Statistical Mechanics of Confined Systems with Rotational Excitations

Werner Ebeling [a]

[a] *Institute of Physics, Humboldt University Berlin, Invalidenstraße 110, D-10115 Berlin, Germany, e-mail:ebeling@physik.hu-berlin.de*

Gerd Röpke [b]

[b] *Department of Physics, University of Rostock, Universitätsplatz 3, D-18055 Rostock, Germany, email: gerd.roepke@physik.uni-rostock.de*

Abstract

New experimental and numerical investigations of confined systems of particles demonstrate the existence of rotational excitations. We develop here a statistical theory of finite systems, including rotational modes, by introducing the angular momentum into the formalism and by constructing the relevant distributions. As special applications we study systems driven to a prescribed kinetic energy by negative friction or by special isokinetic thermostats. Several distribution functions which are solutions of the Liouville or Fokker-Planck equations are given. The theory is applied to Coulomb clusters confined by parabolic forces .

Key words: Confinement, rotational excitations, active Brownian motion, isokinetic thermostats, Coulomb clusters.
PACS: 05.40.-a,05.45.-a, 82.20.Mj

1 Introduction

The development of the statistical mechanics of finite systems starts with the pioneering papers of Gibbs [1]. In the twentieth century the theory of finite systems was developed mainly in connection with the theory of clusters [2]. There exist several examples of finite physical systems which show spontaneous excitation of rotational modes. As examples we mention rotations of grains in confined dusty plasmas and in confined plasmas created by strong laser pulses. Another well-studied example are systems of active Brownian particles, discussed in our previous work [3–6]. What all of these systems have in common is that they are driven by an energy supply to rotational modes. Here we wish to contribute to the general theory of the statistical mechanics of confined finite systems, using special considerations of the angular integrals of motion. In the last decade a new interest arose from new experimental possibilities for holding a finite system of particles in special field configurations using, for example, Paul traps, Penning traps, and heavy ion storage rings [7]. There also is strong interest in the properties of confined plasmas created by strong laser pulses [8]. Recently in dusty plasmas rather large Coulomb clusters have been created [9–12]. Considerable progress has also been achieved in the theoretical description of these phenomena. For example, 2D Coulomb clusters with parabolic confinement were studied by Lozovik, Bedanov and Peeters and others [13]. These authors give a Mendeleev table of the elementary excitations for $N = 2 - 52$. Further, the spectral properties of classical 2-d Coulomb clusters have been investigated [14]. It was shown that for any axial symmetric system, the system as a whole can rotate corresponding to an eigenfrequency $\omega = 0$. We mention also several simulations which demonstrate the dynamics of 2-d Coulomb clusters [15]. The most interesting new effect observed experimentally and theoretically is the excitation of rotational modes, and the present work is devoted to a discussion of this phenomenon. The development of a corresponding statistical theory of finite systems including rotational modes is still in its infancy. As we will show here this requires the introduction of the angular momentum into the formalism of statistical mechanics. In standard statistical mechanics, characterized by canonical distributions, the angular momentum usually does not play a role except for special systems as e.g. rotating stars [16]. Assuming canonical distributions the mean angular momentum is alway zero. This follows from the Maxwell distribution which is peaked around zero velocity. Here we need distribution functions which include the angular momentum explicitly in a non-trivial way. We will profit from four directions in the theory of far from equilibrium systems,

- the theory of relevant distributions [17, 18]
- the theory of canonical-dissipative systems [19–24].
- the theory of active Brownian particles [3–6]
- the theory of thermostats [25, 26].

In all of these different approaches a rather general ensemble theory can be developed. Most of the applications of the theory for nonequilibrium distributions have been to transport theory [17, 18], and the theory of thermostats has largely been applied to molecular dynamics [25, 26]. On the other hand the theory of canonical-dissipative systems and the theory of active Brownian particles mainly concentrated on biological applications, e.g. cell and swarm dynamics [3–6].

2 Construction of Nonequilibrium Ensembles

2.1 Observables describing rotational modes

In this section we develop some aspects the general theory of the classical and quantum statistical mechanics of confined finite systems making a special consideration of the angular integrals of motion. Let us consider an $N-$ particle system with the Hamiltonian:

$$H_S = \sum_i^N \frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} V(\boldsymbol{r}_i - \boldsymbol{r}_j) \ . \tag{1}$$

Including an embedding in surroundings, a heat bath, we have two additional terms in the total Hamiltonian:

$$H_{total} = H_S + H_B + H_{SB}$$

here the bath is modeled by $H_B = H_B(Q,P)$, and the coupling by $H_{SB} = \sum_i^N V(\boldsymbol{r}_i, Q)$. Special cases are the isolated system with $H_{SB} = 0$ and external fields $V^{\rm ext}(\boldsymbol{r}_i)$, modeling traps.
Let us discuss now the observables corresponding to conserved or prescribed quantities. Since the choice of these observables is not clear from the beginning, candidates we consider are the invariants of the dynamics and quantities which are prescribed by the boundary conditions. Among the invariant quantities is the angular momentum of special interest is in our context:

$$\boldsymbol{L}_N = \sum_i^N \boldsymbol{L}_i, \quad \boldsymbol{L}_i = \boldsymbol{r}_i \times \boldsymbol{p}_i \ .$$

Further $\boldsymbol{L}_N^2$ and higher powers of the angular momentum are of interest. The time evolution is given by:

$$\frac{d}{dt}\boldsymbol{L}_N = \frac{i}{\hbar}[H, \boldsymbol{L}_N] = \frac{i}{\hbar}[H_{SB}, \boldsymbol{L}_N] \ . \tag{2}$$

We will assume central forces, so that any change of the angular momentum is due to the "bath". If the coupling H_{SB} is absent or has rotational symmetry then the total angular momentum is a conserved quantity. Alternatively we may prescribe the angular momentum by boundary conditions. For the relaxation time of the angular momentum we find from linear response theory the expression

$$\tau_L \propto \int_0^\infty dt \ \langle \left(\frac{d\boldsymbol{L}_N}{dt}\right)_t \left(\frac{d\boldsymbol{L}_N}{dt}\right)_{t=0} \rangle \ ,$$

i.e. if the torque is weak, the relaxation time is long. The equilibrium correlation function may be evaluated by simulations or by analytical methods like

perturbation expansions.
Among the quantities which may be prescribed by the surrounding, the kinetic energy is of special interest. Due to specific boundary conditions in some situations the individual kinetic energies are prescribed up to certain accuracy. For example, the interaction with a laser beam or with a surrounding plasma may fix the kinetic energies of the individual particles T_i around some value given by the laser intensity

$$T_i = \frac{m_i}{2}\boldsymbol{v}_i^2 \simeq T_0 \ .$$

In a recent paper Trigger and Zagorodny [27] have shown that the charged grains in a dusty plasma have a velocity distribution which is peaked around a characteristic kinetic energy of the grains.

2.2 Distributions for the relevant quantities

As pointed out above, if the coupling H_{SB} is absent or has rotational symmetry the total angular momentum is a conserved quantity. Alternatively we may prescribe it by boundary conditions. Then, in classical or quantum statistical approach

$$\rho = \rho(H_S, N, \boldsymbol{L}_N) \ .$$

Such a distribution is then given by the initial conditions, and this may be a canonical distribution, but also any other forms of functional dependence are possible. Two cases are of special interest:
1) For rotating bodies of N particles which are only weakly coupled to an external heat bath and which otherwise are in internal equilibrium, the distribution is well known. Here the angular momentum $\boldsymbol{L}_N$ is given as a conserved quantity and we may assume an extended Gibbs distribution (see Landau and Lifshits [16]).

$$\rho_{\text{eq}} = \frac{1}{Z_{\text{eq}}} e^{-\beta(H_S - \mu N - \boldsymbol{\omega}\cdot\boldsymbol{L}_N)} \ . \tag{3}$$

here $\boldsymbol{\omega}$ is the angular velocity. 2) If the torque due to the surrounding bath is weak, then $\boldsymbol{L}_N$ is nearly conserved, and it is a long-living mode of the system. In particular this is the case if the cluster and the surroundings have nearly spherical symmetry. Then $\boldsymbol{L}_N$, $\boldsymbol{L}_N^2$, etc. are quasi-conserved and should be included in the relevant distribution [17, 18].
Assuming that several $n-$ order moments of the angular momentum are given at time t

$$\text{Tr}\{\rho_{\text{rel}}(t) L_N^n\} = \langle L_N^n \rangle^t$$

then we find the distribution by maximizing the entropy following standard methods [17, 18]. In our case we get the generalized Gibbs distribution

$$\rho_{\rm rel}(t) = \frac{1}{Z_{\rm rel}(t)} e^{-\beta\left(H_S - \mu N - \sum_n \boldsymbol{\omega}_{(n)}(t) \boldsymbol{L}_N^n\right)} \tag{4}$$

Here the Lagrange multipliers $\boldsymbol{\omega}_{(n)}(t)$ are determined by the prescribed averages as shown in detail e.g. in [17, 18]. Of special importance is the case $n = 2$, i.e. the square of the angular momentum is given.
Now we will consider relevant distributions including kinetic energy and angular momentum. As already mentioned, sometimes the experimental conditions are such that the particles are driven to to a prescribed kinetic energy

$$\boldsymbol{v}_i^2(t) \to v_0^2$$

Examples are charged grains in dusty plasmas [11, 27] or Coulomb clusters driven by a strong laser field. Due to the interaction with the surrounding, in the examples the bath is provided by the plasma ions or the radiation field, and the particles are accelerated to certain kinetic energy. In this case we postulate that the distribution is of the following form

$$\rho_N(\boldsymbol{v}_1, ..., \boldsymbol{v}_N) = \Pi_{i=1}^N \exp\left[-\alpha_v(\boldsymbol{v}_i^2 - v_0^2)^2\right] \tag{5}$$

According to this distribution the most probable squared velocities (kinetic energies) are at the values v_0^2. Here α_v is an appropriate parameter characterizing the dispersion. We denote this type of ensemble "isokinetic ensemble". This notation is borrowed from molecular dynamics, where Gaussian isokinetic ensembles play an important role [25, 26].
This can be generalized to conditions that fix the individual energies H_i of the particles around a given value H_0. This leads to the Gaussian distributions

$$\rho_N(v_1, ..., v_N) = \Pi_{i=1}^N \exp\left[-\alpha_H(H_i - H_0)^2\right] \tag{6}$$

In radially symmetric systems, this driving to v_0^2 or H_0 implies for a special class of systems (an example will be given below) that $\boldsymbol{L}_i$ is also fixed about a certain L_{i0}. This is due to internal connections between the invariants of motion. Therefore we will consider also the distributions

$$\rho_N(L_1, ..., L_N) = \Pi_{i=1}^N \exp\left[-\alpha_L(\boldsymbol{L}_i - L_{i0})^2\right] \tag{7}$$

Let us briefly discuss the physical meaning of probability distributions with prescribed angular momenta.

Where is the probability concentrated in the phase space? We consider as a simple case a rotating 2-dimensional particle in a 4-dimensional phase space (a physical realization will be considered below). Then fixing the total energy $H = E$ defines the surface of a sphere (or a cylinder if the kinetic energy

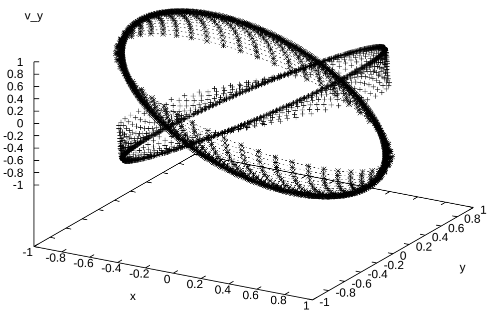

Fig. 1.
Typical distribution of a rotating 2-d particle with fixed angular momentum $\boldsymbol{L}^2 = L_0^2$. *The two possible values of the angular momentum select two tires on the sphere* $H = const.$. *We see a projection of the 4-dimensional phase on the* $x - y - v_y -$ *space.*

is prescribed) in the 4-dimensional space. If, in addition, the square of the angular momentum is prescribed, $\boldsymbol{L}^2 = L_0^2$, we define this way two planes in the phase space which intersect with the sphere on two perpendicular circles. An example is shown in Fig. 1. This way the probability will be concentrated on two "tires" in the phase space.
We used in this section the method of generalized Gibbs distributions [16] and in particular the Zubarev method for constructing relevant distributions [17,18]. These methods are of phenomenological character and connected with the maximum entropy approach. We repeat the basic assumption: Due to the boundary conditions certain averages as e.g. here the angular momentum L_N or L_N^2 are prescribed. This does not mean that the quantities are fixed, only the averages are prescribed and fluctuations around the means which are described by the distribution are possible. In the next section we will develop a more special microscopically oriented method for the construction of nonequilibrium distributions. This method is based on a theoretical model for a special driving mechanism, the model of canonical-dissipative driving.

3 Driven Nonequilibrium Systems

3.1 Driving by canonical-dissipative forces

The term "canonical - dissipative" expresses a special extension of the Hamiltonian dynamics [19–24]. The new equations of motion have Hamiltonian structure but contain additional dissipative terms. These terms, characterizing the driving/dissipation, are fully determined by integrals of the conservative motion. The rather special character of this assumption allows in many cases exact solutions of the dynamical and stochastic equations. The theory of canonical-dissipative systems is closely connected with the theory of invariants of motion. The relation between canonical- dissipative systems and finite systems is based on the fact that in systems of finite particles which are held in a field configuration, the invariants of motion play also a very specific role. In macroscopic systems under normal conditions only the Hamiltonian is relevant and other invariants as e.g. the angular momentum do not exist. This is in part connected with the boundary conditions which forbid e.g. free rotations of macroscopic systems. In driven finite systems of canonical-dissipative type, rotational excitations and distributions of the angular momentum play a special role [6]. In the simplest case the dissipation is determined by the Hamiltonian $I_0 = H$. However we may introduce also other invariants of motion: $I_1, I_2, ..., I_s$ e.g $I_1 = L^2$, ... In the general case we postulate the equations of motion:

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} - \frac{\partial G(I_0, I_1, I_2, ...)}{\partial p_i} \tag{8}$$

This system may be driven to certain bounded manifolds of the phase space, which correspond to relative minima of the generating function G. For example the square of the angular momentum may be prescribed by

$$G(L^2) = d(L^2 - L_1^2)$$

This driving force fixes the angular momentum and concentrates the motion on a submanifold. In the final stationary state which is located on this submanifold, the dissipative terms disappear, i.e. the final trajectories correspond to a Hamiltonian system. The invariants of motion cannot be prescribed in an arbitrary way, but they should be consistent with the target Hamiltonian system and with other given invariants. Therefore prescribing one invariant may fix also several others.
The stochastic theory may be formulated in the standard way by Langevin and Fokker-Planck equations. Considering only 2 invariants H and L^2 the Langevin equations read:

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} - \frac{\partial G(H, L^2)}{\partial p_i} + (2D)^{1/2}\xi_i(t) \tag{9}$$

The Fokker-Planck equations are given by:

$$\frac{\partial \rho}{\partial t} + \sum p_i \frac{\partial \rho}{\partial q_i} - \sum \frac{\partial H}{\partial p_i}\frac{\partial \rho}{\partial p_i} = \sum \frac{\partial}{\partial p_i}\left[\frac{\partial G(H; L^2)}{\partial p_i}\rho + D\frac{\partial \rho}{\partial p_i}\right] \tag{10}$$

The special structure of this partial differential equation allows to find exact stationary solution depending only on H, L^2.

$$\rho_0(q_1...q_f p_1...p_f) = Q^{-1} \exp\left(-\frac{G(H;L^2)}{D}\right) \tag{11}$$

The derivative of ρ_0 vanishes if $G' = 0$. This means the probability is maximal at the surface $H = E_1, L^2 = L_1^2$ where G is minimal. In the limit of small noise $D \to 0$ we get microcanonical ensembles with constant probability density on shells. For special choices of G the distribution (11) may agree with one of the relevant distributions discussed before. Let us discuss as a simple example one particle with

$$H = \frac{\boldsymbol{p}^2}{2m}, \qquad G(H) = \gamma H - \alpha \log(1 + \beta H) \tag{12}$$

This leads to the Langevin equation

$$\frac{d\boldsymbol{p}}{dt} = \left(\frac{\alpha}{1 + \beta \boldsymbol{p}^2/2m} - \gamma\right) \frac{\boldsymbol{p}}{m} + (2D)^{1/2} \boldsymbol{\xi}(t) \tag{13}$$

The stationary distribution which solves the Fokker-Planck equation reads

$$\rho_0(\boldsymbol{p}) = Q^{-1} \left(1 + \frac{\beta \boldsymbol{p}^2}{2m}\right)^{\alpha/D} \exp\left(-\frac{\gamma \boldsymbol{p}^2}{2mD}\right) \tag{14}$$

In the limit of small noise this distribution is sharply peaked around $\boldsymbol{p}^2 = m v_0^2$ with the characteristic velocity

$$v_0^2 = \frac{2}{m}\left(\frac{\alpha}{\gamma} - \frac{1}{\beta}\right) \tag{15}$$

In the limit of small noise $D \to 0$ or strong driving $\beta \to \infty$ the velocity distribution can be approximated by

$$\rho_0(\boldsymbol{v}) = C \exp\left[-\alpha_v (\boldsymbol{v}^2 - v_0^2)^2\right] \tag{16}$$

with $\alpha_v = (\alpha^2/(2\gamma D))$. We notice that this distributions is of the type derived in the previous section from Zubarev's formalism (see eq.(5)). Physically this distribution corresponds to a condition where the kinetic energies of the individual particles are sharply peaked around certain mean values.

The special type of driving described before leads us to the concept of active Brownian motion. This model unifies the idea of Brownian motion with the model of (acoustic) oscillators driven by negative friction [3–5]. We will assume here that the energy supply which drives the system is provided by an energy depot [3, 4]. In order to specify the dissipative forces and equations of motions we consider $2-d$ systems of N masses m $(i = 1, 2, ..., k, ...N)$. The particles are confined by a linear force $-a\boldsymbol{r}$ which attracts to the center of confinement. We postulate a Langevin dynamics ($m = 1$):

$$\frac{d}{dt}\boldsymbol{r}_i = \boldsymbol{v}_i\,; \tag{17}$$

$$\frac{d}{dt}\boldsymbol{v}_i = \boldsymbol{F}_i - a\boldsymbol{r}_i + \sqrt{2D}\boldsymbol{\xi}_i(t) \tag{18}$$

The dissipative forces have the following form:

$$\boldsymbol{F}(e, \boldsymbol{v}) = \boldsymbol{v}(de^n - \gamma_0) \tag{19}$$

where e is the energy content of a depot and d is a conversion parameter. The first term expresses an acceleration in the direction of $\boldsymbol{v}$. The second term $\gamma_0\boldsymbol{v}$ is the usual passive friction, which by assumption is connected with the noise by an Einstein relation $D = \gamma_0 kT$. We assume further that the Brownian particles are able to take up energy, which can be stored in the depot e. This internal energy can be converted into kinetic energy with a momentum dependent rate $de^n v^2$, which results in the acceleration in the direction of movement. The exponent n is free so far. In the first variant of the depot model (SET-model) we assume the exponent $n = 1$ and formulate the balance of the depot energy [3, 4, 28]

$$\frac{de}{dt} = q - ce - d\boldsymbol{v}^2 e \tag{20}$$

Here q is the rate of energy supply and c the rate of internal dissipation. Assuming $q > 0$ and requiring that the internal energy depot relaxes fast compared to the motion of the particle we get in adiabatic approximation the effective dissipative force [3, 4, 28]

$$\boldsymbol{F} = \boldsymbol{v}\left(\frac{dq}{c + dv^2} - \gamma_0\right) \tag{21}$$

For sufficiently large values of q and d the friction function may have a zero at

$$v_0^2 = \frac{q}{\gamma_0} - \frac{c}{d} = \frac{c}{d}\zeta; \qquad \zeta = \frac{qd}{c\gamma_0} - 1 \tag{22}$$

Here ζ is the bifurcation parameter. For $\zeta > 0$ and $|\boldsymbol{v}| < v_0$, we have a free energy input, the system is driven (self-propelling).
We now discuss a second variant of the depot model where the exponent is $n = 1/2$. In this case we assume the following balance of the depot

$$\frac{de}{dt} = q\sqrt{e} - ce - d\boldsymbol{v}^2\sqrt{e} \tag{23}$$

In this second model we get assuming $q > 0$ and requiring that the internal energy depot relaxes fast compared to the motion of the particle in adiabatic approximation

$$\boldsymbol{F} = \boldsymbol{v}\left(\frac{d}{c}(q - v^2) - \gamma_0\right) \tag{24}$$

Now for $dq > c\gamma_0$ a root $v_0^2 = (dq/c) - \gamma_0 > 0$ exists and we get a cubic expression which corresponds to the Rayleigh friction law. Both friction forces have qualitatively the same shape which is shown in Fig. 2. A common way of writing both model laws is

$$\boldsymbol{F} = -\gamma(\boldsymbol{v}^2)\boldsymbol{v}.$$

Here the friction γ is velocity-dependent, containing as a rule a negative part at small velocities. Negative friction provides energy input (pumping) and allows self-organization [22].
It is interesting to notice that the second model has another important limit. Introducing the variable $\gamma(t) = \gamma_0 - d\sqrt{e}$ we find the "dissipative force"

$$\boldsymbol{F} = -\gamma(t)\boldsymbol{v} \tag{25}$$

with a time-dependent friction which satisfies the dynamic equation

$$\frac{d\gamma}{dt} = \frac{d}{2}\left(v^2 - \frac{c}{d}\gamma - q + \frac{c}{d}\gamma_0\right) \tag{26}$$

In the limit $c = 0$ this reduces to a Nose'-Hoover dynamics.
Let us consider now the stochastic distributions. With respect to the stochastic term in the Langevin equation we assume that only the passive friction generates noise $D = \gamma_0 kT$.

In the simplest case of force-free particles, the kinetic energy is a conserved quantity : $v^2 = const.$. This means the system is canonical-dissipative. Consequently we are able to find exact solutions for the probability following the schema described above. For the SET-model we find the stationary distribution:

$$\rho_0(v_1, v_2) = C \exp\left[-\frac{v^2}{2kT} + \frac{q}{2D}\log\left(1 + \frac{d}{c}v^2\right)\right] \tag{27}$$

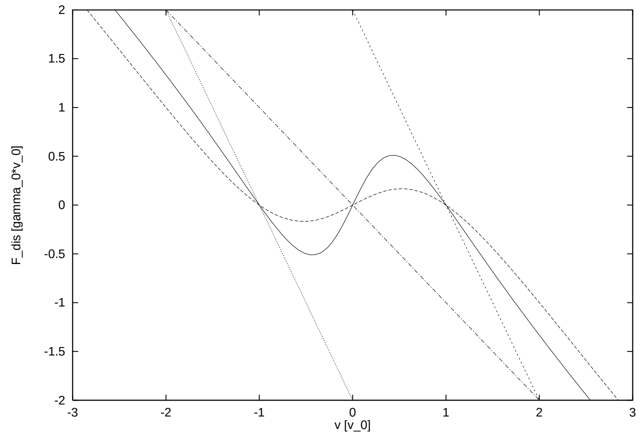

Fig. 2.

Friction force driving active particles: (i) Passive friction force (dash-dotted straight line). (ii) SET-model for different strength of driving $\zeta = 0.5$ *(dashed line);* $\zeta = 2$ *(full line);* $\zeta = \infty$ *(dash-dotted line with a step at zero); (iii) Second model, cubic law of Rayleigh type (dashed line, same curve as for SET with* $\zeta = 0.5$*).*

This distribution corresponds to eq. (14) derived above for the simplest example of a canonical-dissipative system. We notice also the close relation to Lorentz gas distributions [26]. Driving by velocity-dependent dissipative forces may have similar effects as driving by isokinetic thermostats [25]. We have to emphasize, however, that we discussed here only dissipative thermostats.
So far we have not considered rotations. In order to create an angular momentum we combine a driving to prescribed kinetic energies, as described above, with a rotational-symmetric confinement [5].

4 Rotations in confined Coulomb systems

As an application we now consider clusters of highly charged grains confined on a plane in a parabolic well. The theory of the ground state of 2-dimensional clusters of charged particles in parabolic confinement is due to Lozovik, Bedanov, Peeters and others [13,14]. These authors investigated the spectrum of excitations, in particular the rotational modes and derived a Mendeleev table N = 2-52. We mention also the experimental investigations by Melzer et al. [11] and simulations by Bonitz et al. [15]. Here we concentrate on the question of nonequilibrium excitations under conditions of negative friction. Trigger and Zagorodny have shown [27], that charged grains embedded into a plasma behave according to negative friction which is due to the absorption of ions. The friction function derived by Trigger and Zagorodny [27] is at least qualitatively very similar the models discussed in the previous section. Therefore we will use the driving by negative friction of the SET-type described in section 3 as a simple model for the difficult nonequilibrium situation of real plasmas. We study here only a simplified situation with the following properties:

- N grains are confined on a plane by parabolic forces,
- the grains are driven be negative friction to a characteristic velocity v_0.
- the particles repel each other by means of Coulombic interactions

We model the mechanism of driving $v_i^2 \to v_0^2$ by a velocity-dependent dissipative force. Since the friction function derived by Trigger and Zagorodny [27] is rather complicated we will model it here by a SET-like friction function with adapted parameters. Following Trigger and Zagorodny we consider grains with radius a, mass m_g and charge Z which are embedded into an electron-ion plasma with ion density n_i, the ions have the temperature T_i, the mass m_i, the thermal velocity v_{Ti} and the charge Z_i. The parameter of nonideality is defined as

$$\Gamma = \frac{Z Z_i e^2}{k_B T_i a} \tag{28}$$

We assume that $\Gamma > 1$ holds, but on the other side the nonideality is not too large. With these assumptions and notations a reasonable approximation of SET-type of the friction function derived by Trigger and Zagorodny [27] reads:

$$\gamma(v^2) = 2A(\Gamma - 1)\frac{v^2 - v_0^2}{v_0^2 + \delta v^2} \tag{29}$$

where

$$A = \frac{m_i\sqrt{2\pi}}{3m_g} n_i a^2 v_T \tag{30}$$

The fit parameter δ is found to be

$$\delta = \frac{(3\Gamma - 1)v_0^2}{10(\Gamma - 1)v_{Ti}} - 1 \tag{31}$$

and the target velocity is approximated by

$$v_0^2 = v_{Ti}^2 \frac{10\Gamma + 15\Gamma^2 - 25}{15\Gamma - 7} \tag{32}$$

We will assume further that the grains move on a plane and are confined confined in a parabolic well

$$U(r) = \frac{1}{2}\omega^2(x^2 + y^2)$$

These assumptions reflect in some approximation the conditions in the experiments of Melzer, Klindworth and Piel [11]. In order to determine the characteristic features we first consider the case $N = 2$ i.e. 2 grains are confined in a parabolic well. In the ground state $v_0 = 0$ both particles are at rest and have the distance r_0 and the energy E_0 corresponding to equilibrium between Coulomb repulsion and the attraction to the center. In the opposite case of very large excitations $mv_0^2 \gg (Ze)^2/r_0$ the two particles move on high orbits with the radius

$$r_0 \simeq \frac{v_0}{\omega_0}$$

Under these conditions we have equipartition of kinetic and potential energy and find

$$H = \frac{1}{2}(\boldsymbol{v}^2 + \omega_0^2 \boldsymbol{r}^2) \simeq 2v^2 \simeq 2v_0^2$$

Further we find for the angular momentum

$$L^2 \simeq r_0^2 v^2 \simeq \frac{v_0^4}{\omega_0^2}$$

We see that for strong excitations these systems have additional conserved quantities: kinetic energies, potential energies and angular momenta are in fixed relations. These relations are specific for parabolic forces. We will study now N particles and assume that the oscillator energy v_0^2 is very large in comparison to the Coulomb energy. The N particles which are driven to the kinetic energy $v_0^2/2$ will move on circular orbits in the external parabolic potential $U(r)$. The deterministic motion is determined by a balance between centrifugal and attracting forces

$$\frac{v^2}{r} = |U'(r)| \tag{33}$$

This conditions leads to two azimuthal modes corresponding to limit cycle orbits with the radius $r_0 = v_0/\omega_0$ and the angular momenta

$$L_+ = +\frac{v_0^2}{\omega_0}; \qquad L_- = -\frac{v_0^2}{\omega_0}. \tag{34}$$

The special solutions of the deterministic equations describing the rotational modes reads

$$x = r_0 cos(\omega_0 t + \phi); \qquad y = r_0 sin(\omega_0 t + \phi) \tag{35}$$

The second limit cycle with negative angular momentum follows by inversion of the direction of motion. The 2 limit cycles of our problem were represented in Fig. 1. On the limit cycle orbits the following relations are valid

$$H \simeq 2T \simeq Nv^2; \qquad L = \pm H/\omega_0; \qquad L^2 \simeq N r_0^2 v^2 \tag{36}$$

In other words, we have additional invariants of motion and the system is canonical-dissipative on the limit cycle and near to it. This gives us a chance to find analytical solutions for the probability. In order to construct these solutions we use the relations (valid on and near to the limit cycle)

$$\gamma(v^2) \simeq \gamma(H_1) \simeq \gamma(L_1^2/r_0^2)$$

where H_1 and L_1 are given per particle. Introducing this into the known solution for the velocity distribution we get functions of H_1 or L_1 which solve the Fokker-Planck equation. In order to find the physically correct solution we have to fulfill the condition that $\boldsymbol{L}$ is perpendicular to the coordinate plane. This way we find the approximate solution

$$\rho_0(x_1, x_2, v_1, v_2) = C \exp\left[-\frac{H}{kT} + \frac{q}{2D}\log\left(1 + \frac{d}{c}H\right)\right]$$

$$\left[\exp\left(-\delta\left(L + H/\omega_0\right)^2\right) + \exp\left(-\delta\left(L - H/\omega_0\right)^2\right)\right] \quad (37)$$

with a free parameter δ characterizing the dispersion of L^2 around H/ω_0. The probability is concentrated on two tires (around the limit cycles) in the 4-d phase space as demonstrated already in Fig. 1. The distribution of the angular momentum is bistable and is shown in Fig. 3.

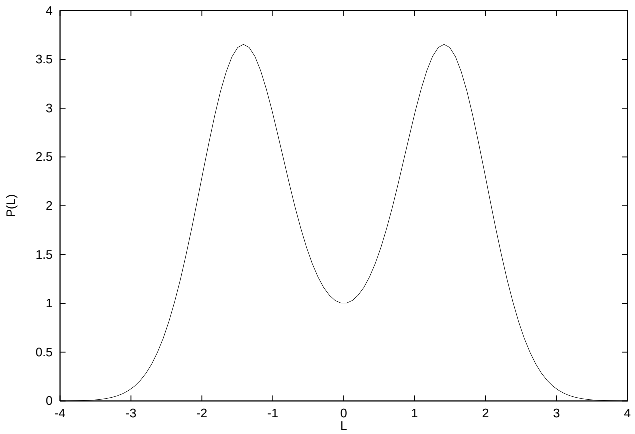

Fig. 3.
Distribution of angular momentum $P(L)$ for strongly driven particles distributed on a ring. SET-model with parameters $v_0 = r_0 = c = d = \gamma_0 = 1; q = 3; D = 1/2$

Now we discuss in brief the effect of Coulombic forces. We begin again with $N = 2$. The Hamiltonian reads

$$H = \frac{1}{2}(v_1^2 + v_2^2) + \frac{1}{2}\omega_0^2(r_1^2 + r_2^2) + \Phi(r) \quad (38)$$

Including screening we have

$$\Phi(r) = \frac{Z^2 e^2}{r}\exp(-\kappa r). \quad (39)$$

Here κ is the screening coefficient [11], which is zero for pure Coulomb interactions. In the ground state $v_1 = v_2 = 0$ and for $\kappa = 0$ we find the stationary distance

$$r_0 = \left[\frac{(Ze)^2}{2\omega_0^2}\right]^{1/3}$$

At finite velocities the situation is much more complicated since the Coulomb interaction influences the excitations. We consider here only the modes of azimuthal excitations, i.e. no radial oscillations are excited. For the stationary orbits we get from the equilibrium condition

$$\frac{v_0^2}{r_0} = \omega_0^2 r_0 + \Phi'(r_0) \tag{40}$$

which yields a nonlinear equation for $r_0(v_0)$. In the Coulomb $\kappa = 0$ case the stationary Hamiltonian and the angular momentum

$$L = (x_1 v_{1y} + x_2 v_{2y}) - (y_1 v_{1x} + y_2 v_{2x})$$

are given by

$$H_0 = 2v_0^2; \qquad L = \pm H/\omega_0 \tag{41}$$

Including noise, we may approximate the stationary distribution by Gaussian functions

$$\rho_0 \simeq \exp\left[-\alpha(H - 2v_0^2)^2\right]\left[\exp\left(-\delta(L + H/\omega_0)^2\right) + \exp\left(-\delta(L - H/\omega_0)^2\right)\right] \tag{42}$$

where α depends on the model for isokinetic driving and δ is a (still unknown) parameter characterizing the dispersion of the relation between L and H. In reality the excitations in excited Coulomb systems are extremely difficult, as one can guess already from he spectrum of the ground state excitations [14]. Here we restricted our study to the azimuthal modes which are connected with rotational excitations.

5 Discussion

The purpose of this paper is to contribute to the general theory of rotating systems. We studied first a general phenomenological theory based on generalized Gibbs distributions, in particular, systems which are driven to a given kinetic energy by negative friction. We used two models of driving:

- negative friction derived from the depot model SET,
- dissipative thermostats which fix the average of individual kinetic energies.

Both these models have in common the feature that the individual particles are driven to distributions centered around prescribed kinetic energies. In order to create an angular momentum we combined this driving mechanism with an rotational-symmetric confinement. Due to internal relations between the invariants of motion these systems typically show rotations. As an application we studied a simple model of 2-dimensional Coulomb clusters confined in parabolic fields. For the case of two particles and also for N particles on a ring we see in the model similar rotation phenomena as observed in experiments [11]. A more realistic model of these phenomena should include the full friction function derived by Trigger and Zagorodny [27], screening phenomena and the interaction of a larger number of grains, corresponding work is in progress.

We thank M. Bonitz, W.G. Hoover, R. Klages, S. Trigger and F. Schweitzer for discussions on these topics.

References

[1] J.W. Gibbs, Collected Works of J. Willard Gibbs, (Yale Univ. Press, New Haven 1902).

[2] J.W.P. Schmelzer, G. Röpke, V.B. Priezzhev (eds.), Nucleation theory and applications, (Publ. JINR, Dubna 2002).

[3] F. Schweitzer, W. Ebeling, B. Tilch, Phys. Rev. Lett. **80** (1998) 5044.

[4] W. Ebeling, F. Schweitzer, B. Tilch, BioSystems **49** (1999) 17.

[5] U. Erdmann, W. Ebeling, L. Schimansky-Geier, F. Schweitzer Eur. Phys. J. B **15** (2000) 105.

[6] F. Schweitzer, W. Ebeling, B. Tilch., Phys. Rev. E **64** (2001) 021110.

[7] W. Paul, Rev. Mod. Phys. **62** (1990) 5.

[8] S. Kulin, T.C. Killian, S.D. Bergeson, S.L. Rolston, Phys. Rev. Lett. **85** (1999) 318.

[9] J.H. Chu, I. Lin, Phys. Rev. Lett. **72** (1994) 4009.

[10] H. Thomas, G.E. Morfill, V. Demmel, J. Goree, B. Feuerbacher, D. Möhlmann, PRL **73** (1994) 652.

[11] A. Melzer, M. Klindworth, A. Piel, Phys. Rev. Lett. **87** (2001) 115002.

[12] V.E. Fortov, A.N. Nefedov, O.F. Petrov, Physics - Usphekhi **40** (1997) 1163.

[13] V.M. Bedanov, F.M. Peeters, Phys. Rev. B **49** (1994) 2667.

[14] V.A. Schweigert, F.M. Peeters, Phys. Rev. B **51** (1995) 7700.

[15] M. Bonitz, V. Golubnychiy, A.V. Filinov, Yu.E. Lozovik, Microelectronic Engineering **62** (2002) 141.

[16] L.L. Landau, E.M. Lifshits, Statistical Physics (Pergamon, Oxford 1959).

[17] Subarew, D.N.: Statistische Thermodynamik des Nichtgleichgewichts, (Akademie-Verlag, Berlin 1976).

[18] D.N. Zubarev, V. Morosov, G. Röpke, Statistical mechanics of nonequilibrium processes, vol. I-II, (Wiley, Berlin 1996/1997).

[19] R. Graham, Springer Tracts in Mod. Phys. **66** (1973) 111.

[20] H. Haken, Z. Phys. **263** (1973) 267.

[21] M.O. Hongler, D.M. Ryter, Z. Phys. B **31** (1978) 333.

[22] R. Feistel, W. Ebeling, Evolution of Complex Systems, (Kluwer, Dordrecht 1989).

[23] Yu.L. Klimontovich, Theory of Open systems, (Kluwer, Dordrecht 1995).

[24] W. Ebeling, Cond. Matter Phys. **3** (2000) 285.

[25] W. G. Hoover, Time reversibility, computer simulation, and chaos, (World Scientific, Singapore 1999.

[26] K. Rateitschak, R. Klages, W.G. Hoover, J. Stat. Phys. **101** (2000) 61.

[27] S.A. Trigger, A.G. Zagorodny, Phys. Rev. Lett., submitted (2002).

[28] C.A. Condat, G.J. Sibona, Physica D **168-169** (2002) 235.