Canonical Transformations and Invariants in time-dependent classical Hamilton Systems

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0. Outline

- Review: Hamilton's variational principle, canonical transformations, extended phase-space
- Canonical transformations in the extended phase-space
- Special class of time-dependent Hamilton systems and its canonical transformation into the equivalent time-independent system
- Invariant of the time-dependent Hamilton system and its physical interpretation
- Example with computer demonstration
- Application: verification of computer simulations of dynamical systems
- Outlook: Classification of dynamical systems

1. Hamilton's variational principle

Starting from the Lagrange function $L(\vec{q}, \dot{\vec{q}}, t)$, the Hamilton function $H(\vec{q}, \vec{p}, t)$ of an explicitly time-dependent system of n degrees of freedom $\vec{q} = (q_1, \ldots, q_n)$, $\vec{p} = (p_1, \ldots, p_n)$ is defined as

$$H(\vec{q}, \vec{p}, t) = \sum_{i=1}^{n} p_i \, \dot{q}_i - L(\vec{q}, \dot{\vec{q}}, t) \, .$$

The system's time evolution ("system path") $\big(\vec{q}(t), \vec{p}(t)\big)$ obeys Hamilton's variational principle

$$\delta \int_{t_1}^{t_2} \left[\sum_{i=1}^{n} p_i(t) \, \dot{q}_i(t) - H\big(\vec{q}(t), \vec{p}(t), t\big) \right] dt = 0 \, .$$

The variation vanishes exactly if the equations of motion ("canonical equations") are fulfilled:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \, , \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} \, , \qquad i = 1, \ldots, n \, .$$

2. Canonical Transformations

A coordinate transformation

$$q_i' = q_i'(\vec{q}, \vec{p}, t)\,, \qquad p_i' = p_i'(\vec{q}, \vec{p}, t)\,, \qquad i = 1, \ldots, n$$

that conserves the form of the canonical equations is called "canonical". This is exactly the case if Hamilton's variational principle is maintained in the new set of (primed) coordinates

$$\delta \int_{t_1}^{t_2} \left[\sum_{i=1}^{n} p_i' \dot{q}_i' - H(\vec{q}\,', \vec{p}\,', t) \right] dt = 0\,.$$

We observe that the time t plays the role of an external parameter that is not subject to transformation.

$\rightsquigarrow$ Canonical transformations that include in addition a transformation of time t are *not* covered by this description.

$\rightsquigarrow$ Generalization is required: canonical transformations in the "extended phase-space".

3. Canon. transformations in the extended phase-space

conventional phase-space: $2n$-dimensional Cartesian space formed by all particle coordinates of the given dynamical system:

$$q_1, \ldots, q_n, p_1, \ldots, p_n$$

extended phase-space: $2n + 2$-dimensional Cartesian space as the Kronecker product with the conjugate variables $(t, -H)$:

$$q_1, \ldots, q_n, p_1, \ldots, p_n, t, -H$$

Justification: Hamilton's variational principle may be written equivalently in terms of an evolution parameter s with $t = t(s)$

$$\delta \int_{s_1}^{s_2} \left[\sum_{i=1}^{n} p_i \frac{dq_i}{ds} - H \frac{dt}{ds} \right] ds = 0\,.$$

In the extended phase-space, the condition for a transformation to be canonical may be formulated as before: Hamilton's variational principle must be maintained by virtue of the transformation.

$$\delta \int_{s_1}^{s_2} \left[\sum_{i=1}^{n} p_i \frac{dq_i}{ds} - H \frac{dt}{ds} \right] ds = \delta \int_{s_1}^{s_2} \left[\sum_{i=1}^{n} p_i' \frac{dq_i'}{ds} - H' \frac{dt'}{ds} \right] ds = 0$$

$\rightsquigarrow$ $-H$ and t can be conceived in a natural sense as canonically conjugate variables p_{n+1} and q_{n+1}.

$\rightsquigarrow$ The integrands may differ at most by a total differential $dF_1(\vec{q}, \vec{q}', t, t')$

$$\sum_{i=1}^{n} p_i \, dq_i - H(\vec{q}, \vec{p}, t) \, dt = \sum_{i=1}^{n} p_i' dq_i' - H(\vec{q}', \vec{p}', t') \, dt' + dF_1(\vec{q}, \vec{q}', t, t') \, .$$

The „generating function" F_1 thus defines the transformation rules between old (unprimed) and new (primed) coordinates:

$$p_i = \frac{\partial F_1}{\partial q_i}\,, \quad p_i' = -\frac{\partial F_1}{\partial q_i'}\,, \quad H = -\frac{\partial F_1}{\partial t}\,, \quad H' = \frac{\partial F_1}{\partial t'}\,.$$

Applying the Legendre transformation

$$F_2(\vec{q}, \vec{p}\,', t, H') = F_1(\vec{q}, \vec{q}\,', t, t') + \sum_{i=1}^{n} q_i' p_i' - t' H'\,,$$

the generating function may be expressed equivalently in terms of the old position and the new momentum coordinates. The corresponding coordinate transformation rules are given by

$$q_i' = \frac{\partial F_2}{\partial p_i'}\,, \quad p_i = \frac{\partial F_2}{\partial q_i}\,, \quad t' = -\frac{\partial F_2}{\partial H'}\,, \quad H = -\frac{\partial F_2}{\partial t}\,.$$

Starting from a generating function F_2, we now canonically transform in the extended phase-space a class of non-linear time-dependent Hamilton functions.

4. Non-linear time-dependent Hamilton system

We now consider the non-linear time-dependent system described by the Hamilton function

$$H(\vec{q},\vec{p},t) = \sum_{i=1}^{n} \tfrac{1}{2} p_i^2 + V(\vec{q},t)\,.$$

$\rightsquigarrow$ In the case of $\partial V/\partial t \neq 0$, H is <u>no</u> constant of motion.

<u>Strategy</u>: the explicitly time-dependent system H will be transformed canonically in the extended phase-space into a time-<u>in</u>dependent (autonomous) system H':

$$H(\vec{q},\vec{p},t) \xrightarrow{\text{canon. transf.}} H'(\vec{q}\,',\vec{p}\,')\,.$$

$\rightsquigarrow$ In the transformed system, H' is a constant of motion.

$\rightsquigarrow$ H' expressed in terms of the old coordinates $\vec{q}$, $\vec{p}$ provides a constant of motion I in the frame of the original system H.

5. Canon. transformation into a time-independent system

The canonical transformation in the extended phase-space be generated by

$$F_2(\vec{q}, \vec{p}', t, H') = \phi_2(\vec{q}, \vec{p}', t) - H' \int_{t_0}^{t} \frac{d\tau}{\xi(\tau)}$$

with

$$\phi_2(\vec{q}, \vec{p}', t) = \frac{1}{\xi(t)} \sum_{i=1}^{n} \left(\sqrt{\xi(t)}\, q_i p_i' + \tfrac{1}{4} \dot{\xi}(t)\, q_i^2 \right) .$$

Then, the following transformation rules $\{q_i, p_i\} \leftrightarrow \{q_i', p_i'\}$ apply

$$\begin{pmatrix} q_i \\ p_i \end{pmatrix} = \begin{pmatrix} \sqrt{\xi(t)} & 0 \\ \dot{\xi}(t)/\sqrt{4\xi(t)} & 1/\sqrt{\xi(t)} \end{pmatrix} \begin{pmatrix} q_i' \\ p_i' \end{pmatrix} .$$

$\xi = \xi(t)$ denotes a differentiable function of time t only that will be determined later.

In the same way, the transformations of time t and Hamilton function H follow from the rules derived above

$$t' = -\frac{\partial F_2}{\partial H'} = \int_{t_0}^{t} \frac{d\tau}{\xi(\tau)}\,, \qquad H = -\frac{\partial F_2}{\partial t} = -\frac{\partial \phi_2}{\partial t} + \frac{H'}{\xi(t)}\,.$$

The transformed Hamilton function H' is obtained expressing H and $\partial\phi_2/\partial t$ in terms of the new variables as

$$H' = \sum_{i=1}^{n} \tfrac{1}{2} {p'_i}^2 + V'(\vec{q}\,', t)\,,$$

with $V'(\vec{q}\,', t)$ the new effective potential

$$V'(\vec{q}\,', t) = \tfrac{1}{4}\left[\ddot{\xi}\xi - \tfrac{1}{2}\dot{\xi}^2\right] \sum_{i=1}^{n} {q'_i}^2 + \xi\, V\!\left(\sqrt{\xi}\,\vec{q}\,', t\right).$$

Question: How do we render V' independent of time explicitly?

Answer: We define the function $\xi = \xi(t)$ appropriately.

$$\frac{\partial V'(\vec{q}\,', t)}{\partial t} \stackrel{!}{\equiv} 0 \quad \Longrightarrow \quad \xi = \xi(t)\,.$$

By virtue of this condition, we obtain the following linear homogeneous third-order differential equation for $\xi(t)$:

$$\dddot{\xi}(t) \sum_{i=1}^{n} q_i^2 + 4\dot{\xi} \left(V + \tfrac{1}{2} \sum_{i=1}^{n} q_i \frac{\partial V}{\partial q_i} \right) + 4\xi \frac{\partial V}{\partial t} = 0\,,$$

referred to as the "auxiliary equation" for $\xi(t)$. In general, this equation depends on all position coordinates $q_i(t)$, $i = 1, \ldots, n$. With $\xi(t)$ a solution of the auxiliary equation, we have $V' = V'(\vec{q}\,')$.
$\rightsquigarrow$ $H' \equiv I$ represents the invariant in question.

Writing I as a function of the old coordinates, we have indeed found the invariant pertaining to the original system:

$$I = \xi(t)\, H(\vec{q}, \vec{p}, t) - \tfrac{1}{2}\dot{\xi}(t) \sum_{i=1}^{n} q_i p_i + \tfrac{1}{4}\ddot{\xi}(t) \sum_{i=1}^{n} q_i^2\,.$$

6. Physical interpretation of the invariant I

Inserting the canonical equations

$$\dot{q}_i = p_i\,, \qquad \dot{p}_i = -\frac{\partial V(\vec{q},t)}{\partial q_i}\,, \qquad i = 1,\ldots,n$$

into dH/dt, we find the energy balance relation

$$\frac{d}{dt}\left[\sum_{i=1}^{n} \tfrac{1}{2}\dot{q}_i^2 + V(\vec{q},t)\right] - \frac{\partial V(\vec{q},t)}{\partial t} = 0\,.$$

$\rightsquigarrow$ The system's total energy change is given by $\partial V/\partial t$. With $\partial V/\partial t$ from the auxiliary equation, this gives the total time derivative

$$\frac{d}{dt}\left[\xi(t)\left(\sum_{i=1}^{n} \tfrac{1}{2}\dot{q}_i^2 + V(\vec{q},t)\right) - \tfrac{1}{2}\dot{\xi}(t)\sum_{i=1}^{n} q_i\dot{q}_i + \tfrac{1}{4}\ddot{\xi}(t)\sum_{i=1}^{n} q_i^2\right] = 0$$

The expression in brackets is the invariant I. It can be interpreted now as the energy conservation law for non-autonomous systems.

7. Physical interpretation of $\xi(t)$

In the extended phase-space, the invariant I can be written as

$$I(\vec{q},\vec{p},t,H) = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\sum_{i=1}^{n} q_i\dot{q}_i + \tfrac{1}{4}\ddot{\xi}(t)\sum_{i=1}^{n} q_i^2 = \text{const.}$$

with $dI = 0$ holding along the system trajectory $\big(\vec{q}(t),\vec{p}(t)\big)$ if $\xi(t)$ is a solution of the auxiliary equation. Explicitly, $dI/dt = 0$ means

$$\left.\frac{\partial I}{\partial t}\right|_{\vec{q},\vec{p},H} + \frac{\partial H}{\partial t}\left.\frac{\partial I}{\partial H}\right|_{\vec{q},\vec{p},t} + \sum_{i=1}^{n}\left(\dot{p}_i\left.\frac{\partial I}{\partial p_i}\right|_{\vec{q},t,H} + \dot{q}_i\left.\frac{\partial I}{\partial q_i}\right|_{\vec{p},t,H}\right) = 0\,.$$

Inserting the canonical equations and the auxiliary equation, we find

$$\left.\frac{\partial I}{\partial H}\right|_{\vec{q},\vec{p},t} = \xi(t)\,,$$

as expected. $\xi(t)$ thus gives the change of the total energy I with respect to the actual system energy H.

- The auxiliary equation can only be integrated in conjunction with the integration of the equations of motion.
- On the solution path $\vec{q}(t)$, the coefficients of the auxiliary equation are functions of time t only: $V = V(\vec{q}(t), t)$.
- Then, the auxiliary equation is an <u>ordinary</u>, linear, homogeneous, third-order differential equation.
- A unique solution function $\xi(t)$ exists, as long as $V(\vec{q}(t), t)$ and its partial derivatives are continuous.
- For the isotropic quadratic potential ($d(t)$ continuous, arbitrary)
$$V(\vec{q}, t) = d(t) \sum_{i=1}^{n} q_i^2$$
the auxiliary equation decouples from the solution functions $q_i(t)$ of the equations of motion.

- With $\xi = \xi(t)$ a solution of the auxiliary equation, the Hamilton function H' embodies a *constant of motion* $I \equiv H'$. Expressed in the old coordinates, I can be interpreted as the generalized energy conservation law for the non-autonomous system H.
- H' describes an autonomous system that is equivalent to H.
- The equivalent autonomous system H' represents a real physical system if and only if $\xi(t) > 0$.
- On the other hand, H' expressed in terms of the old (unprimed) coordinates provides a constant of motion I for the system H for *all* $\xi(t)$ that are solutions of the auxiliary equation.
- For the particular case $\partial H/\partial t \equiv 0$, i.e. for an autonomous system H, $\xi(t) \equiv 1$ is a solution of the auxiliary equation.
  $\rightsquigarrow$ This leads directly to the known result: $I \equiv H$.
  The invariant $\widetilde{I}$ with $\xi(t) \neq$ const. provides a second invariant for autonomous systems H.

8. Example: Time-dependent non-linear oscillator

We now consider the simple case of a non-linear oscillator with time-dependent coefficients. Its Hamilton function is given by

$$H(q,p,t) = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)\,q^2 + a(t)\,q^3\,.$$

Then, the invariant I specializes to

$$I = \xi(t)\Big(\tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)\,q^2 + a(t)\,q^3\Big) - \tfrac{1}{2}\dot{\xi}(t)\,qp + \tfrac{1}{4}\ddot{\xi}(t)\,q^2\,.$$

Correspondingly, the auxiliary equation for $\xi(t)$ is obtained as a special case of the general one

$$\dddot{\xi} + 4\dot{\xi}\omega^2 + 4\xi\omega\dot{\omega} + q(t)\Big(4\xi\dot{a} + 10\dot{\xi}a\Big) = 0\,.$$

We observe that the solution $\xi(t)$ depends on the trajectory $q(t)$. This is caused by the cubic term $a(t)$ of the Hamilton function.
$\rightsquigarrow$ $\xi(t)$ can be determined only if the auxiliary equation is integrated together with the equation of motion.

9. Numerical Example

The equation of motion and the auxiliary equation for the non-linear oscillator

$$\ddot{q} + \omega^2(t)\, q + 3a(t)\, q^2 = 0$$

$$\dddot{\xi} + 4\dot{\xi}\omega^2 + 4\xi\omega\dot{\omega} + q(t)\Big(4\xi\dot{a} + 10\dot{\xi}a\Big) = 0$$

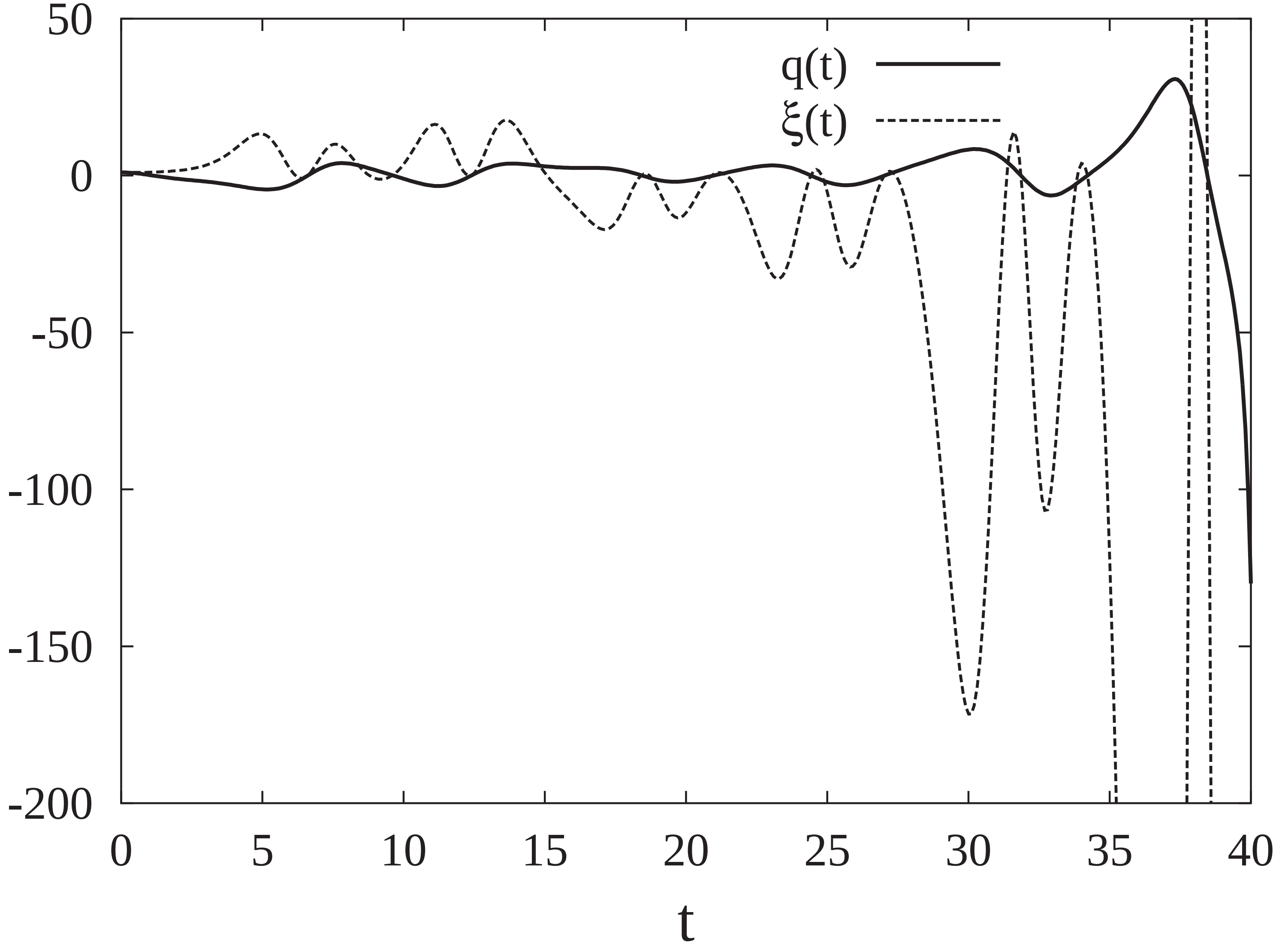
$$\omega(t) = \sqrt{2}\cos(t/2)\,, \qquad a(t) = 5 \times 10^{-2}\,\sin(t/3)$$

are *simultaneously* integrated, with the initial conditions

$$q(0) = 1\,, \quad p(0) = \dot{q}(0) = 0\,, \qquad \xi(0) = 1\,, \quad \dot{\xi}(0) = 0\,, \quad \ddot{\xi}(0) = 0\,.$$

$\rightsquigarrow$ The invariant for this particular particle evaluates to $I(q,p,t) = 1$. In our computer demonstration, we plot

- $q(t)$ and $\xi(t)$ versus t
- the motion in the potential: $V(q(t),t)$ versus $q(t)$
- the motion in phase-space: $p(t)$ versus $q(t)$, and $I(q,p,t) = 1$



q(t)
ξ(t)
50
0
-50
-100
-150
-200
0
5
10
15
20
25
30
35
40
t

10. Verification of Computer simulations

We return the general case and recapitulate:

$$I = \xi(t)\left(\sum_{i=1}^{n} \tfrac{1}{2} p_i^2 + V(\vec{q}, t)\right) - \tfrac{1}{2}\dot{\xi}(t)\sum_{i=1}^{n} q_i p_i + \tfrac{1}{4}\ddot{\xi}(t)\sum_{i=1}^{n} q_i^2$$

is the constant *global* energy, given by the system's energy H <u>and</u> its energy in- and out-flux. It applies for a system whose dynamics are governed by the equations of motion

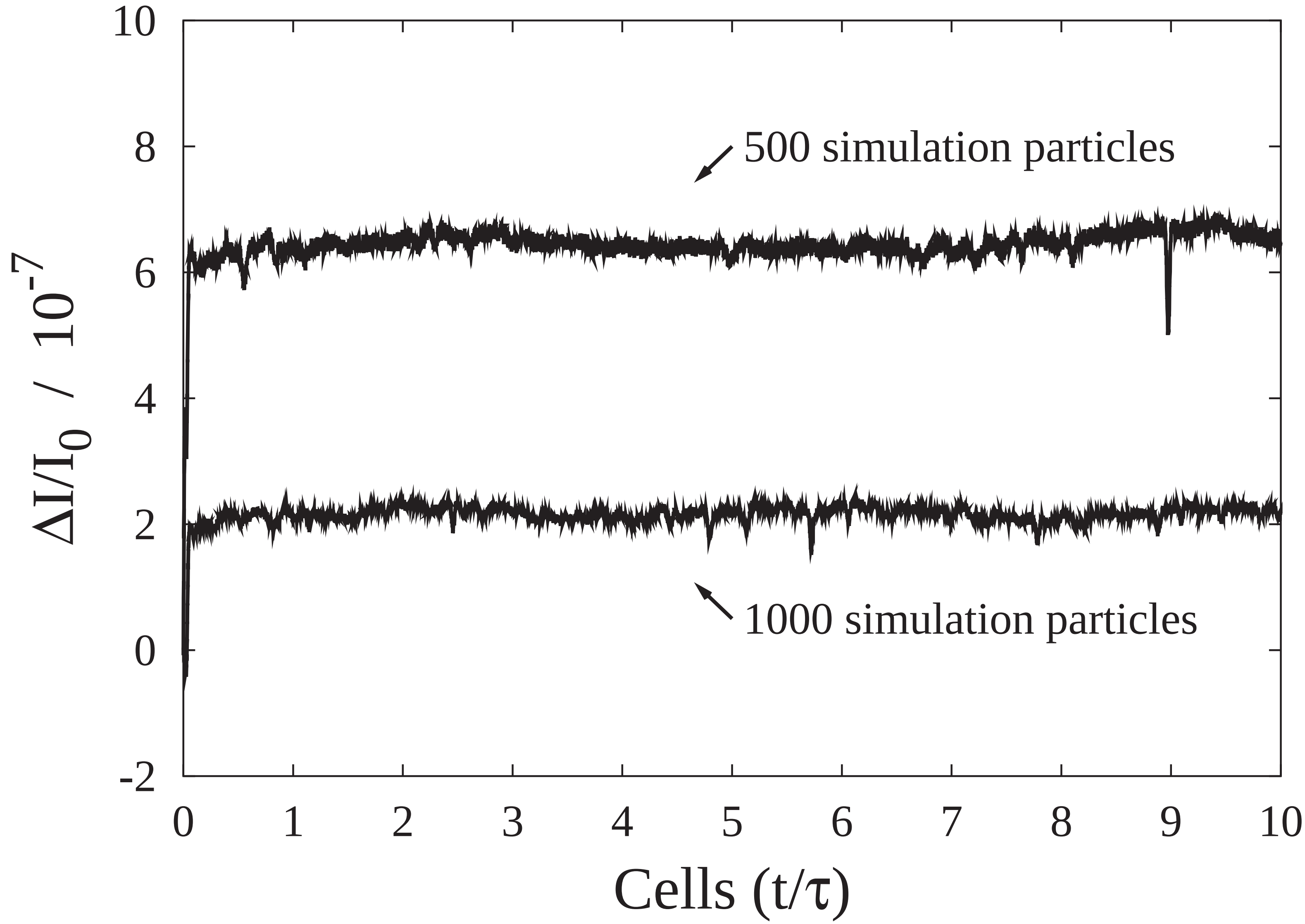
$$\dot{q}_i = p_i\,, \qquad \dot{p}_i + \frac{\partial V(\vec{q}, t)}{\partial q_i} = 0\,, \qquad i = 1, \ldots, n$$

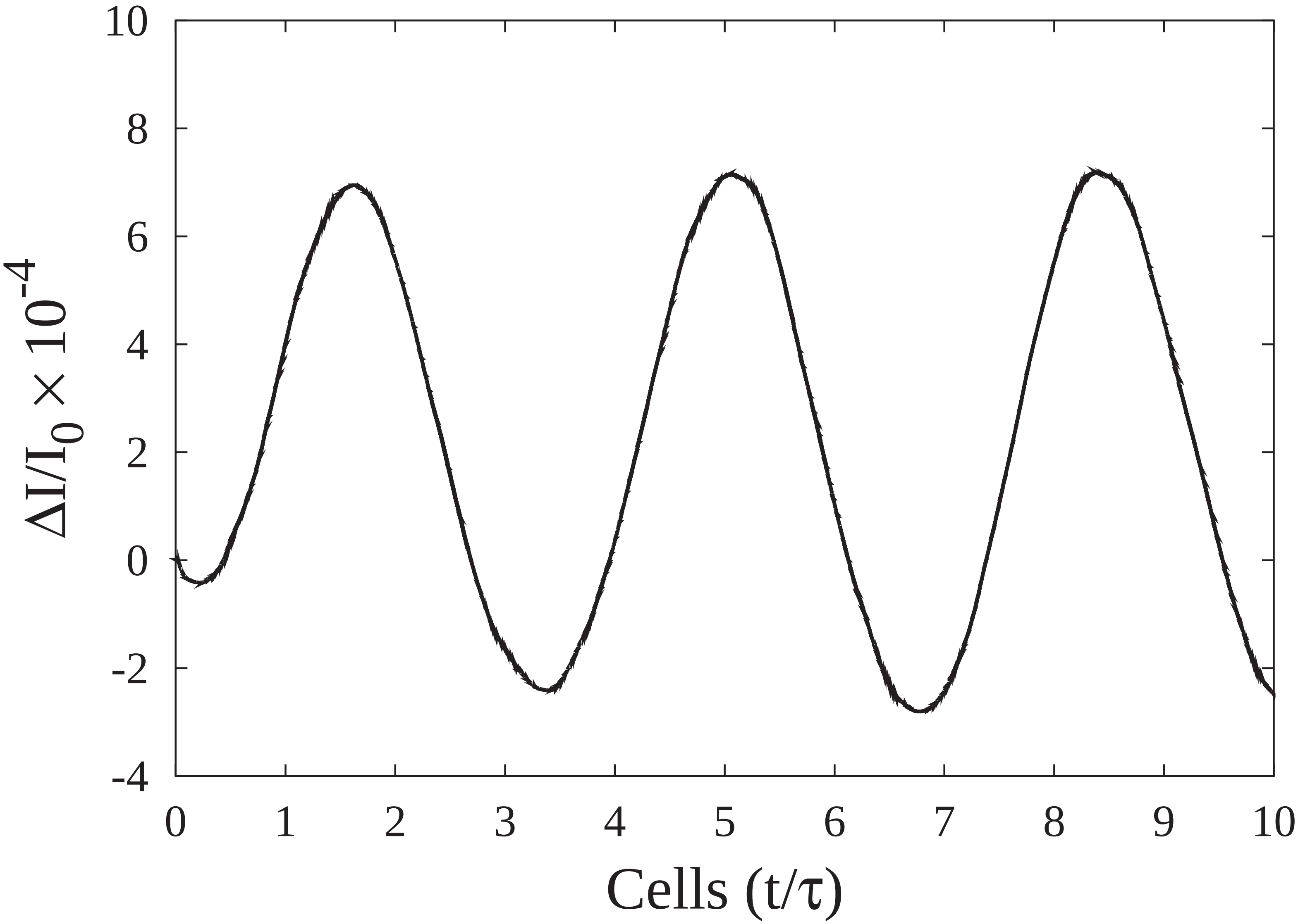
and for $\xi(t)$ a solution of the linear third-order auxiliary equation

$$\dddot{\xi}\sum_{i=1}^{n} q_i^2 + 4\dot{\xi}\left(V + \tfrac{1}{2}\sum_{i=1}^{n} q_i \frac{\partial V}{\partial q_i}\right) + 4\xi\frac{\partial V}{\partial t} = 0\,.$$

<u>Proof</u>: Evaluate dI/dt insert the equations of motion.

- The invariant I is a time integral of the auxiliary equation if $\vec{q}(t)$ and $\vec{p}(t)$ are time integrals of the equations of motion.
- If $\vec{q}(t)$ and $\vec{p}(t)$ follow from Computer simulations, the equations of motion are only approximately satisfied because of the generally limited accuracy of numerical methods.
- If the auxiliary equation is integrated on the basis of simulation results, the quantity I is no longer *strictly* constant.
- The relative deviation $[I(t) - I(0)]/I(0)$ of the numerically calculated $I(t)$ from the exact invariant $I(0)$ can be regarded as „a posteriori" error estimation for the respective simulation.
- This is a generalization of the accuracy test for $H = \text{const.}$ which is applicable for autonomous systems only.


500 simulation particles
1000 simulation particles
ΔI/I0 / 10-7
Cells (t/τ)
10
8
6
4
2
0
-2
0
1
2
3
4
5
6
7
8
9
10

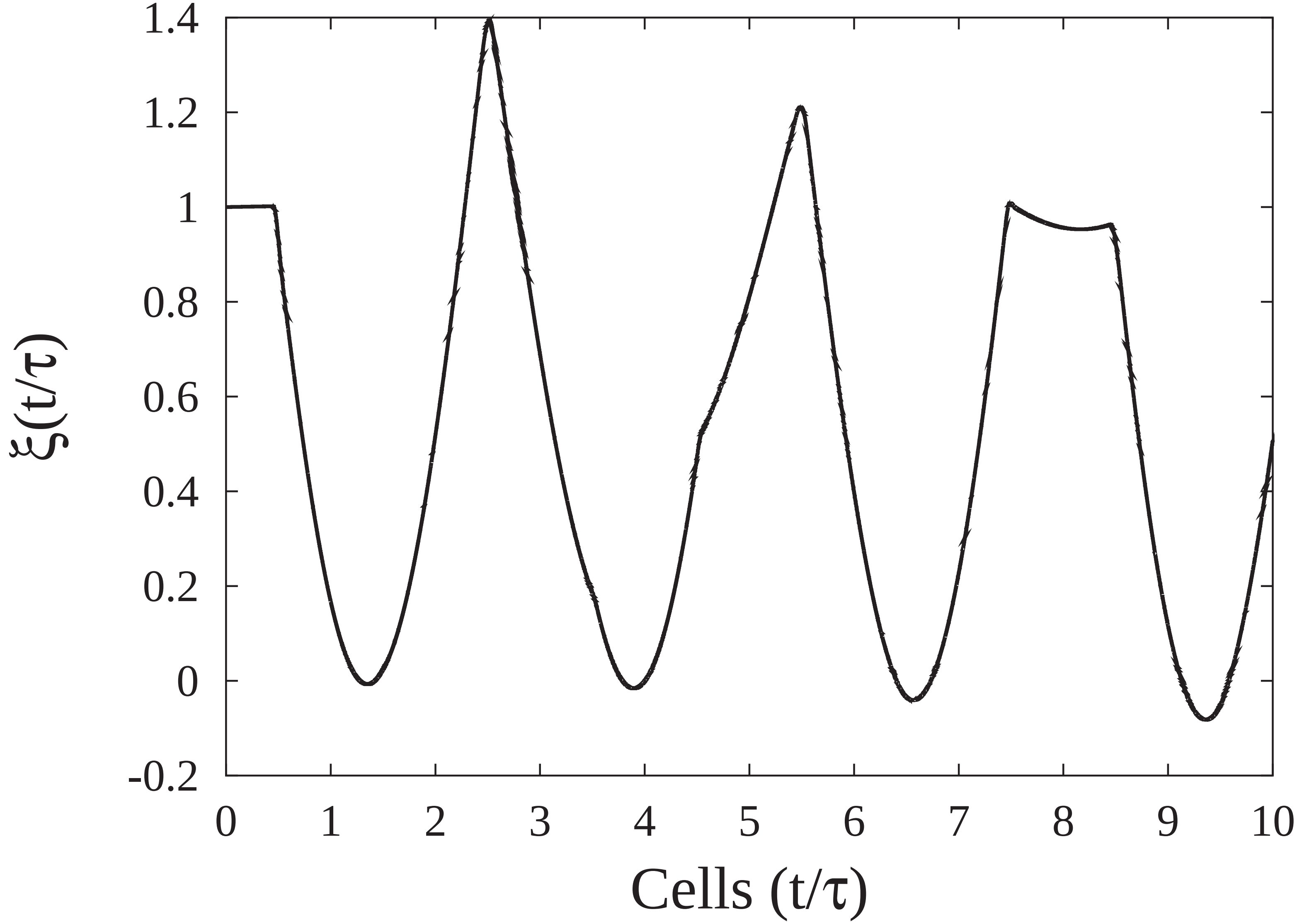

10
8
6
4
2
0
-2
-4
0
1
2
3
4
5
6
7
8
9
10
$\Delta I/I_0 \times 10^{-4}$
Cells (t/τ)

11. Outlook: Classification of dynamical systems

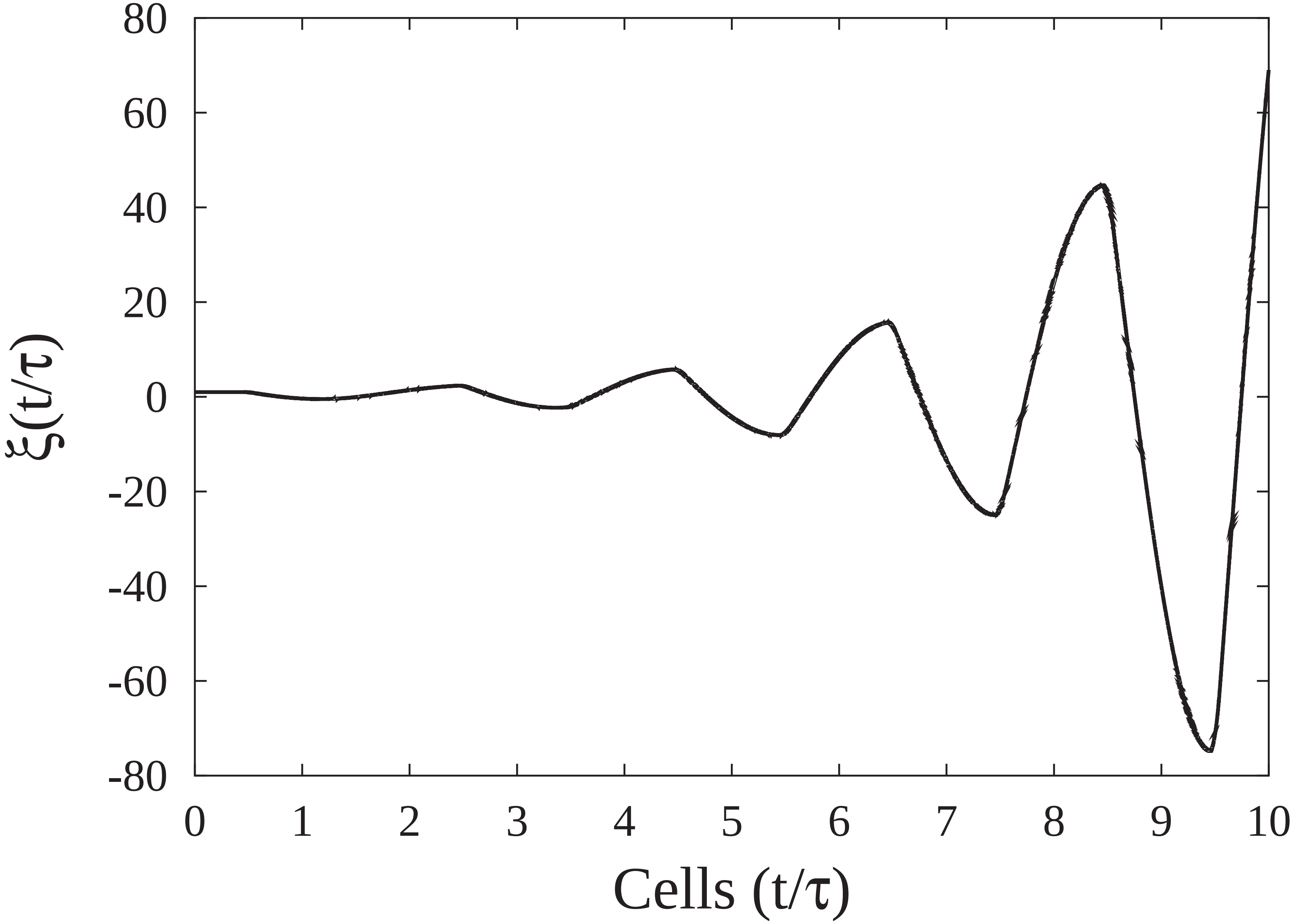
Question: What does it mean if the auxiliary function $\xi(t)$ gets unstable?

Conjecture: Transition from a regular to a chaotic behavior.

$\Longrightarrow$ Halo formation in ion beams



Periodic beam transport at $\sigma_0 = 45°$, $\sigma = 9°$



Periodic beam transport at $\sigma_0 = 60°$, $\sigma = 15°$

Publications:

- Phys. Rev. Lett. **85**, 3830 (2000)
- accepted in principle at Phys. Rev. E