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Nonlinear Dynamics and Fluctuations of Dissipative Toda Chains[1]

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The dynamics of a ring of masses including dissipative forces (passive or active friction) and Toda interactions between the masses is investigated. The characteristic attractor structure and the influence of noise by coupling to a heat bath are studied. The system may be driven from the thermodynamic equilibrium to far from equilibrium states by including negative friction. We show, that overcritical pumping with free energy may lead to a partition of the phase space into attractor regions corresponding to several types of collective motions including uniform rotations, one- and multiple soliton-like excitations and relative oscillations. The distribution functions in the phase space and the correlation functions of the forces and the spectra of nonlinear excitations are calculated. We show that a finite-size Toda ring with weak thermal coupling develops at intermediate temperatures a broadband colored noise spectrum with an $1/f$ tail at low frequencies.

KEY WORDS: $1/f$ noise; soliton like excitations; energy localization; correlation spectrum; activation processes; Active Brownian particles; energy supply; nonlinear friction.

1. INTRODUCTION

The nonlinear excitations in Toda chains coupled to a heat bath or other environments were studied in several recent papers.[1–8] One of the reasons for the special interest in Toda systems is the existence of exact solutions for the dynamics and the statistical thermodynamics. On this basis it was

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shown in refs. 2 and 3 that phonon excitations determine the spectrum at low temperatures and strongly localized soliton excitations are the most relevant at high temperatures. In this paper we study dissipative Toda lattices including noise and passive or active (velocity-dependent) friction. In particular we will investigate far from equilibrium conditions.

In our earlier work we have studied several special effects in Toda rings including noise and passive friction, the influence of non-uniformities and several temperature regimes.[4–8] In subsequent work it was shown by MD-simulations for 1d-, 2d-, and 3d-systems of up to 200 molecules with Morse-interactions and with finite-range Lennard–Jones potentials[9, 10] as well as for the full Lennard–Jones interaction[11] that the basic effects observed in Toda rings, as e.g., the existence of "optimal" temperature regimes persists for typical molecular forces and in higher dimensions. We studied energy localization effects in the spectrum of correlations[7, 8] and the tails of the one-particle distribution function at high energies.[6, 10]

This paper is devoted to the study of dissipative Toda systems including active friction effects and the influence of noise. Models of active Brownian particles were recently used for modeling several new types of complex motion.[12–17] We will study here only one-dimensional systems of N active Brownian particles with Toda interactions, which form a ring. In recent works we already studied several phenomena in Toda rings with passive friction and noise.[7, 8] A first approach to investigate Toda rings of active particles with the aim to model dissipative solitons was given recently.[13] In the mentioned work it was shown theoretically and by simulations that in active Toda rings running excitations may be generated. Here we extend these studies and introduce a more realistic model for active friction according to refs. 12 and 16. First we will investigate the attractor structure for small and for large strength of pumping, illustrating the transition to a multistable attractor regime. Then the influence of noise and in particular the properties of the correlation function of the stochastic forces are investigated. By numerical integration of Langevin equations we find the time correlations of the force fluctuations and the power spectrum. The influence of system size and the role of nonlinear excitations on the low frequency part of the spectrum are discussed. Finally the role of noise beyond the bifurcation point and in particular the destruction of the attractors of coherent motion by noise is discussed.

2. THE MODEL OF DISSIPATIVE TODA CHAINS

Our one-dimensional model of active Brownian particles consists of N point masses m_i located at the coordinates x_i on a ring with the total length L. The particles are connected to their next neighbors at both sides by pair interactions. The Toda spring energy is described by

$$U(r_i; \omega_0, b) = \frac{m\omega_0^2}{b^2} (\exp[-br_i] - 1 + br_i) \tag{1}$$

where $r_i = x_{i+1} - x_i - \sigma$ is the distance to the next particle less the equilibrium distance σ, further b is the stiffness of the springs and ω_0 is the linear oscillation frequency around the equilibrium distance σ.

We assume in the following that all masses have the same value $m = 1.0$ and that all potential parameters have the same values. Closely related to the Toda potential is the exponential potential $U(r_i) = (m\omega_0^2/b^2) \exp[-br_i]$. In both cases the dynamics on a ring is equivalent. We will assume here that the average distance of the particles on the ring is equal to the equilibrium distance σ. This is not an essential restriction, since any change of the average distance may be compensated by a change of other parameters. For any choice of the parameters the global minimum of the potential corresponds to the equal distance of the particles. The dynamics of our Brownian particles is determined by the following Langevin equation for the individual velocities v_i:

$$\frac{dv_i}{dt} - A[e^{-b(x_i - x_{i-1})} - e^{-b(x_{i+1} - x_i)}] = \sqrt{2D}\, \zeta_i(t) - \gamma(v_i)\, v_i \tag{2}$$

where $A = (m\omega_0^2/b) \exp(b\sigma)$. The terms at the l.h.s. are of conservative nature and the terms on the r.h.s are of dissipative origin. The first term on the r.h.s. describes the white noise created by a thermal reservoir

$$\langle \zeta_i(t) \rangle = 0 \qquad \langle \zeta_i(t)\, \zeta_j(t') \rangle = \delta_{ij} \delta(t - t') \tag{3}$$

and the second one the active friction. The parameter D gives the strength of noise. The case where the friction is purely passive, i.e., $\gamma(v) = \gamma_0 = \text{const}$ and there is no external force has been studied in detail in refs. 7 and 8. Here we would like to include the effect of active (negative) friction. As a simple model of active friction we consider the friction function proposed in recent work[12, 14, 16] which aims to model active particles with stationary depots:

$$\gamma(v) = \gamma_0 - \frac{dq}{1 + dv^2} = \gamma_0 \left[1 - d \left(\frac{1 + dV^2}{1 + dv^2} \right) \right] \tag{4}$$

Here γ_0 is the usual passive friction, q is the parameter of pumping strength. The second contribution in Eq. (4) comes from the energy reservoir and we will assume here that this energy input does not fluctuate.

In our model all noise comes from the thermal heat bath. The parameters q, d, V characterize the pumping. If $q > \gamma_0$ then at small velocities $v < V$ the friction is negative. The critical velocity is

$$V = + \sqrt{\frac{\alpha}{d}} \tag{5}$$

where

$$\alpha = \frac{q}{\gamma_0} - 1 \tag{6}$$

plays the role of the bifurcation parameter. The region $\alpha > 0$ where the friction function is negative at $v < V$ corresponds to a pumping with free energy on the cost of the energy reservoir.[12, 16] For simplicity we will assume throughout this paper that the reservoir is stationary and does not fluctuate.

3. NONLINEAR DYNAMICS WITHOUT NOISE

Let us now study the solutions of Eq. (2) in the case of zero noise $D = 0$ considering α as the bifurcation parameter. We have to differ between two different situations: In the simplest case of passive friction $\alpha < 0$, i.e., $q < \gamma_0$ all motions come to rest after a finite relaxation time which is of the order $1/\gamma(0)$. The dynamical system has only one attractor. Any initial condition converges to the only stationary and stable solution

$$v_i = 0, \qquad r_i = \sigma, \qquad i = 1, 2, ..., N \tag{7}$$

corresponding to the rest of all particles on the ring at equal distances. The system has neutral stability with respect to a drift on the ring. Near to the point $\alpha = 0$ we may develop

$$\gamma(v_i) = -\gamma_0(\alpha - d v_i^2 + O(v_i^4)) \tag{8}$$

We see that at $\alpha = 0$ a bifurcation occurs. Due to the degeneration of the problem N of the $2N$ roots of the linear problem disappear. For $\alpha > 0$ we observe the appearance of $N + 1$ coexisting attractors. The attractors posses left-right symmetry with respect to rotations on the ring. The main difference between the attractor states is in qualitative respect given by different average velocities of the particles on the ring

$$\langle v \rangle_t = \frac{1}{\tau} \int_0^\tau \frac{1}{N} \sum_{i=1}^{N} v_i \tag{9}$$

where τ is the largest period of oscillations. We mention that the possibility of non-zero average velocities is connected with the fact that the particles are provided with free energy. The two left-right symmetrical attractors which correspond to the largest mean velocity are

$$v_i = \pm V, \qquad r_i = \sigma, \qquad i = 1, 2, ..., N \tag{10}$$

The particles are located at equal distances with the mean density $\rho = N/L$ on the ring and rotate with the constant velocity V either in clockwise or in counter-clockwise direction. This is a point attractor, the stability follows by an elementary analysis.

The remaining attractors correspond to excitations of two or more local compression pulses. Generally we can say that in areas where the nonlinear interaction forces are smaller than the pumping influence (e.g., around equilibrium distance) the particles aim to reach velocities $v_i = \pm V$. In areas dominated by the interaction the particles are forced to slow down and finally change their directions of motion. In first approximation for large b the combination of $(N-k)$ particles moving clockwise $(v_i > 0)$ and k counter-clockwise prepares an attractor with a temporal mean of velocity per particle

$$\langle v \rangle_t \approx \frac{N-2k}{N} \sqrt{\frac{\alpha}{d}}, \qquad k = 0 \cdots N \tag{11}$$

It depends on the initial conditions, which attractor is finally visited by the system.

Numerical investigations of the deterministic system confirm the existence of these attractors. In case of strongly nonlinear interaction forces we observe for $k > 0$ different combinations of stationary soliton excitations. For a ring with $N = \text{odd}$ we find in addition to the left-right constant rotations $(N-1)$ attractors with non-zero average velocity all having left-right symmetry. The two attractors with the second-largest average velocity are characterized by local compressions which are concentrated mostly on one of the springs and which are running left-right around the ring. This kind of excitation reminds of a dissipative soliton. Soliton-like excitations in a closely related model were investigated in ref. 13. The subsequent attractors show with decreasing average velocity, i.e., increasing k more complicated compression patterns running left-right around the ring. Simulations with stochastic initial conditions (random particle distribution and Gaussian velocity distribution) always lead to one of the attractors and give an idea of the attractor basins (see Fig. 1a). All our computer simulations correspond to $\sigma = 1.0$ and $\omega_0 = 1.0$, in other words these quantities serve as the length and time units. The first and last line in Fig. 1a corresponds to the uniform rotations $(\langle v \rangle_t = \pm V)$. In this case the mean energy is minimal

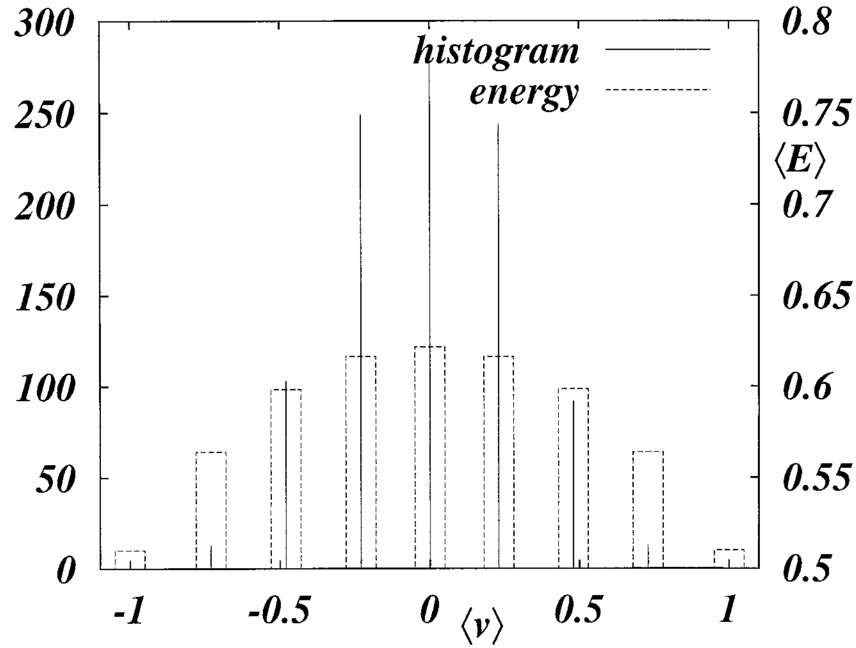

Fig. 1. (a) Attractors for $N=8$, $\rho=1.0$, $m=1.0$ in case of over-critical pumping ($\gamma_0=1.0$, $d=1.0$, $V=1.0$) and strongly nonlinear interaction forces ($b=10.0$). Thin lines represent frequency of appearance per 1000 runs (each with stochastic initial conditions: random particle distribution, initial velocities $v_i(0)=\sqrt{12}\,\zeta$ where ζ is taken from a Gaussian distribution with standard deviation (1.0) vs. characteristic temporal mean of velocity (horizontal) and energy(vertical) per particle. (b) Melting away of discrete attractor structure for $D=0.03$.

(represented by the vertical boxes in Fig. 1a). The second lines, counted from outside, represent stationary one-soliton excitations of the type found in ref. 13. Here we find always one particle moving in opposite direction to the others. For a detailed investigation including the stability analysis of this attractor see ref. 13. While with stochastic initial conditions the already described attractors do not appear very often, the most frequently visited attractor is the central one with $\langle v \rangle_t = 0$ which exists only for $N=$ even. Neighboring particles oscillate opposingly ($v_i = -v_{i-1}$) around the equilibrium distance. Similar to the optical excitations in lattice systems, this attractor is connected to the highest mean energy due to big contributions of potential energy. For stability discussion concerning this attractor we introduce new coordinates $q_i = x_i - x_{i-1} - \sigma$. Because of $x_{i+1} - x_{i-1} \equiv 2\sigma$ the equations of motion for q_i can be written

$$\dot{q}_i = 2v_i, \qquad \dot{v}_i = -\gamma(v_i)\, v_i - 2A \exp\left(-\frac{b}{\rho}\right) \sinh bq_i \tag{12}$$

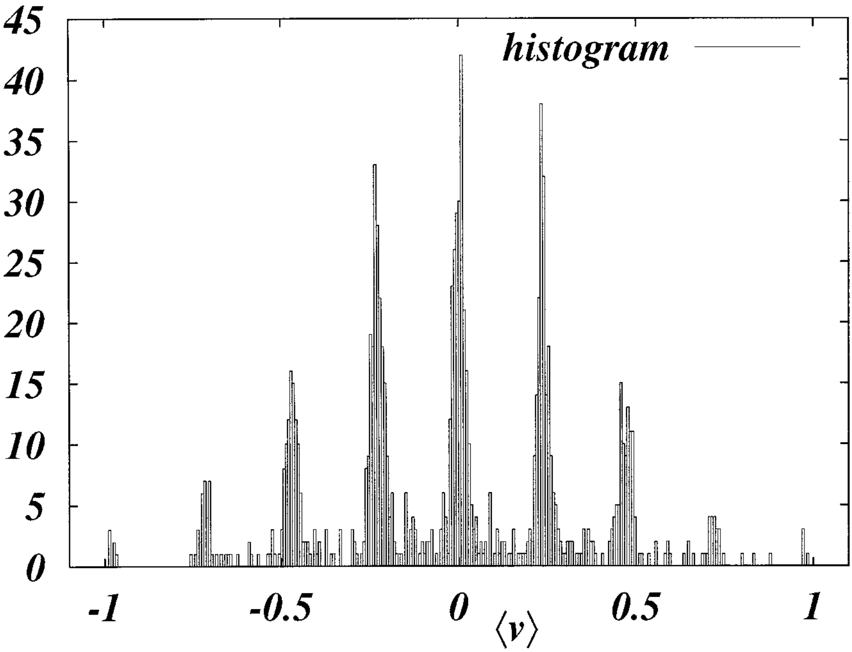

Fig. 1. (*Continued*)

This is equivalent to

$$\frac{dv_i}{dq_i} = -\frac{1}{2}\gamma(v_i) - \frac{A}{v_i}\exp\left(-\frac{b}{\rho}\right)\sinh bq_i \tag{13}$$

For conservative rings ($\gamma(v_i) \equiv 0$) integration of Eq. (13) leads to

$$v_i^2(q_i) = v_{i,0}^2 - \frac{A}{b}\exp\left(-\frac{b}{\rho}\right)(\cosh bq_i - \cosh bq_{i,0}) \tag{14}$$

The last equation describes a periodic motion in the q_i-v-space. The difference between conservative and dissipative vector-field (Eq. (13)) is given by

$$\Delta = -\tfrac{1}{2}\gamma(v) \tag{15}$$

Since $\Delta < 0$ for $V^2 < v^2$ and $\Delta > 0$ for $V^2 > v^2$ the superposition of the conservative vector-field and Δ creates the stable periodic attractor for $k = N/2$ (Fig. 2c).

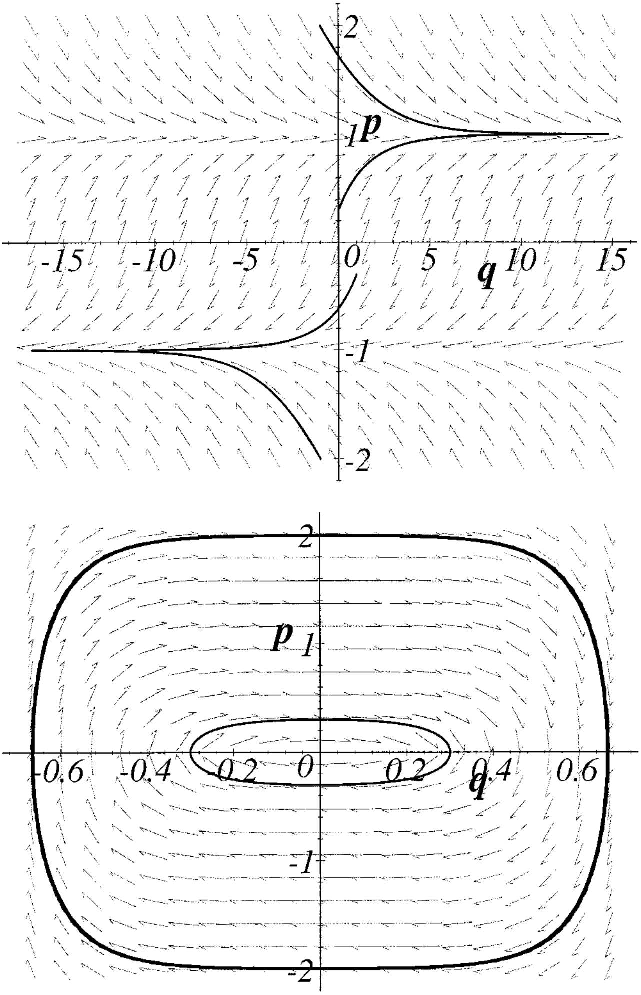

Fig. 2. Phaseportraits of the dynamics of the coordinates $q_i = x_i - x_{i-1} - 1/\rho$ of one particle just with nonlinear friction (a), only with Toda-interaction (b) and the same particle under friction and interaction influences (c). (a) Here it can be seen that moving with $\pm V$ represents a stable attractor basin which will be reached for over-critical pumping.

4. THE INFLUENCE OF NOISE

Let us begin with the discussion of the statistical properties of the first case of purely passive friction ($q = 0$). For under-critical pumping strength $q < \gamma_0$, i.e., $\alpha < 0$ the phenomena are in qualitative respect very similar to the case $q = 0$. As shown above the deterministic attractor corresponds to

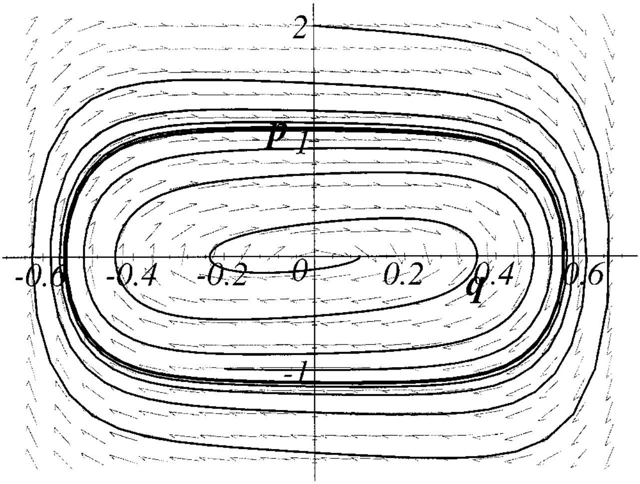

Fig. 2. (*Continued*)

a state where all particles are at rest and have equal distance; the stability is neutral with respect to rotations. Now we add white noise according to Eqs. (2) and (3) and assume the validity of an Einstein relation $k_B T = mD/\gamma_0$. Then the statistical properties are described by a canonical ensemble with given pressure P and temperature T. Explicite calculations were given in refs. 1–8. Let us repeat in short a few of the results: Using the abbreviations

$$X = \frac{\varepsilon}{\sigma b k_B T}, \qquad Y = \frac{P}{b k_B T}, \qquad \varepsilon = \frac{m\omega_0^2 \sigma}{b} \tag{16}$$

the distribution function of a single molecule reads

$$\begin{aligned} f(p, r) &= Z_1^{-1} \exp\left(-\frac{p^2/2m + U_{\text{eff}}}{k_B T} \right) \\ Z_1^{-1} &= \frac{b X^{X+Y}}{\sqrt{2\pi m k_B T}\, \exp(X)\, \Gamma(X+Y)} \end{aligned} \tag{17}$$

with the effective potential

$$U_{\text{eff}}(r) = U(r) + Pr \tag{18}$$

Here k_B denotes the Boltzmann constant and P the pressure. $U(r)$ is the Toda potential according to Eq. (1). All thermodynamical functions follow by derivation of the partition function with respect to the corresponding parameters. The specific heat is given by

$$c_V = k_B \left(\frac{1}{2} + X + Y - \frac{1}{\Psi'(X+Y)} \right) \tag{19}$$

where the trigamma-function Ψ' is defined as usual by the second logarithmic derivative of the Γ-function. This function tends to k_B in the low-temperature regime due to the thermal energy $k_B T$ of each phonon. On the other hand, c_V shows the properties of a 1d hard-sphere gas at high temperatures, i.e., c_V tends to $1/2k_B$. In the middle between the two limits a weak transition occurs from the phonon-determined regime to a soliton-determined regime. We introduced a transition temperature T_{tr} corresponding to $c_V = 3/4k_B$. For $b = 100/\sigma$ we get for example $k_B T_{tr} = 1.6 \cdot 10^{-3} m\omega_0^2 \sigma^2$. In the region around T_{tr} thermal excitations should be described more generally as cnoidal waves which contain both phonons and solitons as special cases in the low- and high- amplitude limit, respectively.[1] Loosely speaking, cnoidal or solitary waves can be considered as deformed phonons with more or less steep compression humps and shallow dilatation valleys between them. In the transition region the interaction between solitary-wave excitations leads to interesting physical effects.

In particular it was shown that a nonlinear Toda chain with periodic boundary condition is able to transform the uncorrelated, white noise of the surroundings into noise of $1/\omega$-type.[8] This is a typical finite size effect which disappears in the thermodynamic limit $N \to \infty$. In Fig. 3 we have shown the force-force time-correlation function obtained from simulations for rings with $N = 5$ and $N = 30$ particles respectively. Both curves show a correlation minimum and a distinct positive peak corresponding to solitary waves moving around the ring. The soliton which moves to lower frequency with increasing particle number on the ring. The power spectrum represented in Fig. 4 shows a high frequency structure beginning with a soliton peak and followed by a broad shoulder which decays at high frequencies. At low values of ω we observe a very specific noise which over a few decades behaves like $1/\omega$. In this respect the type of noise we have observed corresponds to the flicker-noise in small systems investigated by Klimontovich.[18] We observe also a decrease of amplitude with N. Due to the limited accuracy of our calculations in the region of low ω we cannot make a quantitative statement about the scaling with N. Klimontovich derives a scaling with N^{-1}.[18] For Toda rings the $1/f$ spectrum implies a hierarchy of beatings where periods with more energetic compression pulses are more probable to appear at longer time intervals. The internal dynamics is accompanied by a long-term correlated random rotation of the whole ring. This effect is closely connected

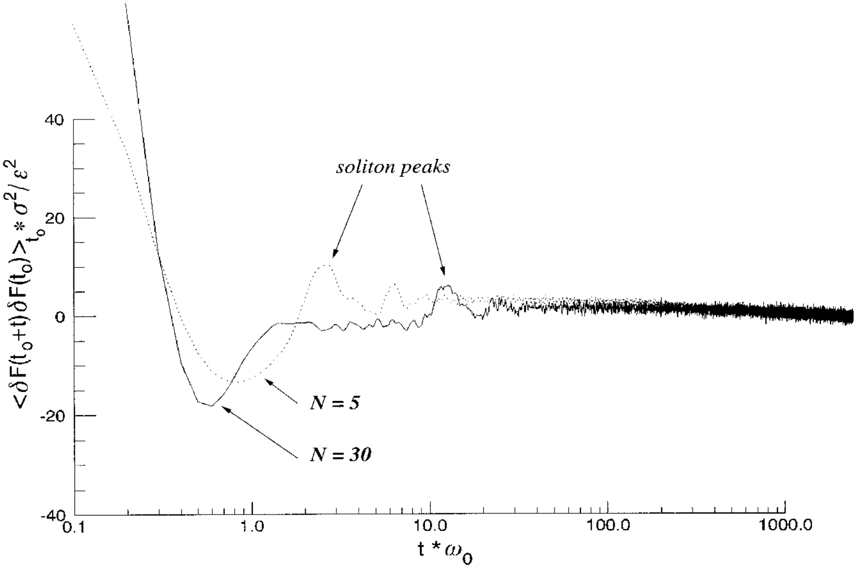

Fig. 3. The influence of the system size on the autocorrelation functions ACF(t) of a random force F demonstrated for a 5-particle (dotted) and a 30-particle (solid) Toda ring (parameters: $b = 100/\sigma$, $k_B T = 0.26\varepsilon$, $\gamma = 10^{-3}\omega_0$). The peaks at $t \approx 2.5\omega_0^{-1}$ for $N = 5$ and at $t \approx 15\omega_0^{-1}$ for $N = 30$ correspond to soliton excitations. Compared to the 5-particle ring, in the 30-particle ring the solitary-wave peak is shifted to the right but also less pronounced because higher frequencies are thermally activated too.

with the neutral stability with respect to rotations of the ring as a whole. These coherent fluctuations of the ring correspond to a diffusion regime. We stress that the Toda ring is in thermal equilibrium and the $1/f$ tail of the spectrum reflects the character of equilibrium fluctuations. The hierarchical order of the fluctuations is due to the superposition of mainly two soliton-like waves of similar amplitude and frequency running in opposite directions. The fluctuations of their amplitudes and frequencies lead to some kind of nonlinear beating phenomenon that is connected to a region of the spectrum that is similar to $1/f$-noise.[8] As shown by Klimontovich flicker-noise may be interpreted as a diffusion regime of the dynamics of finite systems. Typical properties of the flicker-noise of Klimontovich-type are:[18]

(i) The flicker noise appears in small systems at frequencies ω_{fl} bounded from above by the diffusion time L^2/D and from below by the observation time t_{obs}

$$\frac{1}{t_{\mathrm{obs}}} < \omega_{\mathrm{fl}} < \frac{D}{L^2} \tag{20}$$

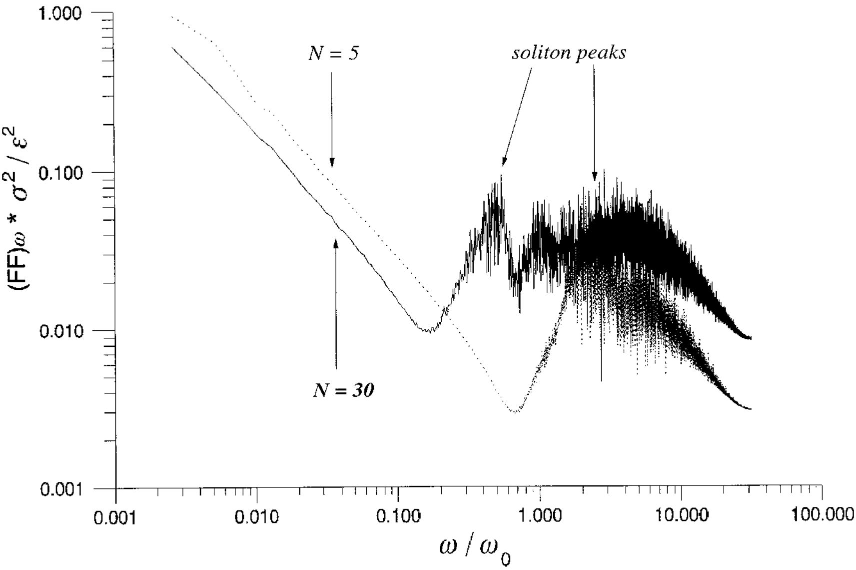

Fig. 4. Spectra $(FF)_\omega$ corresponding to the ACF of the 5-particle (dashed) and the 30-particle (solid) Toda rings presented in Fig. 3. The intensity of the $1/f$ noise at the lower end of the spectrum is clearly diminished in the 30-particle compared to the 5-particle system indicating the finite-size character of the $1/f$ noise.

were D is the diffusion constant (corresponding here to a rotational stochastic motion of the whole ring) and L is the length of the system (corresponding here to $N\sigma$).

(ii) The amplitude of the flicker noise is proportional to $1/(N\omega)$, where N is the particle number.

The $1/f$-noise observed here on finite Toda systems is not connected to a fine-tuning of temperature, structural parameters, particle number, or thermal coupling, but occurs in a wide range of these quantities with varying intensity. The deciding property of the underlying deterministic system is the neutral stability of the ring and the nonlinear coupling between the modes of oscillation.

So far we considered the passive case $q = 0$. We have shown above that with increasing q at $q = \gamma_0$ a bifurcation to multistable attractor regime is observed. Let us now discuss the influence of noise in the case $\alpha > 0$, i.e., $q > \gamma_0$. For that much more complicated case no analytical theory is available. We may expect however that the monomodal momentum distributions in the passive case are replaced by multimodal momentum distributions. As we have shown the deterministic system is characterized by an attractor structure corresponding to discrete temporal means of the average momenta. The fixation of initial conditions corresponds to selection of a certain attractor, which will be approached by the system. Including the white noise term in Eq. (2) by choosing $D > 0$ may allow the system to switch from approaching one attractor in favor of others. This leads to transparent separatrices between the attractors and finally to a loss of the discrete structure in the attractor representation of Fig. 1a, as one can see in Fig. 1b. We observe transitions between the attractor basins of the system, which is far from equilibrium and may switch permanently between the attractor basins. With increasing noise we find a destruction of the deterministic attractor structure beginning with the outer attractors in Fig. 1. In other words the coherent motions of the ring with the highest average velocity are the most sensitive with respect to noise. Figure 5 shoes probability distributions for the mean velocity of $N = 2$ particles in dependence on the noise strength. We see that the outer peaks corresponding to coherent left-right rotations disappear at a noise strength of $D \simeq 0.15$. For larger N qualitatively similar phenomena are observed.

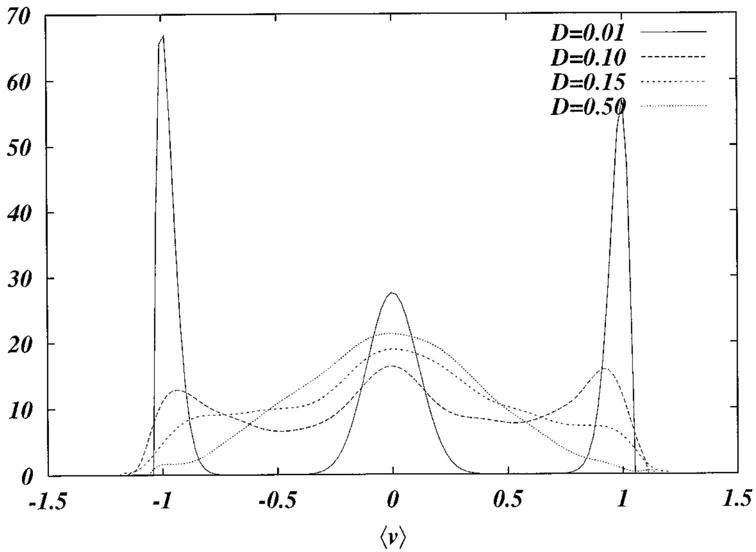

Fig. 5. Stochastic Bifurcation of an active Toda ring with $N = 2$. The outer maxima, which correspond to coherent motions, disappear at a noise level of about $D \simeq 0.15$. The center peak still refers to the most probable attractor because of its bigger width even so it seems to look smaller.

5. DISCUSSION AND CONCLUSIONS

The investigation of the dynamics, the statistical properties and excitation spectra in classical nonlinear chains is of central importance to several branches of physics and chemical kinetics. As simple 1d models of excitations in molecular systems we investigated here Toda systems including velocity-dependent friction which includes negative parts. The advantage of this model is that it admits exact solutions for the dynamics and statistical thermodynamics in the limit of passive friction and on the other hand for strong negative friction the system may be driven to far from equilibrium states.

We have shown, that far from equilibrium beyond critical pumping strength the system develops a rather complicated attractor structure corresponding to more complex nonlinear excitations. In particular we could show that for strong pumping $q > \gamma_0$, single rotations of the ring, solitonic excitations, optical excitations etc. may be realized in dependence of the initial conditions.

The second part of the paper is devoted to the influence of noise. We started with the case of passive friction $\gamma_0 > q$ and investigated in particular $q = 0$. In supplementing the investigations in previous papers[5–11] which were concentrated on energy localization and distribution functions for passive systems we presented here new simulations of the time correlations. We observed a transformation of the uncorrelated noise of a surrounding heat bath into a broadband colored noise with a long tail at low frequencies confirming the previous findings in refs. 7 and 8. This behavior was proven here for finite-size Toda rings of $N = 5$ and $N = 30$ particles with weak thermal coupling in the transition-temperature range. Such systems seem to be ideal hosts for the excitation of special active sites possessing resonance frequencies inside this low frequency band. The finite-size Toda ring with moderate coupling to a surrounding heat bath in the transition-temperature region is perhaps the simplest classical model of a ring-shaped biomolecule in solution. The basic idea, which still has to be worked out, is that the long-term correlated conformational changes which are relevant in context with protein-folding processes and enzyme reactions might be related to dynamical mechanisms similar to those observed in our simple Toda model. We have demonstrated here that the inclusion of energy supply, which in our case could model the ADP/ATP-exchange, leads to a more rich multistable dynamics. Beyond critical pumping i.e., at $q > \gamma_0$ we observed $N + 1$ attractors between which the trajectories may switch under the influence of noise. This way we observed $N + 1$ different stochastic regimes corresponding to the deterministic attractors and stochastic transitions between the regimes. With increasing noise first the coherent motions with the highest average speed of rotation are destroyed as in ref. 19.

We express the hope that the further investigation of the simple model system investigated here in this paper will support the understanding of complex molecular motions, including active motion supported by energy supply.

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