On Brayton-Moser network decomposition and state-space energy based generalization of Nosé-Hoover dynamics

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Abstract: - This paper deals with generalization of the Brayton-Moser network decomposition and related structural properties to a relatively large class of finite dimensional strictly causal systems, which can be described in the state-space representation form. The resulting energy-metric function is defined for dissipative systems and is induced by the output signal dissipation power. It is demonstrated that such a power-oriented approach determines both, the structure of a system representation as well as the corresponding system state space topology. A special form of physically correct internal structure of an equivalent state space representation has been derived as a natural consequence of strict causality, the state-space energy conservation, dissipativity assumption and the state minimality requirement.

Key-Words: - State-space energy, decomposition, dissipation power, active power, reactive power.

1 Introduction

It is well known that a large class of real world systems admits modelling based on *Hamilton`s principle* of clasical mechanics either in the form of *Euler-Lagrange equations* or in the form of *Hamilton canonical equations* [1]. In deriving both the sets of equations a crucial role plays a *representation of the energy storage* in the system. Although the Hamilton principle was originally formulated for mechanical systems only, from a general point of view the *specific physical nature* of the system *is immaterial.* Despite of almost generally accepted opinion that both, the *energy-based paradigm* as well as *system conservativity* are *necessary* for construction of *physically correct system representations,* there are also known some approaches in which a *power-based paradigm* plays the key role. Most of them are based on the general concept of state [2], [3]. One of resulting network models is known as the Brayton-Moser equations [4], [5]. The another one is known as the Nosé-Hoover dynamics

2 Problem Formulation

The well known Brayton-Moser equations, resulting from a *special choice of state variables* in electrical circuits theory, represent one of the most important systematic tools for formulation of *state space equations for nonlinear networks.* The network is considered as an abstract system, i.e. as a collection of components joined to a box inside which all the connections are made. In fact, these connections represent a set of internal and external *interactions* between system components which are considered as a set of *workless constraints* on the *component variables.* There are four kinds of electrical network components: inductors, capacitors, resistors and sources. Because resistors and sources are both specified by *voltage-current constitutive characteristics* it seems natural to consider them as a same kind of components; thus for both the term *converter* will be used.

From a mathematical point of view the dynamical behavior of a nonlinear electrical circuit may in principle be described by a set of *state equations* – set of first order ordinary nonlinear differential equations

$$\dot{x}_i = f_i(x_1, x_2, \cdots, x_n) + v_i,\ i \in \{1, 2, \cdots, n\} \qquad (1)$$

together with *output equations*

$$y_k = h_k(x_1, x_2, \cdots, x_n),\ k \in \{1, 2, \cdots, p\} \qquad (2)$$

where the variables x_1, x_2,...x_n are the *state variables*, the variables v_1, v_2, ... v_n represent the *effect of inputs*, and the variables y_1, y_2,...y_p represent the *observed outputs.*

Any such mathematical structure is called *state space representation* of the electrical network. The state variables may be taken as coordinates of a vector referred to a basis in a Euclidean space of *n* dimensions, called the *state space* of the system representation. Each solution of the state equations determines a *state space trajectory.*

Any state space representation having a particularly *simple* or *useful structure* is called *canonical.* It will be demonstrated that one of the most effective electrical network *canonical state space representations,* the *Brayton-Moser equations,* can be interpreted as a direct consequence of a very *special state space decomposition.*

In this paper, a class of linear and especially nonlinear systems is discussed from the *abstract system state energy* point of view. A conceptually new approach is based on the idea that *abstract state space energy* can be *measured* by a *distance* of the *actual state x(t)* from the *equilibrium.* Thus a *metric* is defined *ρ[x(t), x*]* and used as a key for definition of a new concept of *abstract state-space energy E(x)* [6, 7, 8, 9].

3 Classical form of Brayton - Moser Network State Space Decomposition

Let *v* and *i* be vectors whose entries are the voltages and currents of the network components. The *total network power* is given by *scalar product*

$$P = \langle v, i \rangle \tag{3}$$

Thus for voltage and current variations the corresponding differential in power is given by

$$dP = dG + dJ \tag{4}$$

where *dG* and *dJ* are defined by

$$dG = \langle i, dv \rangle, \quad dJ = \langle v, di \rangle \tag{5}$$

and represent differentials in *total network content* and the *total network co-content*, respectively.

For converters, integrals of these quantities may be interpreted in terms of areas on constitutive characteristics. On the other hand for inductors and capacitors no such interpretation is possible. What is really important is that the total network content and total network co-content, defined by these integrals, are *zero* when evaluated *along any curvilinear arc in the state space.* For any instantaneous value of the state we may put

$$i = C(v)\frac{dv}{dt}, \quad v = L(i)\frac{di}{dt} \tag{6}$$

where *C(v)* and *L(i)* are matrices whose elements are the appropriately evaluated values of an *incremental capacitance* and *incremental inductance*, respectively.

Now, since all the converter variables are determined by the state variables together with the converter constitutive characteristics, we may define a *power-like scalar function Q(i,v)* of currents *i(t)* and voltages *v(t)* [10-12], and use it to derive the *Brayton-Moser canonical form of equations*:

$$L(i)\frac{di}{dt} = -\left[\frac{\partial Q}{\partial i}\right]^T \tag{7}$$

$$C(v)\frac{dv}{dt} = -\left[\frac{\partial Q}{\partial v}\right]^T \tag{8}$$

Example 1. For further motivation and deeper understanding the following example of 6th order *electrical circuit with two nonlinearities,* as introduced in the Fig. 1. seems to be useful.

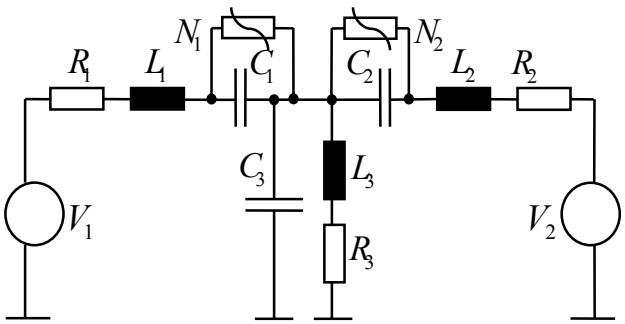

Fig. 1. Example of nonlinear electrical network

The *content* of all *tree converters* reads

$$G_{tree} = \frac{1}{2}R_2 i_{L2}^2 - v_2 i_{L2} + \frac{1}{2}R_3 i_{L3}^2 - v_1 i_{L1} + \frac{1}{2}R_1 i_{L1}^2 \tag{9}$$

the corresponding *co-content* is given by the expression

$$J_{chords} = \int_0^{v_{C1}} f(v_{C1})dv_{C1} + \int_0^{v_{C2}} f(v_{C2})dv_{C2} \tag{10}$$

the *tree structure* is described by the *interaction matrix*

$$D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 1 & -1 \end{bmatrix} \tag{11}$$

and the *power-like function Q* can be specified using the general expression

$$Q = v^T Di + G_{tree} - J_{chords} \tag{12}$$

Its explicit final form for the given network reads

$$Q = v_{C1}i_{L1} + v_{C2}i_{L2} - v_{C3}i_{L1} + v_{C3}i_{L2} - v_{C3}i_{L2} + \frac{1}{2}R_2 i_{L2}^2 - v_2 i_{L2} + \frac{1}{2}R_3 i_{L3}^2 - v_1 i_{L1} + \frac{1}{2}R_1 i_{L1}^2 - \int_0^{v_{C1}} f(v_{C1})dv_{C1} + \int_0^{v_{C2}} f(v_{C2})dv_{C2} \quad (13)$$

It contains all the *necessary information* for specification of the *state equations* of the given nonlinear network in the so called *Brayton-Moser canonical form:*

$$\begin{aligned} L_1\frac{di_{L1}}{dt} &= -\frac{\partial Q}{\partial i_{L1}} = -v_{C1} + v_{C3} + v_1 - R_1 i_{L1} \\ L_2\frac{di_{L2}}{dt} &= -\frac{\partial Q}{\partial i_{L2}} = -v_{C2} - v_{C3} - R_2 i_{L2} + v_2 \\ L_3\frac{di_{L3}}{dt} &= -\frac{\partial Q}{\partial i_{L3}} = v_{C3} - R_3 i_{L3} \\ C_1\frac{dv_{C1}}{dt} &= \frac{\partial Q}{\partial v_{C1}} = i_{L1} - f(v_{C1}) \\ C_2\frac{dv_{C2}}{dt} &= \frac{\partial Q}{\partial v_{C2}} = i_{L2} - f(v_{C2}) \\ C_3\frac{dv_{C3}}{dt} &= \frac{\partial Q}{\partial v_{C3}} = -i_{L1} + i_{L2} - i_{L3} \end{aligned} \quad (14)$$

4 State Space Energy Based Generalization of Conservation Laws for Dissipative Systems

The class of frequently postulated mathematical models of many physical systems is usually ***restricted*** to classical ***conservative Hamiltonian systems***, i.e. without any energy dissipation. In such systems a total stored energy is not allowed to change in time. In many cases such ***restriction is not adequate to*** real situations**.**

Let us now consider an ***abstract structure*** shown in the Fig. 2.

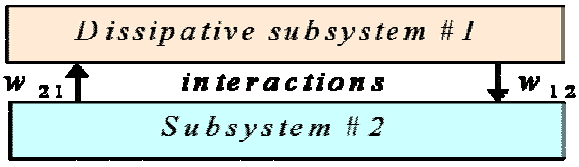

Fig. 2. Decomposition of a system with dissipation

The recently proposed new concept of the *state space energy* (SSE) [8], [9], is closely related to the classical concept of *total system energy* (TSE), but both the notions *must not be confused in general.*

There are at least *three fundamental differences* between them:

• at first, the classical concept of TSE is directly connected to the *knowledge* of a *specific physical nature of the system* under consideration (e.g. physical, biological, chemical, mechanical, etc.), whereas the concept of the SSE is a *pure abstraction* which has been defined *quite independently* of any *priori physical knowledge* .

• at second, the concept of SSE is defined *exclusively* as a *function of state* without any regard to a *set of (physical or abstract) system parameters.*

• at third, the concept of SSE is defined in such a way that *in general* it represents only that *part of the total system energy*, which is *accumulated in the actual state of the system* under consideration, i.e. it represents a *property of the state space* only, and does not include any *effects of actual inputs.* In contrary to the TSE which is closely related to the *total power* the definition of the proposed concept of SSE is based on the so called *output dissipation power* only. We start with some basic ideas of the state space energy based approach [9].

Let $P_0(t) \geq 0$ denotes the *instantaneous value* ***output dissipation power*** of a zero-input causal system with ***informational output*** $y(t)$ defined by:

$$y(t) = \pm\sqrt{P_0(t)},\ P_0(t) \geq 0 \quad (15)$$

Notice that for a ***conservative system***, i.e. for ***zero dissipation power, no information*** can be gained *by measurement the output.*

Let $E(t)$ denotes the *instantaneous value* of the ***state space energy*** stored in a state vector $x(t)$

$$E(t) = \int_{t_0}^{\infty} P_0(\tau)d\tau,\ \forall t:\ t = t_0 \quad (16)$$

The following *differential form* of an abstract ***state space energy conservation principle*** holds

$$\frac{dE}{dt} = \langle \psi(x), f(x) \rangle = -P_0(t) \quad (17)$$

where ψ *is the* ***gradient vector*** *of the* ***state space energy*** *potential field* E, f is the ***state space velocity vector***, and the symbol $\langle .,. \rangle$ *denotes* ***the Lie derivative in form of the dual product operation.***

Because the *choice of origin* and of the *state space coordinate system is free* we can ***without any restriction of generality*** *define* the ***gradient vector*** $\psi(x)$ of the energy E in its ***most simple form***

$$\psi(x) = x^T \rightarrow E = \frac{1}{2}\sum_{i=1}^{n} x_i^2 \quad (18)$$

where n is the ***order of the system representation.***

Example 2. In order to illustrate the idea of the state space energy conservation principle the following 4th order system representation is introduced

$$\begin{aligned}\dot{x}_1 &= -\Delta_1 x_1 + \omega_2 x_2\\ \dot{x}_2 &= -\omega_2 x_1 + \sigma_3 x_3\\ \dot{x}_3 &= -\sigma_3 x_2 + \omega_4 x_4\\ \dot{x}_4 &= -\omega_4 x_3 + \sigma_5 x_5\\ y &= \pm\sqrt{\Delta_1 x_1}\end{aligned} \quad (19)$$

The state space energy $E(t)$ is given by

$$\psi(x)=[x_1,x_1,x_1,x_1]^T \rightarrow E=\frac{1}{2}[x_1^2+x_2^2+x_3^2+x_4^2] \quad (20)$$

the dissipation power $P_0(t)\geq 0$ is defined by:

$$P_0(t) = y^2(t) = \Delta_1 x_1^2 \quad (21)$$

and the state space energy conservation law reads:

$$\begin{aligned}&\frac{dE}{dt}=-\Delta_1 x_1^2+(\omega_2-\omega_2)x_1x_2+\\ &+(\sigma_3-\sigma_3)x_2x_3+(\omega_4-\omega_4)x_3x_4=-P_0(t)\end{aligned} \quad (22)$$

where Δ_1 is the dissipation parameter, ω_2, ω_4 are eigen-frequencies of two oscillating subsystems and σ_3 is the interaction parameter, representing the interaction between both the 2nd order subsystems.

The other terms determine a ***"total exchange power"*** P_E

$$P_E(\xi,\eta)=\xi_1(\eta_1-\eta_3)+\xi_2(\eta_2+\eta_3)-\xi_3\eta_3 \quad (23)$$

where $|\tilde{\omega}_2|$ and $|\tilde{\omega}_4|$ represent absolute values of the ***"frequency fluctuations"*** defined by

$$\begin{aligned}\tilde{\omega}_2 &= s_1|\tilde{\omega}_2| = s_1|\omega_2-\hat{\omega}_2|\\ \tilde{\omega}_4 &= s_3|\tilde{\omega}_4| = s_3|\omega_4-\hat{\omega}_4|\end{aligned} \quad (24)$$

Similarly $|\tilde{\sigma}_3|$ represents an absolute value of the ***"interaction fluctuations"*** defined by

$$\tilde{\sigma}_3 = s_2|\tilde{\sigma}_3| = s_2|\sigma_3-\hat{\sigma}_3|, \quad s_2\in\{-1,1\} \quad (25)$$

and the binary parameters s_k, $k\in\{1,2,\ldots n\text{-}1\}$ define a ***"spin structure".***

Observation 1: It is worthwhile to notice that for all values of the frequency parameters ω_2, ω_4 and for arbitrary value of the interaction parameter σ_3 the positivity condition of the dissipation parameter Δ_1 is necessary and sufficient for strict dissipativity of the complete system representation (19).

Observation 2: Notice that for zero value of the interaction parameter σ_3=0 the system degenerates to two isolated 2nd order subsystems: the first subsystem remains *dissipative*, but the other one will become *conservative*. Thus the same kind of the *state space decomposition appears* as that introduced in connection with *the Brayton-Moser canonical form.*

Observation 3: Notice further that for a special case of zero *dissipation parameter* Δ_1=0 the system representation becomes *conservative for any value of the interaction parameter* σ_3 without any regard to values of *frequency parameters* ω_2, ω_4.

The n^{th} -order system has 2^{n-1} possible sign-combinations of *frequency- and interaction parameters*, i.e. ***spin parameters*** s_k. Thus for the 4th-order system there are just 8 possible ***"spin structures",*** corresponding to 8 different, but ***state equivalent,*** system ***state space representations:***

$$\begin{aligned}\dot{x}_1 &= -\Delta_1 x_1 u(t) + \omega_2 x_2 & \dot{x}_1 &= -\Delta_1 x_1 u(t) - \omega_2 x_2\\ \dot{x}_2 &= -\omega_2 x_1 + \sigma_3 x_3 & \dot{x}_2 &= \omega_2 x_1 + \sigma_3 x_3\\ \dot{x}_3 &= -\sigma_3 x_2 + \omega_4 x_4 & \dot{x}_3 &= -\sigma_3 x_2 + \omega_4 x_4\\ \dot{x}_4 &= -\omega_4 x_3 & \dot{x}_4 &= -\omega_4 x_3\\ y(t) &= \pm\sqrt{\Delta_1 x_1} & y(t) &= \pm\sqrt{\Delta_1 x_1}\end{aligned}$$

$$\begin{aligned}\dot{x}_1 &= -\Delta_1 x_1 u(t) + \omega_2 x_2\\ \dot{x}_2 &= -\omega_2 x_1 - \sigma_3 x_3\\ \dot{x}_3 &= \sigma_3 x_2 + \omega_4 x_4\\ \dot{x}_4 &= -\omega_4 x_3\\ y(t) &= \pm\sqrt{\Delta_1 x_1}\end{aligned} \quad \ldots \text{etc.} \quad (26)$$

The ***courses of the state space energy*** for corresponding ***spin structures*** with parameter values $\omega_2 = \pm 1$, $\sigma_3 = \pm 1$, $\omega_4 = \pm 1$ and for the ***dissipation*** $\Delta_1 = 0.1$, i.e. for $|\omega_2| = 1$, $|\sigma_3| = 1$, $|\omega_4| = 1$, are displayed in the Fig.3. for illustration.

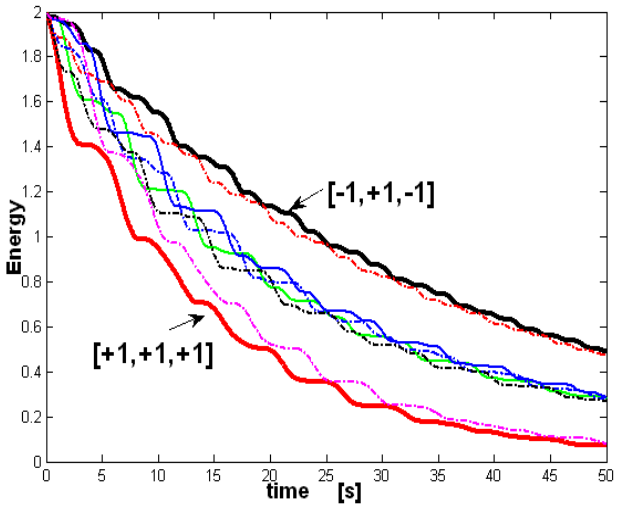

Fig. 3. Courses of the state-space energy $E(t)$.

Let a concept of the *state space hyper-energy* J be defined by integration of the state space energy:

$$J = \int_{t_0}^{t_1} E(\tau) d\tau, \quad t_1 \to \infty \tag{27}$$

It is important to note that the new concept of the state space *hyper-energy J*, divided by the length of the time interval $T=[t_0,t_1]$, defines a ***mean value of the state space energy E[x(t)]*** *on* $[t_0, t_1]$**.**

The *rate of dissipation* of the eight different *state space energy courses,* shown in the Fig. 3. may be *evaluated* by means of the state hyper-energy in dependence on the *8 possible spin structures* as follows from the Table 1.

Spin struct. $\{s_1,s_2,s_3\}$	ω_2 s_1	σ_3 s_2	ω_4 s_3	*Hyper-energy J*	*Normalized inverse of J P*
S1	1	1	1	27.6	1
S2	-1	1	1	49.5	0.56
S3	1	-1	1	68.5	0.4
S4	-1	-1	1	52.6	0.53
S5	1	1	-1	47.6	0.58
S6	-1	1	-1	71.5	0.39
S7	1	-1	-1	50.5	0.55
S8	-1	-1	-1	32.6	0.85

Table 1. Hyperenergy based system evolution and its probabilistic interpretation

Recall that the concept of the hyper-energy has no meaning for Hamiltonian systems. The reason is that for any non–vanishing constant energy $E(x) = \text{const.} > 0$, the definition integral would diverge. Hence due to mathematical reasons, the *dissipativity axiom is necessary.*

Notice that the normalized inverse value of the state space hyper-energy may be interpreted as a ***probabilistic measure P*** *on the complete set of possible state space trajectories.* By this way we can try to decide ***which spin structure*** of the equivalent state space representations is ***the most likely to be realized.***

Observation 4: Possibility of the probabilistic interpretation above, together with a modified Hamilton`s optimality principle, obviously opens new perspectives to blend some fundamental concepts of the ***classical Hamiltonian mechanics,*** (deterministic) ***chaos theory,*** and the (probabilistic) ***quantum theory.***

Observation 5: It is worthwhile to notice that the last equation in (19) says that ***no information about the internal system behavior can be gained by measurement the output, if dissipation parameter*** Δ_1 ***vanishes.***

Observation 6: The last equation in eqn. (19) should be interpreted as a plausible ***signature of necessity*** of ***a Heisenberg-like uncertainty principle*** *not only in the quantum theory.*

The topological structure of the 4th order example of the dissipative system representation (19) is displayed in the Fig. 4. for illustration.

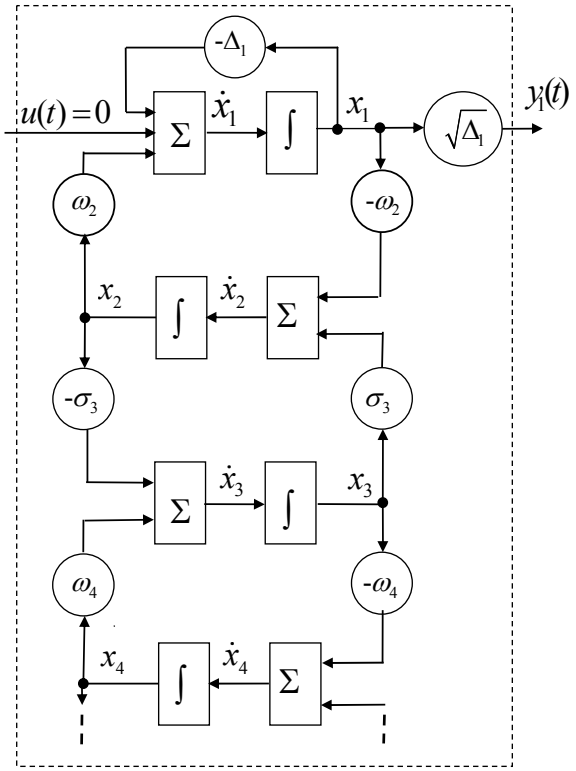

Fig. 4. Topological structure of the 4th order linear dissipative system representation.

If the state representation (19) is given, it is easy to determine the corresponding 4th-order ordinary homogenous differential equation:

$$x^{(4)}(t) + a_1 x^{(3)}(t) + a_2 x^{(2)}(t) + a_3 \dot{x}(t) + a_4 x(t) = 0 \tag{28}$$

where the parameters a_k for k=1,2,3,4 are given by nonlinear parameter space transformation

$$\begin{aligned} a_1 &= \Delta_1 \\ a_2 &= \omega_2^2 + \sigma_3^2 + \omega_4^2 \\ a_3 &= \Delta_1(\sigma_3^2 + \omega_4^2) \\ a_4 &= \omega_2^2 \omega_4^2 \end{aligned} \tag{29}$$

On the other hand, the energy motivated state space representation (19) exists if and only if the corresponding ***parameter space transformation is real and invertible.***

Expressing the ***algebraic structure*** of the state space representation in a semi-linear vector-matrix form as follows

$$\Re\{\varphi\}: \quad \dot{x}(t) = A\,x(t) + B\,u(t) \qquad y(t) = C\,x(t), \tag{30}$$

it becomes obvious that it can be generalized for a general class of ***strictly causal systems of any finite order n*** as follows:

$$A = \begin{bmatrix} -\Delta_1 & \omega_2 & 0 & 0 & 0 & \cdots & 0 & 0 \\ -\omega_2 & 0 & \sigma_3 & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\sigma_3 & 0 & \omega_4 & 0 & \cdots & 0 & 0 \\ 0 & 0 & -\omega_4 & 0 & \sigma_5 & \cdots & 0 & 0 \\ 0 & 0 & 0 & -\sigma_5 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & -\sigma_{n-1} & 0 & \omega_n \\ 0 & 0 & 0 & \cdots & 0 & 0 & -\omega_n & 0 \end{bmatrix} \tag{31}$$

$$C = \begin{bmatrix} \pm\sqrt{\Delta_1} & 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix} \tag{32}$$

Observation 7: From a system-theoretical point of view the strictly Hamiltonian systems, as a limiting case of the dissipative structure (31), (32) for $\Delta_1 \to 0$, have to be excluded because of *impermissible idealization.*

It is of crucial importance to realize that the essential ***structural features*** of the proposed state space energy approach are ***independent of the standard assumptions of linearity and time-invariance.***

Postulating validity of a Hamilton optimality principle, it can be concluded that the ***most probable spin structure to be realized is {1, 1, 1}.*** It corresponds to ***minimum mean value of the state space energy E(x).***

If we interpret normalized inverse state hyper-energy P as a proper probability measure on the space of allowed values of the state energy $E(x)$ *we are able to prove* that even by means of ***a periodic spin structure switching even a controlled quantum-chaotic behavior can appear.***

Example 3: Let us illustrate the idea by applying it to the *Josephson junction,* (as an example of a *nano-structure),* in form of a 4th-order *bilinear system* representing *two oscillators* in a *weak interaction* σ_3:

$$\begin{aligned} \dot{x}_1 &= -\Delta_1 x_1 + u(t)\omega_2 x_2 \\ \dot{x}_2 &= -u(t)\omega_2 x_1 + \sigma_3 x_3 \\ \dot{x}_3 &= -\sigma_3 x_2 + \omega_4 x_4 \\ \dot{x}_4 &= -\omega_4 x_3 \\ y &= \pm\sqrt{\Delta_1 x_1} \end{aligned} \tag{33}$$

Parameters ω_2, ω_4 may be seen as *frequencies* of two isolated *oscillating subsystems.* The *superconductivity* assumption *implies* that $\Delta_1 \to 0$, the system becomes *conservative,* and *behavior* of its *state* becomes *unobservable by the output.*

On the other hand, using *u(t)* as an *external input,* the behavior of *state may be controlled* by a properly chosen *signal u(t),* e.g.:

$$u(t) = \kappa sign[v(t)],\ v(t) = \sin(2\pi ft/30) \tag{34}$$

Some results of simulation experiments for parameter values

$$\omega_2 = \frac{2}{3}\pi, \omega_4 = 1, \kappa = \frac{1}{2} \tag{35}$$

shown in the Fig. 5. and 6. illustrate the essence of the proposed *quantum-chaos oriented* approach. In the 3-D projection shown in the Fig. 5., the ***chaotic-like nature of the system trajectories*** obviously ***dominates.***

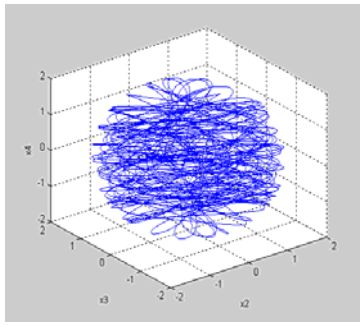

Fig. 5. Projection of the quantum-chaotic-like behavior into a 3-D subspace of the state space.

In contrary, the 2-D projection shown in the Fig. 6. suggests that the ***quantum-like nature of the system behavior should not be ignored, too.***

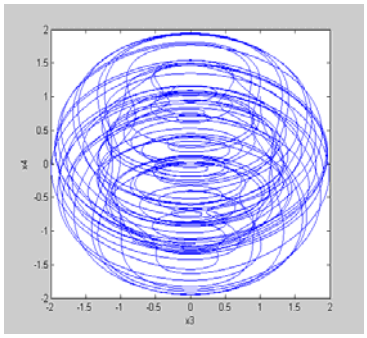

Fig. 6. Projection of quantum-chaotic system behavior into the state plane (x_3, x_4).

It is important to stress that in the example above the chaotic behaviour is *undetectable by the output,* or *externally un-measureable* because of the *conservativity*. In contrary to this, in the *dissipative chaos*, where the system behaviour is *observable by output*, the state space *energy conservation* law holds *in the average only.*

5 State Space Energy Conservation for Brayton-Moser Decomposition

In *general case* the results obtained may be expressed in the following *vector form:*

$$\begin{aligned} \Re(S):\ \dot{x} &= f[x,u] \triangleq Fx + Gu + \phi(x) \\ y &= h[x] \triangleq Hx \end{aligned} \tag{36}$$

For considered example 1. of the Brayton-Moser system decomposition the matrices F and G take the form:

$$F \triangleq \begin{bmatrix} -\alpha_{11} & 0 & 0 & -1 & 0 & 1 \\ 0 & -\alpha_{22} & 0 & 0 & -1 & -1 \\ 0 & 0 & -\alpha_{33} & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 & 0 & 0 \end{bmatrix}, \ G \triangleq \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{37}$$

Thus the *general structure* of *system representations* obtained by *Brayton-Moser canonical state space decomposition* may be *visualized* by the *structural diagram* shown in the Fig. 7.

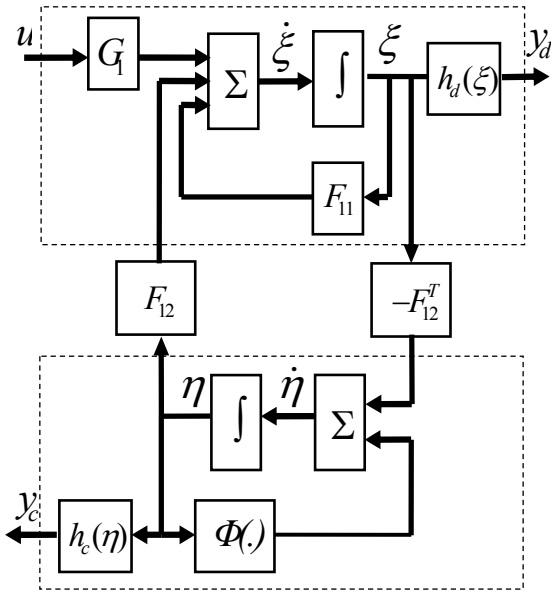

Fig. 7.The Brayton-Moser state space decomposition

As a consequence of the *Brayton-Moser state space decomposition* a corresponding *system decomposition* arises and may *algebraically* be expressed by *matrix decomposition*

$$F = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}, \ F_{21} = -F_{12}^T \tag{38}$$

where the submatrix F_{12} is defined by the matrix D in the form

$$F_{12} = \begin{bmatrix} -1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \tag{39}$$

and represents the *interaction matrix* between two 3rd order *isolated subsystems* characterized by submatrices F_{11}, F_{22}. The submatrix F_{11} represents the ***strongly dissipative subsystem*** with *real negative roots* of the corresponding *characteristic polynomial*

$$\begin{aligned} F_{11}(s) &= \det[sI - F_{11}] = \det\begin{bmatrix} s+R_1 & 0 & 0 \\ 0 & s+R_2 & 0 \\ 0 & 0 & s+R_3 \end{bmatrix} \\ &= (s+R_1)(s+R_2)(s+R_3) \end{aligned} \tag{40}$$

and the second one described by zero matrix $F_{22} = 0$, is ***strongly conservative*** with *zero roots* of the corresponding *characteristic polynomial*

$$F_{22}(s) = \det[sI - F_{22}] = \det\begin{bmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{bmatrix} = s^3 \tag{41}$$

For the two dimensional *vector input signal*

$$u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \tag{42}$$

representing the two voltage sources as displayed in the Fig. 1. we obtain the corresponding *input matrix decomposition* in the form

$$G_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \ G_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{43}$$

Finally the *nonlinear interaction* term, which can be interpreted as a *vector feedback control signal,* is determined by

$$\phi_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \ \phi_2 = \begin{bmatrix} -\phi_1(\eta_1) \\ -\phi_2(\eta_2) \\ 0 \end{bmatrix} \tag{44}$$

As a result the *state space velocity vector field* is given by

$$\begin{aligned} \dot{\xi} &= F_{11}\xi + F_{12}\eta + G_1 v + \phi_1(\xi,\eta) \\ \dot{\eta} &= -F_{12}\xi + F_{22}\eta + G_2 v + \phi_2(\xi,\eta) \end{aligned} \tag{45}$$

and hence, similarly as the *state vector x,* it is *decomposed* into the *dissipative* and *conservative* vector components:

$$\dot{\xi} = \begin{bmatrix} \dot{\xi} \\ \dot{\xi}_2 \\ \dot{\xi}_3 \end{bmatrix}, \quad \dot{\eta} = \begin{bmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \\ \dot{\eta}_3 \end{bmatrix} \tag{46}$$

Because of *skew-symmetry* of the *total interaction matrix*

$$F_I \triangleq \begin{bmatrix} 0 & F_{12} \\ -F_{12}^T & 0 \end{bmatrix} \tag{47}$$

a *nonvanishing interaction* between both the subsystems *exists* but *from energy transfer point of view* it is *completely neutral.* Thus the *state space energy* may be *decomposed:*

$$E(\xi,\eta) = E_D(\xi) + E_C(\eta) \tag{48}$$

$$\begin{aligned} E_D(\xi) &\triangleq \frac{1}{2}\left[\xi_1^2 + \xi_2^2 + \xi_3^2\right], \\ E_C(\eta) &\triangleq \frac{1}{2}\left[\eta_1^2 + \eta_2^2 + \eta_3^2\right] \end{aligned} \tag{49}$$

Computing the *Lie derivative of the state space energy* along the network state space representation

$$\begin{aligned} \dot{\xi}_1 &= -R_1\xi_1 - \eta_1 + \eta_3 + v_1 \\ \dot{\xi}_2 &= -R_2\xi_2 - \eta_2 - \eta_3 + v_2 \\ \dot{\xi}_3 &= -R_3\xi_3 + \eta_3 \\ \dot{\eta}_1 &= \xi_1 - \phi_1(\eta_1) \\ \dot{\eta}_1 &= \xi_2 - \phi_2(\eta_2) \\ \dot{\eta}_3 &= -\xi_1 + \xi_2 - \xi_3 \end{aligned} \tag{50}$$

for the *total power* $P_D(t)$ of the *dissipative subsystem* we obtain the expression

$$\begin{aligned} \left.\frac{dE_D}{dt}\right|_{\Re(S)} &= \left\langle \frac{\partial E_D}{\partial \xi}, \dot{\xi} \right\rangle \Big|_{\Re(s)} \\ &= (\xi_1\dot{\xi}_1 + \xi_2\dot{\xi}_2 + \xi_3\dot{\xi}_3)\big|_{\Re(S)} \\ &= \xi_1(v_1 - R_1\xi_1) + \xi_2(v_2 - R_2\xi_2) - R_3\xi_3^2 - P_E(\xi,\eta) \triangleq P_D(t) \end{aligned} \tag{51}$$

and for the *total power* $P_C(t)$ of the *conservative* one we get

$$\begin{aligned} \left.\frac{dE_C}{dt}\right|_{\Re(S)} &= \left\langle \frac{\partial E_C}{\partial \eta}, \dot{\eta} \right\rangle \Big|_{\Re(s)} \\ &= (\eta_1\dot{\eta}_1 + \eta_2\dot{\eta}_2 + \eta_3\dot{\eta}_3)\big|_{\Re(S)} \\ &= -\eta_1\phi_1(\eta_1) - \eta_2\phi_2(\eta_2) + P_E(\xi,\eta) \triangleq P_C(t) \end{aligned} \tag{52}$$

where the *interaction term*

$$P_E(\xi,\eta) = \xi_1(\eta_1 - \eta_3) + \xi_2(\eta_2 + \eta_3) - \xi_3\eta_3 \tag{53}$$

in contrary to the other *active power components* of both the *individual subsystems* is of a *reactive nature,* and obviously represents the *exchange power* between *these subsystems.*

Because the *internal interactions* of the system are *neutral* both the *reactive powers are compensated,* and thus we obtain:

$$P(\xi,\eta) = P_D(\xi) + P_C(\eta) \tag{54}$$

As a consequence the *total system power* is of *active nature*:

$$\begin{aligned} P(\xi,\eta) &= \xi_1(v_1 - R_1\xi_1) + \xi_2(v_2 - R_2\xi_2) \\ &-\eta_1\phi_1(\eta_1) - \eta_2\phi_2(\eta_2) - R_3\xi_3^2 \end{aligned} \tag{55}$$

and it may be *decomposed* into the *total input signal power* P_{IS}

$$P_{IS}(\xi,v) = \xi_1 v_1 + \xi_2 v_2 \tag{56}$$

delivered by both the *ideal voltage sources,* decreased by the amount of the *total input dissipation power* P_{ID} given by

$$-P_{ID}(\xi) = -[R_1\xi_1^2 + R_2\xi_2^2] \tag{57}$$

by the *total feedback dissipation power* P_{FD}, defined by

$$-P_{FD}(\eta) = -[\eta_1\phi_1(\eta_1) + \eta_2\phi_2(\eta_2)] \tag{58}$$

and by the *total output dissipation power* P_{OD}, defined by the *instantaneous value of the output signal power inducing the output equation* in a *typical form* of the eq. (19), (32) as follows

$$\begin{aligned} -P_{OD}(y) &= -[y(t)]^2 = -R_3\xi_3^2 \\ y(t) &= \sqrt{R_3}\,\xi_3 = \sqrt{\Delta_1}\,\xi_3 \end{aligned} \tag{59}$$

6 Fundamentals of Non-Hamiltonian Nosé-Hoover Dynamics

The interest of scientific community in control of natural processes has along history. In the 20th century numerous challenging control problems of molecular dynamics have been studied, especially in connection with automatic control of nuclear and chemical reactors.

Major *practical difficulties* when controlling processes at the atomic and/or molecular level are closely connected with the *tiny spatial size* and the *fast speed* of the processes in the *micro-world.*

Typically, an *average size* of a molecule of a chemical substance is of the order 10 *nm*, and *average interatomic distance* in a molecule is of order 1 *nm.* An *average period* of natural oscillations of a molecule is of the order 10-100 femto-seconds, i.e. 10^{-14}-10^{-13}s.

Construction of devices for measurement and control at such spatiotemporal scales is an enormously hard scientific and technological problem. In such a way a new scientific-technological field, which became known as the *femto-chemistry*, arose.

There is certainly no surprise that besides of practical difficulties mentioned above also a variety of new challenging *theoretical problems* of the so called *molecular dynamics* appeared. Because of great number of interconnected particles (of the order 10^{23}) new problems in the field of *numerical simulation* required development of *new theoretical approaches*, too. Since the beginning of the 1980s there has been a growing interest in modeling and control problems in *classical* and *quantum-theoretic* formulation. One of the most promising theoretical tools is known as the *Nosé-Hoover dynamics* [13, 14] as a *generalization* of the well known *classical Hamiltonian dynamics.*

It is now widely recognized that a concept of the *geometrical structure* plays a *crucial role* in classical as well as in the quantum-theory based dynamics. For instance, the numerical integration methods for ordinary differential equations *preserving the geometrical structure of the underlying vector fields* are likely to lead to more accurate long-term trajectory behavior than those more traditional methods ignoring the geometrical structure of the corresponding state space [16, 17].

Recall that according the *Liouville`s theorem* for divergenceless vector fields the *time evolution of state trajectories under Hamiltonian dynamics conserves the state space volume element.* Because of such special structure (called *symplectic structure)* the corresponding numerical integration methods are called *symplectic integrators.* Symplectic integrators represent a main tool of the conventional *statistical mechanics* [15], and have been applied to a broad class of Hamiltonian dynamical problems in *classical* as well as in the *quantum-mechanical* setting. The *non-Hamiltonian dynamics* characterized by *non-vanishing divergence* seems, at least from the theoretical point of view, to be significantly more satisfying because of assumed *"state space compressibility"*. Such situations typically arise in the treatment of *non-equilibrium steady states* and/or, for instance when treating *mechanics of "thermostatted systems"*. In order to summarize the main features of the *non-Hamiltonian* approach known as the *Nosé-Hoover dynamics,* consider an *even order state space representation* with the *state vector* $\boldsymbol{x}$:

$$x = [x_1, x_2, \cdots, x_n]^T \tag{60}$$

Following the standard approach of Hamiltonian dynamics, we divide the state variables x_k, $k \in \{1,2,\ldots,n\}$ into *two sub-vectors*: the *vector of coordinates* $\boldsymbol{q}$ and the *vector of moments* $\boldsymbol{p}$ (of dimension $n/2$) [13, 14, 15].

Let the *vector field f* with components f_i reads

$$f_i = \frac{dx_i}{dt} = \dot{x}_i, \quad f(x) = A(x)\frac{\partial H(x)}{\partial x} \tag{61}$$

where *H(x)* is *Hamilton function* representing the *total system energy* and $A(.)$ is n x n *antisymmetric matrix:*

$$A^T(x) = -A^T(x) \tag{62}$$

It follows from anti-symmetry of $A(.)$ that it holds

$$L_f H = \left\langle f, \left(\frac{\partial H}{\partial x}\right)^T \right\rangle = 0 \tag{63}$$

i.e. that *Lie derivative* of the *Hamilton function* according to the *vector field f along the trajectories* induced by the field *f(x) vanishes.* It means that the energy function *H(x)* is conserved along any trajectory generated by any vector field *f(x)*.

It is important to note that the energy function can in general be decomposed as follows:

$$H(x) = \sum_{\alpha=1}^{m} H(\alpha, x) \tag{64}$$

where the *decomposition* is of course *not unique.*

Obviously, the decomposition of the energy induces a corresponding *decomposition of the vector field*

$$f(x) = \sum_{\alpha=1}^{m} f(\alpha, x) \tag{65}$$

and that of the *Lie derivative*

$$L = \sum_{\alpha=1}^{m} L^{\alpha} \tag{66}$$

where the *Lie derivative operation L* is defined by

$$L^{\alpha} = f_i(\alpha)\frac{\partial}{\partial x_i} \tag{67}$$

It is not difficult to recognize that the *Nosé-Hoover approach* is *closely related* to the proposed *state space energy based approach*. In fact, the *essence of the Nosé-Hoover decomposition* can be reduced to the ***special case of the state space energy based structures*** for ***limiting value of the dissipation parameter*** $\Delta_1 = 0$ and for ***properly transformed energy function H.***

For further motivation and deeper understanding several simple examples of closely related 4th-order system representations may be useful.

Example 4. (A 4th –order dissipative structure)

$$A=\begin{bmatrix} -\Delta_{11} & \omega_2 & 0 & 0 \\ -\omega_2 & -\Delta_{22} & \sigma_3 & 0 \\ 0 & -\sigma_3 & -\Delta_{33} & \omega_4 \\ 0 & 0 & -\omega_4 & -\Delta_{44} \end{bmatrix} \quad (68)$$

Two *coupled harmonic oscillators* with *interaction parameter* σ_3, with *four independent dissipation channels* Δ_{kk}, k=1,2,3,4, and with *two eigen-frequences* ω_2, ω_4.

The *characteristic polynomial A(s)* of the matrix *A* is given in the form:

$$\begin{aligned} A(s) =& s^4 + (\Delta_{11}+\Delta_{22}+\Delta_{33}+\Delta_{44})s^3 + \\ & (\omega_2^2+\omega_4^2+\sigma_3^2+\Delta_{11}\Delta_{22}+\Delta_{11}\Delta_{33} \\ & +\Delta_{11}\Delta_{44}+\Delta_{22}\Delta_{33}+\Delta_{22}\Delta_{44}+\Delta_{33}\Delta_{44})s^2 + \\ & (\Delta_{11}\omega_4^2+\Delta_{33}\omega_2^2+\Delta_{22}\omega_4^2+\Delta_{44}\omega_2^2+ \\ & \Delta_{11}\sigma_3^2+\Delta_{44}\sigma_3^2+\Delta_{11}\Delta_{22}\Delta_{33}+\Delta_{11}\Delta_{22}\Delta_{44}+ \\ & \Delta_{11}\Delta_{33}\Delta_{44}+\Delta_{22}\Delta_{33}\Delta_{44})s + \\ & \omega_2^2\omega_4^2+\Delta_{11}\Delta_{22}\omega_4^2+\Delta_{33}\Delta_{44}\omega_2^2+\Delta_{11}\Delta_{44}\sigma_3^2+ \\ & \Delta_{11}\Delta_{22}\Delta_{33}\Delta_{44} \end{aligned} \quad (69)$$

Example 5. (Parametrically minimal canonical structure of the state space energy based dissipative system representation)

$$A=\begin{bmatrix} -\Delta_1 & \omega_2 & 0 & 0 \\ -\omega_2 & 0 & \sigma_3 & 0 \\ 0 & -\sigma_3 & 0 & \omega_4 \\ 0 & 0 & -\omega_4 & 0 \end{bmatrix} \quad (70)$$

Two *coupled harmonic oscillators* with *two eigen-frequences* ω_2, ω_4. with *interaction parameter* σ_3, and with *unigue dissipation channel* $\Delta_1=\Delta_{11}$.

The *characteristic polynomial A(s)* of the matrix *A* is given in the form:

$$\begin{aligned} A(s) = & s^4+\Delta_1 s^3+(\omega_2^2+\omega_4^2+\sigma_3^2)s^2+ \\ & (\Delta_1\omega_4^2+\Delta_1\sigma_3^2)s+\omega_2^2\omega_4^2 \end{aligned} \quad (71)$$

Example 6. (A 4th –order conservative structure)

$$A=\begin{bmatrix} 0 & \omega_2 & 0 & 0 \\ -\omega_2 & 0 & \sigma_3 & 0 \\ 0 & -\sigma_3 & 0 & \omega_4 \\ 0 & 0 & -\omega_4 & 0 \end{bmatrix} \quad (72)$$

Two *coupled harmonic oscillators* with *interaction parameter* σ_3, with *zero dissipation*, and with *two eigen-frequences* ω_2, ω_4.

The *characteristic polynomial A(s)* of the matrix *A* is given in the form:

$$A(s)=s^4+(\omega_2^2+\omega_4^2+\sigma_3^2)s^2+\omega_2^2\omega_4^2 \quad (73)$$

Example 7. (A 4th –order symplectic structure)

$$A=\begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \quad (74)$$

Two *uncoupled harmonic oscillators* with the same *normalized eigen-frequences* $\omega_4=\omega_2=1$
The *characteristic polynomial A(s)* of the matrix *A* is given in the form:

$$A(s)=s^4+2s^2+1 \quad . \quad (75)$$

Example 8. (Structure of a 4th –order Nosé-Hoover system representation)

$$A=\begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & -p \\ 0 & 0 & 0 & 1 \\ 0 & p & -1 & 0 \end{bmatrix} \quad (76)$$

Two *coupled harmonic oscillators* with *interaction parameter p*, with *zero dissipation*, and with *two normalized eigen-frequences* $\omega_4=\omega_2=1$.

The *characteristic polynomial A(s)* of the matrix *A* is given in the form:

$$A(s)=s^4+(2+p^2)s^2+1 \quad (77)$$

Comparing the characteristic polynomials eqn. (77) and (71) it follows that the ***structure*** of the ***Noseé-Hoover system representation*** (76) can be considered as a ***special case of the parametrically minimal canonical structure of the state space energy based dissipative system representation*** (70) for ***vanishing dissipation parameter*** $\Delta_1=0$.

Notice that the *Hamiltonian energy function* corresponding to the *standard Nosé-Hoover dynamics for a single degree of freedom* above is defined by

$$H(x)=\frac{p^2}{2}+\Phi(q)+kT\eta+\frac{p_\eta^2}{2Q} \quad (78)$$

The resulting *state equations of the 4th –order Nosé-Hoover system representation* read:

$$\dot{q} = \frac{p}{m} \quad . \tag{79}$$

$$\dot{p} = -\Phi - \frac{pp_n}{Q} \tag{80}$$

$$\dot{\eta} = \frac{p_n}{Q} \tag{81}$$

$$\dot{p}_\eta = \frac{p^2}{m} - kT \tag{82}$$

and the corresponding *internal structure* can be illustrated by the structural diagram displayed in the Fig. 8.

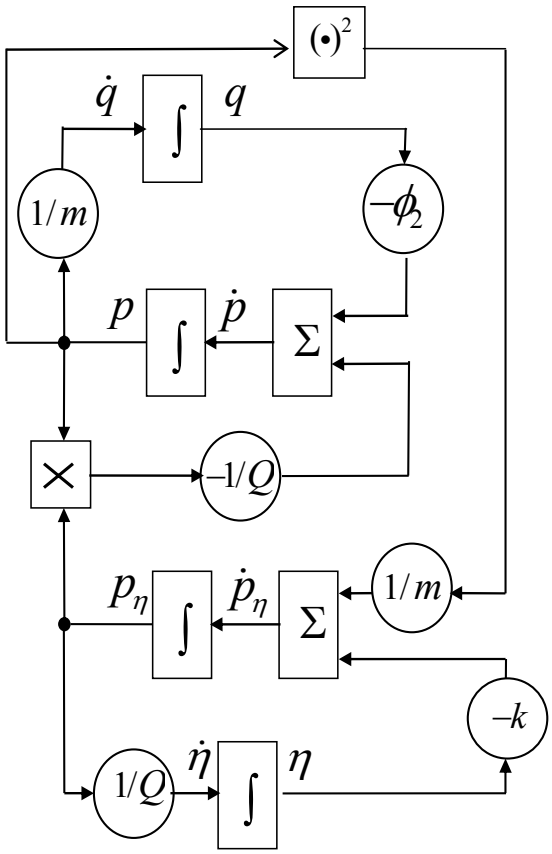

Fig. 8. Structure of the 4th order Nosé-Hoover system

7 Parametric ambiguity of dissipative state representations and parameter space transformations

Notice that *set of binary parameters* s_i, $s_i \in \{-1,+1\}$ appeared as a *consequence* of the fact that the *solution* of the *nonlinear set of equations* (29) resulting from the *state equivalence relation* was *not unique.*

In the given context the *logical variables* s_i *with values* in a binary set play a similar role like *spins* in the *quantum theory*.

Notice that a set of parameters Δ_k, $k = 1, 2,\ldots,n$ represents the well known *set of diagonal minors* of the corresponding *Hurwitz determinant* important in the *asymptotic stability theory* [6, 7, 8].

It is easy to prove that it is the case if and only if all the *diagonal minors* Δ_1, Δ_2, Δ_3, . . Δ_n. of the corresponding *Hurwitz determinant* H_n

$$H_n \triangleq \begin{vmatrix} a_1 & 1 & 0 & 0 & 0 & \ldots & 0 \\ a_3 & a_2 & a_1 & 1 & 0 & \ldots & 0 \\ a_5 & a_4 & a_3 & a_2 & a_1 & \ldots & 0 \\ a_7 & a_6 & a_5 & a_4 & a_3 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & a_n \end{vmatrix} \tag{83}$$

are *real and positive*.

Let a 6-th order system representation is given.

$$\begin{aligned} \Re(S): \quad \dot{x}_1(t) &= -\Delta_1 x_1(t) + \omega_2 x_2(t) \\ \dot{x}_2(t) &= -\omega_2 x_1(t) + \sigma_3 x_3(t) \\ \dot{x}_3(t) &= -\sigma_3 x_2(t) + \omega_4 x_4(t) \\ \dot{x}_4(t) &= -\omega_4 x_3(t) + \sigma_5 x_5(t) \\ \dot{x}_5(t) &= -\sigma_5 x_4(t) + \omega_6 x_6(t) \\ \dot{x}_6(t) &= -\omega\Delta_6 x_5(t) + \ldots \\ y(t) &= \pm\sqrt{\Delta_1} x_1(t) \end{aligned} \tag{84}$$

The corresponding ***transformation of the parameter space*** into the well known so called ***Frobenius structure*** reads:

$$\begin{aligned} a_1 &= \Delta_1 \\ a_2 &= \omega_2^2 + \sigma_3^2 + \omega_4^2 + \sigma_5^2 + \omega_6^2 \\ a_3 &= \Delta_1(\sigma_3^2 + \omega_4^2 + \sigma_5^2 + \omega_6^2) \\ a_4 &= \omega_2^2(\omega_4^2 + \sigma_5^2 + \omega_6^2) + \sigma_3^2(\sigma_5^2 + \omega_6^2) + \omega_4^2\omega_6^2 \\ a_5 &= \Delta_1\sigma_3^2(\sigma_5^2 + \omega_6^2) + \Delta_1\omega_4^2\omega_6^2 \\ a_6 &= \omega_2^2\omega_4^2\omega_6^2 \end{aligned} \tag{85}$$

It easy to find the *unique* solution of the *set of the algebraic equations* (29) with respect to the ***dissipation parameter*** Δ_1, as well as with respect to the set of ***quadrats*** of the unknown ***frequency parameters*** ω_2, ω_4, ω_6, . . . , as well as that of the unknown ***interaction parameters*** σ_3, σ_5, σ_7, . . . in the following form:

$$\begin{aligned}
&\Delta_1 = a_1 ,\\
&\omega_2^2 = \frac{a_1 a_3 - a_3}{a_1} = \frac{\Delta_2}{\Delta_1}\\
&\sigma_3^2 = \frac{a_1 a_2 a_3 - a_3^2 - a_1^2 a_4}{(a_1 a_2 - a_3) a_1} = \frac{\Delta_3}{\Delta_2 \Delta_1}\\
&\omega_4^2 = \frac{\Delta_4 \Delta_1}{\Delta_2 \Delta_3}, \quad \sigma_5^2 = \frac{\Delta_5 \Delta_2}{\Delta_3 \Delta_4},\\
&\omega_6^2 = \frac{\Delta_6 \Delta_3}{\Delta_4 \Delta_5}, \ldots, \sigma_k^2 = \frac{\Delta_k \Delta_{k-3}}{\Delta_{k-2} \Delta_{k-1}}, \ldots,
\end{aligned} \tag{86}$$

It follows that for an n^{th}-order system there exist *n-1 spin numbers* s_i with values in the set {-1,+1} defining N possible combinations of the so called ***spin structures*** $S_i = \{s_1, s_2, ,,. \ . \ ., s_{n-1}\}$, i = 1,2, . . . , N, with $N=2^{n-1}$.

As a consequence a *general analytical solution* in terms of the *(n-1) unknown parameters* ω_k and σ_k is *non-unique* and can be expressed by means of a set of the *(n-1)* ***binary spin parameters*** $\{s_1, s_2, \ldots, s_{n-1}\}$ together with a set of n ***real positive parameters*** $\{\alpha_1, \alpha_2, \ldots, \alpha_n\}$ in the form:

$$\begin{aligned}
&\Delta_1 = \alpha_1 , \ \omega_2 = s_1 \alpha_2 , \sigma_3 = s_2 \alpha_3\\
&\omega_4 = s_3 \alpha_4 , \quad \sigma_5 = s_4 \alpha_5\\
&\omega_6 = s_5 \alpha_6 , \ldots, \sigma_k = s_{k-1} \alpha_k , \ldots,\\
&\alpha_k > 0, k \in \{1, 2..., n\}
\end{aligned} \tag{87}$$

where the parameters α_k and s_k are for general case of any finite order n defined by:

$$\begin{aligned}
&\alpha_1 = a_1 = \Delta_1 > 0,\\
&\alpha_2 = \sqrt{\frac{\Delta_2}{\Delta_1}} > 0,\\
&\alpha_3 = \sqrt{\frac{\Delta_3}{\Delta_2 \Delta_1}} > 0, \alpha_4 = \sqrt{\frac{\Delta_4 \Delta_1}{\Delta_2 \Delta_3}} > 0,\\
&\alpha_5 = \sqrt{\frac{\Delta_5 \Delta_2}{\Delta_3 \Delta_4}} > 0, \alpha_6 = \sqrt{\frac{\Delta_6 \Delta_3}{\Delta_4 \Delta_5}} > 0, \ldots,\\
&\alpha_n = \sqrt{\frac{\Delta_n \Delta_{n-3}}{\Delta_{n-2} \Delta_{n-1}}} > 0, s_k \in \{-1, +1\}
\end{aligned} \tag{88}$$

Consequently the ***output observation equation*** is defined by the matrix C in the form

$$C = \left[\pm\sqrt{\Delta_1}, 0.0, ..., 0 \right] \tag{89}$$

and the tridiagonal matrix A is given by

$$A = \begin{bmatrix}
-\alpha_1 & s_1\alpha_2 & 0 & 0 & 0 & 0\\
-s_1\alpha_2 & 0 & s_2\alpha_3 & 0 & 0 & 0\\
0 & -s_2\alpha_3 & 0 & \ddots & 0 & 0\\
0 & 0 & \ddots & \ddots & s_{n-2}\alpha_{n-1} & 0\\
0 & 0 & 0 & -s_{n-2}\alpha_{n-1} & 0 & s_{n-1}\alpha_n\\
0 & 0 & 0 & 0 & -s_{n-1}\alpha_n & 0
\end{bmatrix} \tag{90}$$

Consequently the representation (31), (32) can be explicitly expressed as follows

$$\begin{aligned}
\Re(S): \quad &\dot{x}_1(t) = -\alpha_1 x_1(t) + s_1\alpha_2 x_2(t)\\
&\dot{x}_2(t) = -s_1\alpha_2 x_1(t) + s_2\alpha_3 x_3(t)\\
&\dot{x}_3(t) = -s_2\alpha_3 x_2(t) + s_3\alpha_4 x_4(t)\\
&\dot{x}_4(t) = -s_3\alpha_4 x_3(t) + s_4\alpha_5 x_5(t)\\
&\dot{x}_5(t) = -s_4\alpha_5 x_4(t) + s_5\alpha_6 x_6(t)\\
&\dot{x}_6(t) = -s_5\alpha_6 x_5(t) + ...\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
&y(t) = \pm\sqrt{\Delta_1} x_1(t),\\
&s_k \in \{-1, +1\}, \Delta_1 = \alpha_1, \alpha_k > 0, k \in \{1, 2..., n\}
\end{aligned} \tag{91}$$

8 State equivalence relation and state space transformations

In order to be able to interpret the obtained results for any given n-th order ordinary differential equation like (28), we need an effective tool to *transform any given state space representation,* such as (31), but *of arbitrary finite order*, into the form like (28), and back.

One straightforward approach suggests to compute *successive derivatives of the output equation* up to the order *n,* combined with *successive elimination all of the state variables* as follows (for n=6):

$$\begin{aligned}
&y(t) = \pm\sqrt{\Delta_1} x_1(t)\\
&\dot{y} + \alpha_1 y = \pm\sqrt{\Delta_1} s_1\alpha_2 x_2\\
&\ddot{y} + \alpha_1\dot{y} + \alpha_2^2 y = \pm\sqrt{\Delta_1} s_1 s_2 \alpha_2\alpha_3 x_3 \ldots\\
&y^{(5)} + \alpha_1 y^{(4)} + (\alpha_2^2 + \alpha_3^2 + \alpha_4^2 + \alpha_5^2)\dddot{y} +\\
&+\alpha_1(\alpha_3^2 + \alpha_4^2 + \alpha_5^2)\ddot{y} +\\
&[\alpha_2^2\alpha_4^2 + \alpha_2^2\alpha_5^2 + \alpha_3^2\alpha_6^2]\dot{y} + \alpha_1\alpha_3^2\alpha_5^2 y =\\
&\pm\sqrt{\Delta_1} s_1 s_2 s_3 s_4 s_5 \alpha_2\alpha_3\alpha_4\alpha_5\alpha_6 x_6
\end{aligned} \tag{92}$$

As a by-product the following *state space transformation relations* have been obtained:

$$x_1 = \frac{1}{\gamma_1} y, \quad \gamma_1 = \pm\sqrt{\Delta_1}, \Delta_1 = \alpha_1 > 0$$
$$x_2 = \frac{1}{\gamma_1 s_1 \alpha_2}\left(\alpha_1 y + \dot{y}\right),$$
$$\gamma_1 = \pm\sqrt{\Delta_1}, \; s_1 = \pm 1, \alpha_2 > 0$$
$$\cdots\cdots \qquad (93)$$
$$x_6 = \frac{1}{\gamma_1 s_1 s_2 s_3 s_4 s_5 \alpha_2 \alpha_3 \alpha_4 \alpha_5 \alpha_6}[\alpha_1\alpha_3^2\alpha_5^2 y +$$
$$+(\alpha_2^2\alpha_4^2 + \alpha_2^2\alpha_5^2 + \alpha_3^2\alpha_6^2)\dot{y} + +\alpha_1(\alpha_3^2 + \alpha_4^2 + \alpha_5^2)\ddot{y} +$$
$$+(\alpha_2^2 + \alpha_3^2 + \alpha_4^2 + \alpha_5^2)\dddot{y} + \alpha_1 y^{(4)} + y^{(5)}],$$
$$\gamma_1 = \pm\sqrt{\Delta_1}, s_k \in \{-1, +1\}, \alpha_1 > 0, \alpha_2 > 0, \alpha_3 > 0, \ldots, \alpha_6 > 0$$

which can be expressed in a vector-matrix form

$$x = T\bar{x}, \quad \bar{x} = T^{-1}x \qquad (94)$$

with an *invertible transformation matrix* T which can be decomposed as follows

$$T = T_S . T_\alpha \qquad (95)$$

where the *signature matrix* T_S is defined by

$$T_S = \begin{bmatrix} 1 & 0 & 0 & 0 & \ldots \\ 0 & s_1 & 0 & 0 & \ldots \\ 0 & 0 & s_1 s_2 & 0 & \ldots \\ 0 & 0 & 0 & s_1 s_2 s_3 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \qquad (96)$$

with $s_{1,2,3\ldots}=\pm 1$, and the *parameter matrix* T_α is defined by

$$T_\alpha = \pm\frac{1}{\sqrt{\Delta_1}} \begin{bmatrix} 1 & 0 & 0 & 0 & \ldots \\ \frac{\alpha_1}{\alpha_2} & \frac{1}{\alpha_2} & 0 & 0 & \ldots \\ \frac{\alpha_2}{\alpha_3} & \frac{\alpha_1}{\alpha_2\alpha_3} & \frac{1}{\alpha_2\alpha_3} & 0 & \ldots \\ \frac{\alpha_1\alpha_3}{\alpha_2\alpha_4} & \frac{\alpha_2^2+\alpha_3^2}{\alpha_2\alpha_3} & \frac{\alpha_1}{\alpha_2\alpha_3\alpha_4} & \frac{1}{\alpha_2\alpha_3\alpha_4} & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \qquad (97)$$

For the inverse matrix T^{-1} we get immediately

$$T^{-1} = (T_s . T_\alpha)^{-1} = (T_\alpha)^{-1}(T_s)^{-1} = T_\alpha^{-1} T_s \qquad (98)$$

where the *parameter matrix* T_α equals to the inverse transpose of *observability matrix* of *the system representation* given by

$$H_o = \left[C^T, \; A^T C^T, (A^T)^2 C^T, \ldots, \; (A^T)^{n-1} C^T\right] \qquad (99)$$

9 Effect of nonlinear state energy feedback transformations

Example 9. In this part, the example of switching system based on energy feedback is presented [18, 19]. In this example the 4th order system described by eq. (33) is used and only sign of parameter Δ_1 is switched so that state space energy values are changed between E_1 and E_2 and mean E_M (desired value) is

$$E_M = 0.5(E_1 + E_2) \qquad (100)$$

In this example E_1=2, E_2=3 and E_M=2.5. The structure diagram of the state space energy controlled feedback system is shown in Fig. 9. and simulation results are in Fig. 10 - 15.

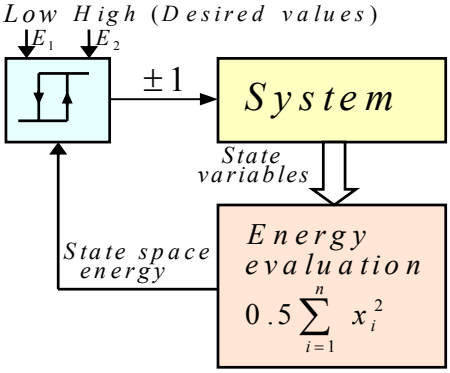

Fig. 9. Structure of state space energy controlled feedback system.

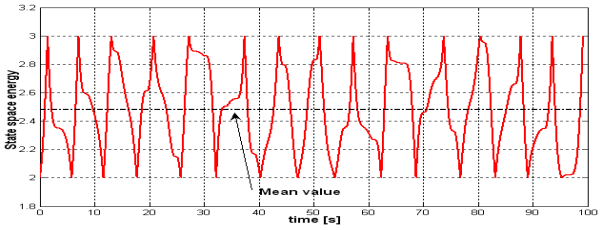

Fig. 10. The state space energy evolution of the state energy feedback controlled system.

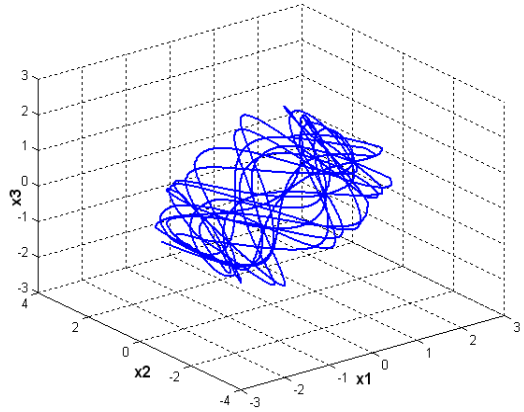

Fig. 11. 3-D projection of a chaotic-like state space trajectory.

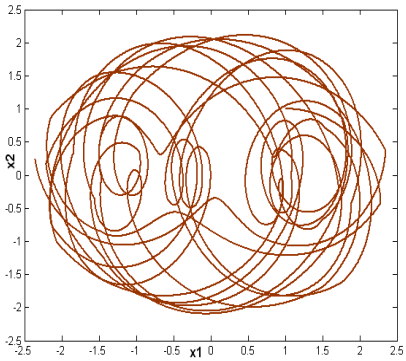

Fig. 12. 2-D projection of an energy quantum-like state space trajectory.

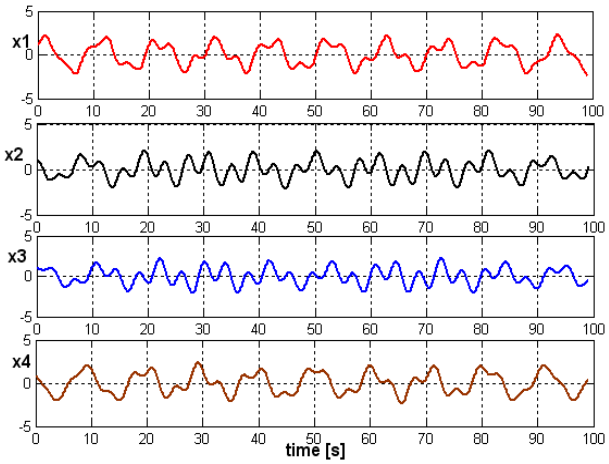

Fig. 13. Time evolution of the state variables.

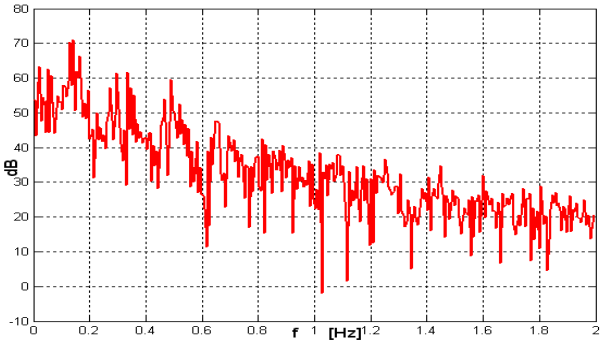

Fig. 14. The frequency spectrum of the state space energy.

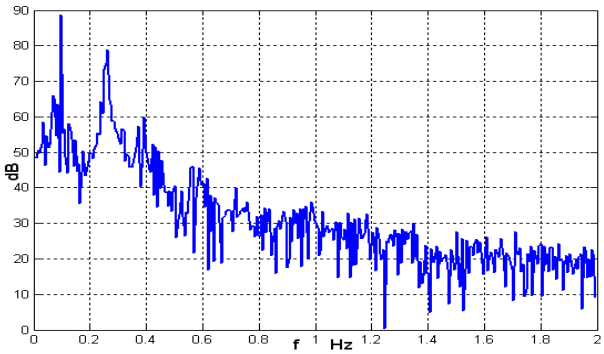

Fig. 15. Frequency spectrum of the output signal x_1.

10 Chaotic behavior of Nosé-Hoover system representations - example

Example 10. In 1995 Hoover pointed out [Hoover, W. G.: Remark on "Some Simple Chaotic Flows". Phys. Rev. E, vol. 51, nr. 1, 759-760, 1995] that the *conservative system* described by the 3rd–order nonlinear differential equation

$$\dddot{y} - \frac{\ddot{y}(y+\ddot{y})}{\dot{y}} - \dot{y}^3 = 0 \qquad (101)$$

found by Sprott is a *special case of the Nosé-Hoover thermostated system* that had earlier been shown in [Posch, H. A., Hoover, W. G., and Vesely, F. J.: Canonical Dynamics of the Nosé Oscillator: Stability, Order, and Chaos. Phys. Rev. A, vol. 33, nr. 6, pp. 4253-4265, 1986] to exhibit *time-reversible Hamiltonian chaos.*

One of the *state space representations* of the given system can be expressed as follows

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 + x_2 x_3 \\ \dot{x}_3 &= 1 - x_2^2 \end{aligned} \qquad (102)$$

where the *observed output signal is not defined.*

In vector-matrix notation we can write

$$\dot{x} = A(x)x + B \qquad (103)$$

where the corresponding matrices *A(x)* and *B* read

$$A(x) = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & x_2 \\ 0 & -x_2 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \qquad (104)$$

Accepting the *state space energy theory point of view,* we may write

$$E(x_1, x_2, x_3) = \frac{1}{2}(x_1^2 + x_2^2 + x_3^2) \qquad (105)$$

for *the state space energy E[x(t)]* and hence the *state space energy conservation principle* reads

$$\begin{aligned} \frac{dE}{dt} &= x_1 x_2 + x_2(-x_1 + x_2 x_3) + x_3(1 - x_2^2) \\ &= x_3 = \\ &= |x_3|\, sign(x_3) = -P_o(t) \end{aligned} \qquad (106)$$

It means that for $|x_3|=0$ the *output dissipation power* $P_0(t)$ *changes its sign.* Consequently the system behaves like *antidissipative* for $x_3 > 0$, and as a *dissipative* one for $x_3<0$. As a result the *state space energy E[x(t)]* has to be *constant in the mean*, i.e. the given ***chaotic Nosé-Hoover system*** has to be classified as ***"conservative in the mean".***

The corresponding *internal structure* of the given ***chaotic Nosé-Hoover system*** is compatible with the ***canonical structure*** derived above for general case of the state space energy motivated approach, and is displayed in the Fig. 16.

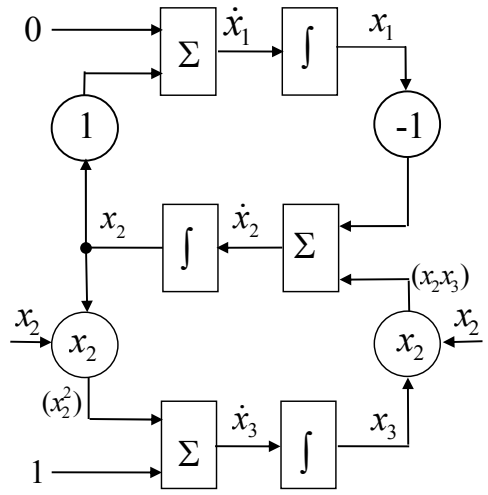

Fig. 16. Structure of the 3rd order Nosé-Hoover system

The theoretical conclusions have been verified by computer experiments. Some of the most typical are illustrated by following figures.

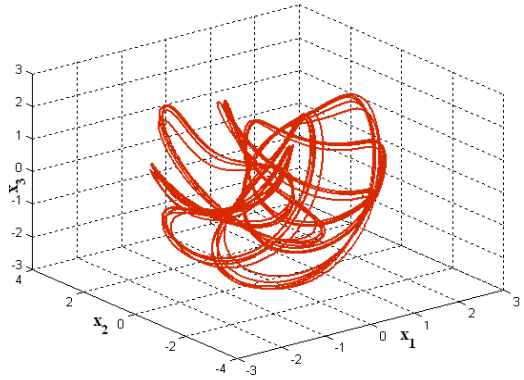

Fig. 17. Typical course of state space trajectories.

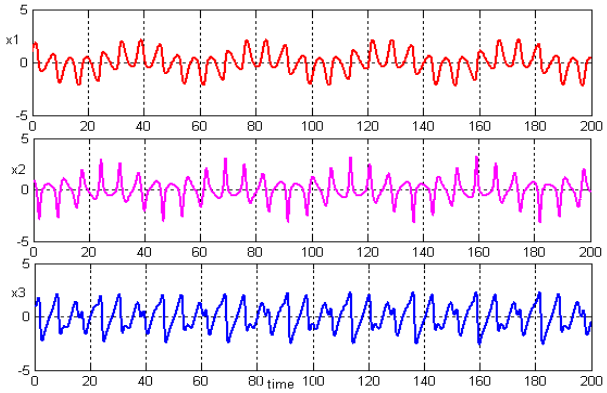

Fig. 18. Time evolution of state space trajectories.

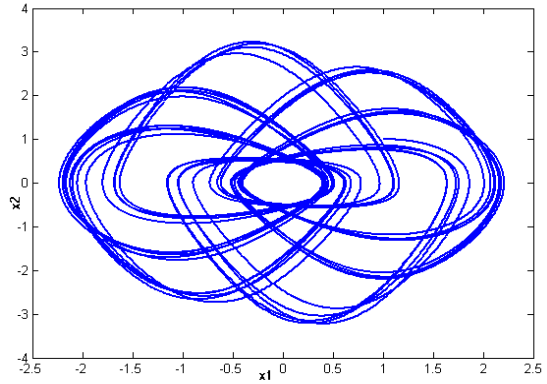

Fig. 19. 2-D projection into the state plane (x_1, x_2)

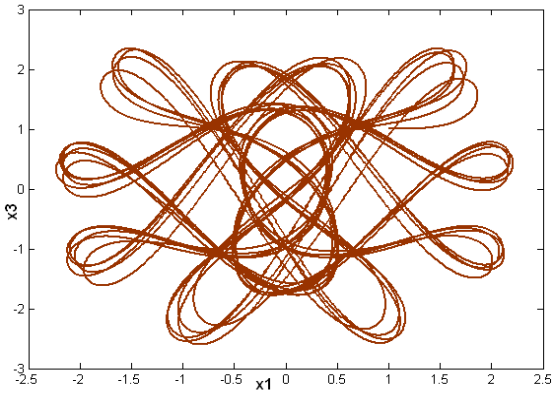

Fig. 20. 2-D projection into the state plane (x_1, x_3)

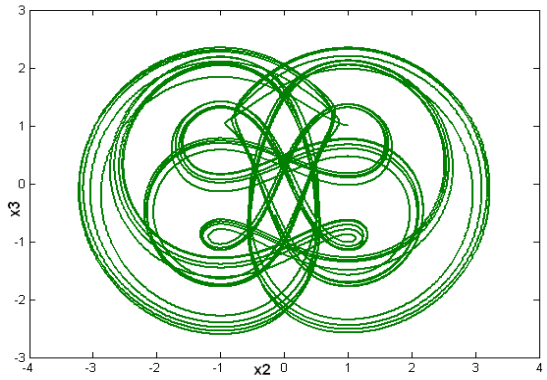

Fig. 21. 2-D projection into the state plane (x_2 , x_3)

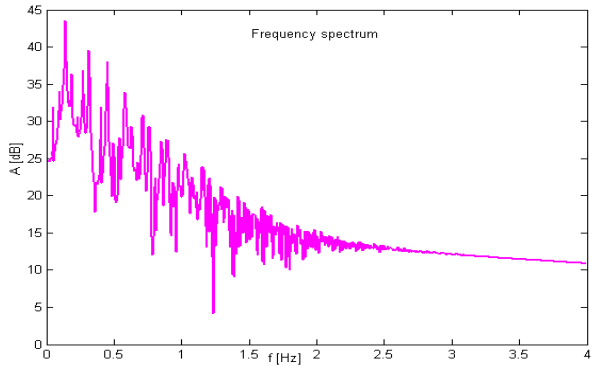

Fig. 22. Frequency spectrum of the output signal x_1.

Note that in the given structure ***chaos occurs for all coefficients equal to unity, and so it is especially simple in that sense.***

11 Conclusions

The proposed state space energy based approach seems to open a new perspective in development of sufficiently universal and more adequate abstract system representations for variety of natural systems. A wave–like form of the hyper-energy, together with the new concept of spin structure provides a new paradigm for research of interactions in nano-scale. It also seems to open promising new directions for further work in the field of quantum-chaotic systems.

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