

Thermostatistics of Overdamped Motion of Interacting Particles

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We show through a nonlinear Fokker-Planck formalism, and confirm by molecular dynamics simulations, that the overdamped motion of interacting particles at $T = 0$, where T is the temperature of a thermal bath connected to the system, can be directly associated with Tsallis thermostatistics. For sufficiently high values of T , the distribution of particles becomes Gaussian, so that the classical Boltzmann-Gibbs behavior is recovered. For intermediate temperatures of the thermal bath, the system displays a mixed behavior that follows a novel type of thermostatistics, where the entropy is given by a linear combination of Tsallis and Boltzmann-Gibbs entropies.

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Nonlinear Fokker-Planck equations (FPEs) [1] are frequently employed to represent macroscopically physical and chemical systems displaying anomalous diffusion behavior [2]. Scientifically and technologically important examples of such systems include, among others, the flow through porous media [3], the dynamics of surface growth [4], the diffusion of polymerlike breakable micelles [5], and the dynamics of interacting vortices in disordered superconductors [6–8]. A typical nonlinear FPE may be written in the general form [1,9]

$$\frac{\partial P}{\partial t} = -\frac{\partial[A(x)\Psi(P)]}{\partial x} + \frac{\partial}{\partial x}\left[\Omega(P)\frac{\partial P}{\partial x}\right], \quad (1)$$

where the external force $A(x)$ is associated with a potential $\phi(x)$ [$A(x) = -d\phi(x)/dx$], and the analyticity of the potential as well as the integrability of the force are assumed to hold in all space. The functionals $\Psi[P(x, t)]$ and $\Omega[P(x, t)]$ satisfy requirements of positiveness, integrability, and differentiability with respect to $P(x, t)$ [9]. Moreover, in order to preserve the probability normalization for all times, one should impose the probability distribution, together with its first derivative, as well as the product $A(x)\Psi[P(x, t)]$, to be zero in the limits $x \rightarrow \pm\infty$.

An important result associated with nonlinear FPEs is the H theorem and its generalizations [1,9–13]. In the case of a system subjected to an external potential, the H theorem leads to a well-defined sign for the time derivative of the free-energy functional,

$$F = U - \gamma S, \quad U = \int_{-\infty}^{\infty} dx \phi(x) P(x, t), \quad (2)$$

where γ represents a positive Lagrange multiplier and the entropy may be considered in a very general form as

$$S[P] = \int_{-\infty}^{\infty} g[P(x, t)] dx, \\ g(0) = g(1) = 0, \quad \frac{d^2 g}{dP^2} \leq 0, \quad (3)$$

with the condition that $g[P(x, t)]$ should be at least twice differentiable. Considering the FPE (1), for $dF/dt \leq 0$ [9,13], we obtain

$$-\gamma \frac{d^2 g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]}. \quad (4)$$

A relevant outcome of Eq. (4) is that the ratio $\Omega[P]/\Psi[P]$ determines an entire class of FPEs associated with a single entropic form [9,13]. Here we are interested on the following type of nonlinear FPE [14,15]:

$$\frac{\partial P}{\partial t} = -\frac{\partial[A(x)P]}{\partial x} + D\nu \frac{\partial}{\partial x}\left[P^{\nu-1} \frac{\partial P}{\partial x}\right], \quad (5)$$

where D is a constant, ν is a real number, and the functionals in Eq. (1) correspond to $\Psi[P(x, t)] = P(x, t)$ and $\Omega[P(x, t)] = D\nu[P(x, t)]^{\nu-1}$. By substituting these quantities in Eq. (4), integrating and using the conditions (3), one obtains Tsallis entropy [9,16,17], for which

$$g[P] = k \frac{[P(x, t)]^\nu - P(x, t)}{1 - \nu}, \quad (6)$$

where $k \equiv D/\gamma$. Considering an external force $A(x) = -\alpha x$ ($\alpha \geq 0$), the solution for Eq. (5) with initial condition $P(x, 0) = \delta(x)$ is given by the distribution

$$P(x, t) = B(t)[1 + \beta(t)(1 - \nu)x^2]_+^{1/(\nu-1)}, \quad (7)$$

where $[y]_+ = y$, for $y > 0$, and zero otherwise. The time-dependent parameters $B(t)$ and $\beta(t)$ are defined in such a way as to preserve the norm and the form of the distribution for all times [14,15,18]. Equation (7) corresponds exactly to the distribution obtained through extremization of Tsallis entropy Eq. (6), for the energy defined as in

Eq. (2), and under standard constraints of probability normalization. It is important to notice that, by substituting $\nu = 2 - q$ in Eq. (7), one recovers precisely the usual distribution of nonextensive statistical mechanics, known as q Gaussian, as obtained through a more general definition for the internal energy [17].

Additionally, the way in which the system evolves dynamically, as well as its stationary state, provides distinctive signatures of anomalous diffusion behavior. For small times $t \ll 1$, it is possible to show that the diffusion propagation front $x(t)$ dictated by Eq. (5) advances as $\langle x(t) \rangle \propto t^{2/(\nu+1)}$ [13]. In the limit $t \rightarrow \infty$, the system approaches the stationary state given by

$$P_{\text{st}}(x) = B^*[1 - \beta^* x^2]_+^{1/(\nu-1)}, \quad (8)$$

depending on the initial time t_0 , $\beta^* = \beta(t_0)[B^*/B(t_0)]^2$, and $B^* = [\alpha B(t_0)^2/2D\nu\beta(t_0)]^{1/(1+\nu)}$. One should stress that this form of stationary distribution holds for any confining potential $\phi(x)$, by simply replacing in Eq. (8) the term x^2 with $\phi(x)$ [14].

Next we show that the microscopic behavior of a system of interacting particles undergoing overdamped motion is fully compatible with a continuum nonlinear diffusion equation. Moreover, we find that such a continuum formulation for a highly dissipative system corresponds to the FPE (5) with $\nu = 2$. We start by considering the equation of motion for a particle i in a system of N overdamped particles,

$$\mu \vec{v}_i = \sum_{j \neq i} \vec{J}(\vec{r}_i - \vec{r}_j) + \vec{F}^e(\vec{r}_i) + \eta(\vec{r}_i, t), \quad (9)$$

where \vec{v}_i is the velocity of the i th particle, μ is the effective viscosity of the medium, the first term on the right accounts for the interactions among particles, $\vec{F}^e(\vec{r}_i)$ represents an external force, and η corresponds to an uncorrelated thermal noise with zero mean and variance $\langle \eta^2 \rangle = k_B T / \mu$. Here we consider a short-range repulsive particle-particle interaction in the form $\vec{J}(\vec{r}) \equiv G(|\vec{r}|/\lambda)\hat{r}$, where \hat{r} is the unit vector along the axis connecting each pair of particles and λ is a characteristic length of the short-range pairwise interaction.

To obtain a continuum description of this system [6], we perform a coarse graining of Eq. (9), starting from the Fokker-Planck equation for the probability distribution of the particle coordinates $\mathcal{P}(\vec{r}_1, \dots, \vec{r}_N, t)$,

$$\mu \frac{\partial \mathcal{P}}{\partial t} = \sum_i \vec{\nabla}_i (-\vec{f}_i \mathcal{P} + k_B T \vec{\nabla}_i \mathcal{P}), \quad (10)$$

where \vec{f}_i is the force on the particle i given by Eq. (9). By introducing the single particle density $\rho(\vec{r}, t) \equiv \langle \sum_i \delta^2(\vec{r} - \vec{r}_i) \rangle$, where the average is made over the distribution $\mathcal{P}(\vec{r}_1, \dots, \vec{r}_N, t)$, one obtains

$$\mu \frac{\partial \rho}{\partial t} = -\vec{\nabla} \left[\int d^2 r' \vec{J}(\vec{r} - \vec{r}') \rho^{(2)}(\vec{r}, \vec{r}', t) + \vec{F}^e(\vec{r}) \rho(\vec{r}, t) \right] + k_B T \nabla^2 \rho(\vec{r}, t), \quad (11)$$

where $\rho^{(2)}(\vec{r}, \vec{r}', t)$ is the two-point density. If we now assume that the approximation $\rho^{(2)}(\vec{r}, \vec{r}', t) \simeq \rho(\vec{r}, t)\rho(\vec{r}', t)$ is valid, we can then coarse grain the particle-particle interaction force to obtain [6]

$$\int d^2 r' \vec{J}(\vec{r} - \vec{r}') \rho(\vec{r}', t) \simeq -a \vec{\nabla} \rho(\vec{r}, t), \quad a \equiv \int d^2 r \vec{r} \cdot \vec{J}(\vec{r})/2, \quad (12)$$

where only length scales larger than λ were considered.

Here we investigate the motion of particles in a two-dimensional narrow channel of size $L_x \times L_y$ under an external force in the x direction, $\vec{F}^e = -A(x)\hat{x}$. We then assume that the concentration is only weakly dependent on the transverse y coordinate, $\rho(\mathbf{r}, t) \approx \rho(x, t)$. After collecting all force terms, we obtain

$$\mu \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left\{ \rho \left[a \frac{\partial \rho}{\partial x} - A(x) \right] \right\} + k_B T \frac{\partial^2 \rho}{\partial x^2}. \quad (13)$$

Interestingly, by introducing the probability $P(x, t) = (L_y/N)\rho(x, t)$, defining $D = (aN)/(\nu L_y)$, and setting $\mu = 1$ and $T = 0$, we recover precisely the FPE (5) for $\nu = 2$. Herein we restrict our study to a restoring harmonic force, $A(x) = -\alpha x$ ($\alpha \geq 0$). In the limit $T = 0$, the steady-state solution of Eq. (13) is given by

$$\rho_{\text{st}} = \frac{\alpha}{2a} (x_e^2 - x^2), \quad |x| < x_e, \quad (14)$$

with $x_e = (3Na/2\alpha L_y)^{1/3}$. This result is identical to Eq. (8) if one adopts $\nu = 2$ and $\beta^* = x_e^{-2}$.

We now show through direct molecular dynamics (MD) simulations that the behavior of a typical overdamped system at $T = 0$ is fully compatible with the solution (14), therefore representing a microdynamical realization of Tsallis thermostatics. As an example, we consider a system of vortex lines moving on a type II superconductor substrate [19,20], but the results presented here could nevertheless be extended to other forms of short-range repulsive interactions [8]. In this case, the effective viscosity is given by $\mu = \Phi_0 H_{c2} / \omega c^2$, where Φ_0 is the magnetic quantum flux, c is the speed of light, ω is the resistivity of the normal phase, and H_{c2} is the upper critical field. Moreover, the commonly adopted vortex-vortex interaction is $\vec{J}(\vec{r}) \equiv f_0 K_1(|\vec{r}|/\lambda)\hat{r}$, where K_1 is a modified Bessel function decaying exponentially for $|\vec{r}| > \lambda$, the prefactor is given by $f_0 = \Phi_0^2 / (8\pi\lambda^3)$, and λ corresponds to the London penetration length [21].

We perform MD simulations with $N = 800$ flux lines placed at random within a two-dimensional channel of sizes $L_x = 100\lambda$, $L_y = 20\lambda$, where periodic boundary conditions are imposed in the y direction. In these

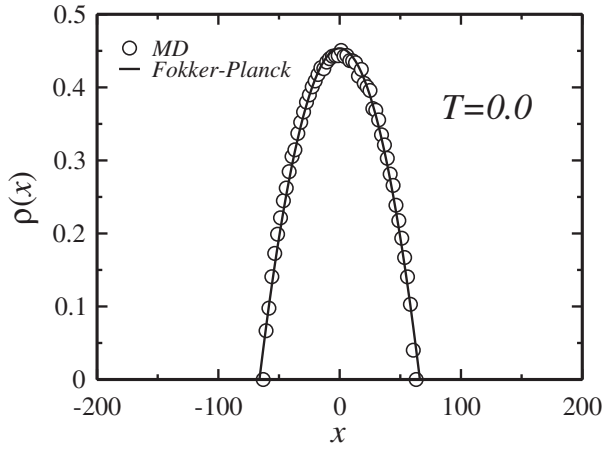


FIG. 1. Profile of the density of particles at stationary state and $T = 0$, obtained from molecular dynamics by integrating Eq. (9) (empty circles), as compared to the theoretical estimate Eq. (14). The best fit to the data of a quadratic function gives the parameter $a = 2.41f_0\lambda^3$ (full line). The position x is measured in units of λ , whereas the steady-state density $\rho(x)$ is expressed in units λ^{-2} .

simulations, we first set $T = 0$, and a confining external force is applied in the x direction with restoring constant $\alpha = 10^{-3}f_0/\lambda$. The equations of motion (9) are numerically integrated and the system evolves in time until a stationary state of mechanical equilibrium is reached, which is identified here in terms of an invariant density profile. As shown in Fig. 1, the obtained stationary profile of particle density is clearly parabolic in shape, in perfect agreement with the theoretical prediction of Eq. (14). The least-squares fit to the simulation data of a quadratic function results in the parameter $a \approx 2.41f_0\lambda^3$. Strictly speaking, the predicted value $a = \pi f_0\lambda^3$, calculated from Eq. (12), is valid only for unconfined systems, if we assume that the density ρ varies slowly within the interaction range of a particle. The discrete character of the interacting particles therefore leads to a correction on this theoretical prediction. In the absence of external forces, i.e., for $\alpha = 0$, our results show that the front propagation at early times evolves as $\langle x(t) \rangle \propto t^{1/3}$ [6]. Once more, the compatibility between this dynamical scaling and the anomalous diffusion behavior intrinsically associated with Eq. (5) for $\nu = 2$ confirms the validity of our approach.

Having shown that overdamped particles in the limit of $T = 0$, typified as interacting flux lines on a type II superconductor substrate, obey Tsallis statistics with an entropic index $\nu = 2$, we now analyze the effect of finite T on this system. From Eq. (13), one can envisage the competition between two types of diffusion, which are associated, respectively, with the strength of interactions between vortices, controlled by the parameter a , or equivalently D , and the temperature of the thermal bath T . In this way, the ratio $k_B T/a$ plays a crucial role in the time evolution of the system. As for the case $T = 0$, in the

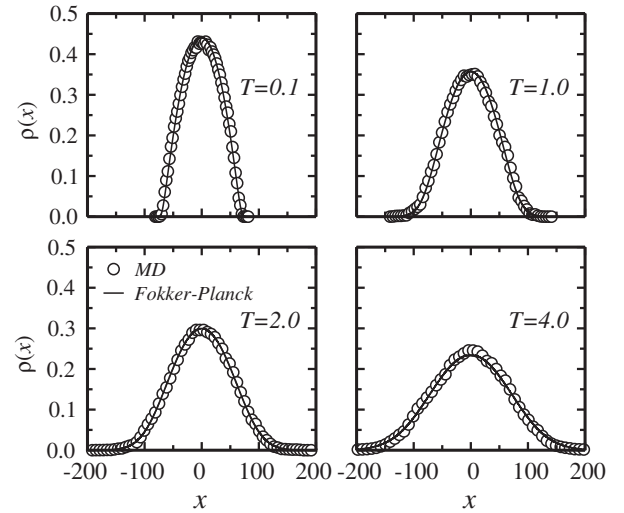


FIG. 2. Comparison between the density of particles profiles in the stationary state obtained from molecular dynamics (empty circles) and the theoretical prediction Eq. (15) (full lines), for different values of the temperature of the thermal bath T . The position x is measured in units of λ , the density is in units λ^{-2} , and T is given in units $(f_0\lambda/k_B)$. The parameter $a = 2.41f_0\lambda^3$ is the same adopted for $T = 0$, whereas $\rho(0)$ is determined by conservation of the total number of particles in the system, $\int_{-L_x/2}^{L_x/2} \rho(x) dx = (N/L_y)$. For low values of T , e.g., $T = 0.1f_0\lambda/k_B$, the density profile is approximately parabolic. At intermediate values of T , the system can be described by a W -Lambert function Eq. (15). At high values of T , the profile becomes typically Gaussian, as illustrated from results at $T = 4f_0\lambda/k_B$.

absence of external forces, i.e., for $\alpha = 0$, the diffusion behavior of the system for $k_B T \ll a$ should be governed by the anomalous features associated with the index $\nu = 2$, namely, $\langle x^2 \rangle \propto t^{2/3}$, whereas normal diffusion prevails for $k_B T \gg a$, i.e., $\langle x^2 \rangle \propto t$. In the presence of a restoring external force and for $T > 0$, a stationary-state analytical solution for Eq. (13) can still be obtained,

$$\rho(x) = \frac{k_B T}{a} W \left\{ \frac{a\rho(0)}{k_B T} \exp \left[\frac{a\rho(0)}{k_B T} - \frac{\alpha x^2}{2k_B T} \right] \right\}, \quad (15)$$

where the W -Lambert function is defined implicitly through the equation $W(z)e^{W(z)} = z$ (see [22] and references therein). In order to test this prediction, extensive MD simulations have been performed for different values of T . As depicted in Fig. 2, we find very good agreement between the continuum model solution Eq. (15) and MD results of density profiles at steady state. For consistency, we consider the same numerical value used to adjust the profile at $T = 0$, namely, $a = 2.41f_0\lambda^3$, while the parameter $\rho(0)$ in Eq. (15) has been determined by a conservation constraint in the total number of particles, $\int_{-L_x/2}^{L_x/2} \rho(x) dx = (N/L_y)$.

The effect of increasing T is to gradually change the density profile from a parabolic to a Gaussian shape.

Indeed these two limits correspond, respectively, to the particular cases of Tsallis distribution with index $\nu = 2$ and the standard Boltzmann-Gibbs statistics. Next we show that the profiles obtained from Eq. (15), for finite T , are in fact associated with a novel type of entropy form. By comparing Eqs. (13) and (1), we obtain that $\Psi[P(x, t)] = P(x, t)$ and $\Omega[P(x, t)] = 2DP(x, t) + k_B T$. Substituting these quantities into Eq. (4), integrating twice, and using the conditions (3), one gets

$$g[P(x, t)] = \frac{D}{\bar{\gamma}} [P(x, t) - P^2(x, t)] - \frac{k_B T}{\bar{\gamma}} [P(x, t) \ln P(x, t)], \quad (16)$$

where $\bar{\gamma}$ is a positive Lagrange parameter defined through a free-energy functional like the one given by Eq. (2), and x is a conveniently rescaled variable. This functional leads to the following entropic form:

$$S[P] = \frac{D}{\bar{\gamma}} \left[1 - \int_{-\infty}^{\infty} dx P^2(x, t) \right] - \frac{k_B T}{\bar{\gamma}} \int_{-\infty}^{\infty} dx P(x, t) \times \ln P(x, t). \quad (17)$$

Equation (17) is precisely the sum of Tsallis entropy with $\nu = 2$, which appears as a consequence of many-body interactions, and Boltzmann-Gibbs entropy, which comes from the thermal noise of the bath. The entropy is zero only for $D = T = 0$. One may now extremize this mixed entropy under the constraints $\int_{-\infty}^{\infty} P(x, t) dx = 1$ and $U = \int_{-\infty}^{\infty} [\phi(x) - \phi_0] P(x, t) dx$, by defining the functional

$$\Sigma[P(x, t)] = \frac{\bar{\gamma}}{k_B T} S[P] - a_1 \int_{-\infty}^{\infty} dx P(x, t) - a_2 \int_{-\infty}^{\infty} dx [\phi(x) - \phi_0] P(x, t). \quad (18)$$

The extreme condition $\delta\Sigma/\delta P = 0$ finally leads to

$$P(x) \exp\left[\frac{2D}{k_B T} P(x)\right] = \exp\{-(1 + a_1) - a_2[\phi(x) - \phi_0]\}, \quad (19)$$

which may be written in terms of W -Lambert's function, i.e., in the same form as Eq. (15), by considering a harmonic potential $\phi(x) = \alpha x^2/2$, multiplying both sides by $2D/(k_B T)$, identifying $a_2 = 1/(k_B T)$, defining z as the right term in Eq. (19), and $W(z) = 2DP(x)/(k_B T)$. This confirms that the entropy Eq. (17) is directly related to the stationary solution Eq. (15) of the FPE (13).

In summary, we have shown through a nonlinear Fokker-Planck formalism and confirmed through MD simulations that a system of interacting particles undergoing overdamped motion at $T = 0$, where T is the temperature of a thermal bath connected to the system, can be considered

as a physical realization of Tsallis thermostatics with an entropic index $\nu = 2$ in Eq. (6). At high values of T , the classical Boltzmann-Gibbs behavior is recovered. At intermediate values of T , our approach, also confirmed by MD simulations, leads to a stationary solution for the corresponding nonlinear FPE that can be expressed in terms of the W -Lambert function. As a consequence, we disclose a novel mixed entropic form based on a linear combination between Tsallis and Boltzmann-Gibbs entropies.

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