Overdamped dynamics of particles with repulsive power-law interactions

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We investigate the dynamics of overdamped D-dimensional systems of particles repulsively interacting through short-ranged power-law potentials, $V(r) \sim r^{-\lambda}$ $(\lambda/D > 1)$. We show that such systems obey a nonlinear diffusion equation, and that their stationary state extremizes a q-generalized nonadditive entropy. Here we focus on the dynamical evolution of these systems. Our first-principle $D = 1, 2$ many-body numerical simulations (based on Newton's law) confirm the predictions obtained from the time-dependent solution of the nonlinear diffusion equation and show that the one-particle space distribution $P(x, t)$ appears to follow a compact-support q-Gaussian form, with $q = 1 - \lambda/D$. We also calculate the velocity distributions $P(v_x, t)$, and, interestingly enough, they follow the same q-Gaussian form (apparently precisely for $D = 1$, and nearly so for $D = 2$). The satisfactory match between the continuum description and the molecular dynamics simulations in a more general, time-dependent framework neatly confirms the idea that the present dissipative systems indeed represent suitable applications of the q-generalized thermostatistical theory.

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Dissipative systems of repulsive particles are representative of many physical phenomena in nature, including, for instance, type-II superconductors [1–7], complex plasmas [8,9], and colloidal systems [10–12]. In the overdamped limit, the equations of motion for such systems take the form of a first-order differential equation, where the velocity of the particles is proportional to the force over them, $\mathbf{v}_i = \mathbf{F}_i/\gamma$. A recent work [13] has shown that, for a wide variety of possible repulsive potentials, the local density $\rho(\mathbf{r}, t)$ of these overdamped repulsive particles should follow a nonlinear diffusion equation in the form

$$\gamma \frac{\partial \rho}{\partial t} = \nabla \cdot \{\rho[\nabla U_{\text{ext}} + a(\rho)\nabla\rho]\}, \tag{1}$$

where $U_{\text{ext}}(\mathbf{r})$ is an applied external potential. The development of a continuum approach allows us to derive the behavior of a system with a large number of particles without having to integrate microscopically the equations of motion of each of these particles.

The function $a(\rho)$ can be obtained from the potential energy U_1 of a particle in the homogeneous state of density ρ [13]:

$$a(\rho) = 2\frac{dU_1}{d\rho} + \rho\frac{d^2U_1}{d\rho^2}. \tag{2}$$

Determining U_1 depends on the knowledge of the interaction potential and on the microscopic structure in which the particles rest in the homogeneous state [13]. As mentioned, the applicability of this approach is restricted to systems of overdamped particles interacting through a short-ranged repulsive potential. More precisely, for large distances r, the interaction potential $V(r)$ should decay faster than r^{-D}, where D is the dimensionality of the system. The form of $a(\rho)$ is also influenced by the way the potential diverges at the origin. If the potential diverges at the origin slower than r^{-D}, $a(\rho)$ should converge to a finite value for densities ρ that are sufficiently large. Conversely, for potentials that diverge faster than r^{-D} at the origin, the energy per particle U_1 grows faster than linearly with the density ρ, and $a(\rho)$ never converges to a fixed value, regardless of the density ρ [13]. In the case where the interaction potential is a power law, $V_{ij} = \epsilon(r_{ij}/\sigma)^{-\lambda}$, with $\lambda > D$, $\sigma > 0$ and $\epsilon > 0$, Eq. (1) can be written as

$$\gamma \frac{\partial \rho}{\partial t} = \nabla \cdot [\rho(\nabla U_{\text{ext}} + C_\lambda \rho^{\frac{\lambda}{D}-1}\nabla\rho)], \tag{3}$$

where the constant C_λ can be computed from the structure of the homogeneous state [13]. More recently, for this family of repulsive potentials, a consistent thermodynamic framework was developed, and thermodynamic potentials, Maxwell relations, and response functions could be obtained [14].

Here we analytically obtain time-dependent solutions of Eq. (3), $\rho(x, t)$, for the case of a parabolic confining potential, $U_{\text{ext}} = -kx^2/2 (k > 0)$, showing that they possess the form of q-Gaussian distributions [15–18]. We have also performed numerical simulations, where the equations of motion for the overdamped dynamics of particles interacting through short-ranged power-law potentials are solved. These two solutions are then compared, and we observe that they are in good agreement. Moreover, our results show that, for the class of solutions we obtain, the velocities of the particles should be proportional to their position, that is, $v_i \sim x_i$. Similar

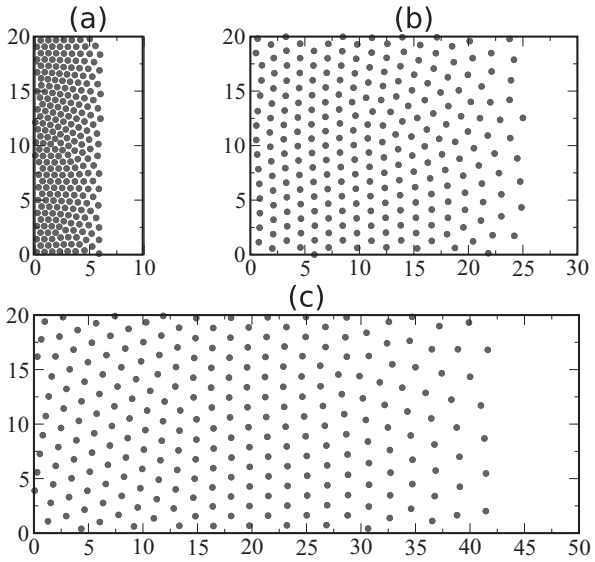

FIG. 1. Snapshots of the configuration of the system in three different moments of the dynamics: (a) $t = 1.0$, (b) $t = 5.88$, and (c) $t = 550$. Due to the symmetry we show only the $x > 0$ half of the system. The particles start in a very narrow region and invade the system as time goes, eventually reaching an equilibrium position. This system comprises $N = 500$ particles, interacting through a potential $V_{ij} = \epsilon(r_{ij}/\sigma)^{-\lambda}$, with $\lambda = 4$, in a cell of lateral length $L_y = 20\sigma$, and confined by an external force $-kx$ with $k = 1 \times 10^{-6}\epsilon/\sigma^2$.

investigations have been performed for models describing the dynamics of type II superconducting vortices [19,20].

In the present work, the systems that we model consist of N particles interacting through the above mentioned potential $V_{ij} = \epsilon(r_{ij}/\sigma)^{-\lambda}$ and confined in the x direction by the external potential U_{ext}. For the case of two dimensions, in the y direction the simulation cell has a finite length L_y, and periodic boundary conditions are imposed. See Fig. 1 for a view of a two-dimensional system in different moments of the dynamics. In this case, it is reasonable to expect the density to be independent on y, so that Eq. (3) can be written as

$$\gamma \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left[\rho\left(kx + C_\lambda \rho^{\frac{\lambda}{D}-1}\frac{\partial \rho}{\partial x}\right)\right]. \tag{4}$$

One may find solutions of Eq. (4) by making use of the similarity hypothesis [21],

$$\rho(x,t) = \frac{g(z)}{f(t)}, \tag{5}$$

with $z = x/f(t)$. Using this in Eq. (4), we obtain

$$\frac{f^{1+\frac{\lambda}{D}}}{C_\lambda}\left(\frac{df}{dt} + kf\right) = -\frac{\frac{d}{dz}\left(g^{\frac{\lambda}{D}}\frac{dg}{dz}\right)}{\frac{d}{dz}(gz)}. \tag{6}$$

The left side of Eq. (6) depends on t, while the right side depends on z. The only possible solution is that both sides are equal to some constant, ν. From that, the left side becomes

$$\frac{df}{dt} = \frac{\nu C_\lambda}{f^{\frac{\lambda}{D}+1}} - kf \tag{7}$$

while the right side can be written as

$$\frac{d}{dz}\left(g^{\frac{\lambda}{D}}\frac{dg}{dz} + \nu g z\right) = 0. \tag{8}$$

In order to solve Eq. (8), we need to consider a proper boundary condition. Since this solution will model a system of particles penetrating a medium, it is reasonable to consider that the density profile $\rho(x,t)$ vanishes at some point, the edge of the profile. Without loss of generality, one may consider that $f(t)$ indicates this edge at all times, $\rho(f(t),t) = 0$ for any t, leading to $g(1) = 0$. With this boundary condition, the solution of Eq. (8) is

$$g = \left[\frac{\lambda\nu}{2D}(1 - z^2)\right]^{\frac{D}{\lambda}}, \tag{9}$$

that is, the shape of the density profile is a q-Gaussian with $q = 1 - \lambda/D$ at any instant of time. The normalization condition, $\int \rho(x,t)\,dx = n$, leads to $\int g\,dz = n$, where $n = N$ for $D = 1$ and $n = N/L_y$ for $D = 2$, remembering that L_y gives the thickness of the simulation cell and N the number of particles. This allows us to determine the value of ν:

$$\nu = \frac{2D}{\lambda}\left[n\frac{\Gamma\left(\frac{3}{2} + \frac{D}{\lambda}\right)}{\Gamma\left(1 + \frac{D}{\lambda}\right)\sqrt{\pi}}\right]^{\frac{\lambda}{D}}. \tag{10}$$

It is also visible from this solution that $f(t)$ is the point where $\rho(f(t),t) = 0$, that is, $f(t)$ is the edge of the distribution. Solving Eq. (7) we obtain

$$f(t) = \left\{\frac{\nu C_\lambda}{k}[1 - e^{-k(\frac{\lambda}{D}+2)(t-t_0)}]\right\}^{\frac{D}{\lambda+2D}}, \tag{11}$$

where t_0 is a free parameter that depends on the initial condition. In fact this solution is not unique. One may note that, for $t = t_0$, it becomes $\rho(x,t_0) = n\delta(x)$; therefore this solution is suitable for this particular initial condition as well as any initial condition that has the form of a q-Gaussian. Moreover, our numerical experiments have shown that, even starting from other initial conditions, the dynamics tend to drive the system towards this behavior after a transient time. In the numerical simulations we present here all particles start confined to a narrow stripe. For this initial condition setting $t_0 = 0$ yields a good fit for our numerical results. In Fig. 2 we show the curves of $f(t)$ and $\dot{f}(t) \equiv df/dt$ for each instant of time t considering $\lambda = 2$ and $\lambda = 3$ in one dimension, and $\lambda = 4$ and $\lambda = 6$ in two dimensions. These curves were obtained from Eq. (11). As we show in what follows, these predictions closely agree with the results from the numerical simulations.

One should expect the stationary state to be in the form of a q-Gaussian. In the context of the continuous model, the overdamped dynamics is minimizing the overall potential energy of the system, $U = \int \rho[kx^2/2 + (DC_\lambda/\lambda)\rho^{\lambda/D}]\,d^Dx$ [13], which can be associated with the q-statistics free energy of a confined ideal gas. In this association, the contribution of the particle-particle interaction, absent in the ideal gas description, is accounted for by the generalized entropy. Therefore the overdamped dynamics should necessarily drive the system towards the state of minimum energy, hence the shape of a q-Gaussian. This distribution has been shown to maximize

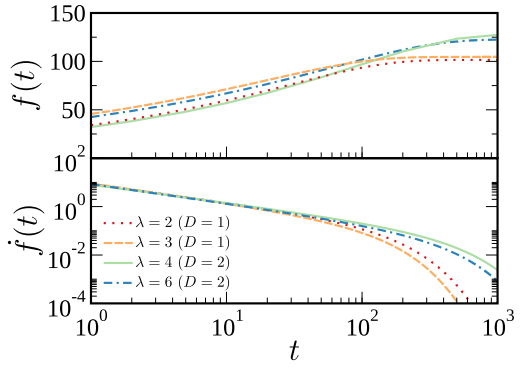

FIG. 2. Curves of $f(t)$ for $D = 1$ ($\lambda = 2$ and 3) and $D = 2$ ($\lambda = 4$ and 6) obtained from Eq. (11) and its derivative $\dot{f}(t)$. In our numerical simulations, we start with all particles confined in a narrow stripe, leading us to use $t_0 = 0$ in Eq. (11). The case $D = 1$ corresponds to $N = 3600$ particles with confining potential strength $k = 3.2 \times 10^{-3}\epsilon/\sigma^2$. The case $D = 2$ corresponds to $N = 4000$ particles, with confining potential strength $k = 1 \times 10^{-3}\epsilon/\sigma^2$, in a cell with transverse size $L_y = 20\sigma$.

the generalized nonextensive entropy S_q, under given constrains [22], and yield well-known particular distributions, such as Student's t ($q > 1$) or r distributions ($q < 1$). Interestingly, this shape is obtained not only at the stationary state, but during most of the dynamics. This is a feature of the confining potential that allows us to find a solution consistent with the similarity hypothesis Eq. (5).

Figure 3 shows the density profile at different moments of the dynamics for one-dimensional systems. To obtain these curves, we performed the Kernel Density Estimation [23] for

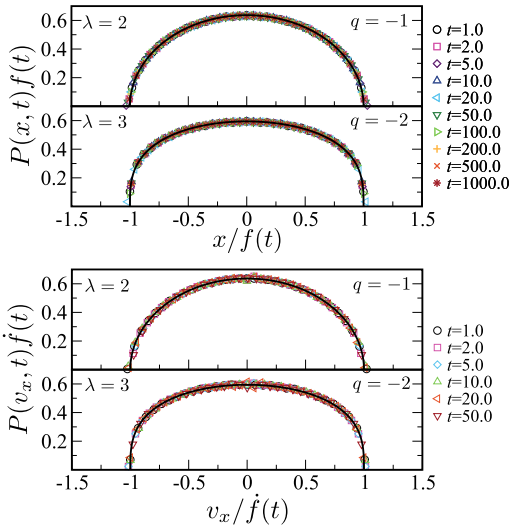

FIG. 3. Distributions of scaled positions and velocities at different moments of the dynamics for the one-dimensional case ($D = 1$). These results concern $N = 3600$ particles interacting through the power-law potential, $V = \epsilon(r/\sigma)^{-\lambda}$, for $\lambda = 2$ ($q = -1$) and $\lambda = 3$ ($q = -2$). The black curves are q-Gaussians. Here we used the strength of the confining potential $k = 3.2 \times 10^{-3}\epsilon/\sigma^2$.

the position of the particles scaled by the length $f(t)$ obtained from Eq. (11). The results from simulation are in perfect agreement with the predicted form given by Eq. (9), showing that, in fact, Eq. (11) yields the correct position $f(t)$ at the edge of the density profile.

Next we proceed to investigate the velocity of particles during the dynamics. To obtain a solution for our nonlinear diffusion, Eq. (4), and considering the similarity hypothesis, Eq. (5), from Eq. (9) it is visible that $g(1) = 0$, that is, $f(t)$ is the position where the density profile vanishes. In fact, Eq. (4) is an instance of the continuity equation in the form, $\partial\rho/\partial t = -\partial(\rho\bar{v})/\partial x$, where $\bar{v}(x,t)$ gives the instantaneous average local velocities of the particles. To be consistent with the similarity hypothesis (5) a similar constraint has to be made to $\bar{v}$:

$$\bar{v}(x,t) = \dot{f}(t)b(z), \quad \text{with } \dot{f}(t) = df/dt. \tag{12}$$

The average velocity of the particles at the edge of the density profile is given by $\bar{v}(f(t),t) = \dot{f}(t)$. By inserting the similarity hypothesis into the continuity equation, we obtain

$$-\frac{\dot{f}}{f^2}\frac{d}{dz}(gz) = -\frac{\dot{f}}{f^2}\frac{d}{dz}(gb), \tag{13}$$

leading to the condition that $\bar{v}(x,t) = (\dot{f}/f)x$, that is, the average velocity is linear with position.

In one dimension there is not more than one particle at each given position x, therefore if $\bar{v}(x,t)$ is linear with x, the

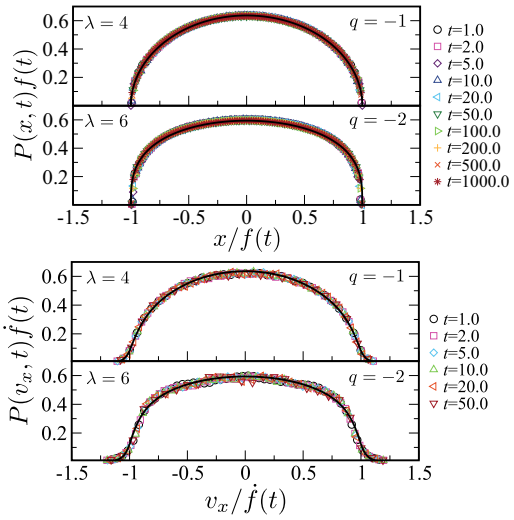

FIG. 4. Distributions of scaled positions and velocities at different moments of the dynamics for the case of two dimensions ($D = 2$). These results concern particles interacting through the power-law potential, $V = \epsilon(r/\sigma)^{-\lambda}$, for $\lambda = 4$ ($q = -1$) and $\lambda = 6$ ($q = -2$). One can compare the density profiles with q-Gaussians (black curves). In the case of the velocity distributions the black curves show convolutions between q-Gaussians and Laplacian distributions, as given by Eq. (15), with the parameter h given by 0.045 and 0.051 for $\lambda = 4$ and 6, respectively. In these simulations we used $N = 4000$ particles in a cell of transverse size $L_y = 20\sigma$ with periodic boundary conditions. In the longitudinal direction (x axis) we imposed a confining force $-kx$ with $k = 1 \times 10^{-3}\epsilon/\sigma^2$.

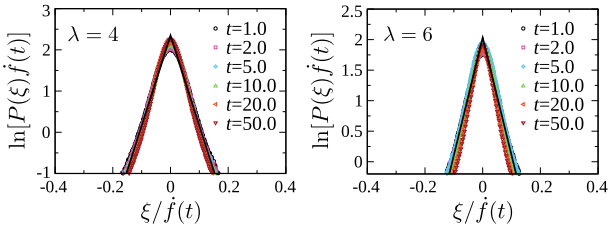

FIG. 5. Distributions of the displacement of the average velocity, $\xi_i = (v_x)_i/\dot{f} - x_i/f$ for some values of times t considering $\lambda = 4$ and $\lambda = 6$ for $D = 2$. The black curves represent Laplacian distributions, $P(\xi) \sim \exp(-|\xi|/h)$, where h is an adjustment parameter, given by 0.045 and 0.051 for $\lambda = 4$ and 6, respectively.

velocity of each particle should be linear with x, leading to the conclusion that they are distributed in the same form, namely, a q-Gaussian. This prediction is consistent with Ref. [24], and confirmed by the results of Fig. 3. In larger dimensionalities there are several particles in the stripe around a given distance x. In this case $\bar{v}(x,t)$ may still be linear with x, but the velocities of each particle may fluctuate around this average.

To test this hypothesis we performed simulations in two dimensions. Figure 4 presents the density profiles and velocity distributions obtained from simulations. As before, positions were scaled by $f(t)$, while velocities were scaled by $\dot{f}(t)$. As exhibited, the density profiles follow closely the q-Gaussian form. The velocity distributions also display an invariant shape for all instants. However, this shape deviates slightly from the expected q-Gaussian form at the largest velocities. Note that to reduce fluctuations in our results we performed averages over 800 sample simulations. To investigate this small difference, we analyze the distribution of the quantity $\xi_i \equiv (v_x)_i/\dot{f} - x_i/f$ among the particles of all samples, which measures how far $(v_x)_i$ is from the expected average $\bar{v}(x_i,t) = (\dot{f}/f)x_i$ for a particle at position x_i at time t. Figure 5 shows the distributions $P(\xi)$ for different values of t. One can see that $P(\xi)$ can be described approximately by a Laplacian distribution,

$$P(\xi) \sim \exp(-|\xi|/h), \tag{14}$$

where the parameter h depends on the particular value of λ. Most likely, these small deviations in the expected value of the velocity are due to the rearrangement of the local spatial structure as the density changes. As we know from the results of Fig. 5, the distribution of positions can be well described as a q-Gaussian, $P(x/f) = G_q(x/[(q-1)f])$. Since $f(t)$ and $\dot{f}(t)$ depend only on time, and $(v_x)_i/\dot{f} = x_i/f + \xi_i$, then the v_x distribution can be found by the convolution [25] between a q-Gaussian and a Laplacian distribution:

$$P\left(\frac{v_x}{\dot{f}}\right) = \frac{1}{2h}\int_{-\infty}^{\infty} d\xi\; G_q\left(\frac{v_x/\dot{f} - \xi}{q-1}\right) e^{-\frac{|\xi|}{h}}. \tag{15}$$

The black curves shown in the Fig. 4 have been obtained from Eq. (15), where the values of h were obtained from the best fits to the molecular simulation data of the Laplace distribution, Eq. (14), as shown in Fig. 5.

We have studied a system of particles interacting through power-law repulsive potentials, and under overdamped motion. In a previous work, through a coarse-graining approximation, this model was related to a nonlinear diffusion equation, whose stationary-state solutions have been shown to be compatible with results obtained from molecular-dynamics simulation [13]. Here we investigate the whole time evolution. Using a similarity hypothesis, we showed that our nonlinear diffusion equation predicts that, for all times, the probability distribution for the positions, $P(x,t)$, is a q-Gaussian with the value of q depending on both the repulsive potential as well as on dimensionality of the system, $q = 1 - \lambda/D$. We present quite satisfactory results from molecular dynamics simulations to give support to the analytic predictions. Moreover, we have also presented results for the x-component velocity probability distribution, $P(v_x,t)$, showing that it is given by a q-Gaussian distribution that, in larger dimensionalities, will be perturbed by a small extra noise well approximated by a Laplacian distribution. We conjecture that these perturbations are due to the rearrangement of the local spatial structure as the density changes. To summarize, we have presented broad evidence that a system of overdamped repulsive particles interacting through a short-range power-law potential constitutes an important physical application for nonextensive statistical mechanics. Both stationary states and time-dependent properties of the systems are fully compatible with the theory.

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