Klimontovich's Contributions to the Kinetic Theory of Nonlinear Brownian Motion and New Developments

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Abstract. We review the concept of nonlinear Brownian motion, originally introduced by Klimontovich, and consider several applications to real systems, including e.g. atoms, molecules or ions laser cooling fields, charged grains in plasmas and interdisciplinary problems. In particular, we also discuss recent developments in the field of active Brownian particles. After summarizing the basic properties of active Brownian particle models, solutions of the corresponding Fokker-Planck equation are analyzed for free motions as well as for motions in confining fields. Furthermore, we study the distributions for finite systems of self-confined particles, interacting via Morse and Coulomb potentials. Finally, applications to clusters of atoms subject to laser cooling as well as to clusters of charged grains in dusty plasmas are discussed.

1. Introduction

Yuri L. Klimontovich devoted a great part of his scientific work to Brownian motions. His interest in this topic was stimulated by numerous inspiring conversations with his colleague and friend Rouslan L. Stratonovich. In particular, he was interested in applications to plasmas, non-ideal gases and interactions with electromagnetic radiation [1, 2, 3, 4, 5]. This way Klimontovich developed the seminal work of Einstein, Smoluchowski, Langevin and others further. The main difference between the standard Brownian motion considered by those pioneers and Klimontovich's nonlinear Brownian motion is the following: Standard Brownian motion is characterized by a linear dissipative (Stokes) force, which acts on the Brownian particle,

$$\boldsymbol{F}_s = -m\gamma_0 \boldsymbol{v}, \tag{1}$$

where m is the mass and γ_0 the collision frequency ($m\gamma_0$ is the friction constant). In contrast, the so-called nonlinear Brownian motion is characterized by nonlinear dissipative forces, expressed e.g. by a collision frequency depending on the velocity and/or the spatial coordinates

$$\boldsymbol{F} = -m\gamma(\boldsymbol{v}, \boldsymbol{r})\boldsymbol{v}. \tag{2}$$

Figure 1 shows an absolute linear dissipative Stokes force for the one-dimensional case and, for comparison, also (nonlinear) velocity-dependent friction forces representing type (2). In particular, we show the friction force of the depot-model (SET-model) introduced in Ref. [6, 7], and a piece-wise linear approximation to it.

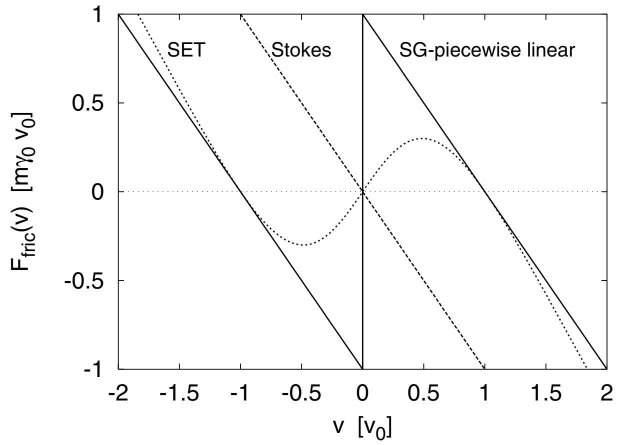

Figure 1. Velocity-dependent dissipative forces for the one-dimensional case. The two most important cases are illustrated: (i) Passive dissipative Stokes force, Eq. (1), with only one zero at $v = 0$. (ii) Active dissipative forces of the SET-depot model, Eq. (9), and a piecewise linear approximation, Eq. (13), with two stable velocities $\pm v_0$ and one unstable velocity $v = 0$ (for the SET-curve parameter values $q = 2, d_0 = c = 1$ were used).

The behavior of usual Brownian particles is completely determined by the (passive) stochastic collisions between the particles and the surrounding medium. In particular this means that there is effectively no active transfer of energy from the medium to the particles. The energetic equilibrium between particles and surrounding medium is expressed in terms of the fluctuation-dissipation theorems. Klimontovich worked out in detail the theory of Brownian motions for the case, where the friction function $\gamma(\boldsymbol{v}, \boldsymbol{r})$ (as well as the corresponding noise strength) is a more or less complicated function of the variables $\boldsymbol{v}$ and $\boldsymbol{r}$. He derived Fokker-Planck equations and provided many special solutions, in particular, for one-dimensional systems of particles with nonlinear friction forces, that were originally derived in the context of self-oscillating systems, as e.g. ensembles of van der Pol oscillators. Extending the ideas of Klimontovich, we want to generalize below to active Brownian particles, which move in 2 dimensions due to an energy input from the surrounding [6, 7, 8, 9, 10].

As already shown by Klimontovich, there exist many applications to non-ideal plasmas and gases [1, 3]. A group of particularly interesting applications includes clusters of atoms/molecules confined in a trap and cooled by laser fields [11]. Naturally, such systems are described by Fokker-Planck equations with nonlinear (non-Stokes) friction [2, 3, 5]. In particular, there exist many recent applications to ultra-cold clusters of atoms/molecules cooled by interaction with laser radiation [14]. Additionally, negative friction has also been observed in investigations of the energy loss (stopping power) of charged particles moving in a plasma [15, 20]. Other interesting applications include charged clusters in microelectronics [16, 17, 18, 19] and charged grains in dusty plasmas [21, 22, 25]. Last but not least, simplified nonlinear Brownian motion models have been used successfully in the past to describe active biological motion [8, 26, 27, 28, 29]. Finally, we also note interesting applications to problems of traffic [30].

2. Dissipative forces, Langevin- and Fokker-Planck equations

The motion of Brownian particles with generalized velocity- and space-dependent friction in a position-dependent potential $U(\boldsymbol{r})$, can be described by the following Langevin equations:

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{v}; \qquad m\frac{d\boldsymbol{v}}{dt} = \boldsymbol{F} - \nabla U(\boldsymbol{r}) + \boldsymbol{\mathcal{F}}(t) \tag{3}$$

Here $\boldsymbol{F}$ is a dissipative force corresponding, in general, to a nonlinear friction law as in Eq. (2). $\boldsymbol{\mathcal{F}}(t) = (\mathcal{F}^i(t))$ is a stochastic force vector with strength S and δ-correlated time dependence, i.e.

$$\langle \boldsymbol{\mathcal{F}}(t) \rangle = 0; \qquad \langle \mathcal{F}^i(t)\mathcal{F}^j(t') \rangle = 2S\,\delta^{ij}\,\delta(t-t'). \tag{4}$$

The noise strength for the momentum, S, is related to the noise strength for the velocities, D_0, via the simple relation $S = m^2 D_0$. In the case of thermal equilibrium systems, corresponding to $\gamma(\boldsymbol{r}, \boldsymbol{v}) = \gamma_0 = \text{const.}$, we may assume that the loss of energy resulting from friction, and the gain of energy resulting from the stochastic force, are compensated on average. In this case the fluctuation-dissipation theorem (Einstein relation) reads

$$S = D_0\, m^2 = m k_B T \gamma_0, \tag{5}$$

where T is the temperature, k_B the Boltzmann constant, and D_0 is a scaled expression for the strength of the stochastic force in velocity space. Below it is sometimes useful to refer to units in which $m = k_B = \gamma_0 = 1$, since then the Einstein relation simplifies to $S = D_0$.

Usually, when dealing with stochastic Langevin equations, one is primarily interested in a statistical description, i.e. in the probability density $P(\boldsymbol{r}, \boldsymbol{v}, t)$ for finding the particle at location $\boldsymbol{r}$ with velocity $\boldsymbol{v}$ at time t. The distribution function, $P(\boldsymbol{r}, \boldsymbol{v}, t)$, which corresponds to the Langevin equation (3), is governed by the Fokker-Planck equation

$$\frac{\partial P(\boldsymbol{r}, \boldsymbol{v}, t)}{\partial t} + \boldsymbol{v}\, \frac{\partial P(\boldsymbol{r}, \boldsymbol{v}, t)}{\partial \boldsymbol{r}} + \nabla U(\boldsymbol{r})\, \frac{\partial P(\boldsymbol{r}, \boldsymbol{v}, t)}{\partial \boldsymbol{v}} = \frac{\partial}{\partial \boldsymbol{v}} \left[\gamma(\boldsymbol{r}, \boldsymbol{v})\, \boldsymbol{v}\, P(\boldsymbol{r}, \boldsymbol{v}, t) + D_0\, \frac{\partial P(\boldsymbol{r}, \boldsymbol{v}, t)}{\partial \boldsymbol{v}} \right]. \tag{6}$$

In the special case of purely passive Stokes friction $\gamma(\boldsymbol{r}, \boldsymbol{v}) = \gamma_0$, the stationary solution of Eq. (6), denoted by $P_0(\boldsymbol{r}, \boldsymbol{v})$, is the Boltzmann distribution:

$$P_0(\boldsymbol{r}, \boldsymbol{v}) \quad = \quad \mathcal{N} \exp\left\{ -\frac{1}{k_B T} \left[\frac{m}{2}\, \boldsymbol{v}^2 \,+\, U(\boldsymbol{r}) \right] \right\}. \tag{7}$$

With regard to nonlinear Brownian motions, a major question is, how this well-known solution changes if we introduce active elements. While for usual Brownian motion the dissipation of energy caused by friction is compensated by the stochastic force, for active particles (e.g. bacteria) there exists an additional influx of energy. In general, one can account for the latter effect by considering more a complex friction function. During the last decade, several models for such self–propelling mechanisms have been proposed [6, 7, 26]. Here, we restrict ourselves to discussing purely velocity-dependent friction, $\gamma(\boldsymbol{r}, \boldsymbol{v}) = \gamma(\boldsymbol{v})$, as a mechanism for accelerating the Brownian motion of particles.

Historically, velocity-dependent friction played an important role already in very early models related to the theory of sound, developed by Rayleigh and Helmholtz. In the simplest case, one may assume the following friction function for the force that acts on an individual Brownian particle (with $\gamma_{1/2}$ being positive constants):

$$\gamma(\boldsymbol{v}) = -\gamma_1 + \gamma_2 \boldsymbol{v}^2 = \gamma_1 \left(\frac{v^2}{v_0^2} - 1 \right) = \gamma_2 (v^2 - v_0^2). \tag{8}$$

This so-called Rayleigh-Helmholtz model is a standard model, which has extensively been studied by Klimontovich in his work on nonlinear Brownian dynamics. We note that $v_0^2 = \gamma_1/\gamma_2$ defines a special absolute velocity value, at which the friction force vanishes.

Another standard model for active friction with a characteristic zero point was empirically found in experiments with moving cells and has been analyzed in detail by Schienbein and Gruler [26]. As shown by these authors, this model allows to describe the active motion of several cell types as e.g. granulocytes.

Further, we consider the so-called depot model [6, 7, 28]. This model is based on the idea that active particles may carry energy depots. By adiabatic elimination of the energy one finds the nonlinear four-parameter friction function (see Fig. 1)

$$\gamma(\boldsymbol{v}) = \gamma_0 - \frac{q}{c + d_0 \boldsymbol{v}^2}, \tag{9}$$

where the four parameters γ_0, q, c and d_0 are assumed to be nonnegative. Evidently, for the depot model the friction function is well-behaved in the full velocity range. Qualitatively, the behavior of the the friction function (9) changes, depending on the value of the bifurcation parameter [8, 9]

$$\zeta = \frac{q}{c\gamma_0} - 1. \tag{10}$$

For positive values $\zeta > 0$ one finds that the friction force vanishes for two absolute velocity values, given by $v_0 = \sqrt{c\zeta/d_0}$ (stable state) and $v_1 = 0$ (unstable). In contrast, for $\zeta < 0$ there is only one stable state corresponding $v_1 = 0$, i.e. in this sub-critical parameter region a particle is damped until it comes to rest.

Let us concentrate on the regime of active motions, $\zeta > 0$. If the velocities are rather small, then we get for the friction law

$$\gamma(\boldsymbol{v}) = \left(\gamma_0 - \frac{q}{c}\right) - \frac{q\,d_0}{c^2}\boldsymbol{v}^2 + \mathcal{O}\left(\boldsymbol{v}^4\right) \tag{11}$$

which, by virtue of

$$\gamma_1 = \frac{q}{c} - \gamma_0; \qquad \gamma_2 = \frac{qd_0}{c^2},$$

corresponds to the Rayleigh-Helmholtz friction discussed above.

For $\zeta > 0$, due to the super-critical pumping, slow particles with $|\boldsymbol{v}| < v_0$ are accelerated and fast particles with $|\boldsymbol{v}| > v_0$ are damped. In the case of two-dimensional motions, for example, the deterministic trajectory ($S = 0$) of our system is attracted by a cylinder in the 4d-space, whose velocity-coordinate projection is given by

$$v_1^2 + v_2^2 = v_0^2, \tag{12}$$

where v_0 is the value of the stationary absolute velocity, reading for the Rayleigh-model or the depot model, respectively,

$$v_0^2 = \frac{\gamma_1}{\gamma_2}; \qquad v_0^2 = \frac{q}{\gamma_0} - \frac{c}{d_0}.$$

With regard to analytical calculations, it is often useful to approximate arbitrary friction models, where the dissipative force has zeros at $|\boldsymbol{v}| = 0$ and $|\boldsymbol{v}| = v_0$, by the piecewise linear force

$$\boldsymbol{F} = -m\gamma(\boldsymbol{v})\boldsymbol{v} \approx -m\alpha\left(1 - \frac{v_0}{|\boldsymbol{v}|}\right)\boldsymbol{v}. \tag{13}$$

For $\alpha = \gamma_0$ this reduces to the Schienbein-Gruler model. In the general case, the constant α has to be fitted to the slope of the nonlinear friction force at the zeros for $|\boldsymbol{v}| = v_0$ as demonstrated in Fig. 1. The piecewise linear approximation admits sometimes simple analytical solutions; however, this model fails to describe the dynamics around $\boldsymbol{v} = 0$ and the transients based on this dynamics. It would be quite interesting to study piecewise linear models with a finite slope in $\boldsymbol{v} = 0$.

3. Free and confined active particles

Let us study first the stationary solutions of the Fokker-Planck equation (6) for the case of free particles. Considering the Rayleigh-model of active friction from Eq. (8) for the case case of free motions (i.e. no external forces), one finds the stationary solution

$$P_0(\boldsymbol{v}) = \mathcal{N} \exp\left[\frac{\gamma_1}{2D_0}\boldsymbol{v}^2 - \frac{\gamma_2}{4D_0}\boldsymbol{v}^4\right], \tag{14}$$

where $\mathcal{N}$ is a normalization constant. The shape of the distribution from Eq. (14) can be seen in Fig. 2. For the piecewise linear model the solution is particularly simple:

$$P_0(\boldsymbol{v}) = \mathcal{N} \exp\left[-\frac{\alpha}{2D_0}\left(|\boldsymbol{v}| - v_0\right)^2\right]. \tag{15}$$

Finally, for the depot-model (sometimes called SET-model) the stationary solution reads

$$P_0(\boldsymbol{v}) = \mathcal{N}\left(1 + \frac{d_0}{c}\,\boldsymbol{v}^2\right)^{q/2D_0} \exp\left[-\frac{\gamma_0}{2D_0}\,\boldsymbol{v}^2\right]. \tag{16}$$

For strong noise, corresponding to high temperatures $D_0 \sim T \to \infty$, the distribution (16) approaches a Maxwellian distribution. In the opposite limit, $D_0 \sim T \to 0$, it reduces to a delta-distribution, peaked at $|\boldsymbol{v}| = v_0$. This limiting behavior is also characteristic for Eqs. (14) and (15), whereas the Maxwellian limit case is not contained in Eqs. (14-15). Figure 2 shows a comparison of the three probability density distributions from Eqs. (14), (15) and (16) for the one-dimensional case.

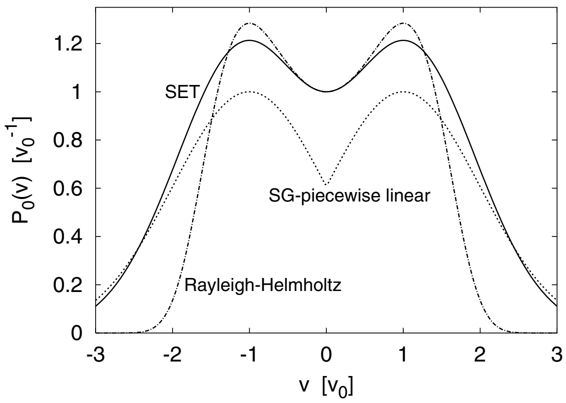

Figure 2. Stationary velocity distribution functions (14)–(16) of active Brownian particles for the one-dimensional case: (i) Rayleigh-Helmholtz model with $\gamma_1 = \gamma_2 = 1$, (ii) Piecewise linear approximation with $\alpha = 1$, and (iii) SET-depot model with over-critical parameter-values $q = 2, d_0 = c = \gamma_0 = 1$. For each curve we have fixed $D_0 = \mathcal{N} = 1$.

If one considers free particles allowed to move in two spatial dimensions, then the stationary probability density is located on a cylinder in the 4- dimensional phase space. Including a confinement in a parabolic trap the particles start to rotate clockwise or counter-clockwise and the probability concentrates on two 'hula-hoop'-like 4-dimensional limit cycles, as demonstrated in Fig. 3.

4. Clusters of atoms or molecules with active friction

Investigations of atoms or molecules confined in a trap and cooled down to very low temperatures have attracted considerable theoretical and experimental interest over the last years [11]. Here we will study finite clusters consisting of a small number of particles (e.g. atoms or molecules), interacting via Morse potentials:

$$\phi(r_{ij}) = A\left[\exp(-ar_{ij}) - 1\right]^2 - A \qquad\qquad a > 0,\ A > 0, \tag{17}$$

where r_{ij} is distance between two particles. Due to the attracting tail of the Morse potentials, the particles can form clusters (self-confinement) at sufficiently low temperatures [12, 13]. Individual particles then move in the collective field of the other molecules, which might be represented by a (self-consistent) mean field approximation [31]. Let us assume that the cluster is subject to laser cooling. This leads to a Fokker-Planck description with active friction very similar to the above models [2, 5, 11, 14]. For simplicity, we shall assume here that the dissipative force

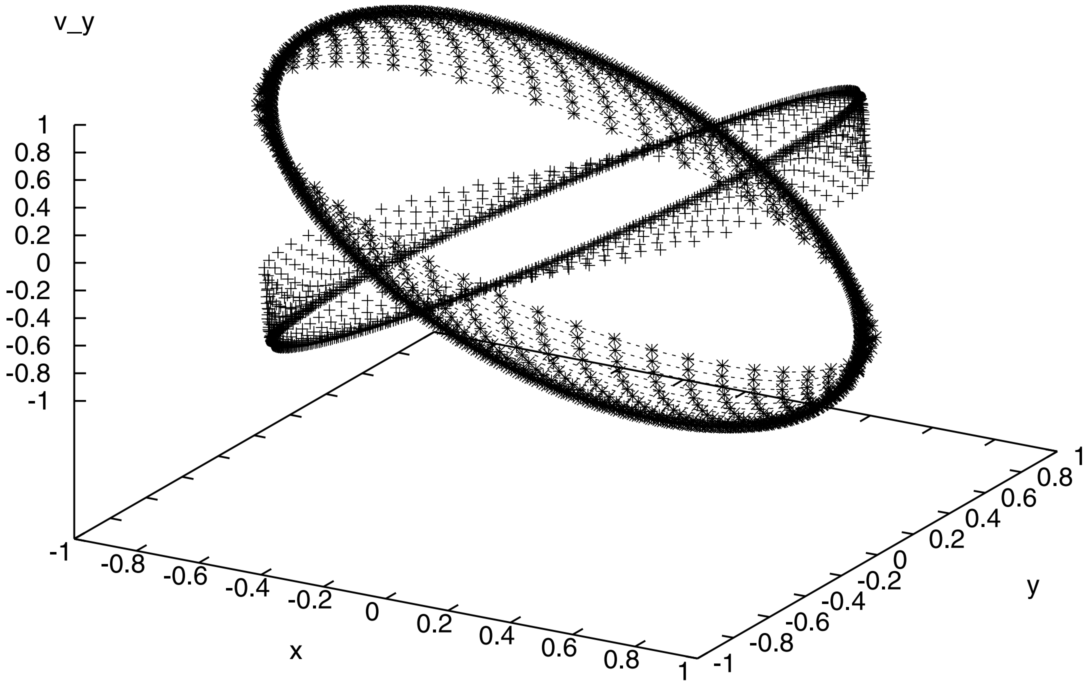

Figure 3. A bundle of stochastic trajectories of active Brownian particles in parabolic confinement near to the limit cycles.

has zeroes at $|\boldsymbol{v}| = v_0$ and, moreover, that the real dissipation function can be approximated the piecewise linear function given in (13). Simulations based on this approximation show that small Morse clusters tend to rotate clockwise or counter clockwise as illustrated in Fig. 4 [31]. Furthermore, larger ensembles of Morse molecules are decomposed into clusters of smaller sizes which may rotate or drift as depicted in Fig. 5.

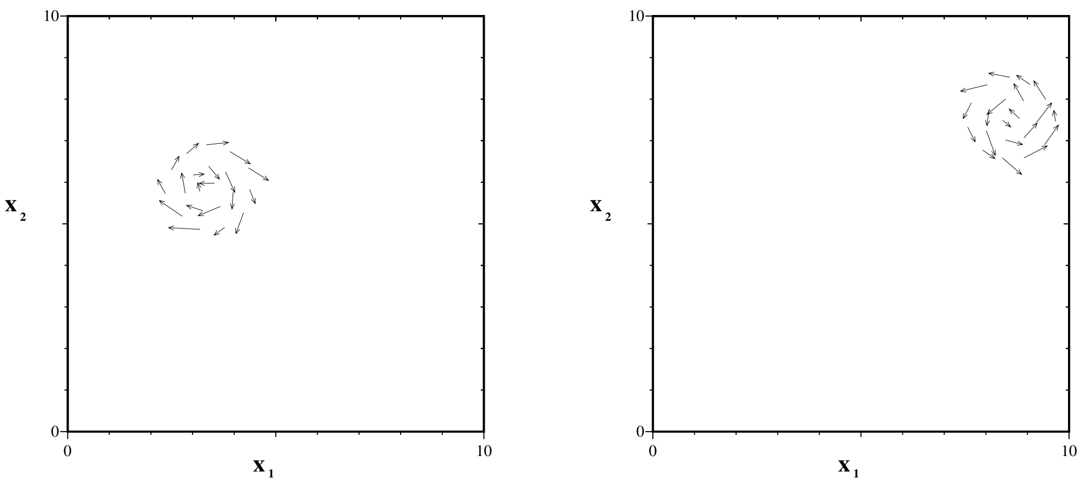

Figure 4. The two possible stationary states of a rotating cluster of 20 particles interacting via Morse forces. The arrows correspond to the velocities of the particles. In the presence of noise the cluster changes from time to time the direction of rotation.

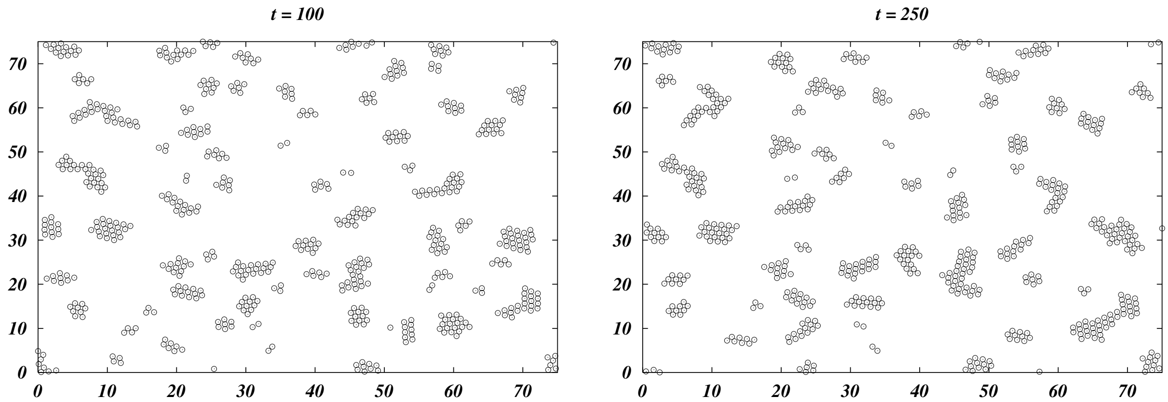

Figure 5. Rotating and drifting clusters of 625 particles with Morse interactions.

5. Coulomb clusters with active friction

Recent investigations of the stochastic dynamics of highly charged Coulomb grains embedded into a plasma have shown that nonlinear friction functions with additional zeroes (negative friction) may possibly occur under very special experimental conditions [21, 22]. The energy influx from a 'depot' is in this case provided by the absorption of ions by the Coulomb grains. The rather complicated dissipation functions derived in [21, 22] can, in principle, again be approximated by a Rayleigh-Helmholtz function or a piecewise linear Schienbein-Gruler friction law.

Let us consider grain-grain interactions, mediated by a screened Coulomb pair interaction potential:

$$\Phi_{ij}^{C}(r) = \frac{Q_i\,Q_j}{4\pi\varepsilon_0}\,\frac{1}{r_{ij}}\,\exp\Big(-\frac{r_{ij}}{\lambda_D}\Big), \tag{18}$$

where λ_D is the Debye screening length, and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$ denotes the distance between two grains located at $\boldsymbol{r}_i = (x_i, y_i)$ and $\boldsymbol{r}_j = (x_j, y_j)$, respectively. Motions perpendicular to the horizontal x-y–plane are neglected. For simplicity, we shall confine ourselves to the case where all grains are identical, i.e.

$$Q_i = Q = -Ze, \qquad\qquad m_i = m \tag{19}$$

for $i = 1, 2, \ldots, N$. If an ensemble of N such particles is confined by an external parabolic potential

$$\Phi^{ex}(\boldsymbol{r}) = \frac{m_g\omega_0^2}{2}\,\boldsymbol{r}^2, \tag{20}$$

then their ground-state configuration corresponds to a regular two-dimensional structure, referred to as Coulomb crystal [17, 18, 24]. These static structures can be classified and a 'Mendeleev' table for the case of pure Coulomb interactions, corresponding to $\lambda_D \to \infty$, was presented in Ref. [16] for particle numbers $N = 2, \ldots, 52$. An analogous analysis for screened potentials of the type (18) can be found in [23].

In [25] we have studied the dynamics of two-dimensional Coulomb clusters confined in a harmonic trap by using a Langevin approach. In particular, we identified the excitations that arise in the presence of negative friction. This was achieved by numerically integrating the Langevin equations of motion

$$m\dot{\boldsymbol{v}}_i \;=\; \boldsymbol{F}_i^{C} + \boldsymbol{F}_i^{ex} - m\gamma(\boldsymbol{v}_i)\boldsymbol{v}_i + \boldsymbol{\mathcal{F}}_i(t), \tag{21}$$

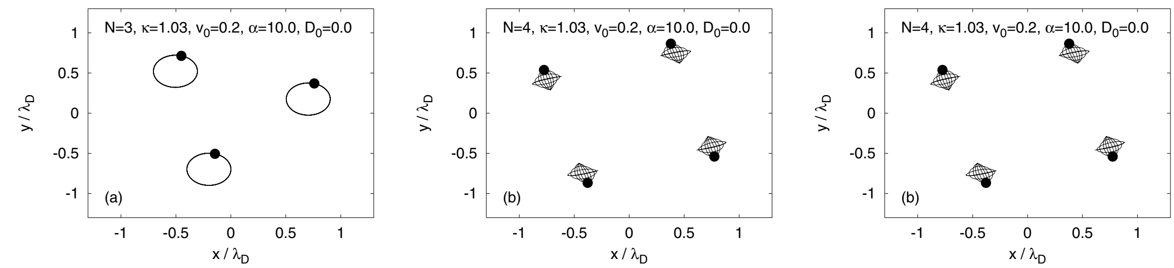

Figure 6. Examples of stationary active motions of Coulomb clusters with $N = 3, 4, 5$ grains and $D_0 = 0$, where the parameter κ is given by $\kappa \equiv Z^2e^2/(4\pi\varepsilon_0 m\omega_0^2\lambda_D^3)$. (a) $N = 3$: This attractor corresponds to an acoustical oscillation. (b) $N = 4$: For this stable optical excitation the stationary orbit of a single grain is very similar to a Lissajous-pattern. (c) $N = 5$: Stationary wave pattern.

where $\boldsymbol{v}_i = \dot{\boldsymbol{r}}_i$ denotes the grain's velocity. In agreement with the Rayleigh-Helmholtz model, the friction function is taken as

$$\gamma(\boldsymbol{v}) = \alpha(\boldsymbol{v}^2 - v_0^2), \qquad\qquad \alpha > 0. \tag{22}$$

From Eq. (20), the external linear force $\boldsymbol{F}_i^{ex}$ modeling the ion trap is obtained as

$$\boldsymbol{F}_i^{ex} = -\nabla_i \Phi^{ex}(\boldsymbol{r}_i) = -m_g\omega_0^2\, \boldsymbol{r}_i, \tag{23}$$

and the screened Coulomb force, acting on the ith grain, is given by

$$\boldsymbol{F}_i^C = \sum_{j=1, j\neq i}^{N} \frac{Z^2e^2}{4\pi\varepsilon_0} \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{r_{ij}^3} \exp\left(-\frac{r_{ij}}{\lambda_D}\right) \left(1 + \frac{r_{ij}}{\lambda_D}\right). \tag{24}$$

Again, in this simplified model the interaction between the grains and the surrounding plasma is encoded in the last two terms in Eq. (21), i.e. by the friction coefficient $\gamma(\boldsymbol{v}_i)$ and the stochastic Langevin force $\boldsymbol{\mathcal{F}}_i(t)$.

Figure 6 shows, for the deterministic limit case $D_0 = 0$, examples of stable stationary excitations in actively driven Coulomb clusters with $N = 3, 4, 5$ grains. Each of these excitations represents a qualitatively different dynamical attractor type of the deterministic system. As discussed in [25], there exists a direct correspondence between the attractors in active Coulomb systems and the so-called normal modes in purely damped Coulomb clusters, recently investigated in experiments by Melzer *et al.* [32].

If the grains are additionally subject to noise, $D_0 > 0$, the stationary dynamics of the model system is not confined to a single attractor basin anymore. If, however, the friction parameter α and the interaction parameter

$$\kappa \equiv \frac{Z^2e^2}{4\pi\varepsilon_0 m\omega_0^2\lambda_D^3} \tag{25}$$

are sufficiently large, then the stochastic trajectories are still spending a relatively long time in the vicinity of the attractor regions of the related deterministic system (with $D_0 = 0$). This is illustrated in Fig. 7 (a), where a stochastic orbit for an actively driven Coulomb cluster with $N = 2$ grains is shown.

Noise-induced transitions between the different attractor regions are, among others, reflected by the probability density $f(L)$ of the absolute angular momentum L. If active friction is

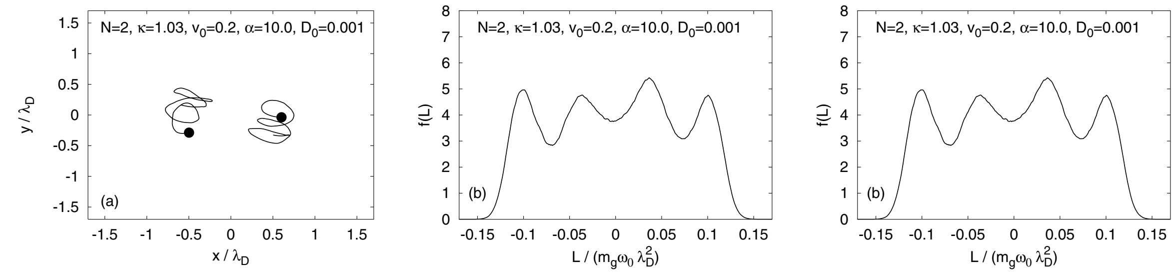

Figure 7. (a) For $D_0 > 0$ the two grains performs a stochastic motion around the center of the trap. Due to the influence of the stochastic force, the system can travel between the different attractor regions of the related deterministic system. (b) Numerically calculated angular momentum probability density $f(L)$ for the case $N = 2$ with active friction. The peaks of the distribution are located at the L-values that characterize the attractors of the corresponding deterministic system with $D_0 = 0$. (c) Numerically calculated function $f(L)$ for purely passive friction $\gamma(v) \equiv \gamma_0 = 1.0$; all other parameters are the same as in (b).

present, then the shape of the function $f(L)$ essentially differs from the approximately Gaussian shape, which is typical of systems with purely passive (positive) friction, compare Fig. 7 (b) and (c). More precisely, as evident from Fig. 7 (b), at sufficiently low (temperature) values D_0 active friction leads to a multi-peaked angular momentum probability density function $f(L)$. The characteristic values $L_1, L_2, \ldots$, at which these peaks occur, are – in lowest order approximation – determined by the mean angular momentum values of the attractors found for the corresponding deterministic system (with $D_0 = 0$).

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