a physically motivated expression for the reaction kernel \( R(b, b') \), depending on the chemistry of the reactive step, the Kac limit of the model, or alternatively the application of homogenization techniques in the long-term regime, provide an expression for the effective reaction coefficient \( k_r \), entering the mean-field model (105). The flexibility of GPK models, especially in their continuous formulation, provides a direct connection between momentum transfer and the collisional efficiency of a reactive process.

In a similar way, it is possible to derive stochastic models for particle/antiparticle production/annihilation accounting for the conservation laws (parity, energy and momentum) of the process. The main physical issue in this case is not the annihilation contribution, which is substantially analogous to a bimolecular reaction, but the production term which intrinsically depends on the vacuum fluctuations and involves the stochastic characterization of zero point energy. The latter issue can be properly formalized in the present theory, embedding CGPK processes within the framework of the second quantization of the electromagnetic field, and its stochastic characterization [32].

6. Concluding remarks

We have introduced the concept of Generalized Poisson–Kac processes, analyzed their structural properties (part I) and addressed their physical implications in statistical physical, hydrodynamics and transport theory (parts II and III).

In its very essence, a GPK process stems from the original intuition of Marc Kac of considering dichotomous velocity fluctuations possessing finite propagation velocity, and considers the fluctuating contribution as a transition amongst a finite number \( N \) of stochastic states immersed in a Markovian structure accounting for the transitions. The primitive statistical description of this process involves \( N \) partial probability density functions \( \{ p_\alpha(x, t) \}_{\alpha=1}^N \) the spatio-temporal evolution of which follows a hyperbolic dynamics, corresponding to a planar wave-motion in the presence of recombination. This is the reason why \( p_\alpha(x, t) \) are also referred to as ‘partial probability waves’, and the resulting macroscopic processes indicated as ‘undulatory transport model’, just to mark the wave-like nature of their basic statistical descriptors.

The nonlinear extension of the theory, as well as the generalization to a continuum of states, provides the natural setting for obtaining straightforwardly a stochastic derivation of the kinetic Boltzmann equation. This result opens up fundamental issues on the underlying physical nature of this equation, alternative to the purely mechanical (Liouvillean) picture. In some sense, the stochastic derivation of the collisional Boltzmann equation concludes the original Kac’s program in kinetic theory starting from the 1954 paper based on a Markovian toy model for gas dynamics, and gives to it new impetus for a thorough exploitation of a fully stochastic formulation of the Boltzmann collisional dynamics.

The GPK approach towards the Boltzmann equation is consistent with the Zermelo objection [22, 23] against the fully mechanical (Hamiltonian) derivation of the Boltzmann equation which, if postulated, leads intrinsically to finite-time Poincaré recurrences and to the lack of a truly irreversible behavior. Albeit sedated by the analysis of the order of magnitude of the recurrence time [33, 34], Zermelo objection persists, from the strict mathematical and logical point of view, as a bleeding wound on the connection between a mechanical (conservative) view of dynamics and the intrinsically irreversible nature of thermodynamics. All these issues on the foundation of Boltzmann collision equation will be hopefully developed in a
subsequence communication. But it is rather intuitive, that the results obtained on the connections between kinetic theory and NFPK models admit powerful implications, not only from a theoretical and thermodynamic point of view, but also in practical applications. The idea of developing a fully stochastic molecular simulator based on NFPK dynamics is not only intriguing, but also feasible and potentially computationally advantageous with respect to the existing methods. Further studies will clarify and quantify the correctness of this possibility.

What is also interesting to observe is that the physical concept of collision amongst molecules corresponds, in the Continuous GPK setting, to a Markovian recombination amongst the partial probability waves \( p(x, v, t) \), induced by the choice of the velocity \( v \) as the stochastic vector-valued variable parametrizing the states of the CGPK process.

Apart from this result, GPK theory provides a simple and tractable class of processes that overcome the intrinsic problems of Wiener-driven stochastic models in describing the physical reality (infinite propagation velocity), and permits to derive out of them new classes of transport equations in the hydrodynamic (continuum) limit. The main qualitative difference between Wiener-driven and GPK stochastic models resides in the regularity issue: the trajectory of GPK processes, for finite values of \( b(c) \) and \( \lambda(c) \), are, with probability 1, almost everywhere smooth curves of time, possessing fractal dimension \( d_f = 1 \), and local Hölder exponent 1. Out of it, finite propagation velocity follows. Moreover, the Kac-limit property provides the natural connection between GPK theory and the classical stochastic formulation of microdynamics based on Brownian motion and Wiener-driven Langevin equations. This connection is not only related to the Kac limit for \( b(c) \), \( \lambda(c) \to \infty \), keeping fixed the nominal diffusivity \( D_{\text{nom}} \), but also as an emergent property in the long-time regime. This justifies while Brownian features can be observed at time-scales much larger than the characteristic recombination scale \( t_{\text{recomb}} = 1/\lambda(c) \). The asymptotic properties of GPK processes represent a bridge between GPK theory and the statistical physics based on Brownian motion and Wiener-driven processes that, as said, can be regarded as an emergent feature for long timescales [35].

The regularity issue of GPK processes admits several implications:

- GPK processes, once extended to space-time stochastic perturbations, provide a valuable tool for approaching, on a rigorous but save way (as singularity issues are concerned), spatio-temporal stochastic dynamics and field-theoretical models (i.e. SPDE) driven by stochastic perturbations. We have outlined several simple linear examples in part II, and the same approach can be extended to work out nonlinear models such as Burgers’ equations, KPZ model, \( \Phi^4 \)-field stochastic quantization, etc.

- The finite propagation velocity of GPK provides a safeguard in the extension of GPK processes to the relativistic case [36, 37].

- Trajectory regularity, characterizing GPK processes, substantially simplifies all the subtleties and technicalities of stochastic (Ito, Stratonovich, Klimontovich etc) calculus, as reduces it to the simplest possible form, namely that of Riemann-Stieltjes integrals.

There is another issue, mentioned throughout this work, that deserves further attention, as it marks a conceptual difference between Wiener-driven Langevin equations and the corresponding stochastic models driven by GPK processes. Consider a Langevin equation driven by a Wiener forcing on the state variable \( x(t) \). The Wiener forcing expresses in a lumped, coarse-grained way, a manifold of small-scale perturbations resulting from the microscopic interactions, internal to the system, and from the interactions with the surrounding. As a result, the associated forward Fokker–Planck equation defines the evolution of the probability density function in which there is no further reference on the state of the stochastic perturbation: this makes this class of models strictly Markovian.
Conversely, in the corresponding GPK case, the statistical description of the process still involves information about the stochastic perturbation: for this reason a system of partial probability densities, \( \{ p_\alpha(x,t) \} \) in the discrete case, \( p(x,t,\alpha) \in D \) in the CGPK case, is required to describe the statistical evolution of the system. The fact that the statistical description of the process keeps memory of the state of the stochastic perturbation, so that system dynamics and stochastic perturbations cannot be decoupled, other than in the Kac limit, is the physical origin of the trajectory regularity of GPK processes. Consequently, GPK processes are not strictly Markovian, which respect to the overall probability density function \( p(x,t) \), but an extended Markovian property can be still established with respect to the complete probabilistic description accounting also for the state of the stochastic perturbation [13].

The consequence of this property, as regards the transport equations in the hydrodynamic limit, is evident: a system driven by GPK fluctuations is fully described in the hydrodynamic limit by a family of partial mass and momentum densities \( \{ \rho_\alpha, \rho_\alpha V_\alpha \} \) and similarly for the other thermodynamic quantities, consistently with the retained information on the state of the stochastic perturbation. This, namely the partial-wave approach towards the coarse-graining of the microdynamic equation of motion, will be analyzed in future works. In any case, it represents a novel and promising alternative to the existing higher-moment expansions, that starting from the well-known Grad’s 13-moment approach [38], have been developed in the current literature on kinetic theory and statistical mechanics.

All the higher-moment expansions, beyond the classical 5-mode approach associated with the collisional invariants, suffer the intrinsic \textit{vulnus}, as regards the lack of positivity, that can be easily interpreted within the Pawula theorem [39]. In this framework, the use of GPK theory, and of its implications in the definition of the hydrodynamic limit, represents not only a new way for approaching the coarse-graining of microscopic dynamics towards the hydrodynamic equations for a continuum, but also the stochastic background for the development of a rigorous, stochastically consistent, formulation of the Extended Thermodynamic Theories of Irreversible Processes, initiated with the works by Müller and Ruggieri, and subsequently elaborated by Jou et al and many others, aimed at generalizing the classical de-Groot Mazur theory of irreversible processes, by introducing a more general definition of the thermodynamic state variables out of equilibrium in order to include the contribution of the fluxes.

References

[1] Giona M, Brasiello A and Crescitelli S 2017 \textit{J. Phys. A: Math. Theor.} \textbf{50} 335002
[2] Giona M, Brasiello A and Crescitelli S 2017 \textit{J. Phys. A: Math. Theor.} \textbf{50} 335003
[3] Zwanzig R 1973 \textit{J. Stat. Phys.} \textbf{9} 215
[4] Van Kampen N G 1981 \textit{J. Stat. Phys.} \textbf{25} 431
[5] McKean H P 1966 \textit{Proc. Natl Acad. Sci.} \textbf{56} 1907
[6] Frank T D 2010 \textit{Nonlinear Fokker–Planck Equations} (Berlin: Springer)
[7] Balescu R 1975 \textit{Equilibrium and Nonequilibrium Statistical Mechanics} (New York: Wiley)
[8] Mischler S and Mouhot C 2013 \textit{Inventroy Math.} \textbf{193} 1
[9] Mischler S 2013 Kac’s chaos and Kac’s program (arXiv:1311.7544)
[10] Wennberg B and Wondmagegne Y 2006 \textit{J. Stat. Phys.} \textbf{124} 859
[11] Carlen E, Mustafa D and Wennberg B 2015 \textit{J. Stat. Phys.} \textbf{158} 1341
[12] Kac M 1956 Foundations of kinetic theory \textit{Proc. 3rd Berkeley Symp. on Mathematical Statistics and Probability} vol 3, ed J Neyman (Berkeley: University of California) p 171
[13] Giona M, Brasiello A and Crescitelli S 2017 \textit{J. Stat. Mech.} \textbf{023205}
[14] Müller I and Ruggeri T 2013 \textit{Rational Extended Thermodynamics} (Berlin: Springer)
[15] Jou D, Casas-Vazquez J and Lebon G 1996 \textit{Extended Irreversible Thermodynamics} (Berlin: Springer)
[16] Jou D, Casas-Vazquez J and Lebon G 1999 \textit{Rep. Prog. Phys.} \textbf{62} 1035
[17] Arnold V I and Khesin B A 1999 Topological Methods in Hydrodynamics (New York: Springer)
[18] Chil M and Childress S 2012 Topics in Geophysical Fluid Dynamics: Atmospheric Dynamics, Dynamo Theory, and Climate Dynamics (New York: Springer)
[19] Wong E and Zakai M 1965 Int. J. Eng. Sci. 3 213
[20] Wong E and Zakai M 1965 Ann. Math. Stat. 36 1560
[21] Shimizu H and Yamada T 1972 Prog. Theor. Phys. 47 350
[22] Zermelo E 1896 Ann. Phys. 57 485
[23] Zermelo E 1896 Ann. Phys. 59 783
[24] Villani C 2006 J. Stat. Phys. 124 781
[25] Parker E N 1979 Cosmological Magnetic Fields: their Origin and their Activity (Oxford: Clarendon)
[26] Busse F H 1976 Phys. Earth. Planet Int. 12 350
[27] Proctor M R E and Gilbert A D (ed) 1994 Lectures on Solar and Planetary Dynamos (Cambridge: Cambridge University Press)
[28] Arnold V I and Korkina E I 1983 Mosk. Vestn. Ser. Mat. Mekh. 1 43
[29] Galloway D J and Proctor M R E 1992 Nature 356 691
[30] de Groot S R and Mazur P 1984 Non-Equilibrium Thermodynamics (New York: Dover)
[31] Naumann W 1985 Physica A 132 339
[32] Milonni P W 1994 The Quantum Vacuum: an Introduction to Quantum Electrodynamics (Boston: Academic)
[33] Boltzmann L 1886 Ann. Phys. 57 773
[34] Chandrasekhar S 1943 Rev. Mod. Phys. 15 85
[35] Laughlin R B and Pines D 2000 Proc. Natl Acad. Sci. 97 28
[36] Giona M 2016 Covariance and spinorial statistical description of simple relativistic stochastic kinematics in preparation
[37] Giona M 2016 Relativistic analysis of stochastic kinematics (arXiv:1612.03057)
[38] Grad H 1949 Commun. Pure Appl. Math. 2 331
[39] Pawula R F 1967 Phys. Rev. 162 186