Cumulant analysis of statistical properties of deterministically thermostatted harmonic oscillator.

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Usual approach to investigate the statistical properties of the deterministically thermostatted systems is to analyze the motion mode of the system. In this work the cumulant analysis are used to study the properties of the stationary probability distribution function of the deterministically thermostatted harmonic oscillators. This approach shifts attention from investigation of the geometrical properties of attractors to study of a probabilistic measure. Three different thermostats, namely Nosé-Hoover, Patra-Bhattacharya and Hoover-Holian ones, were investigated. It was shown that their actual distribution functions are non-canonical because of nonlinearity of the equations of motion. The sufficient conditions for ergodicity were formulated in terms of cumulants.

I. INTRODUCTION

The molecular dynamics approach is widely used to investigate equilibrium thermodynamic properties of many body systems. The thermostats, that is physical equations of motion modified by a dynamic temperature control tool, are commonly used to simulate systems of particles at constant temperature. There are stochastic and deterministic thermostats.

In the case of stochastic thermostat the thermodynamic ensemble is described by a set of stochastic Langevin equations of motion. This approach allow us to create a canonical ensemble. But in some cases this approach is unsuitable because of very slow converging to the equilibrium state.

The deterministic thermostats are alternative way to solve the problem. In this case the ensemble is described by a set of deterministic nonlinear ordinary differential equations in an extended phase space. Additional phase variables are one, two or more pseudo-friction coefficients which obey specific equations of motion. These equations are arranged in such a way that they can control some macroscopic parameters of the ensemble. So, Nosé [1] and Nosé-Hoover (NH) [2] thermostats enhance the phase space by one variable and control the kinetic temperature. More complicated thermostats by Patra-Bhattacharya (PB) [3] and Hoover-Holian (HH) [4] add two variables and control two parameters of the ensemble. As the result of generalizations of these methods in the works [5,6] the families of the thermostats were proposed for which the above-mentioned are special cases. Samoletov and Vasiev [7] propose a dynamic principle underlying a range of thermostats which is derived using fundamental laws of statistical physics. Their approach covers both stochastic and deterministic schemes.

The statistical properties of the stationary dynamical system are described by the stationary probability distribution function (PDF). Such PDF obeys the stationary Liouville continuity equation corresponding to the system considered. For the stationary dynamical system coupled with any deterministic thermostat one of the solution of the equation is PDF which is canonical in the physical phase space and is Gaussian with respect to the additional phase variables. But the actual PDF obtained by solving the equations of motion can be different and it, of course, is not canonical.

The ergodicity of the system is other problem. The system is ergodic if its probabilistic measure is invariant or, in other words, its PDF doesn’t depend on initial conditions. In the case of thermostatted systems usual approach to this problem is to analyze the motion mode of the system. It boils down to study of the geometrical properties of attractors.

In the quasi-periodic mode of motion the system evidently is not ergodic because in this case invariant tori exist that separates the system phase space into invariant domains depending on the initial conditions. The chaotic mode is much more consistent with the concept of ergodicity.

The statistical properties of the deterministically thermostatted systems are investigated mainly on the base of the model of a one-dimensional harmonic oscillator. The authors of the articles [2, 10, 11] showed that under some conditions in the system of the harmonic oscillator coupled with Nosé and NH thermostats there exist invariant tori. The conditions are determined by the system parameters and the initial conditions.

Detailed study of the ergodicity of the singly and doubly thermostatted harmonic oscillators in the chaotic mode gave inconclusive results. The harmonic oscillators coupled with Nosé and NH thermostats were shown [2, 10] to be nonergodic. Patra and Bhattacharya [12], working with the harmonic oscillator coupled with two-chain NH thermostat, find that it does not generate the canonical distribution and does not provide ergodicity of the system. In other papers [13, 17] it was concluded that this thermostat is ergodic and the ergodicity of some other thermostats is discussed. So, the problem of ergodicity of the deterministically thermostatted harmonic oscillator is still open.
In this work the statistical properties of the harmonic oscillator coupled with NH, PB and HH thermostats are studied by means of the cumulant approach. This method make it possible to analyze directly the properties of PDF of the system. The canonicity and ergodicity of the ensembles considered are discussed. In Sec. III the minimal notions of the cumulant approach, which are necessary to understand the matter discussed, are given. The statistical properties of the NH system are considered in Sec. IV In Sec. V the properties of PB and HH thermostats are discussed. In the final section the conclusive considerations are given. In Appendix some intermediate expressions which are referred to in the text are presented.

II. DEGENERATED EQUATIONS FOR CUMULANTS.

The purpose of present work is the statistical analysis of the dissipative dynamical systems whose evolution is given by the equations of motion of the form

\[ \dot{q} = g(q), \]  

where \( q \) are phase variables and \( g \) is a nonlinear differentiable function. Distribution of the system in the phase space is described by PDF \( W(q, t) \). The existence of the stationary limit \( W(q) = W(q, t \rightarrow \infty) \) of this function is assumed.

The characteristic function \( \theta(v, t) \) which is a Fourier transform of the \( W(q, t) \)

\[ \theta(v, t) = \int e^{i\langle qv \rangle}W(q, t) dq \]

is an equivalent way to describe the distribution of the system. Moments and cumulants are coefficients of expansion in a series of the characteristic function and its logarithm respectively

\[ \theta(v, t) = \sum_{m_1, \ldots, m_n=0}^{\infty} \frac{\alpha(t)^{q_1 \ldots q_n}}{m_1! \ldots m_n!} (iv_1)^{m_1} \ldots (iv_n)^{m_n} \]

\[ = \exp \left[ \sum_{m_1, \ldots, m_n=0}^{\infty} \frac{\kappa(t)^{q_1 \ldots q_n}}{m_1! \ldots m_n!} (iv_1)^{m_1} \ldots (iv_n)^{m_n} \right]. \]

Here \( \alpha(t)^{q_1 \ldots q_n} \) is the joint moment and \( \kappa(t)^{q_1 \ldots q_n} \) is the the joint cumulant of \( n \) variables \( q_1, \ldots, q_n \) and \( i \) is the imaginary unit. The full set of moments or cumulants completely represents \( W(q, t) \) as long as the series converges at all \( \{v_i\}_{i=1}^{\infty} \).

In what follows the notion of the cumulant brackets will be need. They are the angle brackets with arguments separated by commas. If arguments are single variables the cumulant bracket coincides with corresponding cumulant, for example \( \langle q_i, q_j, q_k \rangle = \kappa_{2,1}^{q_i, q_j} \). In the case if one or several arguments are functions the operation ”to open cumulant brackets” is need in order to represent a cumulant bracket as a function of cumulants.

The cumulant analysis is widely used for statistical analysis of stochastic differential equations in the theory of Markov processes \[18, 19\]. To analyze deterministic differential equations this approach was applied by V. Kontorovich \[20\]. In cited work a set of degenerated equations for cumulants was obtained as the limit of the full set, in which the amplitudes of random forces tend to zero.

Here we propose simplified derivation of the degenerated equations for cumulants assuming, that all necessary conditions are satisfied. PDF \( W(q, t) \) corresponding to the system \( W(q, t) \) obeys the Liouville continuity equation

\[ \frac{\partial W}{\partial t} + \frac{\partial (\langle qW \rangle)}{\partial q} = \frac{\partial W}{\partial q} + \frac{\partial (\langle K_1 W \rangle)}{\partial q} = 0. \]

The notation \( K_1 = g(q) \) for kinetic coefficients is introduced to bring our designations into accord with \[18–20\]. Let \( f(q) \) be a phase variables function. Then

\[ \frac{d}{dt} \langle f(q) \rangle = \int f(q) \frac{\partial W}{\partial q} dq = \] \[ = - \int f(q) \frac{\partial (\langle K_1 W \rangle)}{\partial q} dq = \left\langle K_1 \frac{\partial f(q)}{\partial q} \right\rangle. \]

where the angle brackets mean the statistical average. In the third term the time derivative is replaced using the Liouville equation \[4\] and the last one is obtained as the result of the integration by parts.

Substituting monomials of variables \( q_i \) instead of \( f(q) \) we arrive at the set of equations for moments

\[ \frac{d}{dt} \langle q_i \rangle = \langle K_{1i} \rangle, \]

\[ \frac{d}{dt} \langle q_i q_j \rangle = \langle q_i K_{1j} \rangle + \langle K_{1i} q_j \rangle = 2 \langle \langle q_i K_{1j} \rangle \rangle, \]

\[ \frac{d}{dt} \langle q_i q_j q_k \rangle = \langle q_i q_j K_{1k} \rangle + \langle q_i K_{1j} q_k \rangle + \langle q_k K_{1j} q_i \rangle = \] \[ = 3 \langle \langle q_i q_j K_{1k} \rangle \rangle, \]

\[ \vdots \]

Here the symbol \( n\{\ldots\}_s \) is the Stratonovich brackets. It denotes completely symmetrical sum of the variables which are put in brackets. A number before the brackets is the number of terms in the expression.

To obtain equations for cumulants one need to use interrelationship of cumulants and moments. In the result the equations get the same form as that for moments if the moment brackets (statistical averaging) are replaced by the cumulant ones \[18, 19\].

\[ \frac{d}{dt} \langle q_i \rangle = \langle K_{1i} \rangle, \]

\[ \frac{d}{dt} \langle q_i q_j \rangle = 2 \langle \langle q_i, K_{1j} \rangle \rangle, \]

\[ \frac{d}{dt} \langle q_i q_j q_k \rangle = 3 \langle \langle q_i, q_j, K_{1k} \rangle \rangle, \]

\[ \vdots \]
In the next sections the stationary statistical properties of the different thermostatted systems are studied. In each case only limited number of stationary equations consisting the set \( \{7\} \) are analyzed.

The phase space dimension of the systems under consideration is three or four. The phase variables are coordinates \( x \), momentums \( p \) and one or two friction coefficients \( \zeta \) and \( \xi \), \( \mathbf{q} = (x, p, \zeta, \xi) \). For the sake of simplicity the upper indices in cumulants are omitted but, instead, the order of the variables in subscripts are fixed, namely

\[
\kappa_{k,l,m}(x,p,\zeta,\xi) = \kappa_{k,l,m}(n).
\] (8)

III. NOSE-HOOVER THERMOSTAT

A. Equations of motion and canonical PDF

Dynamics of a harmonic oscillator which is coupled with NH thermostat obeys the set of three ordinary differential equations of the first order

\[
\begin{align*}
\dot{x} & = \frac{p}{m}, \\
\dot{p} & = -kx - \zeta p, \\
\dot{\zeta} & = \frac{1}{\tau} \left( \frac{p^2}{mT} - 1 \right).
\end{align*}
\] (9)

Here \( \mathbf{q} = (x, p, \zeta) \) are the phase variables, \( m \) and \( \tau \) are the oscillator and the thermostat masses, \( k \) is the coefficient of elasticity and \( T \) is the temperature.

The well known feature of the system \( \{9\} \) is that the stationary PDF

\[
W_c(\mathbf{q}) \propto \exp \left\{ -\frac{p^2}{2mT} - \frac{kx^2}{2T} \right\} \exp \left\{ -\frac{\zeta^2}{2\tau} \right\}
\] (10)

obeys the stationary Liouville continuity equation \( \frac{\partial}{\partial t} \langle \mathbf{q} | W_c(\mathbf{q}) \rangle = 0 \). The marginal PDF in the physical phase subspace \( (x, p) \) is canonical and the whole PDF is Gaussian. Such a function is completely determined by three nonzero cumulants of the second order

\[
\kappa_{2,0,0} = \frac{T}{k}, \quad \kappa_{0,2,0} = Tm, \quad \kappa_{0,0,2} = \frac{1}{\tau}.
\] (11)

All remaining cumulants are equal to zero. Phase variables, distribution of which in phase space are described by such a function, are statistically independent.

B. Equations for cumulants

Kinetic coefficients of the system are

\[
\mathbf{K}_1 = (K_{1x}, K_{1p}, K_{1\zeta}) = \left( \frac{p}{m}, -kx - \zeta p, \frac{1}{\tau} \left( \frac{p^2}{mT} - 1 \right) \right).
\] (12)

The equations for cumulants are an infinite set of nonlinear algebraic equations. In this section the stationary equations corresponding to nonstationary ones with time derivatives from \( \kappa_{1,0,0} \) to \( \kappa_{0,0,4} \) only are analyzed. The number of the equations is 34. But key equations only are written out here. On the left of each equation the corresponding time derivative is written to systematize them.

The first equation is

\[
\dot{\kappa}_{1,0,0} : \quad \langle K_{1x} \rangle = \left( \frac{p}{m} \right) = \frac{1}{m} \kappa_{0,1,0} = 0.
\] (13)

The solution gives zero value of the cumulant \( \kappa_{0,1,0} \). Other representative equation is more complicated

\[
\dot{\kappa}_{0,0,1} : \quad \langle K_{1\zeta} \rangle = \frac{1}{\tau} \left( \frac{\langle p^2 \rangle - 1}{mT} \right) = \frac{1}{\tau} \left( \frac{\kappa_{0,2,0}}{mT} - 1 \right) = 0.
\] (14)

In the last term the dependence of the second moment on cumulants \( \{A.2\} \) and the equality to zero of the cumulant \( \kappa_{0,1,0} \) are taken into account. Thus, equation \( \{14\} \) gives \( \kappa_{0,2,0} = Tm \). The characteristic features of these solutions are that they are completely determined by the equations for cumulants and both of them coincide with corresponding cumulants of the canonical PDF \( \{10\} \).

There are a number of other zero solutions of the equations which have the same features. They are all cumulants of the first order, cumulants \( \kappa_{1,1,0}, \kappa_{1,0,1} \) and \( \kappa_{0,1,1} \) of the second order, all cumulants of the third order with the exception of \( \kappa_{1,1,1} \), and eight cumulants of the fourth order.

The rest of cumulants are the solutions of other type. They obey the set of equations

\[
\begin{align*}
\dot{\kappa}_{1,1,0} : & \quad k\kappa_{2,0,0} + \kappa_{1,1,1} - T = 0, \\
\dot{\kappa}_{2,0,1} : & \quad \frac{1}{\tau T} \kappa_{2,2,0} + 2\kappa_{1,1,1} = 0, \\
\dot{\kappa}_{0,2,1} : & \quad \frac{1}{\tau T} \kappa_{0,4,0} + \frac{2Tm}{\tau} - 2k\kappa_{1,1,1} - 2Tm\kappa_{0,0,2} = 0, \\
\dot{\kappa}_{3,1,0} : & \quad \frac{3}{m} \kappa_{2,2,0} - k\kappa_{4,0,0} = 0, \\
\dot{\kappa}_{1,3,0} : & \quad \frac{1}{m} \kappa_{0,4,0} - 3k\kappa_{2,2,0} - 6Tm\kappa_{1,1,1} = 0, \\
\dot{\kappa}_{1,1,1} : & \quad k\kappa_{2,0,2} + 2k\kappa_{1,1,1}\kappa_{0,0,2} - 4\frac{1}{\tau} \kappa_{1,1,1} = 0
\end{align*}
\] (15)

To obtain these equations the solutions for the canonical cumulants were taken into account. The set contains six equations for seven unknowns. Thus, the set is underdetermined and has infinite number of solutions. To solve these equations one need to take one of the unknowns as a parameter. Let it be \( \kappa_{1,1,1} \). Then

\[
\begin{align*}
\kappa_{2,0,0} = & \quad \frac{T}{k} - k\kappa_{1,1,1}, \\
\kappa_{0,0,2} = & \quad \frac{1}{\tau} + \frac{1}{T} \left( \frac{3}{\tau} - \frac{4k}{m} \right) \kappa_{1,1,1}.
\end{align*}
\] (16, 17)
These cumulants differ from canonical ones [11] because of the summands proportional to $\kappa_{1,1,1}$. The fourth order cumulants, entering into Eqs. (15), are directly proportional to $\kappa_{1,1,1}$. For example
\[ \kappa_{0,4,0} = 6Tm(m - k\tau)\kappa_{1,1,1}. \] (18)
Nonzero value of the cumulant $\kappa_{1,1,1}$ means that the variables $x$, $p$, and $\zeta$ are statistically dependent.

Thus, the analysis of the equations for cumulants shows that all cumulants can be divided into two groups. The first one includes the cumulants which are fixed solutions of the equations. They are $\kappa_{0,2,0}$ and all zero valued cumulants. These cumulants coincide with those of the canonical PDF and in what follows are referred to as canonical. The other group includes the cumulants which depend on a free parameter, similarly to the solutions of Eqs. (15). These cumulants are nonzero because of the statistical dependence of phase variables which is the cause of the difference of the actual PDF from the canonical one. They will be termed as non-canonical.

Further analysis of the equations for cumulants did not give any new information. To achieve further progress in the studying of the system behavior the equations [9] was solved numerically.

C. Numerical approach

The purpose of the numerical approach is to calculate the cumulants of the stationary PDF of the system by means of time averaging of the corresponding combinations of the phase variables along the trajectory of the system motion. Directly calculated averages are asymptotically at $t_{av} \to \infty$ approximate to the moments of PDF
\[ \langle x^k p^m \zeta^n \rangle_t = \lim_{t_{av} \to \infty} \frac{1}{t_{av}} \int_0^{t_{av}} ds \left( x(s)^k p(s)^m \zeta(s)^n \right). \] (19)
Here $t_{av}$ is the time of averaging, $x(s)$, $p(s)$ and $\zeta(s)$ are the values of the phase variables on the system trajectory at instant of time $s$. In order to calculate a cumulant as a time average one need to express it in terms of moments [18, 19] and to average this expression. For example see Eqs. (14, 8, 8).

The motion type of the system is determined by its parameters and initial conditions. The analysis of the system behavior was performed at fixed parameters $k = m = 1$ and $T = 0.5$. The thermostat mass was chosen $\tau = 10$ in regular mode and $\tau = 2$ in chaotic one. The initial conditions are specified later when the results are discussed. To solve the equations [9] the modification of the Verlet algorithm [22] was used with the time step $\Delta t = 0.01$ or 0.001 depending on parameters.

D. Regular motion

The regular motion of the system is ensured by rather large value of the thermostat mass $\tau = 10$ and relatively small values of initial coordinates $x_0$ and momentums $p_0$. Numerical calculations show that the expressions to be averaged converge rather rapidly (the averaging time $t_{av} \sim 10^3 - 10^4$) to the corresponding values resulting from the equations for cumulants. The results of averaging by time of the expressions $\langle x(t) \rangle_t$, $\langle p(t) \rangle_t$ and $\langle x(t), \zeta \rangle_t$ which asymptotically approximates to $\kappa_{2,0,0}$, $\kappa_{0,2,0}$ and $\kappa_{1,1,1}$ are shown in Fig. 1 as functions of $t_{av}$ at initial conditions $x_0 = 0$, $p_0 = 0.1$ and $\zeta_0 = 0$. One can see that these averages are in good agreement with expressions (14) and (16).

![FIG. 1. Dependence of the time averages $\langle x(t) \rangle_t$, $\langle p(t) \rangle_t$ (a) and $\langle x(t), \zeta \rangle_t$ (b) on $t_{av}$ for NH thermostat in the regular mode of motion.](attachment:image.png)

Special attention was payed to the properties of the cumulant $\kappa_{1,1,1}$ which in the numerical analysis is approximated by the time average $\langle x(t), \zeta \rangle_t$. In the previous subsection this value was taken as a free parameter and it cannot be found from the equations. In the numerical approach it is obtained as the average by time along the trajectory and is always determined well. Numerical calculation shows that $\kappa_{1,1,1}$ as well as other cumulants connected with them (14, 16, 18) depend on the initial conditions. The dependence of $\langle x(t), \zeta \rangle_t \approx \kappa_{1,1,1}$ on $x_0$ is shown in Fig. 2 for $\zeta_0 = 0$, different $p_0$ and $t_{av} = 3000$.

Thus, under the condition of regular motion (motion on torus) the system PDF is non-canonical and it depends on the initial conditions, that is the PDF is different on different trajectories. This means that the system is not ergodic. This result is in quite agree with earlier obtained ones [2, 11].
To study the chaotic regime of the system motion the values of the thermostat mass \( \tau \leq 2 \) and the initial values of the oscillator position \( x_0 = 0 \) and 0.5, momentum \( p_0 = 4.0 \), and \( \zeta_0 = 0 \) were chosen. The numerical analysis of the solutions of Eqs. (10) shows that the time averages corresponding to canonical and non-canonical cumulants in this case behave differently.

The averages approximating to the canonical cumulants converge rapidly \((t_{av} \approx 10^3 - 10^4)\) to corresponding solutions of the equations for cumulants. They are \( \langle p, p \rangle_t \), converging to \( \kappa_{0,2,0} \), and all averages converging to zero valued cumulants. As seen in the plots \( \langle p, p \rangle_t \) vs \( t_{av} \) on Fig. 3.

The other time averages approximating to the non-canonical cumulants converge to limiting values very slowly. The time average \( \langle x, p, \zeta \rangle_t \) converging to \( \kappa_{1,1,1} \) is shown on Fig. 4 up to \( t_{av} = 10^9 \) for different \( \tau \) and initial conditions. It is clearly seen that the averaged values are far from their limits.

On the other hand all combinations of the time averages corresponding to the equations for cumulants, including Eqs. (10), converge to their zero values rather quickly \((t_{av} \approx 10^3 - 10^4)\) in spite of the fact that some summands converge very slowly. An example of such behavior can be found on Fig. 3 where the averages \( \langle x, x \rangle_t \), \( \langle p, p \rangle_t \) and \( \langle x, p, \zeta \rangle_t \) are plotted as function of \( t_{av} \). It is seen that these averages at \( t_{av} = 3000 \) satisfy the first equation in the set (10) with good accuracy while the individual terms are far from their stationary values.

In the previous section the dependence of the cumulant \( \kappa_{1,1,1} \) on initial conditions was produced for the case of periodic motion. This was possible due to rapid converging of the time averages. In the case of chaotic motion the situation is more difficult because of their slow converging. It is seen on Fig. 4 that after averaging during time \( t_{av} = 10^9 \) it is still impossible to conclude with certainty wether the limits corresponding to the initial conditions \( x_0 = 0 \) and 0.5 are the same or different. On the other hand at \( \tau = 2 \) the system demonstrate chaotic motion under initial conditions \( x_0 = 0, p_0 = 4, \zeta = 0 \) and periodic one with \( x_0 = 0, p_0 = 0.4, \zeta = 0 \).

In the chaotic regime of special interest is the depen-

\[ \langle x, p, \zeta \rangle_t, \langle p, p \rangle_t \text{ and } \langle x, p, \zeta \rangle_t \text{ on } t_{av} \text{ for NH thermostat in the chaotic mode of motion.} \]
dence of non-canonical cumulants (in particular $\kappa_{1,1,1}$) on the thermostat mass $\tau$. The dependence of $-\langle x, p, \zeta \rangle_1$ on $\tau$ is shown on Fig.4 by open circles in the double logarithmic scale. All points are obtained by averaging in time and the accuracy of the obtained values is small. However the points corresponding to $\tau \leq 0.1$ demonstrate linear dependence in the logarithmic scale. This corresponds to the power law which parameters were found by the mean square method

$$\kappa_{1,1,1} = -0.123 \tau^{0.1}. \quad (20)$$

It is shown on Fig.5 by solid line. Such a behavior of the non-canonical cumulants means that the actual PDF, as $\tau$ decreases, approaches the canonical one.

This feature of the system statistical properties is connected with the existence of two characteristic times. The first one is the characteristic time of mechanical motion of the oscillator in the phase space which is of order $t_{osc} \approx 2\pi \sqrt{m/k}$. The second is the characteristic time of energy exchange between the oscillator and thermostat and is $t_{exch} = \sqrt{T}$. So, the conditions for obtaining good statistical properties of the thermostat is the inequality $t_{exch} \ll t_{osc}$.

![ FIG. 5. Dependence of the time averages $\langle x, p, \zeta \rangle_1$ on the thermostat mass for NH and PB thermostats in the chaotic mode of motion.](image)

**IV. OTHER THERMOSTATS**

In this section the statistical properties of the harmonic oscillator coupled with more complicated thermostats are discussed. The phase spaces of these systems are four-dimensional. Extension of the dimension is due to incorporation of the additional dynamical variable which is one more friction coefficient. Advantage of these thermostats is that they ensure one more cumulant of the actual PDF to be canonical.

The statistical properties of the systems are similar to those discussed in previous section. Therefore, they are discussed in less details. Only the main traits and distinguishing features of the systems are represented. Besides, the statistical properties of the chaotic motion only are discussed.

**A. Patra-Bhattacharya thermostat.**

The dynamical system, which is a harmonic oscillator coupled with PB thermostat [3], can be described by the set of four ordinary differential equations

$$\begin{align*}
\dot{x} &= \frac{p}{m} - \xi x, \\
\dot{p} &= -k x - \zeta p, \\
\dot{\zeta} &= \frac{1}{\tau_1} \left( \frac{p^2}{mT} - 1 \right), \\
\dot{\xi} &= \frac{1}{\tau_2} \left( \frac{kx^2}{T} - 1 \right).
\end{align*} \quad (21)$$

Here the phase variables $q = (x, p, \zeta, \xi)$ form a four-dimensional vector, $\xi$ is additional configurational friction coefficient and $\tau_1$ and $\tau_2$ are the masses of the thermostats.

Gaussian PDF

$$W_c(q) \propto \exp \left\{ -\frac{p^2}{2mT} - \frac{kx^2}{2T} \right\} \exp \left\{ -\frac{\xi^2}{2\tau_1} - \frac{\zeta^2}{2\tau_2} \right\} \quad (22)$$

obeys the stationary Liouville continuity equation corresponding to this system. The marginal PDF in the physical phase space $(x, p)$ is canonical and whole PDF is completely determined by four non-zero cumulants

$$\kappa_{2,0,0,0} = \frac{T}{k}, \quad \kappa_{0,2,0,0} = Tm, \quad \kappa_{0,0,2,0} = \frac{1}{\tau_1}, \quad \kappa_{0,0,0,2} = \frac{1}{\tau_2} \quad (23)$$

The kinetic coefficients of the system are

$$K_1 = (K_{1x}, K_{1p}, K_{1\zeta}, K_{1\xi}) = \left( \frac{p}{m} - \xi x, -k x - \zeta p, \frac{1}{\tau_1} \left( \frac{p^2}{mT} - 1 \right), \frac{1}{\tau_2} \left( \frac{kx^2}{T} - 1 \right) \right). \quad (24)$$

Only three equations for cumulants, which demonstrate main features of PDF, are considered in this section. They are

$$\begin{align*}
\hat{\kappa}_{0,0,1,0} : \quad &\langle K_{1\xi} \rangle = \frac{1}{\tau_1} \left( \frac{p^2}{mT} + \langle p, p \rangle^2 - 1 \right) = 0, \\
\hat{\kappa}_{0,0,0,1} : \quad &\langle K_{1\xi} \rangle = \frac{1}{\tau_2} \left( \frac{kx^2}{T} + k\langle x, x \rangle^2 - 1 \right) = 0, \\
\hat{\kappa}_{1,1,0,0} : \quad &\langle p, K_{1x} \rangle + \langle x, K_{1p} \rangle = \frac{1}{m} \langle p, p \rangle - \langle p, \xi x \rangle - k \langle x, x \rangle - \langle x, \xi p \rangle = 0.
\end{align*} \quad (25)$$

In the two first equations the averages $\langle x^2 \rangle$ and $\langle p^2 \rangle$ were transformed in accordance with Eqs. (A.1) and (A.2). In
order to get resulting expressions it is need to open cumulant brackets \((x, \zeta)\) (A.3) and \((p, \xi x)\) (A.4) and to take into account that all cumulants of the first order are equal to zero. The latter fact follows from the symmetry of the Eqs. (21) and was verified by the numerical calculations.

As a result, Eqs. (25) lead to follow expressions for cumulants
\[
\kappa_{2,0,0,0} = Tm, \\
\kappa_{2,0,0,0} = T/k, \\
k\kappa_{2,0,0,0} = \frac{1}{m} \kappa_{2,0,0,0} \kappa_{1,1,1,0} - \kappa_{1,1,1,0}. \\
\]
(26)
(27)
(28)
The expressions (26) and (27) show that cumulants \(\kappa_{0,2,0,0}\) and \(\kappa_{2,0,0,0}\) are canonical. This means that PB thermostat controls both kinetic and configurational temperatures in contrast to NH thermostat which controls only kinetic one.

The expression (28) together with (26) and (27) result in the equality \(\kappa_{1,1,1,0} = -\kappa_{1,1,1,0}\). Numerical analysis shows that these cumulants are nonzero and the equality is satisfied well at \(t_{av} \geq 1000\). This means that PDF of the PB system is non-canonical because of statistical dependence of the phase variables.

![FIG. 6. Dependence of the time averages \(\langle x, x \rangle_t\) and \(\langle p, p \rangle_t\) on \(t_{av}\) for PB thermostat at initial conditions \(x_0 = 0\), \(p_0 = 4\), \(\zeta_0 = 0\) and \(\xi_0 = 0\).](image)

The numerical solution of Eqs. (21), presented here, was obtained at the model parameters \(k = m = 1\), \(T = 0.5\), \(\tau_1 = \tau_2 \leq 1\) and the initial conditions \(x_0 = 0\) and \(x_0 = 0.5\), \(p_0 = 4\), \(\zeta_0 = 0\) and \(\xi_0 = 0\). The rates of converging of the time averages to canonical and non-canonical cumulants, as well as in the case of NH thermostat, are very different.

The averages \(\langle x, x \rangle_t\) and \(\langle p, p \rangle_t\) approximating to the canonical cumulants \(\kappa_{2,0,0,0}\) and \(\kappa_{1,2,0,0}\) are shown on Fig. 6 as functions of \(t_{av}\). They converge rather rapidly to the configurational and kinetic temperatures \(T = 0.5\). On the other hand, the time average \(\langle x, p, \zeta \rangle_t\) plotted on Fig. 7 converges to \(\kappa_{1,1,1,0}\) much slower.

The dependence of the \(\langle x, p, \zeta \rangle_t\) plotted on Fig. 7 converges to \(\kappa_{1,1,1,0}\) on the thermostat masses \(\tau_1 = \tau_2\) is also established. It is shown on Fig. 6 by open squares. The fitting function
\[
\kappa_{1,1,1,0} = -0.837 \tau^{0.99} \\
\]
(29)
is plotted by the dashed line.

### B. Hoover-Holian thermostat.

The dynamical system which is a linear oscillator, coupled with HH thermostat [4], can be represented by the set of four ordinary differential equations
\[
\dot{x} = \frac{p}{m}, \\
\dot{p} = -kx - \zeta p - \xi p^2, \\
\dot{\zeta} = \frac{1}{\tau_1} \left( \frac{p^2}{mT} - 1 \right), \\
\dot{\xi} = \frac{1}{\tau_2} \left( \frac{p^4}{m^2T^2} - 3\frac{p^2}{mT} \right). \\
\]
(30)
The canonical Gaussian PDF (22) obeys the Liouville continuous equation corresponding to this system and it is completely defined by four nonzero cumulants (23).

The kinetic coefficients of the system are
\[
K_1 = (K_{1x}, K_{1p}, K_{1\zeta}, K_{1\xi}) = \\
= \left( \frac{p}{m}, -kx - \zeta p - \xi p^2, \right. \\
\]
(31)
\[ \frac{1}{\tau_1} \left( \frac{p^2}{mT} - 1 \right) + \frac{1}{\tau_2} \left( \frac{p^4}{m^2 T^2} - \frac{p^2}{mT} \right). \]

The equations for cumulants, which are considered here, are

\[ \kappa_{0,0,0} : \langle K_{12} \rangle = \frac{1}{\tau_1} \left( \langle p, p \rangle + \langle p \rangle^2 - 1 \right) = 0, \]

\[ \kappa_{0,0,1} : \langle K_{13} \rangle = \frac{1}{\tau_2} \left( \langle p^3 \rangle - 3 \langle p \rangle^2 - \frac{p^2}{mT} \right) = 0, \quad (32) \]

\[ \kappa_{1,1,0} : \langle p, K_{13} \rangle + \langle x, K_{1p} \rangle = 0. \]

After opening the cumulant brackets (see Appendix) and taking into account, that all cumulants of the first order and all joined cumulants of the second order are equal to zero (verified by numerical calculations), solutions of the Eqs. (32) take the form

\[ \kappa_{0,2,0,0} = mT, \]

\[ \kappa_{0,4,0,0} = 3\kappa_{0,2,0,0}(mT - \kappa_{0,2,0,0}) = 0, \quad (34) \]

\[ k\kappa_{2,0,0,0} = \kappa_{2,0,0,0} \left( \frac{1}{m} - 3\kappa_{1,1,0,1} \right) - \kappa_{1,1,1,0} - \kappa_{1,1,3,0}. \]

Eq. (33) shows that HH thermostat, as well as NH and PB ones, controls the kinetic temperature of the system. The expression (34) demonstrates the fact that HH thermostat controls additionally the fourth moment \( \langle p^4 \rangle \) Eq. (35) in such a way as to ensure its equivalence to canonical one. In the terms of cumulants this condition corresponds to the equality \( \kappa_{0,4,0,0} = 0 \) (compare it with the same cumulant (18) of NH system PDF).

The properties of the PDF of the harmonic oscillator, coupled with NH, PB and HH thermostats, were analyzed using cumulant approach. It was shown that the PDFs of the systems considered are non-canonical. This is revealed in the fact that a number of cumulants, which are equal to zero in the canonical PDF, are shown to be nonzero. This is a consequence of the statistical dependence of the phase variables because of the nonlinearity of the equations of motion.

\[ \text{FIG. 8. Dependence of the time averages } \langle x, x \rangle_t \text{ and } \langle p, p \rangle_t \text{ on } t_{av}, \text{ for HH thermostat at initial conditions } x_0 = 0, p_0 = 4, \xi_0 = 0 \text{ and } \zeta_0 = 0. \]

The numerical analysis of the statistical properties of the dynamical system (30) shows that its behaviour is qualitatively similar to that of NH and PB thermostats. The time averages approximating to canonical cumulants converge rather rapidly to their equilibrium values (see \( \langle p, p \rangle_t \) on Fig. 8). But the averages approximating to non-canonical cumulants converge much slowly Fig. 9. The nonzero values of these cumulants, as in previous cases, are an effect of the statistical dependence of the phase variables because of the nonlinearity of the equations of motion.

\[ \text{FIG. 9. Dependence of the time averages } \langle x, p, \zeta \rangle_t \text{ and } \langle x, p, \zeta \rangle_t \text{ on } t_{av}, \text{ for HH thermostat with masses } \tau_1 = \tau_2 = 0.1 \text{ at initial conditions } x_0 = 0, p_0 = 4, \xi_0 = 0. \]

The ergodicity is more difficult to analyze. In the case of quasiperiodic motion the situation is clear. The invariant tori exist in this case and PDF of the system depends on initial conditions because of such dependence of the non-canonical cumulants. This means that the system is nonergodic.

The chaotic mode of the systems corresponds to the idea of ergodicity in more degree. But the cumulant method doesn’t allow to identify directly the ergodicity or nonergodicity of the system. It gives only sufficient
conditions of ergodicity. If the set of equations for cumulants is well determined, i.e., all equations are independent and the set is compatible, the system is ergodic. In this case PDF is completely determined by the system parameters and doesn’t depend on the initial conditions for the equation of motion.

It should be noted that now it cannot be ruled out the possibility that these conditions are also necessary. But this statement has to be proved.

The systems analyzed in this work don’t satisfy these conditions. As it was shown in Sec III, the set of equations for cumulants of the NH system splits into two subsets. One subset is quite determined and the other is underdetermined. The solutions of the first subset are canonical cumulants and those of the second one are non-canonical. So, whole set is underdetermined and the PDF of the system is non-canonical and, most likely, non-ergodic.

The PB and HH systems were studied to a less degree. But existence of the rapidly and slowly converging time averages to the canonical and non-canonical cumulants, analogous to that in the NH system, is indirect evidence in favour of the fact that the structure of the sets of equations for cumulants are also analogous.

Thus, on the base of the foregoing we can conclude that PDFs of the deterministically thermostated harmonic oscillators are non-canonical. The degree of non-canonicity are controlled by the type of thermostat and its parameters. The problem of ergodicity of such systems is still open. This statement can be extended to more complex systems because the cause of such properties is the non-linearity of the equations of motion.

Appendix: Expressions referred to in the text.

The opening of the cumulant brackets used in the text.

\[ \langle x^2 \rangle = \kappa_{2,0,0} + \kappa_{1,0,0} \] \hspace{1cm} (A.1)

\[ \langle p^2 \rangle = \kappa_{0,2,0} + \kappa_{0,1,0} \] \hspace{1cm} (A.2)

\[ \langle x, p \rangle = \kappa_{1,1,0} + \kappa_{1,0,0} + \kappa_{0,1,0} + \kappa_{1,0,0} \] \hspace{1cm} (A.3)

\[ \langle p, \xi x \rangle = \kappa_{1,1,0,1} + \kappa_{0,1,1} + \kappa_{0,1,0,1} \] \hspace{1cm} (A.4)

\[ \langle p^4 \rangle = 1 + 3 \kappa_{0,2,0,0} + 4 \kappa_{1,0,0,0} \] \hspace{1cm} (A.5)

The example of the cumulants expressed in terms of the moments

\[ \kappa_{0,2,0} = \langle p, p \rangle = \langle p^2 \rangle - \langle p \rangle^2, \] \hspace{1cm} (A.7)

\[ \kappa_{1,1,1} = \langle x, p, \xi \rangle = \langle x \xi p \rangle - \langle x \rangle \langle p \xi \rangle - \langle p \rangle \langle x \xi \rangle \]

\[ - \langle \xi \rangle \langle px \rangle + 2 \langle x \rangle \langle p \xi \rangle \] \hspace{1cm} (A.8)

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