Nonlinear Dynamics of Active Brownian Particles

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Abstract. We consider finite systems of interacting Brownian particles including active friction in the framework of nonlinear dynamics and statistical/stochastic theory. First we study the statistical properties for $1-d$ systems of masses connected by Toda springs which are imbedded into a heat bath. Including negative friction we find $N+1$ attractors of motion including an attractor describing dissipative solitons. Noise leads to transition between the deterministic attractors. In the case of two-dynamical motion of interacting particles angular momenta are generated and left/right rotations of pairs and swarms are found.

1 Introduction

The main purpose of this work is the study of the dynamics of active Brownian particles including interactions. The friction is modelled by a velocity-dependent function derived from a model of energy supply \cite{1,2,3,4,5}. The interaction between the particles is modelled by Toda potentials (in $1-d$) or Morse potentials (in $2-d$).

Since the classical work of Toda \cite{6} the development of the nonlinear dynamics and statistical thermodynamics of Toda systems has remained a central topic of research. Toda was able to find exact solutions for a special $1-d$ system with an exponential interaction. In particular Toda proved the existence of soliton solutions and calculated the exact partition function. Since that solitons as excitations of nonlinear chains of masses found a remarkable interest. Several interesting results were obtained for the statistical thermodynamics of Toda systems \cite{7,8,9}. We consider here systems with active friction and noise by means of analytical tools and simulations. It was shown in previous work, that there exists a special temperature regime around a transition temperature $T_{tr}$ between the phonon and the soliton regime, in another context called the localization temperature $T_{loc}$, where the interaction of solitons and phonons is strong and has a remarkable influence on several physical phenomena, a special one being energy localization at special sites \cite{13} and another one the excitation of a broadband coloured noise spectrum with an $1/f$ region at low frequencies \cite{14}. Here our main interest is devoted to the influence of negative friction on the properties of Brownian motion. Driving the system by negative friction to far from equilibrium states we find $N+1$ attractors of deterministic motion including an attractor describing dissipative solitons.
Noise leads to transition between the deterministic attractors. In the case of two-dynamical motion of interacting particles positive or negative angular momenta are generated with equal probability. This leads to left/right rotations of pairs, clusters and swarms. We will show that the collective motion of large clusters of driven Brownian particles reminds very much the typical modes of parallel motions in swarms of living entities.

2 Equations of motion, friction and forces

Let us consider a systems of $N$ point masses $m$ with the numbers $1, 2, ..., i, ...N$. We assume that the mass $m$ is connected to the next neighbours at both sides by Toda forces, The distance between the mass $i$ and the mass $i + 1$ is denoted by $R_i$, the equilibrium distance is assumed to be $\sigma$, therefore the spring elongation reads $r_i = R_i - \sigma$. In the following take $\sigma$ as the length unit.

The dynamics of the system is given by the following equation of motion for the elongations

$$\frac{d^2 r_i}{dt^2} = [V'(r_{i+1}) - 2V'(r_i) + V'(r_{i-1})] - \gamma(v_i)v_i + F_i(t) \quad (1)$$

where $F_i(t)$ is a stochastic force with strength $D$ and a $\delta$-correlated time dependence:

$$\langle F_i(t) \rangle = 0; \quad \langle F_i(t)F_j(t') \rangle = 2D \delta(t - t')\delta_{ij} \quad (2)$$

In the case of thermal equilibrium systems we have $\gamma(v) = \gamma(0) = \text{const.}$.

In the general case where the friction is velocity dependent we will assume that the friction is monotonically increasing with the velocity and that the limit for large velocities is a well defined constant:

$$\gamma(v) \to \gamma(0) = \text{const.} \quad (3)$$

Our basic assumption is, that in this limit the loss of energy resulting from friction, and the gain of energy resulting from the stochastic force, are compensated in the average. From this postulat follows the non-equilibrium fluctuation-dissipation theorem:

$$D = k_BT\gamma_0/m \quad (4)$$

Here $T$ is the temperature of the heat bath, $k_B$ is the Boltzmann constant, and $D$ is the strength of the stochastic force. For the case of a passive thermal heat bath $\gamma = \gamma_0$ eq.(3) agrees with the conventional Einstein relation. The validity of a fluctuation-dissipation relation between noise strength and damping strength is assumed in order to guarantee the existence of a stationary or thermal equilibrium, independent on the limit of the friction parameter $\gamma_0 \geq 0$. We note that $\gamma_0 = 0, T = 0$ corresponds to the conservative case.
In the following we will study first the simplest case of passive friction, i.e. we will assume that the friction function is constant \( \gamma(v) = \gamma_0 = \text{const} \). Then more complicated friction functions will be studied. Historically velocity-dependent friction forces were first studied by Rayleigh and Helmholtz. Extensions of these models were investigated in many papers on driven Brownian dynamics \[15\]. A characteristic property of these friction functions is the existence of a zero of friction for a finite velocity \( v_0 \) which defines a kind of attractor in the velocity-space. The model we use here for active friction with an attractor for the velocities \( v_0 \) was introduced in \[1\] and \[2\]. Detailed studies of this so-called energy depot model may be found in \[3,5\]. The case of Rayleigh-friction was analyzed in detail in \[4\]. The depot-model of the friction function is based on a concrete model of Brownian motion with energy supply, storage in a tank and conversion into motion \[1\]. We assumed that the Brownian particle itself is capable of taking up external energy storing some of this additional energy into an internal energy depot, \( e(t) \). Within the energy depot model the depot may be may be altered by three different processes:

1. take-up of energy from the environment; where \( q \) is the pump rate of energy
2. internal dissipation, which is assumed to be proportional to the internal energy. The rate of energy loss is denoted by \( c \).
3. conversion of internal energy into motion, where \( d \) is the rate of conversion of internal to kinetic degrees of freedom. The depot energy is used to accelerate the motion.

Our model of energy supply is motivated by investigations of active biological motion, which relies on the supply of energy. The supplied energy is in part dissipated by metabolic processes, but can be also converted into kinetic energy. The energy depot model leads in an adiabatic approximation to the following friction function

\[
\gamma(v) = \gamma_0 - \frac{q}{1 + dv^2}
\]

For the energy depot model of active friction exists an attracting velocity. This is defined by the zero of the friction function \( \gamma(v_0) = 0 \) which has the value

\[
v_0^2 = \frac{\alpha}{d}; \quad \alpha = \frac{q}{\gamma_0} - 1
\]

Here \( \alpha \) plays the role of the bifurcation parameter. For \( \alpha < 0 \) the friction is purely passive, i.e. in average no energy is supplied. For \( \alpha > 0 \) the friction function has a negative part near to \( v = 0 \) and a zero point which acts as an attracting set in the velocity space.

The interaction between the masses \( i \) and \( i + 1 \) is in the 1d-case modelled by the Toda force

\[
f_i = -V'(r_i) = \frac{\omega^2}{b} (\exp [-br_i] - 1)
\]
Here \( b \) is the stiffness of the springs and \( \omega \) is the linear oscillation frequency around the equilibrium position.

In the harmonic limit the force is given by \( f_i = \omega r_i \). The spring energy is described by the Toda potential

\[
V(r_i; \omega, b) = \frac{m\omega^2}{b^2} (\exp[-br_i] - 1 + br_i)
\]

We will use \( m\omega^2\sigma^2 \) as the energy unit.

In general the calculation of the distribution functions of interacting particles is not a trivial task since it is connected with the solution of a multi-dimensional Fokker-Planck equation. A full solution is available only for the passive case \( \gamma = \gamma_0 = \text{const} \). Then the only attractor of the dynamics is the rest state of the particles and the statistical properties in equilibrium are described by a canonical Toda ensemble under pressure \( P \) and temperature \( T \) \([10, 11, 12]\). The stationary solution of the Fokker-Planck equation which corresponds to our Langevin equation reads

\[
P_0(p_n, r_n) = Z_1^{-1} \exp\left(-\frac{p_n^2}{2m} + \frac{V_{\text{eff}}}{k_BT}\right)
\]

\[
Z_1^{-1} = \frac{bX^{X+Y}}{\sqrt{2\pi mk_BT} \exp(X) \Gamma(X+Y)}
\]

with the effective potential

\[
V_{\text{eff}}(r_n) = V(r_n) + Pr_n
\]

Here \( k_B \) denotes the Boltzmann constant, and \( V(r) \) is the Toda potential defined above. Further we used the abbreviations

\[
X = \frac{m\omega^2}{b^2 k_BT}; \quad Y = \frac{P}{bk_BT}
\]

The elementary excitations in passive Toda rings including the noise spectrum and the structure factor were investigated in detail in the work \([13, 14]\). The investigation of the dynamics of Toda rings with energy supply by active friction is more difficult and only partial solutions are available \([3, 4]\). We discuss here the special case when the supply of energy is given by the depot model in the approximation of a velocity-dependent friction \([12, 13]\). Due to the driving slow particles are accelerated and fast particles are damped. At definite conditions our active friction function has a zero corresponding to stationary velocities \( v_0 \), where the friction disappears. The deterministic trajectory of our system is then attracted by a cylinder in the 4d-space given by

\[
v_1^2 + v_2^2 = v_0^2
\]

where \( v_0 \) is the value of the stationary velocity which is for the depot-model given by \( v_0^2 = \frac{\alpha}{\gamma} \).
In Fig. 1 we see the result of a histogram calculated by J. Dunkel for $N = 8$ particles with Toda interactions. Here the result of 1000 runs with stochastic initial conditions is represented as a function of the average velocity of the particles. The shape of the histogram demonstrates the existence of $N + 1$ attractors of motion. We underline however that the histogram shown in Fig. 1 is the result of finite time runs, so it represents the shape of a finite-time distribution function. In the limit of long runs the distribution may change; we expect e.g. that at long times the statistical weights are shifted from the center of the distribution to the wings.

3 Two-dimensional dynamics

The effects demonstrated in the previous sections are not restricted to $1 - d$ Toda lattices but persist at least qualitatively in more realistic $2 - d$ and $3 - d$ models of dense fluids consisting of solvent and solute molecules with Morse- or Lennard-Jones interactions. Superposition of solitons corresponds to multiple collisions in these systems. In higher dimensions a weak localisation of potential energy was observed also at the bindings of the bath molecules and was connected to a transition between different lattice configurations.

We introduce interactions described by the potential $U(r_1, ..., r_N)$; then the dynamics of Brownian particles is determined by the Langevin equation:

$$\dot{\vec{r}}_i = \vec{v}_i; \quad m\dot{\vec{v}}_i = -\gamma(v_i)\vec{v}_i - \nabla U(r_1, ..., r_N) + \mathcal{F}(t)$$

where $\mathcal{F}(t)$ is a stochastic force with strength $D$ and a $\delta$-correlated time dependence as defined above.

We will discuss now the motion of active particles in a two-dimensional space, $r = \{x_1, x_2\}$. The case of constant external forces was already treated by

![Fig. 1. Probability distribution for 8 active Brownian particles](image-url)
Schienbein and Gruler [20]. Symmetric parabolic external forces were studied in [2,3,5] and the non-symmetric case is being investigated in [21].

Here we will study 2d-systems of \(N \geq 2\) particles (see Fig. 2).

We will begin with the study of a 2-particle problem [21]. Let us imagine two Brownian particles which are pairwise bound by a pair potential \(U(r_1 - r_2)\). The two molecules will form dumb-bell-like configurations. Then the motion consists of two independent parts: The free motion of the center of mass having the coordinates \(X_1 = 0.5(x_{11} + x_{21})\) and \(X_2 = 0.5(x_{12} + x_{22})\).

The relative motion under the influence of the potential is described by the coordinates \(\tilde{x}_1 = (x_{11} - x_{12})\) and \(\tilde{x}_2 = (x_{12} - x_{21})\). The motion of the center of mass \(M\) is described by the equations

\[
\begin{align*}
\dot{X}_1 &= V_1 \\
M \dot{V}_1 &= -\gamma (V_1, V_2) V_1 + F_1(t)
\end{align*}
\]

\[
\begin{align*}
\dot{X}_2 &= V_2 \\
M \dot{V}_2 &= -\gamma (V_1, V_2) V_2 + F_2(t)
\end{align*}
\]

(14)

The stationary solutions of the corresponding Fokker-Planck equation reads [3]

\[
P_0(V) = C (1 + dV^2)^{(a/2D)} \exp \left[ -\frac{\gamma_0}{2D} V^2 \right]
\]

(15)

This corresponds to the driven motion of a free particle located in the center of mass.

The relative motion is described by the equations

\[
\begin{align*}
\dot{\tilde{x}}_1 &= \tilde{v}_1 \\
\mu \dot{\tilde{v}}_1 &= -\gamma (\tilde{v}_1, \tilde{v}_2) \tilde{v}_1 - \partial_1 U + \tilde{F}_1(t) \\
\dot{\tilde{x}}_2 &= \tilde{v}_2 \\
\mu \dot{\tilde{v}}_2 &= -\gamma (\tilde{v}_1, \tilde{v}_2) \tilde{v}_2 - \partial_2 U + \tilde{F}_2(t)
\end{align*}
\]

(16)

Fig. 2. Snapshot of 1000 Brownian particles rotating in a parabolic self-consistent field
with $\mu = m/2$. For simplification we specify now the potential $U(r)$ as a symmetric parabolic potential:

$$U(x_1, x_2) = \frac{1}{2}a (x_1^2 + x_2^2)$$

(17)

First, we restrict the discussion to a deterministic relative motion, which is described by four coupled first-order differential equations. The relative motion of 2 particles corresponds to the absolute motion of 1 particle in an external field. Therefore we will omit now for simplicity the tilde denoting the relative character of the motion and denoting the mass again by $m$ instead of $\mu$:

$$\dot{x}_1 = v_1 \quad m\dot{v}_1 = -\gamma(v_1, v_2) v_1 - ax_1$$
$$\dot{x}_2 = v_2 \quad m\dot{v}_2 = -\gamma(v_1, v_2) v_2 - ax_2$$

(18)

For the one-dimensional case it is well known that this system possesses a limit cycle corresponding to sustained oscillations [15]. For the $2 - d$ case we have shown in [2] that a limit cycle in the $4 - d$ space is developed, which corresponds to left/right rotations with the frequency $\omega_0$. The projection of this periodic motion to the $\{v_1, v_2\}$ plane is the circle

$$v_1^2 + v_2^2 = v_0^2 = \text{const.}$$

(19)

The projection to the $\{x_1, x_2\}$ plane also corresponds to a circle

$$x_1^2 + x_2^2 = r_0^2 = \frac{v_0^2}{\omega_0^2}$$

(20)

The energy for motions on the limit cycle is

$$E_0 = \frac{m}{2} (v_1^2 + v_2^2) + \frac{a}{2} (x_1^2 + x_2^2)$$
$$= \frac{m}{2} v_0^2 + \frac{a}{2} r_0^2$$

(21)

(22)

We have shown in [2], that any initial value of the energy converges (at least in the limit of strong driving) to

$$H \longrightarrow E_0 = m v_0^2$$

(23)

This corresponds to an equal distribution between kinetic and potential energy. As for the harmonic oscillator in $1 - d$, both parts contribute the same amount to the full energy. This result was obtained in [2] based on the assumption that the energy is a slow (adiabatic) variable which allows a phase average with respect to the phases of the rotation. In explicit form we may represent the motion on the limit cycle in the $4 - d$ space by the 4 equations [3]
\[ x_1 = r_0 \sin(\omega_0 t) \quad v_1 = -r_0 \omega_0 \cos(\omega_0 t) \quad (24) \]
\[ x_2 = r_0 \cos(\omega_0 t) \quad v_2 = -r_0 \omega_0 \sin(\omega_0 t) \quad (25) \]

The frequency is given by the time the particle needs for one period moving on the circle with radius \( r_0 \) with constant speed \( v_0 \). This leads to the relation
\[ \omega_0 = \frac{r_0}{v_0} = \left( \frac{m}{\mu} \right)^{1/2} = \omega \quad (26) \]

This means, the particle oscillates (at least in our approximation) with the frequency given by the linear oscillator frequency \( \omega \).

The trajectory on the limit cycle defined by the above 4 equations is like a hula hoop in the \( 4 - d \) space. The projections to the \( x_1 - x_2 \)-space as well as the projections to the \( v_1 - v_2 \)-space are circles. The projections to the subspaces \( x_1-v_2 \) and \( x_2-v_1 \) are like a rod. In the \( 4- d \) space the attractor has therefore the form of a hula hoop. A second limit cycle is obtained by reversal of the velocity. This second limit cycle forms also a hula hoop which is different from the first one, however both limit cycles correspond to opposite angular momenta. \( L_3 = +\mu r_0 v_0 \) and \( L_3 = -\mu r_0 v_0 \).

Applying similar arguments to the stochastic problem we find that the two hoop-rings are converted into a distribution looking like two embracing hoops with finite size, which for strong noise converts into two embracing tyres in the \( 4-d \) space. In order to get the explicit form of the distribution we may introduce the amplitude–phase representation \[ x_1 = \rho \sin(\omega_0 t + \phi) \quad v_1 = -\rho \omega_0 \cos(\omega_0 t + \phi) \quad (27) \]
\[ x_2 = \rho \cos(\omega_0 t + \phi) \quad v_2 = -\rho \omega_0 \sin(\omega_0 t + \phi) \quad (28) \]

where the radius \( \rho \) is now a slow and the phase \( \phi \) is a fast stochastic variable. By using the standard procedure of averaging with respect to the fast phases we get the distribution of the radii \[ P_0(\rho) = C \left( 1 + d\rho \omega_0^2 \right)^{(q/2D)} \exp \left[ -\frac{\gamma_0}{2D} \rho^2 \omega_0^2 \right] \quad (29) \]

The probability crater is located above the two deterministic limit cycles on the sphere \( r_0^2 = \frac{v_0^2}{\omega_0^2} \). Strictly speaking not the whole spherical set is filled with probability but only two circle-shaped subsets on it, which correspond to a narrow region around the limit sets. The full stationary probability has the form of two hula hoop distributions in the \( 4d \) space. This was confirmed by simulations \[ 3 \].

The projections of the distribution to the \( \{ x_1, x_2 \} \) plane and to the \( \{ v_1, v_2 \} \) plane are smoothed \( 2d \)-rings. The distributions intersect perpendicular the \( \{ x_1, x_2 \} \) plane and the \( \{ x_2, v_1 \} \) plane. Due to the noise the Brownian
particles may switch between the two limit cycles, this means inversion of the angular momentum (direction of rotation) \[3,21\].

Summarizing our findings for a 2-particle system forming a dumb-bell system we may state: The center of mass of the dumb-bell will make a driven Brownian motion corresponding to a free motion of the center of mass. In addition the dumb-bell is driven to rotate around the center of mass. What we observe then is a system of rotating Brownian molecules. The internal degrees of freedom are excited and we observe driven rotations.

In this way we have shown that the mechanisms described here may be used also to excite the internal degrees of freedom of Brownian molecules.

An extension of the theory of pairs leads to a theory of the motion of clusters of active molecules \[22,23,21,24\]. In Fig. 3 we see a snapshot of simulations of the stochastic dynamics of a cluster of 1000 active interacting Brownian particles.

In order to simplify the simulations we assumed that the interaction of the molecules in the cluster is given by a van der Waals-like interaction with a relatively long range range. For example we may use the interaction model proposed by Morse

\[
\phi(r) = A \left[ \exp(-ar) - 1 \right]^2 - A
\]  

(30)

Due to the attracting tail the molecules form clusters. The individual molecules move then in the collective (self-consistent) field of the other molecules which might be represented by a mean field approximation

\[
V(\tilde{r}) = \int d\tilde{r}' \phi(\tilde{r} - \tilde{r}') \rho(\tilde{r}')
\]  

(31)

where \( \tilde{r} = (\tilde{x}_1, \tilde{x}_2) \) is the radius vector counted from the center of mass and \( \rho(\tilde{r}') \) is a mean density in the cluster. Approximating \( V \) by quadratic terms

\[
\begin{array}{c}
\text{Fig. 3. Snapshot of the same swarm after one half period of rotation}
\end{array}
\]
only we get
\[ V(\tilde{x}_1, \tilde{x}_2) = V_0 + \frac{1}{2} (a_1 \tilde{x}_1^2 + a_2 \tilde{x}_2^2) + \ldots \] (32)

In this way we arrive again at the harmonic problem we have studied above. We may conclude that the individual molecules in the cluster move at least in certain approximation in a parabolic potential. From this follows that they will make rotations in the field. We have performed simulations with 1000 particles moving in a self-consistent potential of parabolic shape. The driving function has a zero at \( v_0^2 = 1 \). In Figs. 2 and 3 one sees two snapshots of the moving cluster formed by the molecules.

Since the individual particles move in an effective parabolic potential angular momenta are generated, the swarm starts to rotate. Similar as in the case of the dumb-bells the clusters are driven to make spontaneous rotations. Finally a stationary state will be reached which corresponds to a rotating cluster with nearly constant angular momentum (see Fig. 4). Under the influence of noise the cluster may switch to the opposite angular momentum, i.e. to the opposite sense of rotation, the system occurs to be bistable.

In Fig. 4 is shown that in noisy systems of active Brownian particles the two values \( L_3 = -m r_0 v_0, +m r_0 v_0 \) have the maximal probability. Strong coupling of the particles leads to synchronization of the angular momenta, for weak coupling the cluster may be decomposed into groups with different angular momentum \[21,24\]. The rotating swarms simulated in our numerical experiments remind very much the dynamics of swarms studied in papers of Vicsek and collaborators \[22,23\] and in other recent work \[21,24\].

4 Conclusions

We studied here the active Brownian dynamics of a finite number of particles including interactions modelled by Toda or Morse potentials and velocity-dependent friction. Beside analytical investigations we have made a numerical study of relatively small systems. For this we have been investigating 1d-model systems with nonlinear Toda interactions and 2d-models with parabolic confinement. At low enough temperatures we observe only harmonic excitations and the models reduce to systems of coupled harmonic oscillators. However at higher temperatures the dynamics is completely changed and nonlinear excitations of soliton-type come into play. At high temperatures the behaviour of 1d interacting systems is dominated by soliton-type excitations. Including active friction we observe in the 1d-case \( N + 1 \) attractors of nonlinear excitations. For interacting Brownian particles in 2d-case angular momenta are generated (see Fig. 4) and we find rotations of the particles around the center of attraction and collective rotational excitations of swarms.
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Fig. 4. Probability distribution of the angular momentum for active Brownian particles with $v_0^2 = r_0^2 = 1$