# Generalized Fokker-Planck equations derived from nonextensive entropies asymptotically equivalent to Boltzmann-Gibbs

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We derive generalized Fokker-Planck equations (FPEs) based on two nonextensive entropy measures  $S_{\pm}$  that depend exclusively on the probability. These entropies have been originally obtained from the superstatistics framework, therefore they regard nonequilibrium systems outlined by a long-term stationary state in view of a spatiotemporally fluctuating intensive quantity. Moreover, entropies  $S_{\pm}$  as well as Boltzmann-Gibbs (BG) entropy  $S_B$  both pertain to the same asymptotical equivalence class, thus suggesting that  $S_{\pm}$  could depict a consistent thermodynamic generalization of BG. For these reasons, we assert that transport phenomena to be accounted for by our models shall coincide with the portrait given by the conventional FPEs for systems comprehending short-range interactions or a high number of accessible microstates, whereas, for systems composed of a small number of microstates, or those with long-range interactions, the governing equations of motion are to be the FPEs here derived, as long as the system fulfills the attributes mentioned above. We discuss the anomalous diffusion exhibited by the two generalized FPEs and also present some numerical applications. In particular, we find that there are models regarding biological sciences, for the study of congregation and aggregation behavior, the structure of which coincides with the one of our models.

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# I. INTRODUCTION

The concept of entropy occupies a central role in deriving the probability distributions (MaxEnt distributions) that govern the microscopic behavior of general statistical systems. In the traditional theory, for instance, the thermodynamics of short-range, weakly interacting systems composed of a large number of microstates is successfully described by the Boltzmann-Gibbs (BG) probability distribution—in turn obtained by maximizing the BG entropy subject to certain constraints. For complex systems, however, the story becomes different since their dynamics are no longer conducted by typical BG-like distributions but instead generalized entropies have to be introduced [1–7].

Different forms of entropies as a function of probabilities, and possibly additional parameters, have been proposed in order to describe the thermodynamics of complex, nonequilibrium, or strong interacting systems, namely, out of the thermodynamic limit [8,9]. The behavior of those systems is, in general, described by a non-BG probability distribution, meaning that the functional form of the entropy that governs the related dynamics depends on the probability in a different way than  $S_B$  does. Some interesting consequences emerge from nonextensive entropies; for instance, it has been nicely shown in Ref. [10] that the self-similar structures derived from the scaling properties in the Yang-Mills theories behave as fractals, from which one obtains a nonextensive statistical scheme. This approach has been applied to the parameter dependent entropy of Tsallis. Although, in general, the framework does also support some other entropies that convey complexity.

In recent years, by following the superstatistics formalism [11], it has been proposed in Ref. [12] a pair of general entropic forms  $S_{\pm}$  that depend only on the probability and, in consequence, furnish generalized probability distributions. The thermodynamic systems that obey these generalized statistics are *slightly* out of equilibrium, although there exists temporally local equilibrium within each of the cells that sub-divide the system. In other words, the generalized entropies  $S_{\pm}$  give rise to a long-term stationary state in view of a spatiotemporally fluctuating intensive quantity, such as the inverse temperature  $\beta$  in our case. The physical consequences are that the system shall feel an effective interaction represented by an extra attractive (repulsive) contribution in the case of  $S_+$  ( $S_-$ ) (see [13,14]).

As previously stated, in this paper we are to consider systems *slightly* out of thermodynamic equilibrium since the long-term stationary states assure, in a way, that the amplitudes of the fluctuations remain small even when they are subject to small variations in the initial conditions. This stable behavior also confers universality to the scheme; that is, the corrections to the standard Boltzmann factor are to be nearly the same for all superstatistics. In our case the corrections to BG delivered by  $S_{\pm}$  are monotonically subdominant. We remark that this is an interesting attribute since such tendency indicates that  $S_{\pm}$  and  $S_B$  will coincide asymptotically, making it possible to resemble the standard theory when  $S_{\pm}$ 

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encompass a large number of accessible states, whereas for a reduced number of them a modest difference between both approaches is found.

Assuming a more formal attitude, these latter facts can be put in the spirit of the asymptotic classification stated in Ref. [15] where, as an attempt to understand the nature of a wide number of entropies, it has been formulated a classification according to their limiting behavior. In that sense, the entropies that fulfill the first three Shannon-Khinchin (SK) axioms (SK1, continuity; SK2, maximality; SK3, expandability; SK4, additivity) [16,17] become characterized uniquely by a pair of critical exponents (c, d). For instance, in the case of entropies  $S_B$  and  $S_{\pm}$ , they pertain to the class (c, d) = (1, 1). It is possible that other entropic forms  $g(\rho)$  could belong to the equivalence class (1,1), although to our knowledge no others than  $S_{\pm}$  have been proposed with the particularity of fulfilling axioms SK1-SK3 while a violation of SK4 arises at some scale. Even if such were the case, those entropies would provide nearly the same corrections to BG for the reason that  $S_{\pm}$  already draw nonequilibrium systems with stable long-term fluctuations, implying universality according to the superstatistics formulation.

Inspired by the axiomatic classification made in Ref. [15] another critical exponent was introduced in order to take into account the time scaling of time-dependent probability distributions [18]. Those probabilities are encountered in stochastic processes, for instance, in the anomalous diffusive phenomena described by the generalized Fokker-Planck equations (FPEs) useful in describing the movement of particles and living subjects [19–21]. The generalized Fokker-Planck equations and the corresponding asymptotic scalings were derived for several generalized entropic forms in Refs. [18,22]. In this paper we are to adopt such an approach and derive the Fokker-Planck equations associated with  $S_{\pm}$ .

Below we are to review the corresponding asymptotic analysis for the entropic forms that depend only on the probability [12,23,24]. These entropies, as the ones considered in Refs. [15,18], do not fulfill SK4 but we have surprisingly found that they possess the same asymptotic exponents as the BG entropy; namely, they fall into the same equivalence class. Besides the asymptotic analysis, we also construct the generalized FPEs in the Fickian form and make a general analysis of their solutions and scaling behavior. Moreover, it is worth mentioning that the kind of Fokker-Planck equations derived here emerge, as well, in several stochastic processes studied in biological sciences [19,20]. We will also show that the usual FPE is consistently recovered from our generalizations.

The rest of our discussion is organized as follows. In Sec. II we formally introduce the generalized entropies  $S_{\pm}$  to be considered in this paper. Based on the axiomatic classification proposed in Ref. [15], we briefly analyze these entropies in the asymptotic limit to show that they belong to the same equivalence class as BG entropy [25]. In Sec. III, we derive the generalized FPEs corresponding to the generalized entropies  $S_{\pm}$ . In Sec. IV, we compute numerical solutions to FPEs and discuss some properties of their stationary solutions. The anomalous diffusion portrayed by these equations is also discussed. Finally, Sec. V is devoted to conclusions and a general discussion of our results.

# **II. GENERALIZED ENTROPIC FORMS**

In this section we introduce a generalized family of entropies on the basis of the asymptotic analysis made in Ref. [15] that allows us to establish a classification of entropies in terms of scaling exponents. Particular cases of especial interest in this paper are surveyed.

The kind of generalized entropies to be considered in this paper adopt the general form [26]

$$S[\rho] = \sum_{i}^{W} g(\rho_i), \qquad (1)$$

where *W* represents the number of states with corresponding densities of probability denoted by  $\rho_i$ , such that  $\rho_i \in \rho$  for i = 1, ..., W, and *g* is a generic entropic form. The notation  $S[\rho]$  signifies the evaluation of *S* over the whole set of  $\rho$ .

As stated by the authors in Ref. [15], it is possible to establish a distinction and a classification of entropies of the general form (1) by observing the SK axioms [16,17]. For instance, if  $S[\rho]$  is such that it does satisfy the four SK axioms and is of the form (1), then it corresponds univocally to BG entropy  $S_B$ , in which case  $g(\rho) = -\rho \ln \rho$ .

Yet, entropies associated with strong interacting systems are known to satisfy SK1–SK3, whereas there is a violation to SK4. Remarkable examples of this kind of entropies are, for instance, the ones of Tsallis, Rényi, and Kaniadakis (for a general review, we encourage the reader to see the classification in Ref. [15] and its generalization [25]). In this paper, however, we limit our analysis to the two entropies

$$S_{\pm}[\rho] = \sum_{i}^{W} \left( \pm 1 \mp \rho_{i}^{\pm \rho_{i}} \right), \tag{2}$$

and by association with the general form of entropy (1) the respective entropic forms of  $S_{\pm}[\rho]$  are identified as

$$g_{\pm}(\rho) = \pm 1 \mp \rho^{\pm \rho},\tag{3}$$

and it can be shown that they satisfy SK1–SK3 [25]. Furthermore, these particular forms arise in the formalism of superstatistics [11,12] by considering local temperature fluctuations averaged by a specific real distribution  $H(\beta)$ , addressing to a generalized Boltzmann factor

$$B(E) = \int_0^\infty d\beta \, H(\beta) e^{-\beta E},\tag{4}$$

where E is the energy of a microstate associated with each of the considered cells. From the integral transform (4), we can deduce generalized entropies of the form (1) through the formula [27]

$$g(\rho) = \int_0^{\rho} dx \, \frac{E(x) + \delta}{1 - E(x)/E^*},\tag{5}$$

where E(x) is the inverse function of  $B(E) / \int_0^\infty dE' B(E')$ and  $E^* = \max\{E(x)\}$ . In particular, Eq. (3) is recovered by characterizing  $H(\beta)$  with a generalized gamma distribution; in other words,  $S_{\pm}$  have a well defined thermodynamic limit.

We are to discuss ahead how the properties adjudicated to the entropies (2) serve as a motivation for considering them in modeling nonequilibrium effects; for instance, whenever an equipartition configuration is assumed, these entropies differ from the BG entropy when the number of accessible states (microstates) W is considerably small [25]; nonetheless, when W is large, the three entropies are asymptotically equivalent.

As we have already mentioned, several generalized entropies have been proposed in order to model a number of complex systems, provided they do not behave in accordance with BG statistics. Several of these general entropies, satisfying only SK1–SK3, were originally classified in terms of their asymptotic properties in Ref. [15] whereas a wider class of entropies, comprising  $S_{\pm}$ , can be found in Ref. [25]. In the following, we are to explain the asymptotic laws that give rise to the universal exponents; then our purpose is to state to which equivalence class belong the generalized entropies defined in Eq. (2).

For systems characterized by any general entropic form  $g(\rho)$  depending only on the (density of) probability  $\rho$  (and even on other parameters), such that the axioms SK1–SK3 (except SK4) are all fulfilled, the first scaling function is given by [15]

$$f(z) = \lim_{\rho \to 0} \frac{g(z\rho)}{g(\rho)} = z^c, \quad (0 < z < 1), \tag{6}$$

with  $0 < c \leq 1$ . The associated asymptotic law is given by

$$\lim_{W \to \infty} \frac{S_g(\lambda W)}{S_g(W)} = \lambda^{1-c}.$$
 (7)

The second asymptotic law is found by substituting  $\lambda \rightarrow W^a$ , hence the resulting scaling function is defined as

$$h_c(a) = \lim_{\rho \to 0} \frac{g(\rho^{1+a})}{\rho^{ac}g(\rho)} = (1+a)^d, \quad (a, d \in \mathbb{R}).$$
(8)

Every entropy is characterized by the pair of numbers (c, d); in consequence those entropies with the same (c, d) belong to the same equivalence class. In particular for the entropic form  $g(\rho) = -\rho \ln \rho$  that corresponds to BG entropy, Eqs. (6) and (8) lead to (c, d) = (1, 1). Likewise, the asymptotic constants related to  $S_{\pm}$ , with entropic forms (3), are given in the case of  $S_{\pm}$  by

$$\lim_{\rho \to 0} \frac{1 - (z\rho)^{(z\rho)}}{1 - \rho^{\rho}} = z,$$
(9)

where l'Hôpital's rule is used to easily calculate this limit, determining the first constant c = 1 [see Eq. (6)]. Analogously, the second exponent is given by

$$\lim_{\rho \to 0} \frac{1 - \rho^{(1+a)\rho^{1+a}}}{\rho^a (1 - \rho^\rho)} = (1+a), \tag{10}$$

where this implies that d = 1. Then, we have that for  $S_+$  the scaling exponents are (c, d) = (1, 1); we have the same result for  $S_-$ . Therefore, both entropies belong to the same equivalence class as that of the BG entropy. It is in this sense that the entropies  $S_{\pm}$  are consistently, asymptotically equivalent to the BG entropy (or to the Shannon entropy in the context of information theory).

The scaling exponents c and d are of such importance for they enable a classification of generalized entropies according to their asymptotic behavior. The exponent d is responsible for the regime of stability adjudicated to an entropy. With respect to the exponential c, it can assume values in (0,1], otherwise the axioms SK2 or SK3 could be compromised [15].

Even more, the exponential c has a further implication. It was noted by the authors in Ref. [18] that c can be interpreted as a degree of deviation from a stochastic (Markovian) system in a stationary state—in turn characterized by c = 1. Yet, the question whether this exponential may also participate in the classification of dynamical systems has an affirmative response.

The idea has its origin in the known fact [28] that transport phenomena can be phenomenologically classified in accordance with the rescaling of a given distribution  $\rho(\mathbf{x}, t)$  by a factor  $\tau^{-\gamma}$ , under the condition that

$$\rho(\mathbf{x},t) = \tau^{-\gamma} \rho\left(\frac{\mathbf{x}}{\tau^{\gamma}}, \frac{t}{\tau}\right)$$
(11)

remains invariant [29,30], leading to the dynamical equation in terms of the flux J(x, t):

$$\boldsymbol{\tau}^{-(\gamma+1)}\partial_t \rho = -\boldsymbol{\tau}^{-\gamma(c+2)} \nabla \cdot \mathbf{J},\tag{12}$$

which is an FPE as long as both members are equivalent [18,22,31], hence  $\gamma = 1/(c+1)$  has to be fulfilled. The result suggests the relevance of *c* in the classification of dynamical systems.

Inspired by these arguments, our purpose from now on is to find the generalized FPEs corresponding to  $S_{\pm}$  by following the methods stated in Ref. [18]. Since  $S_{\pm}$  belong to the equivalence class (1,1), the resulting FPEs will coincide asymptotically with the linear FPE that governs the dynamics of a memoryless, short-range interaction process, i.e., with  $\gamma = 1/2$ . However, as will be evident soon, there is a regime where nonlinear effects arise naturally, which suggests their contribution may be in charge of some interesting consequences.

# **III. GENERALIZED FOKKER-PLANCK EQUATIONS**

Let us begin by stating the general form of the FPEs that we are to consider hereafter, namely,

$$\partial_t \rho = \nabla \cdot [D(\rho)\nabla F[\rho] + \nu \chi(\rho)\nabla \Phi], \tag{13}$$

where  $D(\rho)$  and  $\nu \chi(\rho)$  are the diffusion and drift (or mobility) coefficients,  $F[\rho]$  is an effective density, and  $\Phi(\mathbf{x})$  is the potential field where the Brownian particles are assumed to move. Alternatively, Eq. (13) can also be put in its conservative Fickian form by replacing the right-hand side by the negative divergence of an effective current of probability **J** as

$$\partial_t \rho = -\nabla \cdot \mathbf{J}$$
  
=  $-\nabla \cdot (\mathbf{J}_{\text{diffusion}} + \mathbf{J}_{\text{drift}}).$  (14)

To get a handle in the following discussion we are to make use of both representations.

In the following discussion we focus on the general case in three plus one dimensions; however, for a number of problems as in Sec. IV, we limit our attention to the *x* axis as the only direction of movement,  $\rho(\mathbf{x}, t) = \rho(x, t)$ ; then FPE (13) becomes

$$\partial_t \rho(x,t) = D \partial_x^2 F[\rho(x,t)] - D \nu \partial_x \{ \chi[\rho(x,t)] \partial_x \Phi(x) \},$$
(15)

having assumed  $D(\rho) = D = \text{const}$  as well as the presence of an attractive field  $\Phi(x) \rightarrow -D\Phi(x)$ . Also note that the term  $\partial_x^2 \rho(x, t)$  in the usual diffusion model has been replaced by  $\partial_x^2 F[\rho(x, t)]$  to account for anomalous (or generalized) diffusion [18,22].

Now, we are interested in pursuing an entropic formulation to derive FPEs of the form (13); to this aim we need the notion of generalized logarithm  $\Lambda(\rho)$  [32]. This function permits us to construct effective densities  $F[\rho]$  that shall be used to compute the spatial variations of the corresponding FPE (13). In fact, each term in Eqs. (13) and (14) is uniquely characterized by the entropy functional; hence there exists a unique FPE for each entropy. For instance, from the standard BG entropy, one obtains the usual FPE.

In what follows we are to make use of entropies (2) to derive FPEs that are thermodynamically compatible with the usual mean-field FPE (as for BG), although there exists a regime where our models differ from the standard case for the reason that they possess nonlinear terms the contribution of which accounts for anomalous diffusion. This is due to the fact that  $S_{\pm}$  are nonextensive entropies that describe systems slightly out of thermodynamic equilibrium. Then, it seems reasonable to suggest that the resulting FPEs may describe the early stages of processes that tend to balance their inner influences in order to reach the equilibrium as a function of time.

To proceed, the first ingredient we need is to variate a functional of the form

$$\Upsilon = g(\rho) - \alpha \rho - \beta w(\rho) E, \qquad (16)$$

where *E* is the internal energy of the system,  $\alpha$  and  $\beta$  are Lagrange multipliers, and  $w(\rho) \in C^1$  is a monotonically increasing function univocally related to the entropy inasmuch as statistical completeness is guaranteed. It can be computed directly by solving for E(y) from the effective Boltzmann factor (4) and then substituting into the formula

$$w(x) = (1 + \alpha/E^*) \int_0^x \frac{dy}{1 - E(y)/E^*},$$
 (17)

where  $\alpha = -\int_0^1 dy E(y)$  and  $E^*$  is the minimum value of E(y) (see [27]). Note that the MaxEnt functional (16) consists of the entropic form  $g(\rho)$  subject to the constraints of normalization of probability (second term) and conservation of energy (third term); from the theory of ensembles such a functional represents a canonical configuration.

Differentiating (16) with respect to  $\rho$  and equating to zero, the generalized logarithm is identified as  $\Lambda(\rho) \equiv E$ , that is,

$$\Lambda(\rho) = E = \frac{G'(\rho) - \alpha}{\beta w'(\rho)},$$
(18)

subject to the conditions  $\Lambda(1) = 0$  and  $\Lambda'(1) = 1$ .

Once the generalized logarithm has been constructed, and assuming that the stationary condition  $\partial_t \rho = 0$  is fulfilled, it is possible to compute explicitly the effective density  $F[\rho]$  via the formula [18]

$$F[\rho] = -\beta \int_0^\rho dx \, x \partial_x \Lambda(x). \tag{19}$$

This functional is, in general, nonlinear in  $\rho$  and possesses the needed information to account for the changes in

TABLE I. Some models that can be characterized through the mean-field Eq. (13).

Model	$D(\rho)$	$F[\rho]$	νχ(ρ)	$\Phi_{\text{ext}}$
Smoluchowski	D	ρ	νχ	Φ
Debye and Hückel	D	ρ	νχ	$\Phi_{\text{electric}}$
Diffusion	D	ρ		0
Porous medium	D	$\rho^{\gamma}$		0
Plastino	D	$ ho^{\gamma}$	$\nu\chi(\rho^{\gamma})$	Φ

diffusion throughout the space. The particular case  $F[\rho] = \rho$  corresponds to the mean-field FPE that describes regular (nonanomalous) diffusion as long as the accompaniment coefficient is constant.

Even more, as we mentioned already, the diffusion and drift terms in Eq. (14) are uniquely determined by the entropy. For the diffusion term, the recipe to compute the effective density  $F[\rho]$  is given by formula (19). It remains to find the appropriate drift coefficient that modulates the intensity of the force  $\nabla \Phi$ . To this aim we use the relation provided by Chavanis [22]:

$$-g''(\rho) = \frac{D(\rho)}{\nu\chi(\rho)} \ge 0, \tag{20}$$

where  $g(\rho)$  is the entropic form given by (1). For example, in the particular case of BG entropy, one gets  $-g''(\rho) = -1/\rho$ . Then, if one assumes a constant diffusion coefficient  $D(\rho) = D$ , it follows that the drift coefficient is proportional to  $\rho$  and the (mean-field) current of probability reads  $\mathbf{J} = -[D\nabla\rho + \nu'\rho\nabla\Phi]$ , with  $\nu'$  a constant.

Further models can be obtained from the mean-field equation (13); we mention a few of them in Table I.

### A. Our model

We are now in the position to derive the corresponding FPEs to the nonextensive entropies  $S_{\pm}$ . These differential equations are, in general, nonlinear, although they will become mean field and linear once the processes of generalized diffusion and drift have attained the equilibrium—at this stage the system will be described by a stationary state.

To begin with, we are to obtain the generalized logarithms  $\Lambda_{\pm}(\rho)$  that are associated with  $S_{\pm}$  via the MaxEnt functional (16). In this case the entropic form  $g(\rho)$  has to be characterized by (3) and, from formula (17), the proper weighting functions have to be characterized by

$$w_{\pm}(\rho) = \rho^{\rho \pm 1}$$

A straightforward calculation leads to the generalized logarithms

$$\Lambda_{+}(\rho) = \frac{1}{\beta} \frac{1 - \rho^{-\rho} + \ln \rho}{1 + \rho + \rho \ln \rho},$$
(21)

$$\Lambda_{-}(\rho) = \frac{1}{\beta} \frac{1 - \rho^{\rho} + \ln \rho}{1 - \rho - \rho \ln \rho}.$$
(22)

With the aid of the generalized logarithms  $\Lambda_{\pm}(\rho)$  we can now compute the effective densities  $F_{\pm}[\rho]$  as follows. In the case of  $F_{+}[\rho]$ , one merely substitutes (21) into (19) and performs the integration to obtain

$$F_{+}[\rho] = \int_{0}^{\rho} dq \left( \frac{1 + x^{1-x} + x^{1-x} \ln x}{1 + x + x \ln x} - \frac{(\ln x + 2)(x - x^{1-x} + x \ln x)}{(1 + x + x \ln x)^{2}} \right)$$
$$= \rho + \frac{\rho^{2}}{4} + \frac{\rho^{3}}{27} + \frac{\rho^{4}}{128} + \cdots$$
(23)

In an analogous way, for the other case we have

$$F_{-}[\rho] = \int_{0}^{\rho} dx \left( \frac{1 - x^{1+x} - x^{1+x} \ln x}{1 - x - x \ln x} + \frac{(\ln x + 2)(x - x^{1+x} + x \ln x)}{(1 + x + x \ln x)^{2}} \right)$$
$$= \rho - \frac{\rho^{2}}{4} + \frac{\rho^{3}}{27} - \frac{\rho^{4}}{128} + \cdots$$
(24)

Note that the nonlinear terms are monotonically subdominant provided the density  $\rho$  is normalized and the coefficients diminish progressively; therefore the contribution of these terms becomes negligible, especially whenever the density  $\rho$  comprises a large number of accessible states or, as will be evident soon, after the system has reached the equilibrium.

It only remains to compute the effective drift terms  $\nu \chi_{\pm}(\rho)$  to complete our FPEs. To this end we assume that *D* and  $\nu$  are constants. Then, by substituting (3) into (20) and integrating, we get

$$\chi_{\pm}(\rho) = \pm \frac{\rho^{1 \mp \rho}}{(\ln \rho + 2)\rho \ln \rho + \rho \pm 1},$$
 (25)

that completes the procedure to finally write the nonlinear FPEs that govern the dynamical fluctuations of the effective densities  $F_{\pm}[\rho]$ , namely,

$$\partial_t \rho = -\nabla \cdot \mathbf{J}_{\pm}$$
  
=  $\nabla \cdot [D \nabla F_{\pm}[\rho] + \nu \chi_{\pm}(\rho) \nabla \Phi],$  (26)

noting that the standard Smoluchowski equation (see Table I) is directly recovered at first order approximation, namely,  $F_{\pm}[\rho] = \rho + O(\rho^2)$  and  $\chi_{\pm}(\rho) = \rho + O(\rho^2)$ .

In this paper we limit our interest to external potentials  $\Phi$  as for Eqs. (26). However, interesting aspects can take place when the potential arises self-consistently by means of the interaction of particles themselves (see, for instance, [33]), in which case the resulting potential is given by  $\Phi = \int d^3x' F[\rho']\phi'(|\mathbf{x} - \mathbf{x}'|)$ , with  $\phi'$  the interaction potential.

The conservative representation of (26) in terms of the effective current  $\mathbf{J}_{\pm}$  must guarantee the conservation of the mass distribution  $M = \int d^3x \rho$  such that the normal component of each  $\mathbf{J}_{\pm}$  vanishes at the boundary; hence by simply application of the divergence theorem to (26) one gets

$$\partial_t \int_V d^3 x \, \rho = -\oint_S d\mathbf{S} \cdot \mathbf{J}_{\pm}.$$
 (27)

One can note from Eq. (27) that the generalized current vanishes for systems the mass of which does not depend on time, hence leading to stationary solutions. Yet, in a more general scenario, when statistical systems are thermodynamically open they become subject to the exchange of energy and matter with the environment, in which case the analysis of the solutions can be put in terms of the free energy A in turn having the form of a Lyapunov function for any potential (see [22,33]). Unfortunately, regarding the FPEs expressed in Eq. (26) we cannot give general closed solutions in the presence of a potential, but only semianalytical solutions when the potential has been neglected—as presented in the section below– -, but instead in Sec. IV some numerical solutions are studied and discussed for some idealized physical models.

## **B.** Generalized diffusion equation

As a special case of the FPE (26), in this section we study the generalized diffusion equation arisen by neglecting the drift term, that is,

$$\partial_t \rho = \nabla \cdot (D \nabla F_{\pm}[\rho]); \qquad (28)$$

these models exhibit the interesting aspect of containing the usual diffusion model plus a diffusion-drift term [see Eq. (34)], capable to produce anomalous diffusion in some regimes, as we are to discuss ahead.

Notice that the effective densities in Eqs. (23) and (24) can also be expressed in the form

$$F_{\pm}[\rho] = \int_{0}^{\rho} dx R_{\pm}(x);$$
(29)

following this notation the generalized flux becomes

$$\mathbf{J}_{\pm}(\rho) = -D\nabla \left[\int_{0}^{\rho} dx R_{\pm}(x)\right],\tag{30}$$

which is proportional to the gradient of the chemical potential  $\mu(\rho)$  [34], namely,  $\mathbf{J}_{\pm}(\rho) = -D\nabla\mu_{\pm}(\rho)$ . Furthermore, the chemical potential  $\mu(\rho)$  comes from the gradient of some function  $f[\rho]$ , namely,  $\mu(\rho) = f'(\rho)$  (see [34]). Hence we can identify  $f'_{\pm}[\rho] = \int_0^{\rho} dx R_{\pm}(x)$ ; therefore the continuity equation transforms into

$$\partial_t \rho = \nabla [DR_{\pm}(\rho) \nabla \rho]; \qquad (31)$$

from this expression we can recognize the generalized diffusion coefficient of our model:

$$D_{\pm}(\rho) = DR_{\pm}(\rho); \qquad (32)$$

the standard diffusion coefficient is recovered at first order approximation from the effective density in either Eq. (23) or Eq. (24).

Please note that the generalized, nonlinear diffusion equation (31) corresponds to the generalized FPE derived from the entropies  $S_{\pm}$ . It can be expressed in terms of  $f_{\pm}[\rho]$  as

$$\partial_t \rho = D\nabla [\partial_{\rho\rho} f_{\pm}[\rho] \nabla \rho]. \tag{33}$$

At this point the reader can be aware that the linear diffusion equation is recovered by considering the first term in the expansions (23) and (24), yet an interesting aspect arises from simply observing that for  $S_{\pm}$  we have  $f_{\pm}[\rho] = \rho^2/2 \pm \rho^3/12 + \cdots$ ; therefore the generalized diffusion equation becomes

$$\partial_t \rho = D(\triangle \rho + \varphi(\rho) \nabla \rho), \tag{34}$$

where  $\triangle$  is the Laplacian operator and  $\varphi(\rho)$  contains all the  $\rho$ -dependent terms in  $f''(\rho)$ . Additionally, we notice that (I)

the generalized diffusion equation (34) induces in a natural way a density-dependent drift term weighted by  $\varphi(\rho)$  and (II) the form of the drift term can be connected to congregation diffusion models which take into account interactions that tend to form aggregates or to separate the particles [19], as we are to discuss in Sec. IV B.

# **IV. NUMERICAL SOLUTIONS**

In this section, we are to present numerical experiments based on the nonlinear FPEs (26) being characterized by some specific external potentials  $\Phi = \Phi_{ext}$ . To serve as comparison with other models we also look for effective potentials  $\Phi_{eff}$ that approximate the behavior prescribed by Eqs. (26). We shall distinguish between the solutions of each FPE in Eq. (26) using the notation  $\rho_+$  and  $\rho_-$ ; when there is no risk of confusion we simply write  $\rho$ . Additionally we explore generalized diffusivity models and contrast them with the chemotaxis-aggregation approach studied in Ref. [19]. Finally we consider a transient diffusivity modification into our models that results in agreement with experiment and with the respective phenomenological model whenever long relaxation times are appointed in our nonequilibrium approach. In all of our numerical simulations we have fixed  $D = \nu = 1$ .

# A. Beyond the mean field

In general, Eqs. (26) are non-mean-field models for a set of random variables the values of which are such that the asymptotic limit,  $\rho \rightarrow 0$ , is far below their regime. Otherwise one is allowed to use the mean-field approximation,  $F_{\pm}[\rho] \approx$  $F_{BG}[\rho] = \rho$ , related to the BG entropy. This fact becomes evident from the expansion of the generalized currents  $\mathbf{J}_{\pm}$  in Eq. (26), yielding

$$\mathbf{J}_{\pm} = -[D\nabla\rho + v\rho\nabla\Phi] \mp \left[\frac{1}{4}D\nabla\rho^{2} - v\rho^{2}\nabla\Phi\right] \\ - \left[\frac{1}{27}D\nabla\rho^{3} + v\rho^{3}\nabla\Phi\right] + \cdots;$$
(35)

the first term is directly related to the standard case  $J_{BG}$ , whereas higher-order terms can be interpreted as a result of advection and generalized forces. Other terms arising from nonlinear combinations of variables have been kept aside from the expansion since they belong to higher-order statistics, used in the estimation of skewness and kurtosis, for instance.

We now would like to compare the behavior between the corresponding models to  $S_{BG}$  and  $S_{\pm}$ . To this end we have computed numerical solutions in one plus one dimensions using a linear potential  $\Phi = x$ , for the non-mean-field Eqs. (26) as well as for the particular mean-field case.

The results are shown in the above panel of Fig. 1, where a stronger influence of the drift terms for both  $\rho_+$  and  $\rho_$ than the one related to  $\rho_{BG}$  is observed. Hence, it becomes natural to find higher velocities of propagation for  $\rho_{\pm}$  than for  $\rho_{BG}$ , a situation depicted in the respective phase portrait, in the bottom panel. This fact can be interpreted as the influence of the additional repulsive forces considered in the non-meanfield models, thus obliging the system to move faster towards the diffusion as compared with the customary equation of motion.



FIG. 1. (a) Normalized density profiles belonging to the nonmean-field Eqs. (26) as well as the particular mean-field case  $F_{BG} = \rho$ . Solutions were computed using a linear potential  $\Phi = x$ . (b) Phase portrait corresponding to the solutions depicted in panel (a). The presence of the drift term induces a higher propagating velocity for  $\rho_{\pm}$  than for  $\rho_{BG}$ .

However, if the corresponding BG model were individually characterized by an effective potential  $\Phi_{eff} = 1.45x$ —which means subject to a stronger repulsive field force while keeping the potential  $\Phi = x$  for the  $S_{\pm}$  models—then the dynamical behavior of  $\rho_{BG}$  would approximately coincide with the behavior of  $\rho_{\pm}$  but under the influence of  $\Phi$ ; in that case their centers of mass would nearly agree. This situation is shown



FIG. 2. (a) Density profiles. As for the BG model, it moves under the influence of an effective field  $\Phi_{\text{eff}} = 1.45x$ , while the  $S_{\pm}$  associated models move in the field  $\Phi = x$ . (b) Phase portrait corresponding to the solutions depicted in panel (a). The three densities feel approximately the same repulsive force; note that their diffusion velocities (below zero) are in agreement with their respective behavior, higher for  $\rho_+$  and lower for  $\rho_-$ .

in Fig. 2, where one can observe the spatial evolution of the density profiles.

#### **B.** Anomalous diffusion

In this section, we are to compare our diffusion models (28)—alternatively represented as (33) or (34)—with the nonlinear, diffusion aggregation prototype proposed in Ref. [19] for the study of random walks of length  $\lambda$ , average time  $\tau$ , and



FIG. 3. In the plot we show the effective densities (23) and (24) truncated to second order, as well as the density of aggregation as for Eq. (36). The latter case is characterized by  $\kappa = -2$  and  $\omega = 7/5$ . Note that when the aggregation model exhibits a critical density  $\omega = 9/2$  and  $\kappa = 1/4$  the generalized diffusion model associated with  $S_+$  is recovered.

a maximum degree of attraction bias  $k_0$ , which reads

$$\partial_t \rho = \Delta \left[ D\rho - \kappa \rho^2 + \frac{2\kappa}{3\omega} \rho^3 \right]$$
$$= \Delta F_{agg}, \qquad (36)$$

where  $\kappa = k_0 \lambda^2 / \tau$  and  $\omega$  stands for the critical density that turns the movement from attractive into repulsive.

To outperform this comparison we are to consider only the first three terms in the expansion of the effective densities  $F_{\pm}$ , (23) and (24) (that is,  $F_{\pm}[\rho] \approx \rho \pm \rho^2/4 + \rho^3/27$ ), for the reason that the nonlinear terms in Eq. (36) obey the same power law as those for the truncated  $F_{\pm}$ . Our diffusion models exhibit nonlinear diffusion for regions of space where the system experiences a sort of faint interactions before reaching the equilibrium, in other words, those regions where the confined constituents are arranged such that the resulting interaction forces are not entirely negligible.

The behaviors of the effective densities F for the models (33) and (36) are shown in Fig. 3. Please note that, regarding the aggregation model, two stages are exhibited if one chooses the particular values  $\kappa = 2$  and  $\omega = 5/4$ . In that case, for some regions of  $\rho$  the dynamical description will be linked to subdiffusion phenomena, while for other regions of  $\rho$  the transport picture will behave anomalously, corresponding to a congregative mode of movement [19]. The latter is a typical case of strong congregation given that  $F_{agg}$  has a minimum and a maximum, hence differing from weak congregation for which there is only one extremal point. Each of these extrema,  $F'_{agg} = 0$ , are equilibrium points.



FIG. 4. Numerical solutions of Eqs. (33) and (36). Density profiles at t = 4 in dimensionless time units. As for the aggregation model (36) we have selected  $\kappa = -2$  and  $\omega = 7/5$ .

From Fig. 3 one can also observe that  $F_{\pm}$  is devoid of global extremal points, which suggests that Eqs. (28) cannot describe strongly congregation movements for the reason that  $F'_{\pm} > 0$  for any region of  $\rho$ . Yet, whether congregations can arise or not depends entirely on the aggregative force  $\kappa \omega$ . As an example, the effective densities  $F_{\pm}$  are related to the forces  $\kappa \omega = \pm 9/8$ , hence showing a repulsive and an attractive behavior, respectively, as shown in Fig. 3.

We now would like to compare the evolution of the density profiles for each case by numerically solving the differential models (28) and (36). To compute the solutions, we have considered normalized, stretched Gaussians (in terms of the exponential functions  $\exp_{\pm}$  defined in the Appendix), as initial conditions, and stretched cosines as boundary conditions. These stretched cosines are defined as  $\cos_{\pm}(x) =$  $\frac{1}{2}[\exp_{\pm}(ix) + \exp_{\pm}(-ix)]$ . The numerical solutions are computed using the method of lines with a spatial domain  $x \in$ [0, 10] and a temporal domain  $t \in$  [0.01, 10]. The resulting density profiles are shown in Fig. 4.

In the realm of ecology and biology, aggregation and chemotaxis models receive a wide application [20]. In such contexts the nonlinear terms in the effective density functions,  $F_{agg}$  or  $F_{\pm}$ , are regarded as effective fluctuating forces resulting from the interaction between the individual and its surrounding. The reason is that the movement of a given animal species through a certain distance could be facilitated (or impeded) by the current conditions of the environment (predators, food, climate). Nonetheless, when the effect of the interactions is incorporated in the dynamical description, the behavior of the species or individuals could be seen as externally influenced.

For instance, the parameter  $\kappa$  in Eq. (36) indicates the tendency to move away from conspecifics, if  $\kappa > 0$ , or to move towards conspecifics, if  $\kappa < 0$ . By direct comparison, the effective density  $F_+$  characterizes an attractive movement between conspecifics for a fixed critical density  $\omega < 0$ , whereas  $F_-$  describes a repulsive movement for  $\omega > 0$ . Furthermore, notice that, as for  $F_+$ , the nonlinear terms  $\rho^2/4 + \rho^3/27$  are always positive, thus concentring high densities. On the other hand, for the case  $F_-$ , the nonlinear terms  $-\rho^2/4 + \rho^3/27$  are always negative, meaning they represent low densities. In practice, however, organisms usually aggregate at low densities and avoid them at high densities [19], meaning there is a density-dependent response that can be modeled with the

diffusion-aggregation Eq. (36). In particular, respecting  $F_{agg}$  as shown in Fig. 4, the nonlinear terms are  $-2\rho^2 + 40\rho^3/21 < 0$  in the interval  $\rho \in [0, 1]$ , although unlike  $F_-$  these do not exhibit a monotonically decreasing behavior, meaning that there is a slight tendency to aggregate even at low densities. Our numerical tests show that regarding the pair of parameters  $\kappa = -2$  and  $\omega = 7/5$  characterizing Eq. (36) the probability of finding an individual at point x < 3 at time t = 4 is less than that estimated by the other two models,  $\rho_+$  and  $\rho_-$  (while  $\rho_{agg}$  is appreciably greater than  $\rho_{\pm}$  for 3 < x < 8). This is a direct consequence of the nonmonotonicity portrayed by the nonlinear terms in  $F_{agg}$ , which predict that there could be a certain distance at which the individuals congregate or aggregate regardless of the seminal type of movement.

### C. Transient diffusion

Alternatively, one can even explore transient diffusivity models characterized as in Eq. (33); to this aim let us make the substitution  $D\eta(\rho) \rightarrow D_0 + D_+(t)$  into the model characterizing the density  $F_+$  in Eq. (23).

In what follows, we want to analyze the transport of excited carriers considering an electron mobility  $\mu$  with fundamental charge *e*. Hence the Einstein relation [35] becomes  $D_0 = \mu k_B T_0/e$ , where  $k_B$  is the Boltzmann constant and  $T_0$  is the environment temperature (for numerical purposes 300 K). On the other hand, when the excess energy of the excited carriers is taken into account, there arises the transient diffusivity term,  $D_+(t) = \mu k_B T^*(0) \exp_+(-t/\tau)/e$ , where  $T^*(0)$  is the initial carrier temperature ( $T^*(0) \gg T_0$ ) and  $\tau$  is the relaxation time (see [36]).

In recent years, scanning ultrafast electron microscopy has been successfully implemented to observe a transient superdiffusivity behavior in the dynamics of electrons and holes in Si after excitation with a short pulse laser [37]. The phenomenological model introduced by the authors reads

$$\partial_t \rho_c = [D_0 + D^*(t)] \nabla^2 \rho_c, \qquad (37)$$

where  $\rho_c$  denotes the distribution associated with the carriers and  $D^* = \mu k_B T^*(0) \exp(-t/\tau)/e$ . Furthermore, as for definitions of the stretched exponentials  $\exp_{\pm}$  (see the Appendix) one is aware that  $\exp_{+}(-t/\tau)$  decays slower than  $\exp(-t/\tau)$ , although both vanish after a brief relaxation time  $\tau$ .

We solved numerically Eqs. (33) and (37) using different initial conditions. in Ref. [37] Eq. (37) is configured with a relaxation time  $\tau = 77$  ps and an initial carrier temperature  $T^*(0) = 4 \times 10^5$  K when regarding electrons, and  $\tau = 161$  ps and  $T^*(0) = 2.7 \times 10^5$  K for holes. Here we set these same



FIG. 5. (a) Normalized distributions characterizing the transport of excited carriers. (b) Square mean deviation for transient diffusivity observed from noninteracting carriers  $\rho_c$  and for interacting carriers  $\rho_+$ .

values as for Eq. (37) but we are to choose different values for Eq. (33).

In case of holes, we have considered an initial temperature  $T^*(0) = 2.16 \times 10^5$  K and a relaxation time  $\tau = 40$  ns, i.e., more than 300 times the relaxation time originally adjusted for model (37). The results are shown in the top panel of Fig. 5. Notice that the behavior of both distributions as well as the square mean deviation, bottom panel, is roughly the same for both cases, exhibiting a transient superdiffusivity that increases monotonically in both models at early times (less than 250 ps); eventually, as time elapses, a steady-state diffusivity is attained.

Yet, the manifested behavior of Eq. (33) is a consequence of its high relaxation time if compared with the values given for models in Ref. [37]. The reason is that this parameter is associated with the time that the sample needs to reach the equilibrium with the medium after the excitation with the laser pulse. Recall that Eq. (33) comes from a nonequilibrium background, involving nonlinear forces and other interactions that have been neglected in Eq. (37); thus our model inherently needs a larger amount of time to reach the equilibrium. However, for higher laser intensities feeding the sample, the electron-electron interactions would not be inappreciable anymore and a description provided by Eq. (37) alone might fall into controversial results. Indeed, our model has, among its attributes, the flexibility to describe a nonequilibrium stage for early times, converging on the region of steady states for larger periods of relaxation time.

## **V. CONCLUSIONS**

We have pursued the entropic derivation of FPEs proposed in Refs. [18,22] to obtain the two generalized FPEs (26) associated with the nonextensive entropies  $S_{\pm}$ . The resulting models include nonlinear terms which can be also interpreted as corrections to the usual mean-field FPE, either directly derivable from the BG entropy or recovered by truncating Eqs. (26) to first order—see, for instance, the expansion in Eq. (35).

Unlike other nonextensive entropies, the pair of entropies  $S_{\pm}$  is nonparametric, but only depends on the probability; thus its associated Fokker-Planck equations do provide distributions exempt of parameters as well.

Furthermore, as we have shown, these sets of entropies belong to the classes (c, d) = (1, 1) and  $\gamma = 1/2$ , indicating that they are thermodynamically compatible with BG entropy. This is an interesting result, and let us reason that Eqs. (26) provide the suitable corrections to the BG model when regarding a system of few accessible microstates [25]. This argument can be supported by simply noting that the first two nonlinear terms in the series representation of the effective densities  $F_{\pm}[\rho]$  indeed correspond to the corrections introduced in the aggregation prototype of movement  $F_{agg}[\rho]$  (see [19]).

As noted from (26), the potential term is weighted by a function  $\nu \chi_{\pm}$  depending only on the distribution density  $\rho$ . This function is univocally determined from the entropic form, an aspect that deserves consideration since every modified Fokker-Planck equation derived by means of the entropic formulation must take into account the very specific weight to the drift potential in order to be in agreement with the respective stochastic equation.

To compare the dynamical Eqs. (26) with other models, we have also computed numerical solutions portraying different circumstances. In the first place we have found that the weighted potential term in Eq. (26) is equivalent to an effective potential. In particular, we note that the drift term as seen from  $\nu \chi \pm (\rho) \nabla \Phi$  has a subtle but stronger influence on the distribution  $\rho$  than the standard term  $\rho \nabla \Phi$ . This behavior enables us to conclude that for systems characterizing a small number of microstates the degree of heterogeneity is such that the interaction among its constituents produces non-negligible effective forces, which tend to vanish as the sample is increased substantially to enlarge the homogeneity.

The generalized diffusion model (28) displays nonlinear anomalous diffusion. As mentioned above, we have found that these models are directly comparable with the segregation models studied in Refs. [19,20] although derived by other means. We stress that, with respect to Eqs. (28), the nonlinear terms associated with interactions between individuals in the biological context arise naturally as a consequence of the generalized entropies  $S_{\pm}$  (see Fig. 4).

Finally, we have also reproduced numerically the general properties of the distributions that suit the transient diffusion model in Eq. (37) originally proposed in Ref. [37]. In our framework, this model is rewritten in terms of our generalized FPE (33). We have observed interesting deviations in the superdiffusivity regime, mainly in the relaxation time. According to our model, differences in the relaxation time will be due to nonequilibrium effects as well as the intrinsic nonlinearities. It is also observed that the steady state is recovered after the superdiffusivity regime, which is in agreement with the recovering of the BG distribution in the long-time scale [25]. A more complete analysis regarding this interesting model will be reported in a future work.

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TABLE II. Coefficients  $a^{\pm}$ .

	$a_j^+$	$a_j^-$
j = 8	-0.000157095	0.000105402
j = 7	0.00373467	-0.00211934
j = 6	-0.0362676	0.0166679
j = 5	0.186358	-0.0675544
j = 4	-0.546751	0.16867
j = 3	0.905157	-0.317048
j = 2	-0.709322	0.3725
j = 1	0.0228963	0.0147449
j = 0	1	1

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# APPENDIX: COEFFICIENTS FOR GENERALIZED EXPONENTIALS

The generalized exponentials  $\exp_{\pm}$ , are indeed stretched exponentials with no closed form known at present. Instead, a numerical approximation has to be pursued. In this paper we have considered the approximation

$$\exp_{\pm}(-x) \equiv \exp(-x) \sum_{j=0}^{\infty} a_j^{\pm} x^j, \quad a_j^{\pm} \in \mathbb{R},$$
(A1)

the first nine coefficients  $a_i^{\pm}$  of which are given in Table II.

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