

GENERALIZED POISSON–KAC PROCESSES AND THE REGULARITY OF LAWS OF NATURE*

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The meaning and the features of Generalized Poisson–Kac processes are analyzed in the light of their regularity properties in order to show how the finite propagation velocity, characterizing these models, permits to eliminate the occurrence of singularities in transport models. Apart from a brief overview on their spectral properties, on the regularization of boundary-value problems, and on their origin from simple Lattice Random Walk models, the article focuses on their application in the study of stochastic partial differential equations, and how their use permits to eliminate the divergence of low-order moments that characterizes the corresponding field equations in the presence of spatially δ -correlated stochastic perturbations, and to ensure positivity whenever needed. A simple reaction-diffusion system subjected to a stochastically intermitted flux and the Edwards–Wilkinson model are used to show these properties.

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*“Not only does God play dice with the world.
He does not let us see what He has rolled.”*
Stanisław Lem (from *Golem XIV*)

1. Introduction

Each first-rank scientist left a program (an “ideology” or an “aesthetics of science”, depending on the personal tastes) beyond his specific findings, corresponding to his personal views on the physical reality and outlining future research directions to be explored. Marian Smoluchowski is not an

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exception to this rule. He marked the beginning of the last century with a new approach to statistical physics paving the way to the birth of new research fields, such as colloidal science, soft-matter physics, *etc.*

The legacy of Marian Smoluchowski has been clearly outlined by Ulam in a 1957 article commemorating the 40th anniversary of his death [1]. It resides essentially in having clarified the importance of statistical fluctuations (and not only of averaged quantities) in understanding the properties of interacting particle systems, and in having identified in the regularity (“uniformity”) properties of natural laws a general principle applicable also at the fluctuational level.

Hundred years after his departure, this scientific program is still actual and “progressive”, in the epistemological meaning given to this term by Lakatos [2], and gravid of potentially revolutionary concepts not only in statistical physics, but in physics as a whole.

This article analyzes the implications of Generalized Poisson–Kac processes, (GPK, for short), recently introduced in [3–6] in the analysis of transport phenomena, and extending the simple and powerful paradigm due to Kac [7] of a process on the line possessing finite propagation velocity and driven by Poissonian perturbations. Indeed, the connection with the above mentioned *Smoluchowski program* is not a gentle tribute, suitable to the occasion, to his scientific figure, but a strict epistemic connection. GPK processes represent a simple and extremely versatile class of stochastic dynamics, defined in any spatial dimension, possessing finite propagation velocity, approximating the Langevin dynamics driven by Wiener processes in the long-term/large distance limit, and converging to them in Kac limit, see Section 3.

The original one-dimensional model studied by Kac was motivated by the problem of finding a stochastic model justifying the Cattaneo hyperbolic heat transport equation [8] (see also the review article [9]), *i.e.*, a stochastic dynamics the probability density of which was a solution of the Cattaneo equation. Subsequently, the Kac model has been object of an intense investigation in statistical physics, see *e.g.* [10–15], just to mention few relevant contributions and review articles. Retrospectively, it is not too far from truth the reflection that the research in the 80s and 90s on stochastic dynamics involving the original Kac’s process was primarily motivated by the fact that this process is the simplest and analytically approachable example of colored noise possessing an exponentially decaying correlation function with time [16, 17]. Moreover, it was taken as a paradigmatic example of bounded noise, simply because the stochastic perturbation flips amongst two values, and consequently it has been often referred to as “dichotomous noise” [18–20].

While all these properties characterize the original Kac model (and, with some caution, also GPK processes, at least when the number of stochastic states is finite), the use of the Poisson–Kac model, as a simple paradigm for colored noise, overlooks the main signature of this class of processes, namely the finite propagation velocity or, equivalently, the regularity (almost everywhere) of the trajectories. The latter two properties mark a straight connection with the Smoluchowski program, involving the extension of the regularity (“uniformity”) laws of nature even at the fluctuational level.

The connections between the original Kac’s stochastic dynamics and the Cattaneo equation is a fortunate accident occurring solely in the one-dimensional spatial case. In higher spatial dimensions, there is no stochastic process admitting the Cattaneo equation as the evolution for its probability density function. Indeed, the Cattaneo equation, in spatial dimensions higher than one, does not even fulfil the requirement of positivity (*i.e.*, the solution of this equation can attain negative values starting from non-negative initial conditions in the free-space propagation) [21]. In point of fact, positivity problems may arise also in the one-dimensional case, whenever bounded domains (intervals) are considered, depending on the way boundary conditions are set [22]. The statistical properties of stochastic processes possessing finite propagation velocity have been mathematically approached by Kolesnik in a brilliant way in a series of articles [23–26]. Focusing on the evolution equations for the overall probability density function, Kolesnik showed that these equations are governed by extremely complex (hyperparabolic) operators. The application of these equations, whenever transport problems in bounded domains are considered, makes the setting of the proper boundary conditions extremely cumbersome.

The failure of a stochastic interpretation of the Cattaneo equation in higher spatial dimensions and his lack of positivity imply that all the transport and thermodynamic theories grounded on the Cattaneo equation as a building block expressing the constitutive equations for fluxes, suffer the same conceptual/physical shortcomings (see Section 2). GPK theory as developed in [3–6] is specifically aimed at providing the stochastic background for hyperbolic theories of transport, in which the finite propagation velocity of the fluctuations is assumed as the fundamental physical Ansatz (it corresponds to a “weak relativity principle” for any physical field evolving in a Minkowskian space-time), and the positivity is automatically fulfilled.

The aim of this article is to describe how the GPK approach matches the Smoluchowski program of regularity. At the end, any scientific program, no matter how progressive and elegant in terms of its internal mathematical structure is, should match experimental evidence. Micro- and nanofluidic experiments on the motion of single particles both in gas and liquid confirm the regularity of fluctuations at short time/length scales [27–29].

The article is organized as follows. Section 2 develops a preliminary analysis on different pathways in non-equilibrium thermodynamics associated with the generalization of Fickian constitutive equations to Cattaneo-like ones. Section 3 introduces the formalism of GPK processes, and some of their main qualitative properties. Section 4 is dedicated to the study of their regularity properties, starting from their derivation from simple Lattice Random Walks. Spectral properties and elimination of singularities in boundary-layer theory are briefly discussed. This section is essentially a succinct review of results that can be found in published (or not yet published) articles, but presented in a slightly new light. Section 5 presents new material, namely the application of Poisson–Kac and GPK processes, as physically meaningful mollifiers of noise-perturbations in stochastic partial differential equations. The latter issue is of current interest due to the recent developments in the theory of stochastic partial differential equations due to Hairer [30] and to the growing application of fluctuating hydrodynamics in the understanding of chemical–physical properties at nanoscales [31].

2. Pathways in non-equilibrium thermodynamics

The commonly accepted approach to non-equilibrium thermodynamics, used in the overwhelming majority of engineering and physical applications, is expressed by the Theory of Irreversible Processes (TIP) crystallized in the monograph by de Groot and Mazur [32]. TIP, starting from the assumption of smoothness for the five fields, mass density $\rho(\mathbf{x}, t)$, velocity $\mathbf{v}(\mathbf{x}, t)$ and energy density $e(\mathbf{x}, t)$, couples mechanical balances with thermodynamic laws by enforcing for the latter the expressions derived at equilibrium. The latter assumption implies to extend the Gibbs equation for the specific entropy production at equilibrium (Eq. (1.4) in [33]) also to non-equilibrium conditions. Enforcing the second principle of thermodynamics, *i.e.*, the non-negativity of the entropy source contributions, TIP derives the thermodynamic constraints for the fluxes of the transported entities (mass, momentum and energy), the so-called “phenomenological equations”, that within the TIP paradigm should be proportional via non-negative phenomenological coefficients (diffusivity, viscosity, thermal conductivity) to the gradients of the associated fields (density, velocity, temperature) with reverse sign.

In terms of microscopic dynamics, this phenomenological picture corresponds to a stochastic model expressed in terms of the Langevin equations driven by the Wiener processes, the simplest example of which is given by

$$d\mathbf{x}(t) = \mathbf{v}(\mathbf{x}(t)) dt + \sqrt{2D} d\mathbf{w}(t), \quad (2.1)$$

where $\mathbf{x} \in \mathbb{R}^n$, $d\mathbf{w}(t)$ are the increments of a n -dimensional vector-valued Wiener process [34], $\mathbf{v}(\mathbf{x})$ a deterministic field, and D the (constant) diffusiv-

ity. The probability density function associated with Eq. (2.1) is a solution of the parabolic Fokker–Planck equation

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\nabla \cdot [\mathbf{v}(\mathbf{x}) p(\mathbf{x}, t)] + D \nabla^2 p(\mathbf{x}, t) \tag{2.2}$$

from which it follows that the probability flux $\mathbf{J}_p(\mathbf{x}, t) = \mathbf{J}_p^c(\mathbf{x}, t) + \mathbf{J}_p^d(\mathbf{x}, t)$ is the sum of a convective $\mathbf{J}_p^c(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}) p(\mathbf{x}, t)$, and of a diffusive contribution

$$\mathbf{J}_p^d(\mathbf{x}, t) = -D \nabla p(\mathbf{x}, t) \tag{2.3}$$

related to the stochastic perturbation, and of Fickian structure. In the light of this analogy, it is not devoid of significance to claim that Wiener fluctuations represent the paradigmatic model of equilibrium fluctuations in thermodynamic systems.

The formal structure of the TIP theory, albeit internally consistent and able to solve a huge and diversified variety of practical problems, is indeed unsatisfactory from a theoretical point of view, at least for two main reasons:

- it does not provide any insight into the thermodynamic regimes characterizing out-of-equilibrium conditions. The properties of non-equilibrium fluctuations are flattened out to those characterizing equilibrium by the constitutive Ansatz of this theory;
- it contains intrinsically fundamental paradoxes (inconsistencies), such as the occurrence of infinite propagation velocity in the evolution of the physical field variables (density, momentum, temperature).

The latter problem has been tackled by Müller and Ruggeri, by expanding, in the form of a thermodynamic theory, the original observation due to Cattaneo [8, 9] of modifying the Fickian phenomenological laws. In the Cattaneo approach, memory effects are included in the constitutive equations for the fluxes, in order to restore a finite propagation velocity, thus obtaining balance equations of hyperbolic, instead of parabolic, nature. This radical shift in the mathematical structure of the balance equations marks the birth of Extended Thermodynamics [33], lately evolved in the Rational Extended Thermodynamics [35] by including in the theory concepts and formalism derived by the Rational Thermodynamics of Truesdall and Noll [36].

In Extended Thermodynamic theories, the fluxes, say $\mathbf{J}_p(\mathbf{x}, t)$, are expressed by constitutive equations of Cattaneo-type with respect to the concentration $p(\mathbf{x}, t)$ that, in the simplest case, are of the form of

$$\tau \frac{\mathbf{J}_p(\mathbf{x}, t)}{\partial t} + \mathbf{J}_p(\mathbf{x}, t) = -D \nabla p(\mathbf{x}, t), \tag{2.4}$$

where τ is the characteristic relaxation time. This form of phenomenological laws derives essentially by generalizing the Gibbsian expression for the specific entropy by including quadratic terms in the fluxes, see *e.g.* Eq. (2.8) in [33].

3. GPK processes

3.1. Introduction

The 1974 article by Kac [7], containing the probabilistic interpretation of the Cattaneo equation, provided a first insight into the stochastic background underlying extended thermodynamic theories. The model considered by Kac is defined on \mathbb{R} by the equation of motion

$$dx(t) = b_0(-1)^{\chi(t,\lambda)} dt, \quad (3.1)$$

where b_0 is a constant having the dimension of a velocity and $\chi(t, \lambda)$ is a Poisson process characterized by the transition rate λ . Indicate with $X(t)$ the stochastic process associated with Eq. (3.1) at time t . Its overall probability density function $p(x, t)$ is a solution of the Cattaneo equation

$$\tau \frac{\partial^2 p(x, t)}{\partial t^2} + \frac{\partial p(x, t)}{\partial t} = D \frac{\partial^2 p(x, t)}{\partial x^2}, \quad (3.2)$$

where $\tau = 1/2\lambda$ and $D = b_0^2/2\lambda$. This result stems from the fact that the statistical description of the non-Markovian process $X(t)$ involves the two partial probability density functions $p_{\pm}(x, t)$, where

$$p_{\pm}(x, t) dx = \text{Prob} \left[X(t) \in (x, x + dx), \quad (-1)^{\chi(t,\lambda)} = \pm 1 \right] \quad (3.3)$$

satisfying the hyperbolic system of equations

$$\frac{\partial p_{\pm}(x, t)}{\partial t} = \mp b_0 \frac{\partial p_{\pm}(x, t)}{\partial x} \mp \lambda [p_+(x, t) - p_-(x, t)]. \quad (3.4)$$

Out of Eq. (3.4), the evolution equation (3.2) for the overall probability density function $p(x, t) = p_+(x, t) + p_-(x, t)$ follows.

It is worth mentioning that the use of stochastic processes characterized by a bounded velocity was already addressed by Goldstein in 1951 [39] and referred by him to as *persistent random walk*, reworking an original idea due to Taylor associated with the description of turbulent diffusion [40]. After elaborate calculations, Goldstein proved that the Laplace transform of the probability density function associated with the persistent random walk satisfies a telegrapher's equation, The 1974 article by Kac is written in a very simple and apparently non-technical way. It is just the simplicity

and the far-reaching physical insights that make this article the cornerstone in the theory of stochastic processes possessing finite propagation velocity.

The final comment by Kac in [7] is indeed interesting. After showing that the Laplace transform of the probability density function associated with the process (3.1) is a solution of the telegrapher’s equation, he concluded:

“The same proof goes also for higher number of dimensions. Again it is simply a matter of writing the Laplace transform and verifying the same formula.”

There are several ways of interpreting this observation, that essentially is a classical, ritual sentence for concluding an article throwing a bridge towards more general and future developments. If interpreted *verbatim*, it suggests that exactly the same approach leading to the one-dimensional Cattaneo equation from stochastic grounds can be extended to higher spatial dimensions without problems.

But this is not the case. Even for simple two-dimensional systems, generalizing Eq. (3.1), such as

$$dx(t) = b_0 (-1)^{\chi_1(t,\lambda)} dt, \quad dy(t) = b_0 (-1)^{\chi_2(t,\lambda)} dt, \quad (3.5)$$

where $\chi_1(t, \lambda)$ and $\chi_2(t, \lambda)$ are two independent Poisson processes characterized by the same transition rate λ , the resulting overall probability density function does not satisfy a Cattaneo equation [41]. This result is even more evident from the mathematical elaborations by Kolesnik [23, 24] for relatively simple processes in the plane.

In spatial dimensions higher than one, the Green function for the Cattaneo equation attains negative values [21]. This clearly indicates that it cannot represent an evolution equation for the probability density function of any stochastic process, and that the one-dimensional problem considered by Mark Kac constitutes a “lucky dimensional singularity” for the Cattaneo equation. This observation has significant implications in extended thermodynamic theories, as it indicates that the Cattaneo building blocks in the formulation of the constitute equations should be replaced by other formal structures, consistent with the positivity requirement, and providing, at the end, hyperbolic transport equations.

A way for achieving this program is to start from a stochastic dynamics, possessing finite propagation velocity and sufficiently flexible to be easily extended in any spatial dimension and for any problem of physical interest. This is the physical motivation for the introduction of GPK processes.

3.2. Structure of GPK processes

GPK processes have been introduced in order to provide a stochastic background to transport theories characterized by a finite value of the ve-

locity of propagation of physical fields, with the further consistency condition, that in some limit, the Kac limit, they provide the same quantitative description of classical Langevin equations driven by Wiener perturbations [3–6].

The starting point is to consider an arbitrary number N of stochastic states, the transitions amongst them being described by a Markov-chain dynamics. This is the meaning of the N -state finite Poisson process $\chi_N(t, \Lambda, \mathbf{A})$, as a stochastic process attaining N possible states $\alpha = 1, \dots, N$, characterized by a vector of transition rates $\Lambda = (\lambda_1, \dots, \lambda_N)$, $\lambda_\alpha > 0$, and by a transition probability matrix $\mathbf{A} = (A_{\alpha,\beta})_{\alpha,\beta=1}^N$, which is a left-stochastic matrix, *i.e.*,

$$A_{\alpha,\beta} \geq 0, \quad \sum_{\alpha=1}^N A_{\alpha,\beta} = 1, \quad \forall \beta = 1, \dots, N. \quad (3.6)$$

The statistical description of $\chi_N(t, \Lambda, \mathbf{A})$ satisfies a Markov chain defined by Λ and \mathbf{A} . More precisely, let $\tilde{P}_\alpha(t) = \text{Prob}[\chi_N(t, \Lambda, \mathbf{A}) = \alpha]$, $\alpha = 1, \dots, N$, the evolution equation for the probabilities $\tilde{P}_\alpha(t)$ is expressed by

$$\frac{d\tilde{P}_\alpha(t)}{dt} = -\lambda_\alpha \tilde{P}_\alpha(t) + \sum_{\beta=1}^N A_{\alpha,\beta} \lambda_\beta \tilde{P}_\beta(t). \quad (3.7)$$

To complete the construction, a family of N constant velocity vectors $\{\mathbf{b}_\alpha\}_{\alpha=1}^N$ of \mathbb{R}^n should be introduced, corresponding to the characteristic velocities in each of the N stochastic states. A GPK process $\mathbf{X}(t)$ in \mathbb{R}^n is thus defined simply by the stochastic evolution equation

$$d\mathbf{x}(t) = \mathbf{b}_{\chi_N(t,\lambda,\mathbf{A})} dt \quad (3.8)$$

corresponding to a stochastic convective motion, where the bounded velocities switch at the pace of $\chi_N(t, \Lambda, \mathbf{A})$. The process so defined is statistically characterized by a system of N partial probability densities $p_\alpha(\mathbf{x}, t)$, where $p_\alpha(\mathbf{x}, t) d\mathbf{x} = \text{Prob}[\mathbf{X}(t) \in (\mathbf{x}, \mathbf{x} + d\mathbf{x}), \chi_N(t, \Lambda, \mathbf{A}) = \alpha]$, that are solutions of the system of hyperbolic equations

$$\frac{\partial p_\alpha(\mathbf{x}, t)}{\partial t} = -\mathbf{b}_\alpha \cdot \nabla p_\alpha(\mathbf{x}, t) - \lambda_\alpha p_\alpha(\mathbf{x}, t) + \sum_{\beta=1}^N A_{\alpha,\beta} \lambda_\beta p_\beta(\mathbf{x}, t). \quad (3.9)$$

The basic quantities, namely Λ , \mathbf{A} and $\{\mathbf{b}_\alpha\}_{\alpha=1}^N$, defining an N -state GPK process in \mathbb{R}^n , are not completely independent, if the consistency requirement with respect to the Wiener limit should be met. This issue is thoroughly analyzed in [4], and here is briefly reviewed, in a simple case. Let $\mathbf{b}_\alpha = b_0 \tilde{\mathbf{b}}_\alpha$, $\lambda_\alpha = \lambda_0 \tilde{\lambda}_\alpha$, where $O(|\tilde{\mathbf{b}}_\alpha|) = O(\tilde{\lambda}_\alpha) = 1$, and for making

the analysis notationally simpler consider $\tilde{\lambda}_\alpha = 1$. Assume the following conditions: (i) the dyadic tensor $\tilde{\mathbf{b}}_\alpha \tilde{\mathbf{b}}_\alpha$ is isotropic

$$\frac{1}{N} \sum_{\alpha=1}^N \tilde{\mathbf{b}}_\alpha \tilde{\mathbf{b}}_\alpha = \kappa \mathbf{I}, \tag{3.10}$$

where $\kappa > 0$, and \mathbf{I} is the identity tensor, and (ii) there is a constant $\delta < 1$ such that

$$\sum_{\alpha=1}^N \mathbf{b}_\alpha A_{\alpha,\beta} = \delta \mathbf{b}_\beta. \tag{3.11}$$

These two conditions are fulfilled for typical GPK schemes as discussed in [4]. Next, consider the evolution for the overall probability density function $p(\mathbf{x}, t) = \sum_{\alpha=1}^N p_\alpha(\mathbf{x}, t)$,

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = -\nabla \cdot \mathbf{J}_p(\mathbf{x}, t), \tag{3.12}$$

where the probability flux vector $\mathbf{J}_p(\mathbf{x}, t) = \sum_{\alpha=1}^N \mathbf{b}_\alpha p_\alpha(\mathbf{x}, t)$ satisfies the equation

$$\begin{aligned} \frac{\partial \mathbf{J}_p(\mathbf{x}, t)}{\partial t} &= -b_0^2 \nabla \cdot \left(\sum_{\alpha=1}^N \tilde{\mathbf{b}}_\alpha \tilde{\mathbf{b}}_\alpha p_\alpha(\mathbf{x}, t) \right) \\ &\quad - \lambda_0 \mathbf{J}_p(\mathbf{x}, t) + \lambda_0 \sum_{\alpha,\beta=1}^N \mathbf{b}_\alpha A_{\alpha,\beta} p_\beta(\mathbf{x}, t). \end{aligned} \tag{3.13}$$

Equation (3.13) is still a constitutive equation “with memory” for the flux $\mathbf{J}_p(\mathbf{x}, t)$, as the time-derivative of the flux is involved, but not of the Cattaneo-type. Consider the limit of this equation for $b_0, \lambda_0 \rightarrow \infty$, keeping constant the value $b_0/2\lambda_0 = D_{\text{nom}}$, that can be viewed as the “nominal” diffusivity of the GPK scheme. This corresponds to the Kac limit of the process for unbounded propagation velocities. For arbitrarily large λ_0 , the recombination dynamics amongst the N partial probability waves is arbitrarily fast so that

$$p_\alpha(\mathbf{x}, t) = \frac{p(\mathbf{x}, t)}{N} + O(\lambda_0^{-1}), \tag{3.14}$$

where $O(\lambda_0^{-1})$ is a quantity going to zero for $\lambda_0^{-1} \rightarrow 0$. Applying Eq. (3.10), the first term at the r.h.s. of Eq. (3.13) can be expressed as

$$\begin{aligned} \nabla \cdot \left(\sum_{\alpha=1}^N \tilde{\mathbf{b}}_\alpha \tilde{\mathbf{b}}_\alpha p_\alpha(\mathbf{x}, t) \right) &= \nabla \cdot \left(\frac{1}{N} \sum_{\alpha=1}^N \tilde{\mathbf{b}}_\alpha \tilde{\mathbf{b}}_\alpha p(\mathbf{x}, t) \right) + O(\lambda_0^{-1}) \\ &= \kappa \nabla \cdot (\mathbf{I} p(\mathbf{x}, t)) + O(\lambda_0^{-1}) = \kappa \nabla p(\mathbf{x}, t) + O(\lambda_0^{-1}). \end{aligned} \tag{3.15}$$

Enforcing the transition condition (3.11) amongst the velocity vectors \mathbf{b}_α , Eq. (3.13) simplifies in the Kac limit as

$$\mathbf{J}_p(\mathbf{x}, t) = -\frac{b_0^2 \kappa}{\lambda_0(1-\delta)} \nabla p(\mathbf{x}, t) = -\frac{2\kappa D_{\text{nom}}}{1-\delta} \nabla p(\mathbf{x}, t). \quad (3.16)$$

It follows from Eqs. (3.12), (3.16) that the overall probability density function $p(\mathbf{x}, t)$ is a solution, in the Kac limit, of the diffusion equation $\partial p(\mathbf{x}, t)/\partial t = D_{\text{eff}} \nabla^2 p(\mathbf{x}, t)$ with an effective diffusion coefficient given by $D_{\text{eff}} = 2\kappa D_{\text{nom}}/(1-\delta)$. This means that $p(\mathbf{x}, t)$ coincides with the solution (for the same initial conditions) of the forward Fokker–Planck equation associated with the classical Langevin equation $d\mathbf{x}(t) = \sqrt{2D_{\text{eff}}} d\mathbf{w}(t)$ driven by a vector-valued n -dimensional Wiener process, the increments of which in the interval dt are $d\mathbf{w}(t)$.

GPK processes can be easily extended to include the presence of a deterministic velocity field $\mathbf{v}(\mathbf{x})$, to a continuum of stochastic states, and to the dependence of both $\mathbf{b}_\alpha(\mathbf{x})$ and $\lambda(\mathbf{x})$ on the state variable \mathbf{x} (conceptually analogous to the case of non-linear Langevin equations). The analysis of these extensions can be found in [4–6].

What is important to point out in the present analysis is that the GPK process (3.8) does not only approach a Wiener dynamics in the Kac limit, but also in its long-term dynamics, for any value of the parameter b_0 and λ_0 . This means that all the equilibrium properties and the associated results (*e.g.* the fluctuation–dissipation relations), that in statistical mechanics are derived from the equilibrium properties of Langevin equations driven by Wiener perturbations, can be equally well interpreted within the GPK formalism, with the further conceptual advantage that the latter does possess regularity properties at short timescales, and is immune from the unpleasant paradox of infinite propagation velocity typical of parabolic transport models.

4. Regularity properties

This section briefly addresses how the constraint of finite propagation velocity permits to regularize classical transport problems eliminating unphysical divergences characterizing parabolic models.

Preliminarily, next paragraph analyzes how GPK process naturally arises in the statistical description of systems of interacting particles, whenever continuous hydrodynamic limits, respectful of the requirement of finite propagation velocity, are considered.

4.1. “A good old boy”: origin of GPK from LRW

Lattice Random Walk (LRW, for short) is probably the simplest model of stochastic particle dynamics and represents one of the milestones in statistical physics [42]. Consider a lattice \mathbb{Z} of points on \mathbb{R} with lattice spacing $\delta > 0$, and assume that at regular time instants $t_n = n\tau$, $n = 1, 2, \dots$, $\tau > 0$, particles perform random jumps to one of the nearest neighboring sites with probability $r_1 > 0$ (to the right) and $r_2 > 0$ (to the left), see Fig. 1. Particle

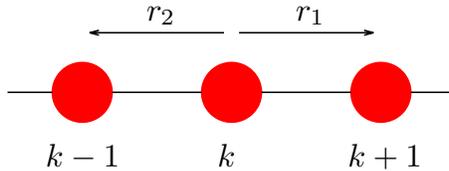


Fig. 1. Schematic representation of the asymmetric LRW.

motion is specified by the three parameters δ , τ and $r = r_1 - r_2 \in [0, 1)$, and described by the evolution equation

$$x_{n+1} = \begin{cases} x_n + \delta & \text{with Prob. } r_1, \\ x_n - \delta & \text{with Prob. } r_2, \end{cases} \tag{4.1}$$

where x_n is the particle position at the discrete time $t_n = n\tau$. Indicating with $p(x_k, t_n)$ the probabilities of finding at time t_n a particle at lattice position x_k , from Eq. (4.1) it follows that this system of probabilities satisfies the evolution equation

$$p(x, t) = r_1 p(x - \delta, t - \tau) + r_2 p(x + \delta, t - \tau) = \mathcal{M}_\tau[p(x, t)] \tag{4.2}$$

that defines the Markov operator \mathcal{M}_τ of the discrete lattice model.

One of the main issues in LRW as well as in any model of interacting particles is to define a continuous limit for Eq. (4.2). This is usually performed by letting the lattice parameters δ and τ go to zero, assuming a suitable rescaling for them, *i.e.*, a relation of the form $\delta = g(\tau)$ connecting the space and time scales of the process as $\delta, \tau \rightarrow 0$. Two cases are typical. By assuming a purely convective rescaling, *i.e.*, $\delta/\tau = b_0 = \text{const.}$, the hydrodynamic limit of Eq. (4.2) is expressed by the continuity equation

$$\frac{\partial p(x, t)}{\partial t} = -v \frac{\partial p(x, t)}{\partial x}, \tag{4.3}$$

where

$$v = r b_0 = (r_1 - r_2) \frac{\delta}{\tau}. \tag{4.4}$$

Conversely, if a diffusive rescaling $\delta^2/2\tau = D_0 = \text{const.}$ is assumed, and if the hopping probabilities depend on δ ,

$$r_1 = \frac{1 + \alpha \delta}{2}, \quad r_2 = \frac{1 - \alpha \delta}{2}, \quad (4.5)$$

where $\alpha = v/2D_0$, then the hydrodynamic limit of Eq. (4.2) is the advection–diffusion equation for $p(x, t)$

$$\frac{\partial p(x, t)}{\partial t} = -v \frac{\partial p(x, t)}{\partial x} + D_0 \frac{\partial^2 p(x, t)}{\partial x^2}. \quad (4.6)$$

All this is well-known [43]. In the latter case (diffusive rescaling), the lattice velocity b_0 diverges. The paradox of infinite propagation velocity for the solutions of Eq. (4.6) is, therefore, an artifact of the approach used to obtain the hydrodynamic limit (4.6), while it is completely absent in the original lattice particle model.

It is, therefore, natural to ask whether it would be possible to derive continuous hydrodynamic equations without performing the limit for $\delta, \tau \rightarrow 0$, consistently with the bounded value of the lattice velocity b_0 [44]. This effort is also reasonable in the light of elementary physical considerations. Consider LRW as a “crude” lattice model of a particle gas system. In this case, both δ and b_0 are physical quantities related to the mean free path and to the root mean square velocity, and ultimately depending on temperature and pressure. The physics of the system indicates that both δ and τ attain finite values for given thermodynamic conditions.

The construction of the continuous model is essentially based on two key steps:

- a continuation of the lattice random walk both in space and time in order to consider $x \in \mathbb{R}$ and $t \in \mathbb{R}^+$. As regards the spatial coordinate, this can be easily achieved by assuming uncertainty in the initial conditions. This means that the initial condition $x(t = 0) = x_0$ is a random variable defined by the probability density function $p_{x_0}(x_0)$ possessing compact support in $(-\delta/2, \delta/2)$. For the time variable, its continuation involves solely the linear continuation of particle trajectories between two subsequent lattice positions x_n and x_{n+1} , as $x(t) = x_n + (x_{n+1} - x_n)(t - t_n)/(t_{n+1} - t_n)$, $t \in [t_n, t_{n+1})$. This linear continuation of the trajectories bears some analogies with the classical Wong–Zakai interpolation of Wiener processes [45].
- While the original lattice model (4.1) is strictly Markovian, as results from Eq. (4.2), the continuous extension introduced above defines a non-Markovian process for $X(t)$. This stems from the fact that in

order to keep a continuous description of particle trajectories, also the local velocity direction s should be considered as a state variable, attaining values $s = 1$ (motion towards positive x -values) or $s = -1$ (motion towards negative x -values).

Starting from the two conceptual steps described above, the development of a continuous statistical description is essentially a matter of “mathematical–physical technology” and is thoroughly addressed in [44]. The final result of this analysis can be summarized as follows. The continuous hydrodynamic equations involve the two partial probability densities $p_{\pm}(x, t) = P_{x,s}(x, s = \pm 1, t)$ that are solutions of the hyperbolic equations

$$\begin{aligned} \frac{\partial p_+}{\partial t} &= -b_0 \frac{\partial p_+}{\partial x} - \frac{2}{\tau} p_+ + \frac{2}{\tau} \left[\frac{(1+r)}{2} p_+ - \frac{(1+r)}{2} p_- \right], \\ \frac{\partial p_-}{\partial t} &= b_0 \frac{\partial p_-}{\partial x} + \frac{2}{\tau} p_- + \frac{2}{\tau} \left[\frac{(1-r)}{2} p_+ + \frac{(1-r)}{2} p_- \right] \end{aligned} \tag{4.7}$$

and contain solely the lattice parameters δ and τ , as $b_0 = \delta/\tau$, and r . The overall probability density function is $p(x, t) = p_+(x, t) + p_-(x, t)$. Equation (4.7) corresponds to the statistical description of a GPK process on the real line possessing two states $\alpha = 1, 2$ corresponding respectively to $s = \pm 1$ and defined by

$$dx(t) = b_{\chi_2(t, \Lambda, \mathbf{A})} dt, \tag{4.8}$$

where $b_1 = b_0, b_2 = -b_0, \Lambda = (2/\tau, 2/\tau)$, and a probability transition matrix

$$\mathbf{A} = \frac{1}{2} \begin{pmatrix} 1+r & 1+r \\ 1-r & 1-r \end{pmatrix}. \tag{4.9}$$

Figures 2 and 3 depict the comparison between the stochastic simulation of LRW at $r = 0.8$ ($\delta = \tau = 1$ a.u.), and the solution of the continuous hyperbolic hydrodynamic model (4.7), as regards the lower-order moments, (mean and squared variance in Fig. 2) and the overall probability density function $p(x, t)$ at the initial stage of the process (Fig. 3).

The lattice simulations involve an ensemble of $N_p = 10^8$ particles initially located at $x_0 = 0$. Correspondingly, the initial conditions for Eq. (4.7) are $p_{\pm}(x, 0) = p_{\pm}^0 \delta(x)$, where, assuming balanced initial conditions, p_{\pm}^0 are the entries of the Frobenius eigenvector $\mathbf{p}^0 = (p_+^0, p_-^0)$ of the matrix \mathbf{A} , $\mathbf{A} \mathbf{p}^0 = \mathbf{p}^0, p_{\pm}^0 \geq 0, p_+^0 + p_-^0 = 1$.

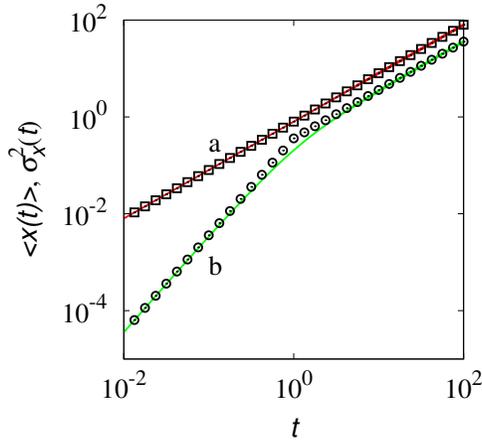


Fig. 2. Mean value $\langle x(t) \rangle$ and squared variance $\sigma_x^2(t)$ for the time-continued asymmetric LRW at $r = 0.8$, $\delta = \tau = 1$, starting from $x(0) = 0$. Lines are the results obtained from the moments of the hyperbolic hydrodynamic limit (4.7), symbols are the theoretical results for the time-continued LRW. Line (a) and (\square) correspond to $\langle x(t) \rangle$, line (b) and (\circ) to $\sigma_x^2(t)$.

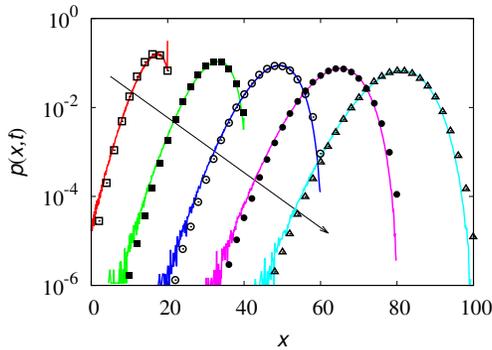


Fig. 3. Probability density function $p(x, t)$ for the asymmetric LRW at $r = 0.8$, $\delta = \tau = 1$, starting from $p(x, 0) = \delta(x)$. Solid lines correspond to the solution of the hyperbolic continuous model, symbols to the results of lattice simulations, normalized in a continuous way (see the main text). The arrow indicates increasing time instants $t = 20, 40, 60, 80, 100$.

Observe that the hyperbolic continuous model not only provides a correct quantitative reproduction of the scaling characterizing the time-continued version of LRW, including the initial ballistic behavior $\sigma_x^2(t) \sim t^2$, induced by the linear continuation of the trajectories, but accurately reproduces the particle density function $p(x, t)$ even at the early stages of the process, as can be observed from the data depicted in Fig. 3.

At these short-time scales, the probability density function of the LRW process is a combination of a relatively small number, $2t + 1$, of impulsive contributions, $p(x, t) = \sum_{k=-t}^t p_k(t) \delta(x - k \delta)$ of intensity $p_k(t)$, but solely a small fraction of these terms admits appreciable intensities $p_k(t)$. Conversely, the overall probability density function of the associated GPK process is an almost smooth function of x . In order to achieve a graphically meaningful comparison of the two models, the impulsive probability density functions associated with LRW processes have been interpolated smoothly in a logarithmic way in each interval $[k \delta, (k + 1) \delta]$, where $p_k(t)$ and $p_{k+1}(t)$ are different from zero (logarithmic linear interpolation means that $\log p(x, t)$ is linearly interpolated in each elementary interval), and the resulting values have been probabilistically normalized to unit integral over the real line.

Moreover, the classical continuous limit (4.6) can be viewed as the Kac limit of Eq. (4.7) for $b_0, 1/\tau \rightarrow \infty$ keeping constant the value $D_0 = \delta^2/2\tau$.

4.2. Physical regularity properties

The occurrence of a finite propagation velocity characterizing GPK processes and the associated transport models has several physical implications as regards the regularity of physical observables. Two simple paradigmatic examples are reviewed below taken from [46, 47], considering for simplicity one-dimensional spatial models.

To begin with consider the original Poisson–Kac model defined by Eq. (3.4). In the Kac limit, it converges to the parabolic diffusion model on the real line with a diffusivity equal to $D = b_0^2/2\lambda$. The eigenfunction of the Kac-limit operator $Dd^2\psi(x)/dx^2 = \mu\psi(x)$ are obviously $\phi_k(x) = e^{ikx}$, $i = \sqrt{-1}$, and the corresponding eigenvalue spectrum is expressed by

$$\mu(k) = -Dk^2, \quad k \in \mathbb{R}. \tag{4.10}$$

The real part of the eigenvalues (indeed the eigenvalues are real by self-adjointness of the operator) diverges to $-\infty$ for high wavenumbers k . This phenomenon determines that the evolution operators $S_t = \exp(tD\partial^2/\partial x^2)$ associated with the solutions of the parabolic diffusion equation form a semi-group of transformations defined solely for $t \geq 0$. Conversely, the eigenfunction spectrum of the Poisson–Kac operator

$$\mathcal{L}_{\text{PK}} = \begin{pmatrix} -b_0\partial/\partial x - \lambda & \lambda \\ \lambda & b_0\partial/\partial x - \lambda \end{pmatrix} \tag{4.11}$$

is still given by vector-valued planar-wave functions $\psi_k(x) = (\psi_{k,0}^+, \psi_{k,0}^-) e^{ikx}$, but the corresponding eigenvalues

$$\mu(k) = -\lambda \pm \sqrt{\lambda^2 - k^2 b_0^2} \tag{4.12}$$

possess negative real part lower-bounded by -2λ for any wavenumber k . Specifically, high-frequency spatial modes decay in time at most exponentially as $e^{-\lambda t}$. As a consequence of this property, the corresponding evolution operators, parametrized with respect to time t , form a group of transformations defined also for $t < 0$. There are several thermodynamic implications of this result, and some of them are addressed in [46].

Another typical example of the regularization induced by the finite propagation velocity involves boundary layer theory. Singularities in the expression of the interfacial fluxes often appear in boundary layer problems governed by parabolic transport models, associated with the occurrence of concentration discontinuities. The hyperbolic formulation of the same problems eliminates the singularities as far as the propagation velocity is kept bounded.

Consider the simplest example of thermal boundary layer: a material medium extending for $x \in (0, \infty)$ and initially at temperature T_{in} , say $T_{\text{in}} = 0$ upon a suitable shift of the temperature scale, is heated by a solid boundary located at $x = 0$ and kept at temperature $T_0 > 0$. Indicating with $D = k/\rho c_p$ the ‘‘thermal diffusivity’’, the classical parabolic model for heat conduction, $\partial T/\partial t = D\partial^2 T/\partial x^2$, $T|_{x=0} = T_0$, $T|_{t=0} = 0$, predicts an interfacial flux at $x = 0$ given by

$$J_0(t) = \sqrt{\frac{D}{\pi t}} T_0 \quad (4.13)$$

that is singular at $t = 0$ just because of the initial discontinuity in the temperature profile deriving from the mismatch between initial and boundary conditions at $x = 0$ and $t = 0$.

Next, consider the hyperbolic formulation of the same problem based on the Poisson–Kac transport formalism. In this case, the temperature field is described by the two partial waves $T_{\pm}(x, t)$, solution of Eq. (3.4), with $p_{\pm}(x, t)$ replaced by $T_{\pm}(x, t)$. The overall temperature is $T(x, t) = T_+(x, t) + T_-(x, t)$, the parameters b_0 and λ satisfy the condition $b_0^2/2\lambda = D$, and the heat flux is expressed by the relation $J(x, t) = b_0 [T_+(x, t) - T_-(x, t)]$. The hyperbolic equations (3.4) for $T_{\pm}(x, t)$ are equipped with the boundary and initial conditions $T_+(x, 0) + T_-(x, 0) = 0$ for $x > 0$ and $T_+(0, t) + T_-(0, t) = T_0$ for $t > 0$. This model can be solved analytically and the expression for the interfacial flux $J_0(t) = J(0, t)$ is [47]

$$J_0(t) = b_0 e^{-b_0^2 t/2D} I_0 \left(\frac{b_0^2 t}{2D} \right) T_0, \quad (4.14)$$

where $I_0(\cdot)$ is the modified Bessel function of first kind and order zero. It follows from Eq. (4.14) that the interfacial flux $J_0(t)$ is bounded by

$$J_0(t) \leq b_0 T_0. \quad (4.15)$$

Moreover, enforcing the asymptotic expansion for the Bessel function entering Eq. (4.14), one obtains

$$J_0(t) = \sqrt{\frac{D}{\pi t}} T_0 \left[1 + O\left(\frac{2D}{b_0^2 t}\right) \right]. \tag{4.16}$$

Equations (4.15)–(4.16) imply that, while the initial singularity of the interfacial flux is cured by the finite-propagation velocity characterizing the hyperbolic model, the long-term properties (corresponding to time scales $t \gg 2D/b_0^2$) are quantitative the same of the classical parabolic model based on the Fourier law.

5. Regularizing stochastic partial differential equations

Langevin equations driven by vector-valued Wiener noise represent the prototypical model of evolution equations for a physical system driven by a deterministic velocity field in the presence of superimposed stochastic fluctuations. The statistical nature of a Wiener process $w(t)$ (possessing uncorrelated increments $w(t + \delta) - w(t)$, $\delta > 0$, characterized by Gaussian probability density function with zero mean and variance equal to the time interval δ), can be regarded as the natural legacy of a large number Ansatz, in which the effects of many unknown and uncorrelated perturbations justify the Gaussian nature for the statistics of the increments of the stochastic forcing.

Analogously, in dealing with stochastic field equations (stochastic partial differential equations),

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \mathcal{N}[\phi(\mathbf{x}, t)] + a(\phi(\mathbf{x}, t)) f_s(\mathbf{x}, t), \tag{5.1}$$

where \mathcal{N} is a non-linear operator of the field variable $\phi(\mathbf{x}, t)$, the most common assumption for the stochastic spatio-temporal forcing $f_s(\mathbf{x}, t)$ is that it possesses zero mean and δ -correlated increments both in space and time

$$\langle f_s(\mathbf{x}, t) \rangle = 0, \quad \langle f_s(\mathbf{x}, t) f_s(\mathbf{x}', t') \rangle = \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'), \tag{5.2}$$

where $\langle \cdot \rangle$ indicates the mean value with respect to the probability measure, For this reason, this term can be “formally” viewed as the “derivative” of a Wiener process. This is the classical model adopted in stochastic field theory [48–50].

However, the δ -correlated structure of the stochastic fluctuations, especially as regards their spatial dependence, poses several consistency issues:

- in the case the field $\phi(\mathbf{x}, t)$ represents a concentration (mass density, a molar concentration, or temperature expressed in absolute units), the evolution equation should satisfy the positivity requirement. Problems with the lack of positivity often arise in the presence of stochastic perturbation satisfying Eq. (5.2) [51, 52];
- for δ -correlated perturbations $f_s(\mathbf{x}, t)$, even in the presence of simple functionals such as $\mathcal{N}[\phi] = \nabla^2\phi + V(\phi)$ (where $V(\phi)$ is a function of ϕ , such as in the Schrödinger equation), the solutions may not exist from a mathematical point of view, or their lower-order moments may diverge, depending on the dimensionality of the space coordinate (see Section 5.2).

In this framework, the use of Poisson–Kac or GPK processes for modeling the stochastic perturbations $f_s(\mathbf{x}, t)$ provides a physically reasonable and simple alternative to the “harsh” δ -correlated processes, possessing from the one hand the same long-term properties, and from the other hand regularizing the short-scale behavior, with the effect of eliminating the mathematical problems associated with positivity, with the non-existence of solutions or of their lower-order moments. Two simple examples are thoroughly addressed in order to elucidate this claim.

5.1. Positivity: a simple transport problem

In many transport problems, the stochastic fluctuations should satisfy positivity requirements. Below, a simple but non-trivial problem is addressed. Consider transport and reaction of a reactant inside a catalytic pore of length L . Let D be the reactant diffusivity and k_r the reaction rate constant (assuming a first-order reaction and isothermal conditions). In non-dimensional form, the balance equation reads

$$\frac{\partial c(x, t)}{\partial t} = \frac{\partial^2 c(x, t)}{\partial x^2} - \phi^2 c(x, t), \quad (5.3)$$

where $\phi^2 = k_r L^2 / D$ is the square Thiele modulus, $x \in (0, 1)$ and t is a non-dimensional time corresponding to the physical time rescaled with respect to the diffusion time L^2 / D . Let us further assume that initially the reactant is absent, and that for $t > 0$ a stochastic feeding occurs at the open pore boundary (the other boundary $x = 0$ is impermeable to transport), corresponding to a reactant flux equal to $J_0 \mu(t)$, where J_0 is a constant and

$\mu(t)$ a stochastic process. This means that Eq. (5.3) fulfills the initial and boundary conditions (see Fig. 4)

$$c(x, 0) = 0, \quad \left. \frac{\partial c(x, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial c(x, t)}{\partial x} \right|_{x=L} = \gamma \mu(t), \quad (5.4)$$

where $\gamma = J_0 L / D C_{\text{ref}}$, and C_{ref} is some reference concentration value. The stochastic process $\mu(t)$ is, by definition, non-negative, as reactant is fed into the catalyst pore, and this ensures that the solutions of the stochastic equation (5.3) are also non-negative, owing to the maximum principle for the Laplacian operator. A simple way for achieving this is to model $\mu(t)$ via Poisson–Kac processes in the form of

$$\mu(t) = \frac{1 - (-1)^{\chi(t, \lambda)}}{2}, \quad (5.5)$$

where the Poisson process $\chi(t, \lambda)$ is characterized by its transition rate λ , that controls the exponential decay of correlations of $\mu(t)$. In this way, $\mu(t)$ attains solely the values 0 or 1, depending on the parity of $\chi(t, \lambda)$.

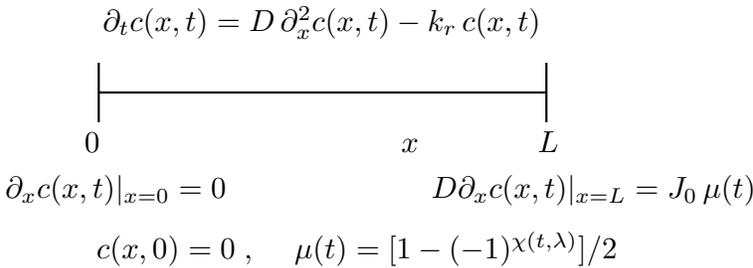


Fig. 4. Overview of the reaction-diffusion model considered in the presence of a stochastic reactant flux at the boundary of a catalytic pore. In this picture, the quantities x , t and $c(x, t)$ are dimensional.

Introduce the auxiliary field $u(x, t)$ as

$$c(x, t) = u(x, t) + \mu(t) c^*(x), \quad (5.6)$$

where $c^*(x)$ is the stationary solution of the corresponding problem in which the stochastic inlet condition is substituted by $dc^*(x)/dx|_{x=L} = \gamma$

$$c^*(x) = \frac{\gamma \cosh(\phi x)}{\phi \sinh(\phi)}. \quad (5.7)$$

The auxiliary field $u(x, t)$ satisfies the equation

$$\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2} - \phi^2 u(x, t) - \mu'(t) c^*(x), \quad (5.8)$$

where $\mu'(t) = d\mu(t)/dt$, equipped with homogeneous boundary conditions $\partial u(x, t)/\partial x|_{x=0,1} = 0$, and with the initial condition $u(x, 0) = -\mu(0) c^*(x)$. Expressing the solution in the eigenbasis $\{\psi_n(x)\}_{n=0}^\infty$ of the diffusion-reaction operator $\mathcal{L} = \partial^2/\partial x^2 - \phi^2$, $\mathcal{L}[\psi_n(x)] = -\nu_n^2 \psi_n(x)$, $\nu_n^2 = n^2 \pi^2 + \phi^2$, $n = 0, 1, \dots$, $(\psi_m(x), \psi_n(x))_{L^2([0,1])} = \delta_{m,n}$

$$u(x, t) = \sum_{n=0}^\infty u_n(t) \psi_n(x), \tag{5.9}$$

the Fourier coefficients $u_n(t)$ satisfy the stochastic system of equations

$$\frac{du_n(t)}{dt} = -\nu_n^2 u_n(t) - \mu'(t) c_n^*, \tag{5.10}$$

where $c_n^* = (c^*(x), \psi_n(x))_{L^2([0,1])}$, $c_0 = \gamma/\phi^2$, $c_n^* = \sqrt{2} \gamma (-1)^n / (n^2 \pi^2 + \phi^2)$, $n = 1, 2, \dots$. The solution of Eqs. (5.3)–(5.4) thus reads

$$c(x, t) = \sum_{n=0}^\infty c_n^* \nu_n^2 \int_0^t \mu(\tau) e^{-\nu_n^2(t-\tau)} d\tau \psi_n(x) \tag{5.11}$$

and the integral in Eq. (5.11) is simply a stochastic Riemann integral. Since the averages of the noise boundary perturbations are

$$\langle \mu(t) \rangle = \frac{1}{2}, \quad \langle \mu(t) \mu(t') \rangle = \frac{1}{4} \left[1 + e^{-2\lambda|t-t'|} \right], \tag{5.12}$$

it follows that the mean concentration $\langle c(x, t) \rangle$ at x in the long-time regime equals $\langle c(x, t) \rangle = c^*(x)/2$ as intuitively expected from the structure of the stochastic perturbation. The pointwise square concentration variance $\sigma_c^2(x, t) = \langle c^2(x, t) \rangle - \langle c(x, t) \rangle^2$ in the long-time limit takes the expression

$$\sigma_c^2(x, t) = \frac{1}{2} \sum_{m=0}^\infty \sum_{n=0}^\infty \frac{\nu_m^2 \nu_n^2 c_m^* c_n^*}{\nu_m^2 + \nu_n^2} \left(\frac{1}{\nu_m^2 + 2\lambda} + \frac{1}{\nu_n^2 + 2\lambda} \right) \psi_m(x) \psi_n(x). \tag{5.13}$$

Indicating with C and V the average concentration and squared variance over all domain, one obtains in the long-term limit

$$C = \int_0^1 \langle c(x, t) \rangle dx = \frac{\gamma}{2\phi^2}, \quad V^2 = \int_0^1 \langle \sigma_c^2(x, t) \rangle dx = \frac{1}{4} \sum_{n=0}^\infty \frac{\nu_n^2 (c_n^*)^2}{\nu_n^2 + 2\lambda}. \tag{5.14}$$

Figure 5 depicts some realization of the process, *i.e.*, the concentration value at the mid-point $x^* = 1/2$ and the associated probability density functions $P_c(x; x^*)$ for the pointwise concentration c at x^* in the long-term regime, for different values of the Thiele modulus ϕ . These data have been obtained by considering 10^5 realizations of the process.

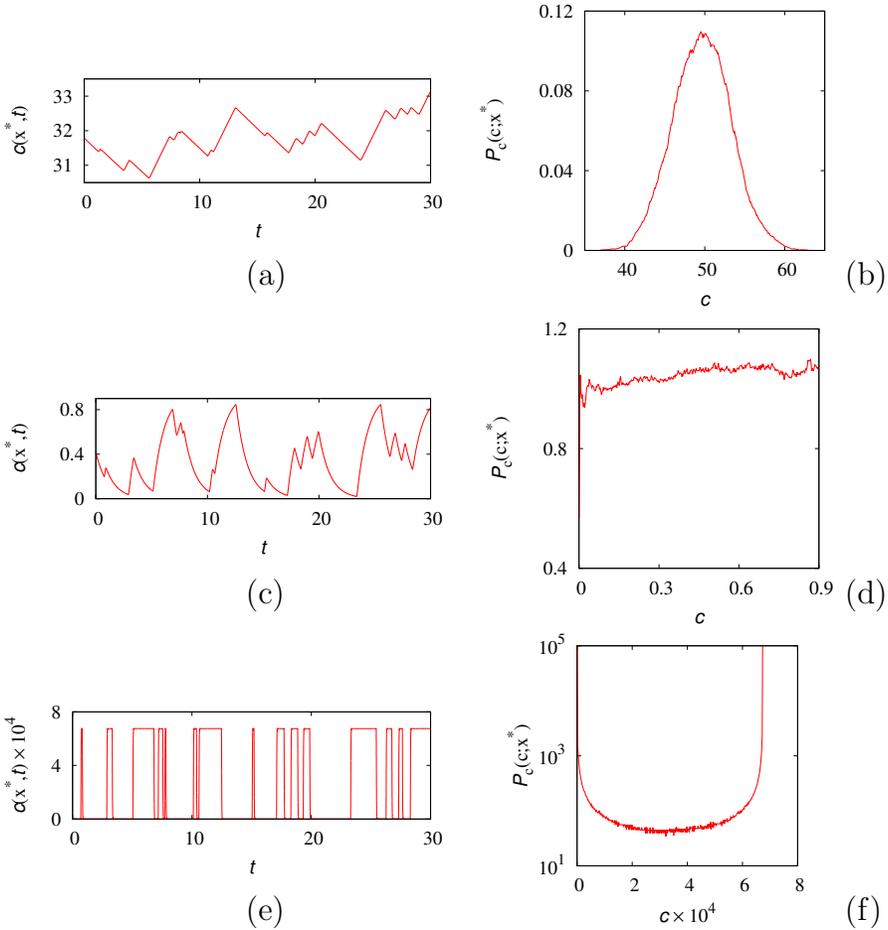


Fig. 5. Realizations, panels (a), (c) and (e), of the stochastic reaction–diffusion model considered in the main text at $x^* = 0.5$, $\gamma = 1$ for different values of the Thiele modulus. Panels (b), (d) and (e) represent the corresponding density functions $P_c(c; x^*)$ for the concentration values c at x^* . Panels (a) and (b) refer to $\phi = 0.1$, (c) and (d) to $\phi = 1$, and (e) and (f) to $\phi = 10$.

Depending on the value of the Thiele modulus, the density functions associated with the local concentration values attain extremely different shapes, ranging from almost Gaussian profiles at low ϕ values (panel (b)), to almost flat distributions (panel (d)) at intermediate $\phi \sim O(1)$ values corresponding to the transition from reaction-controlled to diffusion-controlled regimes, to singular ones, peaked at two characteristic concentrations for high ϕ values (panel (f)), corresponding to the dichotomous behavior of the local concentration values (see panel (e) in Fig. 5).

A final comment refers to the noise-to-signal ratio V/C , expressed as the ratio of the variance to the mean concentration and its dependence on ϕ . The behavior of this global quantity is depicted in Fig. 6 for several values of λ .

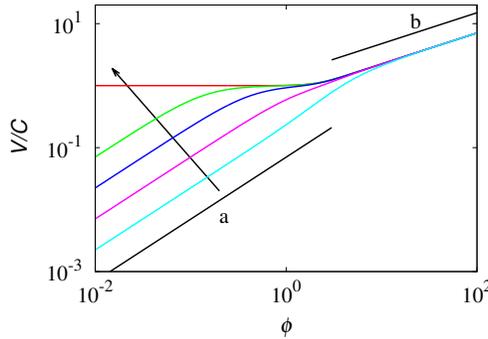


Fig. 6. Noise-to-signal ratio V/C vs. the Thiele modulus ϕ at $\gamma = 1$. The arrow indicates decreasing values of $\lambda = 10, 1, 0.1, 0.01, 0$. Line (a) represents the scaling $V/C \sim \phi$, line (b) $V/C \sim \phi^{1/2}$.

Two observations follow from the inspection of these data. The overall statistical behavior of the process is characterized by the occurrence of three different scaling regimes: (i) $V/C \sim \phi$ at small values of ϕ , (ii) $V/C \sim \text{const.}$ at intermediate values, and (iii) $V/C \sim \phi^{1/2}$ at large values of ϕ . Moreover, the ratio V/C can attain arbitrarily large values for large ϕ , corresponding to an arbitrarily large variance compared to the mean, still keeping rigorously the positivity of the concentration field.

5.2. Convergence of lower-order moments: the Edwards–Wilkinson model

The Edwards–Wilkinson model (EW, for short) corresponds to the diffusion equation in the presence of a stochastic forcing, and is a classical model for surface growth [57–59]. In non-dimensional form it reads as

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = \nabla^2 u(\mathbf{x}, t) + \kappa \xi(\mathbf{x}, t), \tag{5.15}$$

where $\mathbf{x} \in \Omega \subset \mathbb{R}^n$, κ is a constant parameter and $\xi(\mathbf{x}, t)$ is a white-noise stochastic perturbation, satisfying conditions (5.2), i.e., $\langle \xi(\mathbf{x}, t) \rangle = 0$, $\langle \xi(\mathbf{x}, t) \xi(\mathbf{x}', t') \rangle = \delta(t - t') \delta(\mathbf{x} - \mathbf{x}')$. In the present analysis $\Omega = [0, 1]^n$, and the problem is equipped with periodic boundary conditions. Without loss of generality set $\kappa = 1$.

This means that the eigenfunctions of the Laplacian are $\psi_{\mathbf{k}}(\mathbf{x}) = e^{i2\pi\mathbf{k}\cdot\mathbf{x}}$, and the corresponding eigenvalues are $\nu_{\mathbf{k}} = -4\pi^2|\mathbf{k}|^2$, where $\mathbf{k} = (k_1, \dots, k_n)$, k_h integers. Without loss of generality, assume vanishing initial conditions $u(\mathbf{x}, 0) = 0$.

In the presence of δ -correlated stochastic perturbations, the EW model admits bounded lower-order moments (variance) solely for $n = 1$ [53, 54]. The solution of Eq. (5.15) can be expanded in the Laplacian eigenfunctions $u(\mathbf{x}, t) = \sum_{\mathbf{k}} u_{\mathbf{k}}(t) \psi_{\mathbf{k}}(\mathbf{x})$, where the Fourier coefficients $u_{\mathbf{k}}(t)$ are given by

$$u_{\mathbf{k}}(t) = \int_0^t e^{-\nu_{\mathbf{k}}(t-\tau)} \xi_{\mathbf{k}}(\tau) d\tau \tag{5.16}$$

and

$$\xi_{\mathbf{k}}(t) = (\xi(\mathbf{x}, t), \psi_{\mathbf{k}}(\mathbf{x}))_{L^2([0,1]^n)} = \int_{[0,1]^n} \xi(\mathbf{x}, t) e^{-i2\pi\mathbf{k}\cdot\mathbf{x}} d\mathbf{x} \tag{5.17}$$

are characterized by

$$\langle \xi_{\mathbf{k}}(t) \rangle = 0, \quad \langle \xi_{\mathbf{k}}(t) \xi_{\mathbf{m}}(t') \rangle = \delta(t-t') \tilde{\delta}(\mathbf{k} + \mathbf{m}), \tag{5.18}$$

where $\tilde{\delta}(\mathbf{k}) = 1$ for $\mathbf{k} = 0$ and zero otherwise.

In the applications to surface growth, where $u(\mathbf{x}, t)$ is the local height of the surface, the quantity of interest is the deviation $w(\mathbf{x}, t)$ from the overall spatial mean value, *i.e.*,

$$w(\mathbf{x}, t) = u(\mathbf{x}, t) - \frac{1}{\text{meas}(\Omega)} \int_{\Omega} u(\mathbf{x}, t) d\mathbf{x}, \tag{5.19}$$

where $\text{meas}(\Omega)$ indicates the measure of Ω , in the present case, $\text{meas}([1, 0]^n) = 1$. The Fourier coefficients of $w(\mathbf{x}, t)$ with respect to the Laplacian basis are related to those of $u(\mathbf{x}, t)$ by the relation

$$w_{\mathbf{k}}(t) = \begin{cases} 0, & \mathbf{k} = 0, \\ u_{\mathbf{k}}(t), & \mathbf{k} \neq 0. \end{cases} \tag{5.20}$$

Obviously $\langle w(\mathbf{x}, t) \rangle = 0$, while for the spatially averaged squared variance $W^2(t)$ one obtains

$$W^2(t) = \int_{[0,1]^n} \langle w^2(\mathbf{x}, t) \rangle d\mathbf{x} = \sum_{\mathbf{k} \neq 0} \frac{1 - e^{-2\nu_{\mathbf{k}}^2 t}}{2\nu_{\mathbf{k}}^2}. \tag{5.21}$$

In practical calculations, the expression for $W^2(t)$ is truncated to a finite number of modes, *e.g.* by considering $|k_h| \leq N$, $h = 1, \dots, N$. This corresponds to considering $2N + 1$ Fourier modes per coordinate. Figure 7 depicts the behavior of $W^2(t)$ *vs.* t for several values of the truncation order N in the two- and three-dimensional case. As it is well-known [53], the variance of $w(x, t)$ depends on the number of Fourier modes chosen, and this represents a serious inconvenience of the EW model. This phenomenon is clearly depicted in Fig. 8 that shows the asymptotic limit value $W_*^2(N) = \sum_{\mathbf{k} \neq 0, |\mathbf{k}_h| \leq N} 1/2\nu_{\mathbf{k}}^2$ as a function of the modal resolution N .

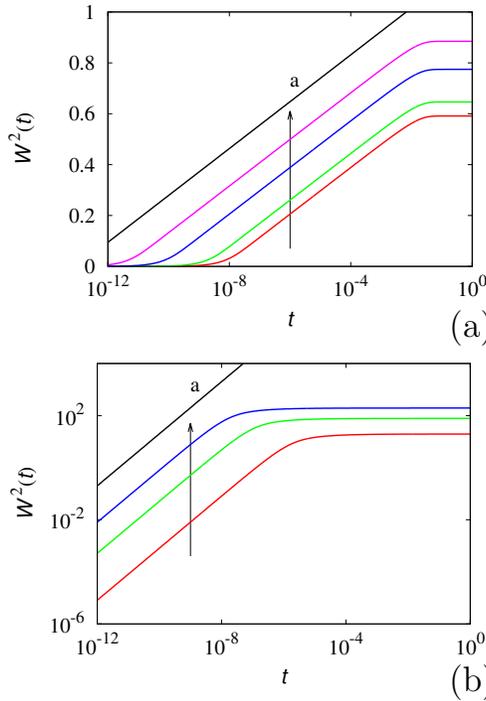


Fig. 7. Behavior of $W^2(t)$ *vs.* t for $n = 2$ (panel (a)) and $n = 3$ (panel (b)), for different values of the truncation order N . The arrows indicate increasing values of N . Panel (a) $N = 10^3, 2 \times 10^3, 10^4, 4 \times 10^4$. Line (a) represents the scaling $W^2(t) \sim \log t$. Panel (b) $N = 10^2, 4 \times 10^2, 10^3$. Line (a) represents the scaling $W^2(t) \sim t$.

The lack of convergence of the squared variance is a consequence of the assumption of δ -correlated noise, especially as regards the dependence on the spatial coordinates, that is “too rough” to ensure convergence for $n > 1$. A similar problem arises *a fortiori* in the case of non-linear stochastic partial differential equations driven by δ -correlated stochastic perturbations.

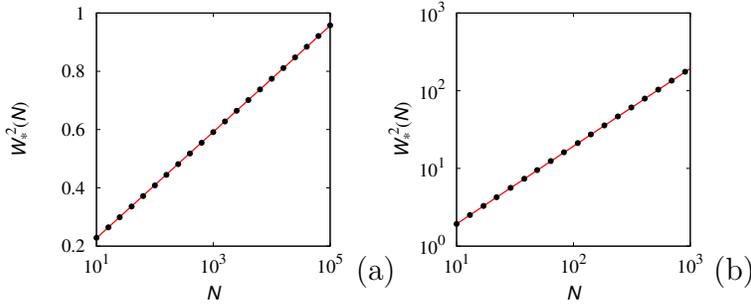


Fig. 8. Behavior of $W_*^2(N)$ vs. N (symbols \bullet) for the two-dimensional and three-dimensional EW model. Panel (a) $n = 2$. The solid line represents the scaling $W_*^2(N) \sim \log N$. Panel (b) $n = 3$. The solid line represents the scaling $W_*^2(N) \sim N$.

The divergence of the EW model can be cured by considering a Poisson–Kac representation for the stochastic perturbation. The simplest way for achieving this is to consider for $\xi(\mathbf{x}, t)$ the following expression in n -dimensional spatial problems:

$$\xi(\mathbf{x}, t) = \Lambda (-1)^{\chi_0(t, \lambda_0)} \prod_{h=1}^n (-1)^{\chi_h(x_h, \lambda_h)}, \quad \lambda = \sqrt{\lambda_0 \prod_{h=1}^n \lambda_h}, \quad (5.22)$$

where $\mathbf{x} = (x_1, \dots, x_n)$, and $\chi(t, \lambda_0)$, $\chi_h(x_h, \lambda_h)$, $h = 1, \dots, n$ are, obviously, independent Poisson processes with respect to time and space coordinates, characterized by the transition rates λ_0 , λ_h , $h = 1, \dots, n$, respectively. Model (5.22) can be viewed as a mollification of the original δ -correlated process, converging to it for $\lambda_0, \lambda_h \rightarrow \infty$.

Expressed in the Fourier modes, the formal solution for $u_{\mathbf{k}}(t)$ is given by

$$u_{\mathbf{k}}(t) = \Lambda B_{\mathbf{k}} \int_0^t e^{-\nu_{\mathbf{k}}^2(t-\tau)} (-1)^{\chi_0(\tau, \lambda_0)} d\tau, \quad (5.23)$$

where

$$B_{\mathbf{k}} = \prod_{h=1}^n \left[\int_0^1 (-1)^{\chi_h(x_h, \lambda_h)} e^{-i2\pi k_h x_h} dx_h \right] = \prod_{h=1}^n B_{k_h}. \quad (5.24)$$

Assuming as initial condition for all the processes $\text{Prob}[\chi_h = 0] = \text{Prob}[\chi_h = 1] = 1/2$, then $\langle u(\mathbf{x}, t) \rangle = 0$. In terms of the $w(\mathbf{x}, t)$ process, $\langle w(\mathbf{x}, t) \rangle = 0$, while the squared variance is given by

$$\langle w^2(\mathbf{x}, t) \rangle = \Lambda^2 \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{m} \neq 0} \langle B_{\mathbf{k}} B_{\mathbf{m}} \rangle C(t, \lambda_0, \mathbf{k}, \mathbf{m}) e^{i2\pi(\mathbf{k}+\mathbf{m}) \cdot \mathbf{x}}, \quad (5.25)$$

where

$$C(t, \lambda_0, \mathbf{k}, \mathbf{m}) = \int_0^t d\tau \int_0^t d\tau' e^{-\nu_{\mathbf{k}}^2(t-\tau)} e^{-\nu_{\mathbf{m}}^2(t-\tau')} e^{-2\lambda_0 |\tau-\tau'|} \tag{5.26}$$

and the correlations $\langle B_{\mathbf{k}} B_{\mathbf{m}} \rangle$ factorize

$$\langle B_{\mathbf{k}} B_{\mathbf{m}} \rangle = \prod_{h=1}^n \tilde{B}(\lambda_h, k_h, m_h), \tag{5.27}$$

where the function $\tilde{B}(\lambda, a, b)$ entering Eq. (5.27) is given by

$$\begin{aligned} \tilde{B}(\lambda, a, b) &= \int_0^1 dx \int_0^1 dy e^{-2\lambda|x-y|} e^{-i2\pi(ax+by)} \\ &= \frac{\lambda}{2} \left(\frac{1}{\lambda^2 + \pi^2 a^2} + \frac{1}{\lambda^2 + \pi^2 b^2} \right) \tilde{\delta}(a+b) \\ &\quad + \frac{1}{2} \frac{\lambda^2 - \pi^2 ab}{(\lambda^2 + \pi^2 ab)^2 + \lambda^2 \pi^2 (a-b)^2} (1 - e^{-2\lambda}), \end{aligned} \tag{5.28}$$

where $\tilde{\delta}(a) = 1$ for $a = 0$ and zero otherwise. The spatially averaged squared variance $W^2(t)$ takes the simpler expression

$$W^2(t) = A^2 \sum_{\mathbf{k} \neq 0} \prod_{h=1}^n \tilde{B}(\lambda_h, k_h, -k_h) C(t, \lambda_0, \mathbf{k}, \mathbf{m}), \tag{5.29}$$

where from Eq. (5.28)

$$B(\lambda, k, -k) = \frac{\lambda}{\lambda^2 + \pi^2 k^2} + \frac{1}{2} \frac{\lambda^2 - \pi^2 k^2}{\lambda^2 + \pi^2 k^2} (1 - e^{-2\lambda}). \tag{5.30}$$

This completes the statistical analysis of the Poisson–Kac EW model as regards its lower-order moments. Let us analyze the convergence and the scaling properties of this model. To begin with, consider the one-dimensional spatial case ($n = 1$), for which the δ -correlated EW model converges. Figure 9 depicts the behaviour of $W^2(t)$ for a very high value of the temporal transition rate $\lambda_0 = 10^9$, and for increasing values of the spatial transition rate λ_1 .

As expected, for sufficiently high values of λ_1 , the behavior of the δ -correlated process is exactly reproduced by its Poisson–Kac counterpart. For the time scales considered, $t \geq 10^{-8}$, this implies to choose $\lambda_1 \sim O(10^9)$.

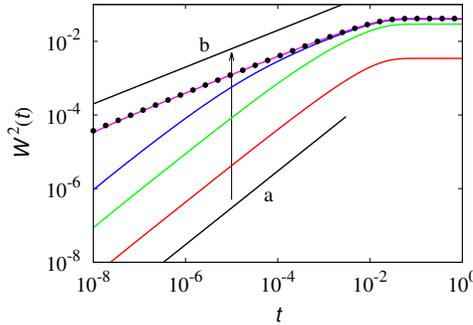


Fig. 9. $W^2(t)$ vs. t for the one-dimensional Poisson–Kac EW model at $\lambda_0 = 10^9$ for several values of λ_1 . The arrow indicates increasing values of $\lambda_1 = 1, 10^1, 10^2, 10^9$. Symbols (●) correspond to the solution of the δ -correlated EW model. Line (a) represents the scaling $W^2(t) \sim t$, while line (b) represents $W^2(t) \sim t^{1/2}$.

The occurrence of three different scalings can be observed: (i) an initial linear scaling $W^2(t) \sim t$, corresponding to the situation where the effects of spatial roughness of $\xi(x, t)$ are negligible, and the squared variance of $w(x, t)$ scales with time as classical Brownian motion; (ii) an intermediate $W^2(t) \sim t^{1/2}$, which is the typical signature of the universality class of the EW model in space dimension one, and (iii) finally, the saturation towards a constant value W_*^2 .

Of course, the convergence of the Poisson–Kac model towards the δ -correlated EW dynamics applies also in higher spatial dimensions, provided that the model is truncated to a finite number of spatial modes. This phenomenon is depicted in Fig. 10, considering the two-dimensional case ($n = 2$) as an example, and $\lambda_1 = \lambda_2$.

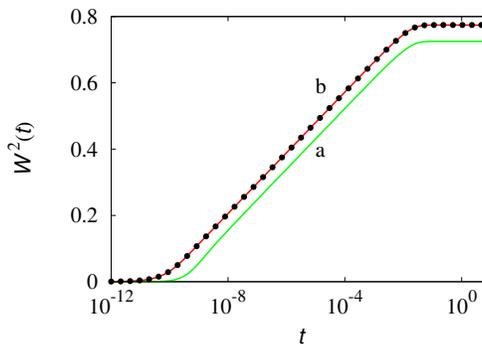


Fig. 10. The two-dimensional truncated Poisson–Kac EW model, using $N = 10^4$ as modal resolution. Line (a) refers to $\lambda_0 = \lambda_1 = 10^9$, line (b) to $\lambda_0 = \lambda_1 = 10^{12}$. Symbols are the results of the corresponding δ -correlated EW process at the same modal resolution.

Contrarily to δ -correlated EW processes, the Poisson–Kac counterparts possess, for finite values of λ_0 and λ_h s, convergent and bounded lower-order moments in any spatial dimension n .

Figure 11 illustrates the behavior of the saturation value W_*^2 (by considering a sufficiently high number of modes to ensure convergence) as a function of the transition rate λ_0 for fixed values of $\lambda_1 = \lambda_2$. It is interesting to observe the occurrence of a crossover behavior: for small values of λ_0 , $W_*^2 \sim \lambda_0$, while for large values of λ_0 , keeping λ_1 bounded, W_*^2 saturates towards a constant value. The analogous plot as a function of $\lambda_1 = \lambda_2$, for fixed λ_0 , is depicted in Fig. 12. It can be observed a non-trivial scaling $W_*^2 \sim \lambda_1^3$ occurring from small values of λ_1 .

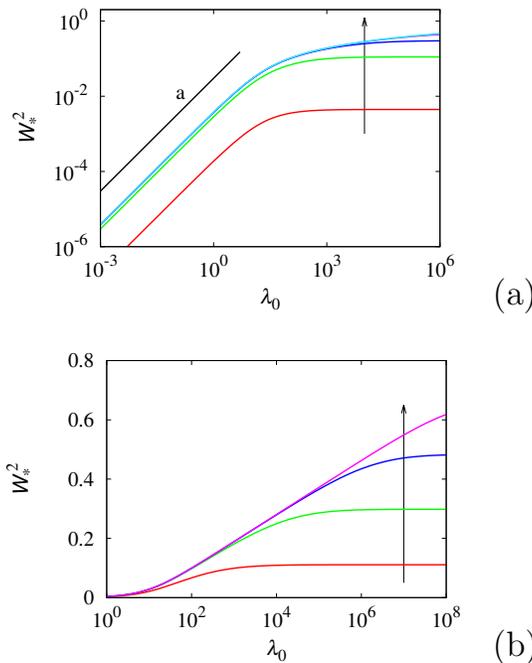


Fig. 11. Behavior of the saturation value W_*^2 for the two-dimensional Poisson–Kac EW model as a function of λ_0 , for different values of λ_1 . The arrows indicate increasing values of $\lambda_1 = \lambda_2$. Panel (a) log–log plot, $\lambda_1 = 1, 10^1, 10^2, 10^3, 10^4$. Line (a) represents the scaling $W_*^2 \sim \lambda_0$. Panel (b) log–normal plot, $\lambda_1 = 10^1, 10^2, 10^3, 10^4$.

To conclude, the use of Poisson–Kac perturbations in stochastic field theories permits to avoid the occurrence of unpleasant divergences induced by δ -correlated spatial perturbations. The extension to non-linear models, such as the Kardar–Parisi–Zhang equation [60] will be developed in forthcoming works.

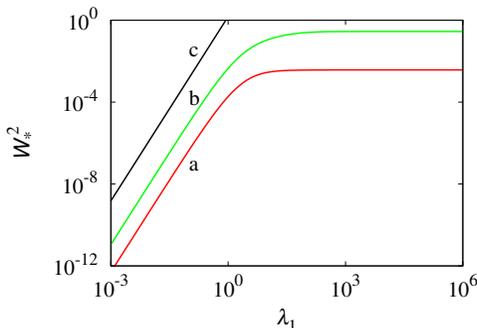


Fig. 12. Behavior of the saturation value W_*^2 for the two-dimensional Poisson–Kac EW model as a function of $\lambda_1 = \lambda_2$, for different values of λ_0 . Line (a) refers to $\lambda_0 = 1$, line (b) to $\lambda_0 = 10^4$. Line (c) corresponds to the scaling $W_*^2 \sim \lambda_1^3$.

6. Concluding remarks

In the light of the regularity Ansatz characterizing the Smoluchowskian approach to statistical physics, this article has analyzed the properties of Poisson–Kac and GPK processes focusing on the role of finite propagation velocity, peculiar of this models, in regularizing stochastic dynamics.

It is important to stress that GPK processes emerge naturally from the analysis of simple particle systems, as addressed in Section 4 using the asymmetric LRW as a paradigmatic example. The extension of the GPK formalism to system of interacting particles, in which interaction potentials are included in the statistical description of particle dynamics, is particularly promising and will be developed in forthcoming works.

The application of Poisson–Kac processes in field-theoretical models is also worth attention in order to mollify the stochastic perturbations and to ensure the existence of the solutions and of their lower-order moments. The classical Edwards–Wilkinson model has been analyzed in this article, but the extension of this approach to non-linear model is feasible and, in principle, will provide an alternative tool to renormalization methods [30] in order to define properly the solutions of stochastic partial differential equations. This is particularly compelling in all those models (*e.g.* emerging from fluctuational hydrodynamics [31]), in which a mathematical solution of the stochastic partial differential equations does not exist *sensu stricto* in the presence of δ -correlated noise, and physical approximations involve the use of coarse numerical methods.

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