Noether's Theorem and Invariants for time-dependent Hamilton-Lagrange Systems

Jürgen Struckmeier

j.struckmeier@gsi.de

Kolloquiums-Vortrag

im Institut für Theoretische Physik
der Johann Wolfgang Goethe-Universität

Frankfurt am Main, 10. Januar 2002

Outline

- Review of Noether's theorem
- Noether's theorem in the Hamiltonian formulation
- Invariant derived from Noether's theorem
- Example 1: 1D harmonic oscillator, time-independent and time-dependent
- Ex. 2: 1D time-dependent non-linear oscillator
- Ex. 3: 2D time-dependent harmonic oscillator
- Ex. 4: System of Coulomb-interacting particles
- Application: verification of computer simulations
- Conclusions

Review of Noether's theorem

Noether's theorem: relates conserved quantities I to infinitesimal point transformations that leave the Lagrange action $L(\vec{q}, \dot{\vec{q}}, t)dt$ invariant.

$\leadsto$ transformation that "does not change the physics".

Review of Noether's theorem

Noether's theorem: relates conserved quantities I to infinitesimal point transformations that leave the Lagrange action $L(\vec{q}, \dot{\vec{q}}, t)dt$ invariant.

$\rightsquigarrow$ transformation that "does not change the physics".

A point transformation maps "points" into "points"

$$(\vec{q}, t) \mapsto (\vec{q}', t')$$

$\rightsquigarrow$ the point transformation uniquely determines the mapping of the velocity vector

$$\dot{\vec{q}} \mapsto \dot{\vec{q}}'$$

Definition of an infinitesimal point transformation of an n-degree-of-freedom Lagrangian system:

$$t' = t + \delta t + \ldots = t + \varepsilon\xi(t) \quad + \ldots$$

$$q'_i = q_i + \delta q_i + \ldots = q_i + \varepsilon\eta_i(q_i, t) \quad + \ldots$$

$$\dot{q}'_i = \dot{q}_i + \delta\dot{q}_i + \ldots$$

$$\xi(t) = \left.\frac{\partial t'}{\partial\varepsilon}\right|_{\varepsilon=0}, \qquad \eta_i(q_i, t) = \left.\frac{\partial q'_i}{\partial\varepsilon}\right|_{\varepsilon=0}.$$

Definition of an infinitesimal point transformation of an n-degree-of-freedom Lagrangian system:

$$t' = t + \delta t + \ldots = t + \varepsilon \xi(t) \qquad + \ldots$$
$$q_i' = q_i + \delta q_i + \ldots = q_i + \varepsilon \eta_i(q_i, t) + \ldots$$
$$\dot{q}_i' = \dot{q}_i + \delta \dot{q}_i + \ldots$$

$$\xi(t) = \left.\frac{\partial t'}{\partial \varepsilon}\right|_{\varepsilon=0}, \qquad \eta_i(q_i, t) = \left.\frac{\partial q_i'}{\partial \varepsilon}\right|_{\varepsilon=0}.$$

The mapping $\dot{\vec{q}} \mapsto \dot{\vec{q}}'$ is hereby uniquely determined

$$\dot{q}_i' = \frac{dq_i'}{dt'} = \frac{dq_i + \varepsilon d\eta_i}{dt + \varepsilon d\xi} = \frac{\dot{q}_i + \varepsilon \dot{\eta}_i}{1 + \varepsilon \dot{\xi}} = \dot{q}_i + \varepsilon \dot{\eta}_i - \varepsilon \dot{\xi} \dot{q}_i + \mathcal{O}(\varepsilon^2),$$

Definition of an infinitesimal point transformation of an n-degree-of-freedom Lagrangian system:

$$\begin{aligned} t' &= t + \delta t + \ldots = t + \varepsilon\xi(t) + \ldots \\ q_i' &= q_i + \delta q_i + \ldots = q_i + \varepsilon\eta_i(q_i, t) + \ldots \\ \dot{q}_i' &= \dot{q}_i + \delta\dot{q}_i + \ldots \end{aligned}$$

$$\xi(t) = \left.\frac{\partial t'}{\partial\varepsilon}\right|_{\varepsilon=0}, \qquad \eta_i(q_i, t) = \left.\frac{\partial q_i'}{\partial\varepsilon}\right|_{\varepsilon=0}.$$

The mapping $\dot{\vec{q}} \mapsto \dot{\vec{q}}'$ is hereby uniquely determined

$$\dot{q}_i' = \frac{dq_i'}{dt'} = \frac{dq_i + \varepsilon d\eta_i}{dt + \varepsilon d\xi} = \frac{\dot{q}_i + \varepsilon\dot{\eta}_i}{1 + \varepsilon\dot{\xi}} = \dot{q}_i + \varepsilon\dot{\eta}_i - \varepsilon\dot{\xi}\dot{q}_i + \mathcal{O}(\varepsilon^2),$$

which means that to first order the variation $\delta\dot{q}_i$ is

$$\delta\dot{q}_i = \varepsilon\left(\dot{\eta}_i - \dot{\xi}\dot{q}_i\right).$$

Definition of an infinitesimal point transformation of an n-degree-of-freedom Lagrangian system:

$$t' = t + \delta t + \ldots = t + \varepsilon\xi(t) + \ldots$$

$$q_i' = q_i + \delta q_i + \ldots = q_i + \varepsilon\eta_i(q_i, t) + \ldots$$

$$\dot{q}_i' = \dot{q}_i + \delta\dot{q}_i + \ldots = \dot{q}_i + \varepsilon\left(\dot{\eta}_i - \dot{\xi}\dot{q}_i\right) + \ldots$$

$$\xi(t) = \left.\frac{\partial t'}{\partial\varepsilon}\right|_{\varepsilon=0}, \qquad \eta_i(q_i, t) = \left.\frac{\partial q_i'}{\partial\varepsilon}\right|_{\varepsilon=0}.$$

The mapping $\dot{\vec{q}} \mapsto \dot{\vec{q}}'$ is hereby uniquely determined

$$\dot{q}_i' = \frac{dq_i'}{dt'} = \frac{dq_i + \varepsilon d\eta_i}{dt + \varepsilon d\xi} = \frac{\dot{q}_i + \varepsilon\dot{\eta}_i}{1 + \varepsilon\dot{\xi}} = \dot{q}_i + \varepsilon\dot{\eta}_i - \varepsilon\dot{\xi}\dot{q}_i + \mathcal{O}(\varepsilon^2),$$

which means that to first order the variation $\delta\dot{q}_i$ is

$$\delta\dot{q}_i = \varepsilon\left(\dot{\eta}_i - \dot{\xi}\dot{q}_i\right).$$

We now consider the subset of infinitesimal point transformations that leave Ldt invariant

$$L\left(\vec{q}, \dot{\vec{q}}, t\right) dt \stackrel{!}{=} L'\left(\vec{q}', \dot{\vec{q}}', t'\right) dt' \, .$$

We now consider the subset of infinitesimal point transformations that leave Ldt invariant

$$L\big(\vec{q},\dot{\vec{q}},t\big)\,dt \overset{!}{=} L'\big(\vec{q}',\dot{\vec{q}}',t'\big)\,dt'\,.$$

The *functional* relation between L' and L may be expressed introducing an auxiliary function $\dot{f}_0(\vec{q},t)$

$$L'\big(\vec{q}',\dot{\vec{q}}',t'\big) = L\big(\vec{q}',\dot{\vec{q}}',t'\big) - \varepsilon\dot{f}_0(\vec{q},t) + \mathcal{O}(\varepsilon^2)\,.$$

We now consider the subset of infinitesimal point transformations that leave Ldt invariant

$$L\left(\vec{q},\dot{\vec{q}},t\right)dt \stackrel{!}{=} L'\left(\vec{q}',\dot{\vec{q}}',t'\right)dt' \, .$$

The *functional* relation between L' and L may be expressed introducing an auxiliary function $\dot{f}_0(\vec{q},t)$

$$L'\left(\vec{q}',\dot{\vec{q}}',t'\right) = L\left(\vec{q}',\dot{\vec{q}}',t'\right) - \varepsilon\dot{f}_0(\vec{q},t) + \mathcal{O}(\varepsilon^2) \, .$$

On the other hand, we may express $L\left(\vec{q}',\dot{\vec{q}}',t'\right)$ in terms of a truncated Taylor expansion of $L\left(\vec{q},\,\dot{\vec{q}},t\right)$

$$L(\vec{q}',\dot{\vec{q}}',t') = L(\vec{q},\dot{\vec{q}},t) + \frac{\partial L}{\partial t}\delta t + \sum_{i=1}^{n}\left[\frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\right] + \ldots$$

We now consider the subset of infinitesimal point transformations that leave Ldt invariant

$$L\left(\vec{q},\dot{\vec{q}},t\right)dt \stackrel{!}{=} L'\left(\vec{q}',\dot{\vec{q}}',t'\right)dt'\,.$$

The *functional* relation between L' and L may be expressed introducing an auxiliary function $\dot{f}_0(\vec{q},t)$

$$L'\left(\vec{q}',\dot{\vec{q}}',t'\right) = L\left(\vec{q}',\dot{\vec{q}}',t'\right) - \varepsilon\dot{f}_0(\vec{q},t) + \mathcal{O}(\varepsilon^2)\,.$$

On the other hand, we may express $L\left(\vec{q}',\dot{\vec{q}}',t'\right)$ in terms of a truncated Taylor expansion of $L\left(\vec{q},\,\dot{\vec{q}},t\right)$

$$L\left(\vec{q}',\dot{\vec{q}}',t'\right) = L\left(\vec{q},\dot{\vec{q}},t\right) + \frac{\partial L}{\partial t}\delta t + \sum_{i=1}^{n}\left[\frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta\dot{q}_i\right] + \ldots$$

Inserting δt, δq_i, and $\delta \dot{q}_i$, we obtain an equation for $f_0(\vec{q}, t)$ that is uniquely determined by the $\xi(t)$, $\eta_i(\vec{q}, t)$

$$\dot{f}_0(\vec{q}, t) - \dot{\xi}\, L(\vec{q}, \dot{\vec{q}}, t) - \xi\, \frac{\partial L}{\partial t} - \sum_{i=1}^{n} \left[\eta_i \frac{\partial L}{\partial q_i} + \left(\dot{\eta}_i - \dot{q}_i \dot{\xi} \right) \frac{\partial L}{\partial \dot{q}_i} \right] = 0$$

Inserting δt, δq_i, and $\delta \dot{q}_i$, we obtain an equation for $f_0(\vec{q}, t)$ that is uniquely determined by the $\xi(t)$, $\eta_i(\vec{q}, t)$

$$\dot{f}_0(\vec{q}, t) - \dot{\xi}\, L(\vec{q}, \dot{\vec{q}}, t) - \xi\, \frac{\partial L}{\partial t} - \sum_{i=1}^{n} \left[\eta_i \frac{\partial L}{\partial q_i} + \left(\dot{\eta}_i - \dot{q}_i \dot{\xi} \right) \frac{\partial L}{\partial \dot{q}_i} \right] = 0$$

The terms can be split into a total time derivative and a sum containing the Euler-Lagrange equations

$$\frac{d}{dt} \left[f_0(\vec{q}, t) - \xi\, L + \sum_{i=1}^{n} (\xi \dot{q}_i - \eta_i)\, \frac{\partial L}{\partial \dot{q}_i} \right] + \sum_{i=1}^{n} (\xi \dot{q}_i - \eta_i) \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) = 0$$

Inserting δt, δq_i, and $\delta \dot{q}_i$, we obtain an equation for $f_0(\vec{q}, t)$ that is uniquely determined by the $\xi(t)$, $\eta_i(\vec{q}, t)$

$$\dot{f}_0(\vec{q}, t) - \dot{\xi}\, L(\vec{q}, \dot{\vec{q}}, t) - \xi \frac{\partial L}{\partial t} - \sum_{i=1}^{n} \left[\eta_i \frac{\partial L}{\partial q_i} + \left(\dot{\eta}_i - \dot{q}_i \dot{\xi} \right) \frac{\partial L}{\partial \dot{q}_i} \right] = 0$$

The terms can be split into a total time derivative and a sum containing the Euler-Lagrange equations

$$\frac{d}{dt} \left[f_0(\vec{q}, t) - \xi\, L + \sum_{i=1}^{n} (\xi \dot{q}_i - \eta_i) \frac{\partial L}{\partial \dot{q}_i} \right] + \sum_{i=1}^{n} (\xi \dot{q}_i - \eta_i) \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) = 0$$

$\rightsquigarrow$ $[\ldots]$ constitutes a conserved quantity I along the solution $\big(\vec{q}(t), \dot{\vec{q}}(t)\big)$ of the Euler-Lagrange equations

$$I = f_0(\vec{q}, t) - \xi\, L + \sum_{i=1}^{n} (\xi \dot{q}_i - \eta_i) \frac{\partial L}{\partial \dot{q}_i} \qquad \Longleftrightarrow \qquad \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0,\ i = 1, \ldots, n$$

Hamiltonian formulation

A Legendre transformation relates a given $L(\vec{q}, \dot{\vec{q}}, t)$ with the corresponding Hamiltonian $H(\vec{q}, \vec{p}, t)$

$$L(\vec{q}, \dot{\vec{q}}, t) = \sum_{i=1}^{n} p_i \, \dot{q}_i - H(\vec{q}, \vec{p}, t) \, , \quad p_i = \frac{\partial L}{\partial \dot{q}_i} \, , \quad \dot{p}_i = \frac{\partial L}{\partial q_i} \, , \quad \frac{\partial L}{\partial t} = -\frac{dH}{dt}$$

Hamiltonian formulation

A Legendre transformation relates a given $L(\vec{q}, \dot{\vec{q}}, t)$ with the corresponding Hamiltonian $H(\vec{q}, \vec{p}, t)$

$$L(\vec{q}, \dot{\vec{q}}, t) = \sum_{i=1}^{n} p_i \, \dot{q}_i - H(\vec{q}, \vec{p}, t) \,, \quad p_i = \frac{\partial L}{\partial \dot{q}_i} \,, \quad \dot{p}_i = \frac{\partial L}{\partial q_i} \,, \quad \frac{\partial L}{\partial t} = -\frac{dH}{dt}$$

Applying these rules to the Noether invariant, we find

$$I = \xi(t) \, H(\vec{q}, \vec{p}, t) - \sum_{i=1}^{n} \eta_i(q_i, t) \, p_i + f_0(\vec{q}, t)$$

Hamiltonian formulation

A Legendre transformation relates a given $L(\vec{q}, \dot{\vec{q}}, t)$ with the corresponding Hamiltonian $H(\vec{q}, \vec{p}, t)$

$$L(\vec{q}, \dot{\vec{q}}, t) = \sum_{i=1}^{n} p_i \, \dot{q}_i - H(\vec{q}, \vec{p}, t) \,, \quad p_i = \frac{\partial L}{\partial \dot{q}_i} \,, \quad \dot{p}_i = \frac{\partial L}{\partial q_i} \,, \quad \frac{\partial L}{\partial t} = -\frac{dH}{dt}$$

Applying these rules to the Noether invariant, we find

$$I = \xi(t) \, H(\vec{q}, \vec{p}, t) - \sum_{i=1}^{n} \eta_i(q_i, t) \, p_i + f_0(\vec{q}, t)$$

The *conditional equation* for $f_0(\vec{q}, t)$ translates into

$$\frac{d}{dt} \left[\xi(t) \, H(\vec{q}, \vec{p}, t) - \sum_{i=1}^{n} \eta_i(q_i, t) \, p_i + f_0(\vec{q}, t) \right] = 0 \quad \Longleftrightarrow \quad \frac{dI}{dt} \stackrel{!}{=} 0$$

Invariant

We now work out the Noether invariant for a class of explicitly time-dependent Hamiltonians $H(\vec{p}, \vec{q}, t)$

$$H = \tfrac{1}{2}\sum_{i=1}^{n} p_i^2 + V(\vec{q}, t)\,, \qquad \dot{q}_i = p_i\,, \quad \dot{p}_i = -\frac{\partial V}{\partial q_i}$$

Invariant

We now work out the Noether invariant for a class of explicitly time-dependent Hamiltonians $H(\vec{p}, \vec{q}, t)$

$$H = \tfrac{1}{2}\sum_{i=1}^{n} p_i^2 + V(\vec{q}, t)\,, \qquad \dot{q}_i = p_i\,, \quad \dot{p}_i = -\frac{\partial V}{\partial q_i}$$

We insert $H(\vec{p}, \vec{q}, t)$ into the equation $dI/dt = 0$ and equate to zero the terms proportional to p_i^2, p_i^1, and p_i^0

$$p_i^2 : \qquad \tfrac{1}{2}\dot{\xi}(t) - \frac{\partial \eta_i(q_i, t)}{\partial q_i} = 0$$

$$p_i^1 : \qquad \frac{\partial f_0(\vec{q}, t)}{\partial q_i} - \frac{\partial \eta_i(q_i, t)}{\partial t} = 0$$

$$p_i^0 : \qquad \dot{\xi}(t) V(\vec{q}, t) + \xi \frac{\partial V}{\partial t} + \frac{\partial f_0}{\partial t} + \sum_i \eta_i \frac{\partial V}{\partial q_i} = 0$$

Combining these equations, we easily eliminate the functions $\eta_i(q_i, t)$ and $f_0(\vec{q}, t)$ to obtain a third-order "auxiliary equation" for $\xi(t)$ that does not depend on $\vec{p}$

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

Combining these equations, we easily eliminate the functions $\eta_i(q_i, t)$ and $f_0(\vec{q}, t)$ to obtain a third-order "auxiliary equation" for $\xi(t)$ that does not depend on $\vec{p}$

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

The Noether invariant I for the particular Hamiltonian system $H(\vec{p}, \vec{q}, t) = \sum_i p_i^2/2 + V(\vec{q}, t)$ writes

$$I = \xi(t)\; H - \tfrac{1}{2}\dot{\xi}(t) \;\sum_i p_i\, q_i + \tfrac{1}{4}\ddot{\xi}(t) \;\sum_i q_i^2$$

Prior to presenting examples 1a, 1b, 2, 3, and 4, we'll discuss the meaning of I and the equation for $\xi(t)$.

We summarize:

- The auxiliary equation for $\xi(t)$ depends on $\vec{q}(t)$.

We summarize:

- The auxiliary equation for $\xi(t)$ depends on $\vec{q}(t)$.
- $\leadsto$ The auxiliary equation can only be integrated *in conjunction* with the canonical equations.

We summarize:

- The auxiliary equation for $\xi(t)$ depends on $\vec{q}(t)$.
- $\rightsquigarrow$ The auxiliary equation can only be integrated *in conjunction* with the canonical equations.
- The $2n$ first-order canonical equations form together with the three first-order equations of the auxiliary equation a closed coupled set of $2n+3$ first-order equations that uniquely determine $\vec{q}(t)$, $\vec{p}(t)$, and $\xi(t)$ — and hence the invariant I.

We summarize:

- The auxiliary equation for $\xi(t)$ depends on $\vec{q}(t)$.
- $\leadsto$ The auxiliary equation can only be integrated *in conjunction* with the canonical equations.
- The $2n$ first-order canonical equations form together with the three first-order equations of the auxiliary equation a closed coupled set of $2n+3$ first-order equations that uniquely determine $\vec{q}(t)$, $\vec{p}(t)$, and $\xi(t)$ — and hence the invariant I.
- The invariant cannot ease the problem of integrating the system's equations of motion.

We summarize:

- The auxiliary equation for $\xi(t)$ depends on $\vec{q}(t)$.
- $\rightsquigarrow$ The auxiliary equation can only be integrated *in conjunction* with the canonical equations.
- The $2n$ first-order canonical equations form together with the three first-order equations of the auxiliary equation a closed coupled set of $2n + 3$ first-order equations that uniquely determine $\vec{q}(t)$, $\vec{p}(t)$, and $\xi(t)$ — and hence the invariant I.
- The invariant cannot ease the problem of integrating the system's equations of motion.
- In the special case of autonomous systems, the function $\xi(t) = 1$ is always a solution of the auxiliary equation. With this solution, the invariant I coincides with the Hamiltonian H.

1D harmonic oscillator

Hamiltonian:

$$H(q,p) = \tfrac{1}{2}p^2 + V(q)\,, \qquad V(q) = \tfrac{1}{2}\omega_0^2 q^2$$

Invariant:

$$I = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\,pq + \tfrac{1}{4}\ddot{\xi}(t)\,q^2$$

with $\xi(t)$ a solution of the 3rd-order auxiliary equation

$$\dddot{\xi}(t) + 4\omega_0^2\,\dot{\xi}(t) = 0$$

1D harmonic oscillator

Hamiltonian:

$$H(q,p) = \tfrac{1}{2}p^2 + V(q)\,, \qquad V(q) = \tfrac{1}{2}\omega_0^2 q^2$$

Invariant:

$$I = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\,pq + \tfrac{1}{4}\ddot{\xi}(t)\,q^2$$

with $\xi(t)$ a solution of the 3rd-order auxiliary equation

$$\dddot{\xi}(t) + 4\omega_0^2\,\dot{\xi}(t) = 0$$

General solution with a, b, c the integration constants:

$$\xi(t) = a + b\cos 2\omega_0 t + c\sin 2\omega_0 t$$

(1) Case $a = 1$, $b = 0$, $c = 0$:

$$\xi(t) = 1 \quad \Longrightarrow \quad I_1 = H$$

(2) Case $a = 0$, $b = 1$, $c = 0$:

$$\xi(t) = \cos 2\omega_0 t \quad \Longrightarrow \quad I_2 = \frac{1}{2}\left(p^2 - \omega_0^2 q^2\right)\cos 2\omega_0 t + \omega_0 pq \sin 2\omega_0 t$$

(3) Case $a = 0$, $b = 0$, $c = 1$:

$$\xi(t) = \sin 2\omega_0 t \quad \Longrightarrow \quad I_3 = \frac{1}{2}\left(p^2 - \omega_0^2 q^2\right)\sin 2\omega_0 t - \omega_0 pq \cos 2\omega_0 t$$

(2) Case $a = 0$, $b = 1$, $c = 0$:

$$\xi(t) = \cos 2\omega_0 t \quad \Longrightarrow \quad I_2 = \tfrac{1}{2}\left(p^2 - \omega_0^2 q^2\right)\cos 2\omega_0 t + \omega_0 pq \sin 2\omega_0 t$$

(3) Case $a = 0$, $b = 0$, $c = 1$:

$$\xi(t) = \sin 2\omega_0 t \quad \Longrightarrow \quad I_3 = \tfrac{1}{2}\left(p^2 - \omega_0^2 q^2\right)\sin 2\omega_0 t - \omega_0 pq \cos 2\omega_0 t$$

The mutual Poisson brackets yield

$$[I_2, I_1] = 2\omega_0 I_3\,, \qquad [I_1, I_3] = 2\omega_0 I_2\,, \qquad [I_2, I_3] = 2\omega_0 I_1$$

Defining $E_1 = T - V$, $E_2 = 2\sqrt{TV}$, the invariants I_2 and I_3 follow as

$$\begin{pmatrix} I_2 \\ I_3 \end{pmatrix} = \begin{pmatrix} \cos 2\omega_0 t & -\sin 2\omega_0 t \\ \sin 2\omega_0 t & \cos 2\omega_0 t \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \end{pmatrix}$$

Only two invariants are functionally independent:

$$I_1^2 = I_2^2 + I_3^2$$

We summarize:

- Autonomous system: $\xi(t) = 1$ is a solution of the auxiliary equation. With this solution, the invariant I_1 coincides with the Hamiltonian H, hence provides the conserved total energy.

We summarize:

- Autonomous system: $\xi(t) = 1$ is a solution of the auxiliary equation. With this solution, the invariant I_1 coincides with the Hamiltonian H, hence provides the conserved total energy.
- The other invariants I_2, I_3 are associated with $\xi(t) \neq \text{const.}$

We summarize:

- Autonomous system: $\xi(t) = 1$ is a solution of the auxiliary equation. With this solution, the invariant I_1 coincides with the Hamiltonian H, hence provides the conserved total energy.
- The other invariants I_2, I_3 are associated with $\xi(t) \neq$ const.
- The invariants I_2 and I_3 are related to the time evolution of both the kinetic energy T and the potential energy V, starting from the particular initial energies T_0 and V_0.

We summarize:

- Autonomous system: $\xi(t) = 1$ is a solution of the auxiliary equation. With this solution, the invariant I_1 coincides with the Hamiltonian H, hence provides the conserved total energy.
- The other invariants I_2, I_3 are associated with $\xi(t) \neq$ const.
- The invariants I_2 and I_3 are related to the time evolution of both the kinetic energy T and the potential energy V, starting from the particular initial energies T_0 and V_0.
- 1D linear system: the $q(t)$-dependence of the auxiliary equation cancels — in contrast to the general case.

Hamiltonian of the *time-dependent* linear oscillator:

$$H(q,p,t) = \tfrac{1}{2}p^2 + V(q,t)\,, \qquad V(q,t) = \tfrac{1}{2}\omega^2(t)\,q^2$$

Invariant:

$$I = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\,pq + \tfrac{1}{4}\ddot{\xi}(t)\,q^2$$

with $\xi(t)$ a solution of the auxiliary equation

$$\dddot{\xi}(t) + 4\omega^2(t)\,\dot{\xi}(t) + 4\omega\dot{\omega}\,\xi(t) = 0$$

Hamiltonian of the *time-dependent* linear oscillator:

$$H(q,p,t) = \tfrac{1}{2}p^2 + V(q,t)\,, \qquad V(q,t) = \tfrac{1}{2}\omega^2(t)\,q^2$$

Invariant:

$$I = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\,pq + \tfrac{1}{4}\ddot{\xi}(t)\,q^2$$

with $\xi(t)$ a solution of the auxiliary equation

$$\dddot{\xi}(t) + 4\omega^2(t)\,\dot{\xi}(t) + 4\omega\dot{\omega}\,\xi(t) = 0$$

We observe:

- Non-autonomous system: all invariants are associated with $\xi(t) \neq$ const.
- 1D linear system: the auxiliary equation is *not* coupled to the canonical equations.
- The auxiliary equation agrees with the equation for $q^2(t) \rightsquigarrow$ we may identify $\xi(t) = \sum_i q_i^2(t)$ in this 1D linear case.

1D non-linear oscillator

Hamiltonian:

$$H(q,p,t) = \tfrac{1}{2}p^2 + V(q,t)\,, \qquad V(q,t) = \tfrac{1}{2}\omega^2(t)\,q^2 + a(t)\,q^3 + b(t)\,q^4$$

Invariant:

$$I = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\,pq + \tfrac{1}{4}\ddot{\xi}(t)\,q^2$$

$\xi(t)$ is now a solution of the auxiliary equation

$$\dddot{\xi} + 4\dot{\xi}\,\omega^2 + 4\xi\,\omega\,\dot{\omega} + 2q(t)\left[2\xi\,\dot{a} + 5\dot{\xi}\,a\right] + 4q^2(t)\left[\xi\,\dot{b} + 3\dot{\xi}\,b\right] = 0$$

1D non-linear oscillator

Hamiltonian:

$$H(q,p,t) = \tfrac{1}{2}p^2 + V(q,t)\,, \qquad V(q,t) = \tfrac{1}{2}\omega^2(t)\,q^2 + a(t)\,q^3 + b(t)\,q^4$$

Invariant:

$$I = \xi(t)\,H - \tfrac{1}{2}\dot{\xi}(t)\,pq + \tfrac{1}{4}\ddot{\xi}(t)\,q^2$$

$\xi(t)$ is now a solution of the auxiliary equation

$$\dddot{\xi} + 4\dot{\xi}\,\omega^2 + 4\xi\,\omega\,\dot{\omega} + 2q(t)\left[2\xi\,\dot{a} + 5\dot{\xi}\,a\right] + 4q^2(t)\left[\xi\,\dot{b} + 3\dot{\xi}\,b\right] = 0$$

- Non-autonomous system: a solution $\xi(t) = \text{const}$ does not exist.
- Non-linear system: the canonical equations and the auxiliary equation are now coupled.
  $\rightsquigarrow$ The auxiliary equation can only be integrated *simultaneously* with the canonical equations.

2D linear oscillator

Hamiltonian:

$$H(\vec{p},\vec{q},t) = \frac{1}{2}\left(p_x^2 + p_y^2\right) + V(\vec{q},t)\,, \qquad V(\vec{q},t) = \frac{1}{2}\left(\omega_x^2(t)\,q_x^2 + \omega_y^2(t)\,q_y^2\right)$$

Invariant:

$$I = \xi(t)\,H - \frac{1}{2}\dot{\xi}(t)\,(p_x q_x + p_y q_y) + \frac{1}{4}\ddot{\xi}(t)\left(q_x^2 + q_y^2\right)$$

The auxiliary equation for this case reads

$$\dddot{\xi}\left(q_x^2 + q_y^2\right) + 4\dot{\xi}\left(\omega_x^2 q_x^2 + \omega_y^2 q_y^2\right) + 4\xi\left(\omega_x\dot{\omega}_x q_x^2 + \omega_y\dot{\omega}_y q_y^2\right) = 0$$

2D linear oscillator

Hamiltonian:

$$H(\vec{p},\vec{q},t) = \frac{1}{2}\left(p_x^2 + p_y^2\right) + V(\vec{q},t)\,, \qquad V(\vec{q},t) = \frac{1}{2}\left(\omega_x^2(t)\,q_x^2 + \omega_y^2(t)\,q_y^2\right)$$

Invariant:

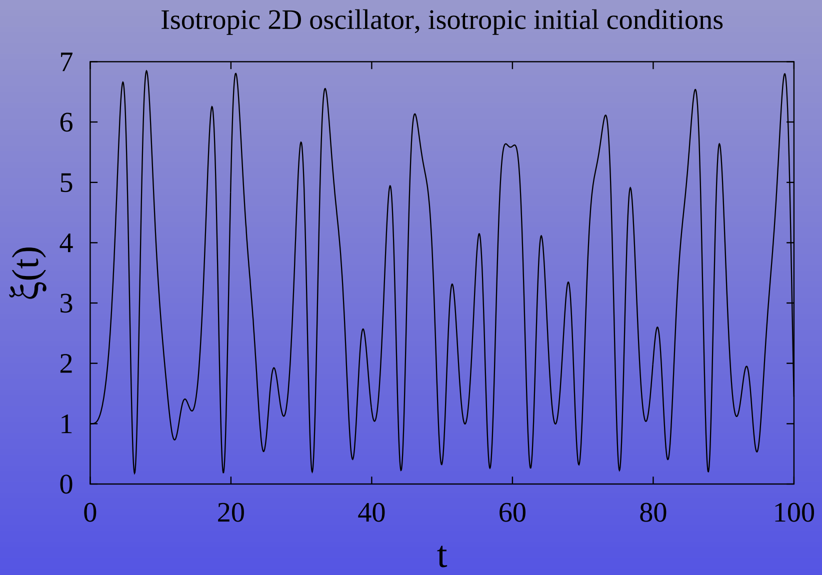
$$I = \xi(t)\,H - \frac{1}{2}\dot{\xi}(t)\,(p_x q_x + p_y q_y) + \frac{1}{4}\ddot{\xi}(t)\left(q_x^2 + q_y^2\right)$$

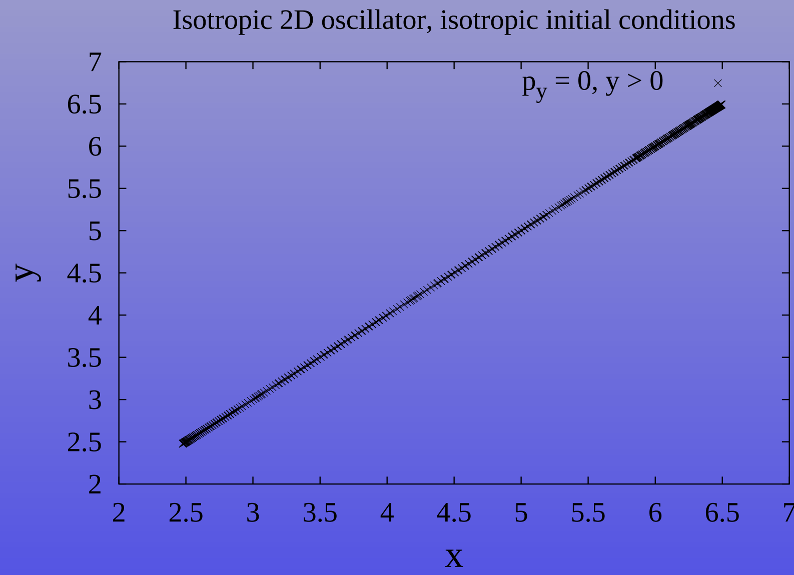
The auxiliary equation for this case reads

$$\dddot{\xi}\left(q_x^2 + q_y^2\right) + 4\dot{\xi}\left(\omega_x^2 q_x^2 + \omega_y^2 q_y^2\right) + 4\xi\left(\omega_x\dot{\omega}_x q_x^2 + \omega_y\dot{\omega}_y q_y^2\right) = 0$$

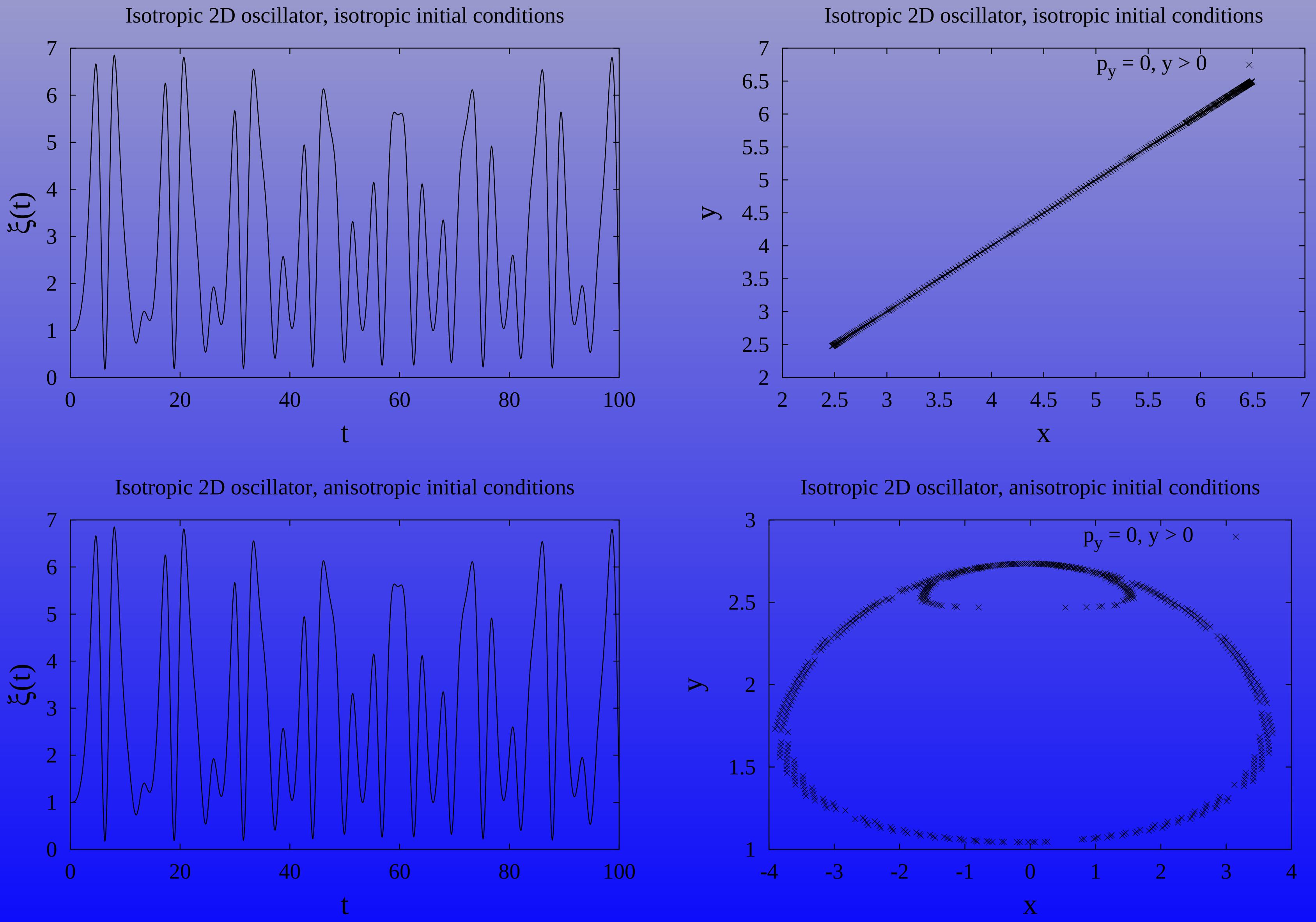
- Non-autonomous system: a solution $\xi(t) = \text{const}$ does not exist.
- 2D system: the auxiliary equation depends on $\vec{q}(t)$.
- The auxiliary equation couples the degrees of freedom.
- The solution $\xi(t)$ may be unstable even if $q_x(t)$ and $q_y(t)$ are stable.

Isotropic 2D Oscillator

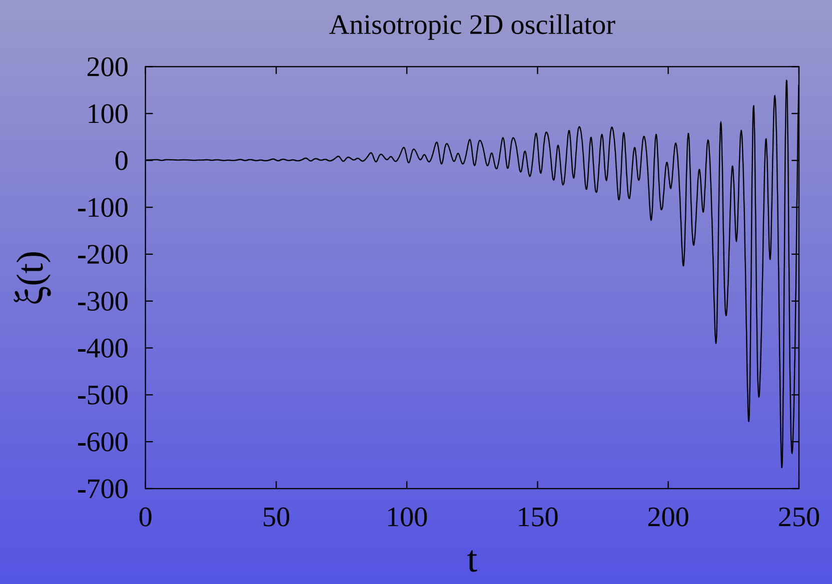


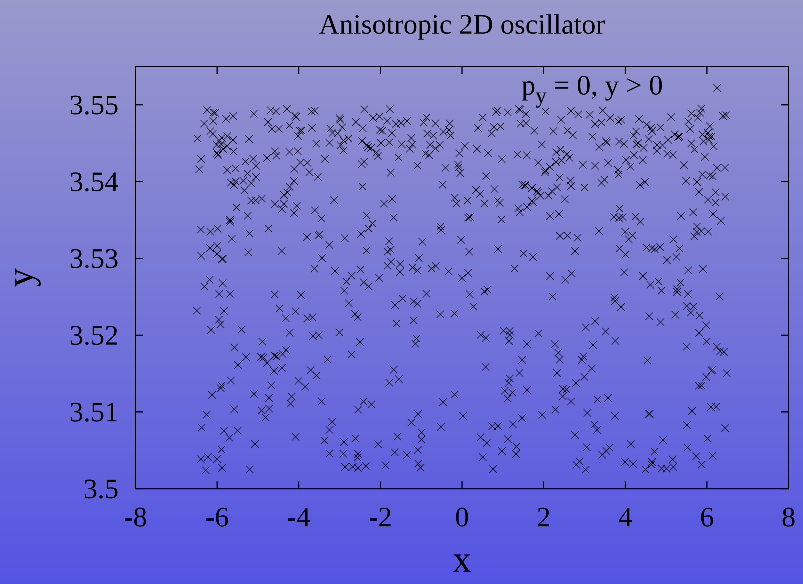


Isotropic 2D Oscillator

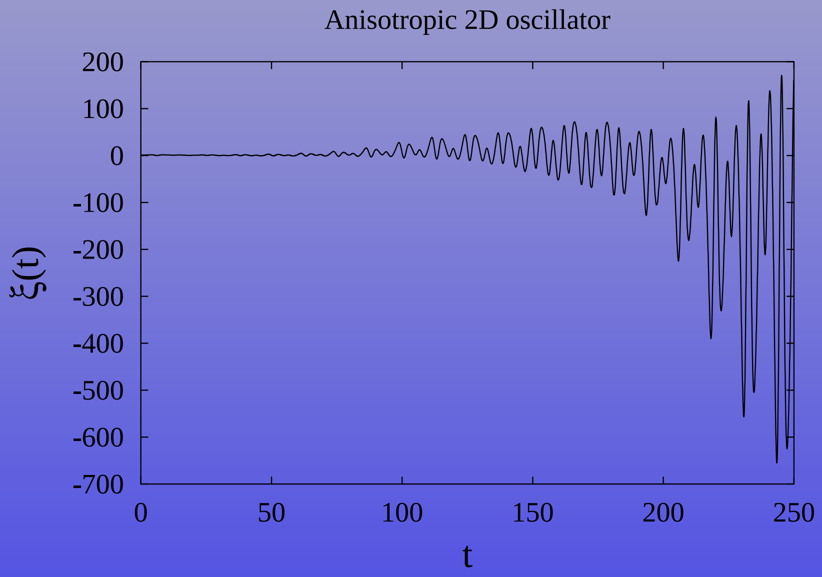


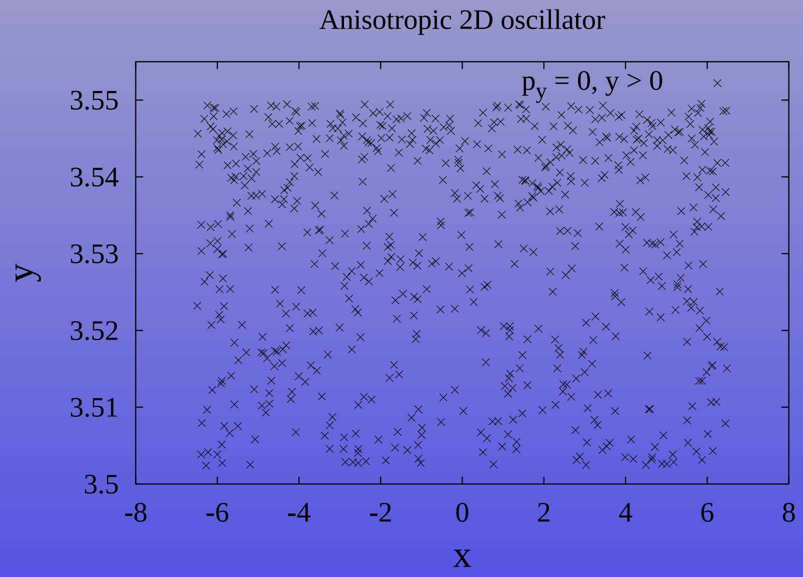
Anisotropic 2D Oscillator

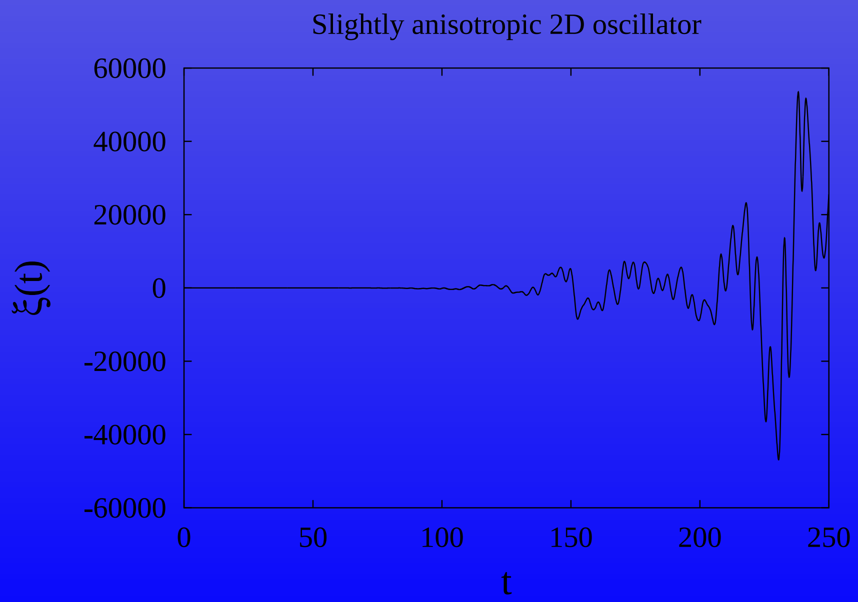


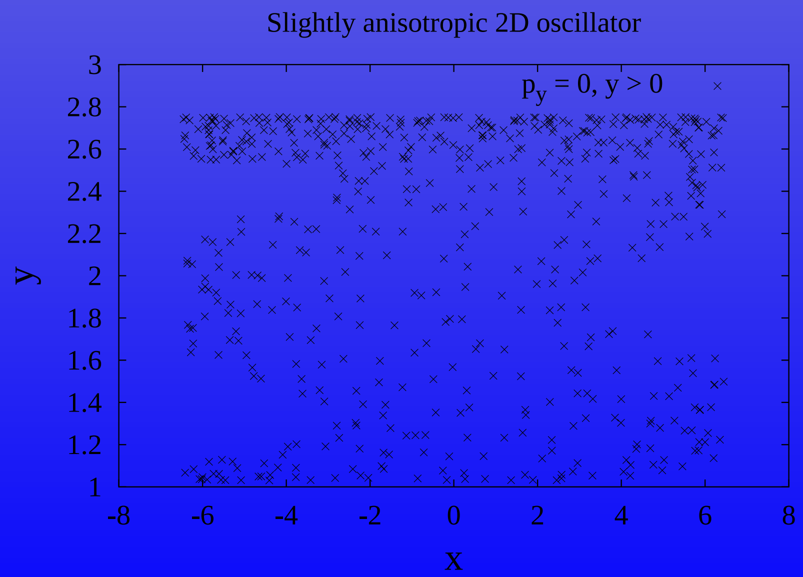


Anisotropic 2D Oscillator









Coulomb-interacting particles

Hamiltonian:

$$H = \sum_{i=1}^{N} \tfrac{1}{2}\left(p_{x,i}^2 + p_{y,i}^2 + p_{z,i}^2\right) + V\left(\vec{x}, \vec{y}, \vec{z}, t\right)$$

The effective potential V contained herein be given by

$$V\left(\vec{x}, \vec{y}, \vec{z}, t\right) = \tfrac{1}{2} \sum_{i=1}^{N} \left[\omega_x^2(t)\, x_i^2 + \omega_y^2(t)\, y_i^2 + \omega_z^2(t)\, z_i^2 + \sum_{j \neq i} \frac{c_1}{r_{ij}}\right]$$

with $c_1 = q^2/4\pi\varepsilon_0 m$ and $r_{ij}^2 = \left(x_i - x_j\right)^2 + \left(y_i - y_j\right)^2 + \left(z_i - z_j\right)^2$.
The invariant has the usual form

$$I = \xi(t)\, H - \tfrac{1}{2}\dot{\xi} \sum_{i=1}^{N} \left(x_i\, p_{x,i} + y_i\, p_{y,i} + z_i\, p_{z,i}\right) + \tfrac{1}{4}\ddot{\xi} \sum_{i=1}^{N} \left(x_i^2 + y_i^2 + z_i^2\right)$$

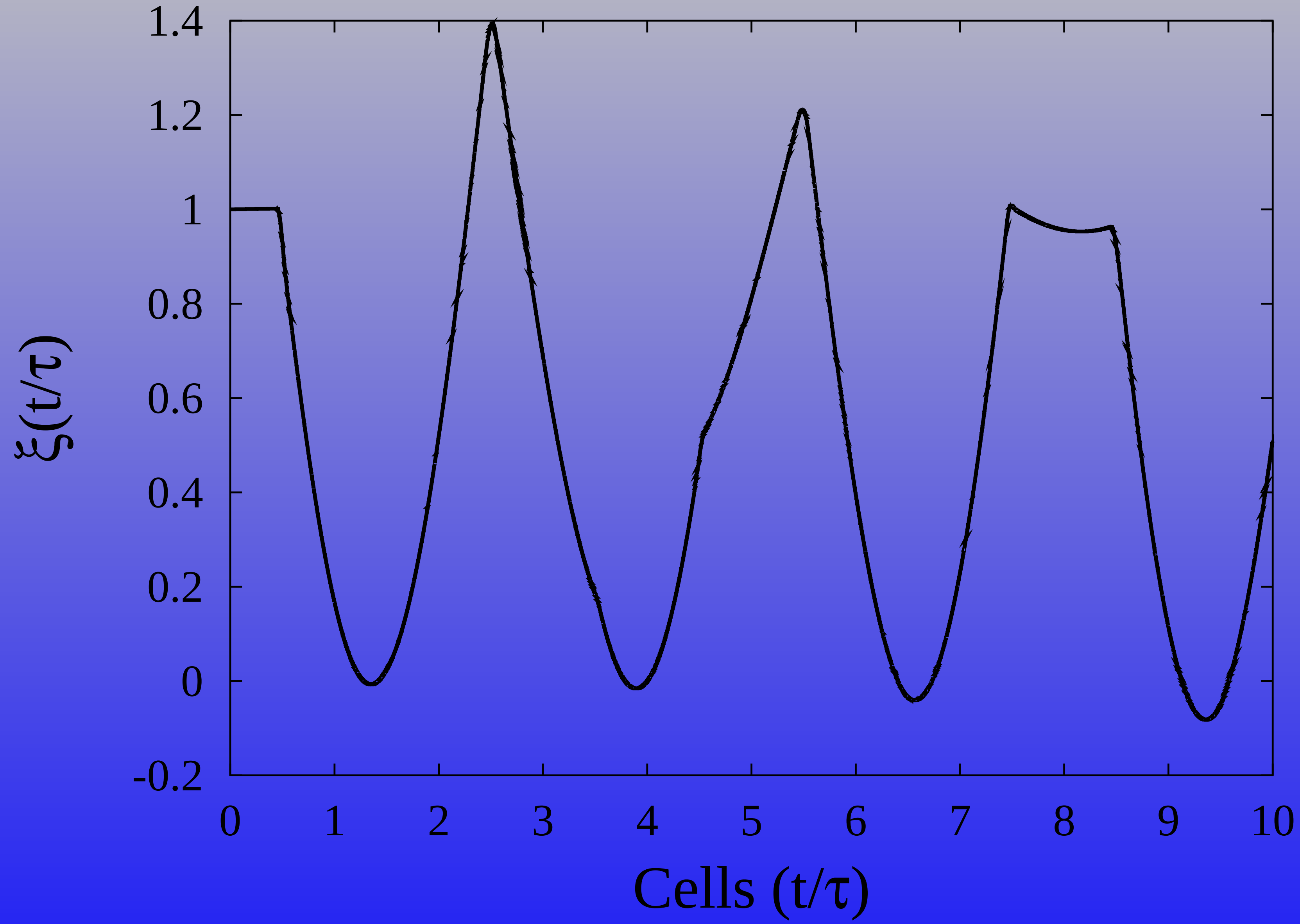
Here, the 3rd-order auxiliary equation for $\xi(t)$ specializes to

$$\sum_i \left[x_i^2 \left(\dddot{\xi} + 4\dot{\xi}\omega_x^2 + 4\xi\omega_x\dot{\omega}_x\right) + y_i^2 \left(\dddot{\xi} + 4\dot{\xi}\omega_y^2 + 4\xi\omega_y\dot{\omega}_y\right) + z_i^2 \left(\dddot{\xi} + 4\dot{\xi}\omega_z^2 + 4\xi\omega_z\dot{\omega}_z\right) + \dot{\xi}\sum_{j\neq i}\frac{c_1}{r_{ij}}\right] = 0\,.$$

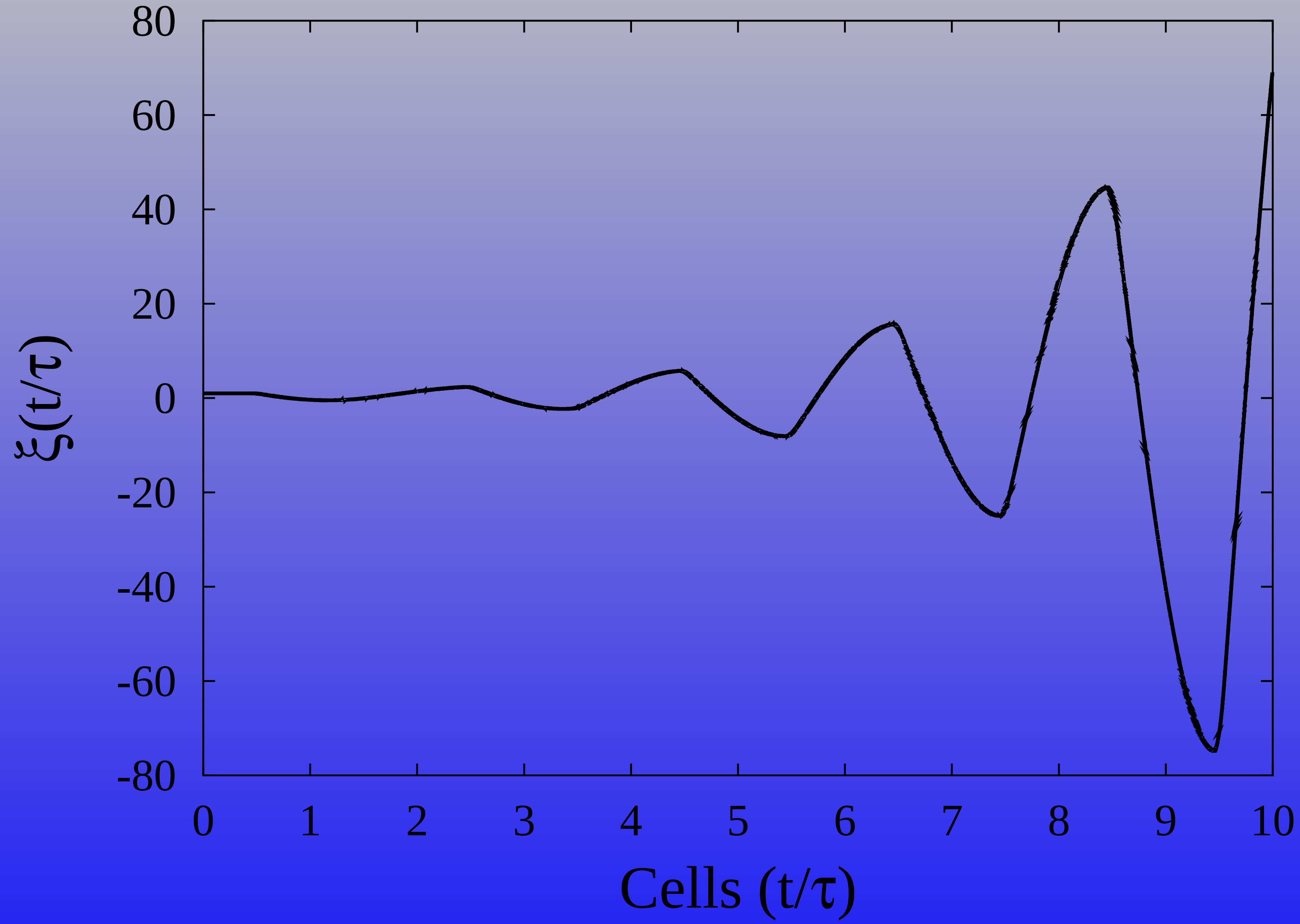
Here, the 3rd-order auxiliary equation for $\xi(t)$ specializes to

$$\sum_i \Big[x_i^2 \left(\dddot{\xi} + 4\dot{\xi}\omega_x^2 + 4\xi\omega_x\dot{\omega}_x\right) + y_i^2 \left(\dddot{\xi} + 4\dot{\xi}\omega_y^2 + 4\xi\omega_y\dot{\omega}_y\right) + z_i^2 \left(\dddot{\xi} + 4\dot{\xi}\omega_z^2 + 4\xi\omega_z\dot{\omega}_z\right) + \dot{\xi}\sum_{j\neq i}\frac{c_1}{r_{ij}}\Big] = 0\,.$$

- Non-autonomous system: a solution $\xi(t) = \text{const}$ does not exist.
- $3N$-degree-of-freedom system: the auxiliary equation depends on $\vec{x}$, $\vec{y}$, and $\vec{z}$.
- The particular evolution of $\xi(t)$ characterizes the dynamical behavior of the system as a whole.
- $\xi(t)$ may be unstable even if the dynamical system itself is stable. Then, the hyper-surface $I = \text{const}$ becomes increasingly distorted.



$\xi(t)$ as stable solution of the auxiliary equation for $\sigma_0 = 45^\circ$, $\sigma = 9^\circ$.



$\xi(t)$ as unstable solution of the auxiliary equation for $\sigma_0 = 60^\circ$, $\sigma = 15^\circ$.

We summarize:

- First time that an invariant I has been derived for such a high-dimensional time-dependent non-linear system.

We summarize:

- First time that an invariant I has been derived for such a high-dimensional time-dependent non-linear system.
- Price: the auxiliary equation for $\xi(t)$ depends on all particle coordinates.

We summarize:

- First time that an invariant I has been derived for such a high-dimensional time-dependent non-linear system.
- Price: the auxiliary equation for $\xi(t)$ depends on all particle coordinates.
- $\xi(t)$ reflects the collective evolution of the N-particle system.

We summarize:

- First time that an invariant I has been derived for such a high-dimensional time-dependent non-linear system.
- Price: the auxiliary equation for $\xi(t)$ depends on all particle coordinates.
- $\xi(t)$ reflects the collective evolution of the N-particle system.
- Example: stability analysis of the auxiliary equation for the time-dependent linear oscillator $\rightsquigarrow$ regimes of oscillatory versus chaotic time evolution of charged particle beam envelopes.

We summarize:

- First time that an invariant I has been derived for such a high-dimensional time-dependent non-linear system.
- Price: the auxiliary equation for $\xi(t)$ depends on all particle coordinates.
- $\xi(t)$ reflects the collective evolution of the N-particle system.
- Example: stability analysis of the auxiliary equation for the time-dependent linear oscillator $\leadsto$ regimes of oscillatory versus chaotic time evolution of charged particle beam envelopes.
- Further investigations on this issue are necessary.

Verification of simulations

We return the general case and recapitulate Noether's theorem:

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

is an invariant for a system whose time evolution follows from

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

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

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

This can also be shown directly if we evaluate dI/dt and insert the auxiliary equation. The remaining terms vanish exactly if the canonical equations hold.

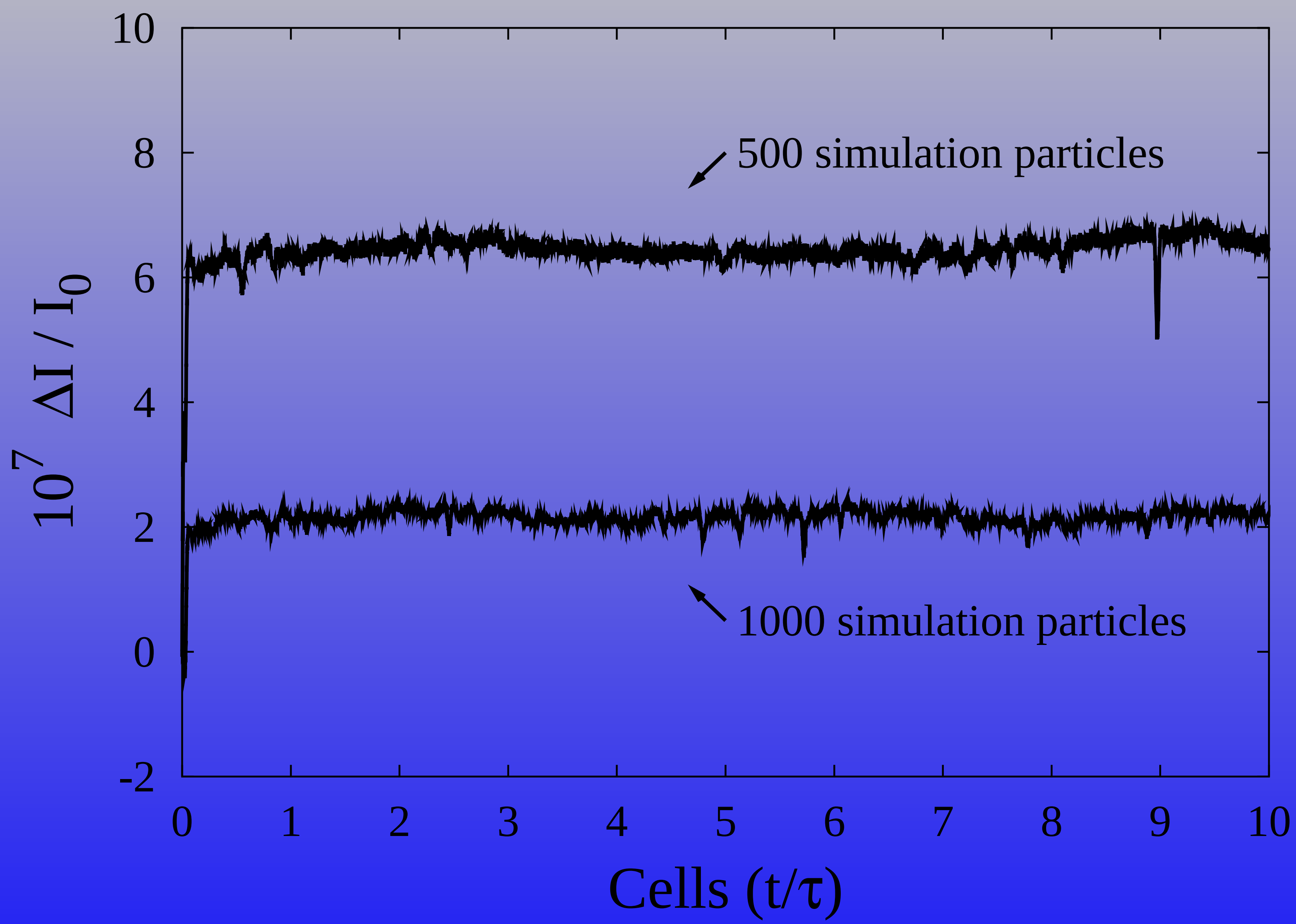
- The invariant I is a time integral of the auxiliary equation if $\vec{q}(t)$ and $\vec{p}(t)$ are time integrals of the canonical equations.

- The invariant I is a time integral of the auxiliary equation if $\vec{q}(t)$ and $\vec{p}(t)$ are time integrals of the canonical equations.
- If $\vec{q}(t)$ and $\vec{p}(t)$ follow from computer simulations, the canonical equations are only approximately satisfied because of the generally limited accuracy of numerical methods.

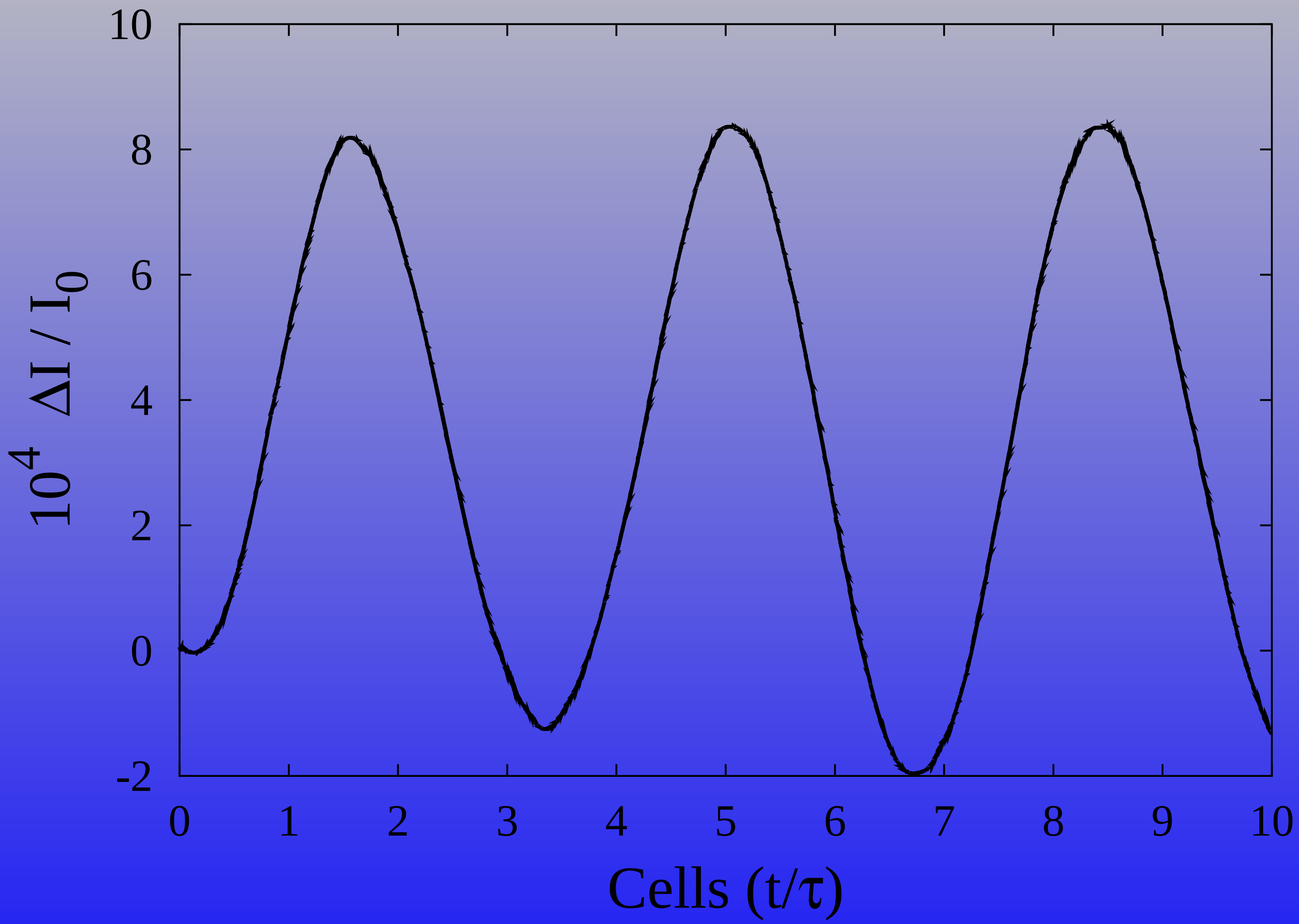
- The invariant I is a time integral of the auxiliary equation if $\vec{q}(t)$ and $\vec{p}(t)$ are time integrals of the canonical equations.
- If $\vec{q}(t)$ and $\vec{p}(t)$ follow from computer simulations, the canonical equations are only approximately satisfied because of the generally limited accuracy of numerical methods.
- $\leadsto$ If the canonical equations and the auxiliary equation are integrated numerically, the quantity I is no longer *strictly* constant.

- The invariant I is a time integral of the auxiliary equation if $\vec{q}(t)$ and $\vec{p}(t)$ are time integrals of the canonical equations.
- If $\vec{q}(t)$ and $\vec{p}(t)$ follow from computer simulations, the canonical equations are only approximately satisfied because of the generally limited accuracy of numerical methods.
- $\leadsto$ If the canonical equations and the auxiliary equation are integrated numerically, the quantity I is no longer *strictly* constant.
- $[I(t) - I(0)]/I(0)$: relative deviation of the calculated $I(t)$ from the exact invariant $I(0)$. $\leadsto$ "A posteriori" error estimation for the simulation.

- The invariant I is a time integral of the auxiliary equation if $\vec{q}(t)$ and $\vec{p}(t)$ are time integrals of the canonical equations.
- If $\vec{q}(t)$ and $\vec{p}(t)$ follow from computer simulations, the canonical equations are only approximately satisfied because of the generally limited accuracy of numerical methods.
- $\rightsquigarrow$ If the canonical equations and the auxiliary equation are integrated numerically, the quantity I is no longer *strictly* constant.
- $[I(t) - I(0)]/I(0)$: relative deviation of the calculated $I(t)$ from the exact invariant $I(0)$. $\rightsquigarrow$ "A posteriori" error estimation for the simulation.
- $\rightsquigarrow$ Generalization of the accuracy test $H = \text{const}$, which applies for autonomous systems only.



Relative invariant error $\Delta I / I_0$ for 3D simulations of a charged particle beam with different numbers of macro-particles.



Relative invariant error $\Delta I/I_0$ for a 3D simulation of a charged particle beam with a systematic 5 %-error in the space-charge force calculations.

Conclusions

- For explicitly time-dependent Hamiltonian systems, invariants I that depend on the canonical variables only do not exist. All invariants are associated with solutions $\xi(t)$ of an auxiliary equation.

Conclusions

- For explicitly time-dependent Hamiltonian systems, invariants I that depend on the canonical variables only do not exist. All invariants are associated with solutions $\xi(t)$ of an auxiliary equation.
- Apart from very specific cases, the auxiliary equation for $\xi(t)$ depends on the canonical coordinates $\vec{q}(t)$. This induces a coupling of the auxiliary equation to the canonical equations.

Conclusions

- For explicitly time-dependent Hamiltonian systems, invariants I that depend on the canonical variables only do not exist. All invariants are associated with solutions $\xi(t)$ of an auxiliary equation.
- Apart from very specific cases, the auxiliary equation for $\xi(t)$ depends on the canonical coordinates $\vec{q}(t)$. This induces a coupling of the auxiliary equation to the canonical equations.
- The coupled $(2n+3)$-system of $2n$ first-order canonical equations and the 3 first-order auxiliary equations determines both the system's time evolution *and* its symmetries.

- This coupling is the reason why the strategy to simplify the solution of a given dynamical system by finding invariants generally does not work.

- This coupling is the reason why the strategy to simplify the solution of a given dynamical system by finding invariants generally does not work.
- In the $(2n+3)$-dimensional space, the invariant I represents a hyper-surface on which the motion takes place. It can be interpreted as the energy surface that includes the energy flow into and from the Hamiltonian system $H(\vec{p}, \vec{q}, t)$.

- This coupling is the reason why the strategy to simplify the solution of a given dynamical system by finding invariants generally does not work.
- In the $(2n+3)$-dimensional space, the invariant I represents a hyper-surface on which the motion takes place. It can be interpreted as the energy surface that includes the energy flow into and from the Hamiltonian system $H(\vec{p}, \vec{q}, t)$.
- The solution $\xi(t)$ of the auxiliary equation may be unstable even if the dynamical system itself is stable. The stability analysis of the the auxiliary equation may provide a direct method to classify a Hamiltonian system with respect to *chaotic* and *non-chaotic* behavior.

Publications

- Phys. Rev. Lett. **85**, 3830 (2000)
- Phys. Rev. E **64**, 026503 (2001)
- Ann. Phys. (Leipzig) **11**, 15 (2002)
- Habilitation thesis (submitted Dec. 2001)
- This talk is available under "http://www.gsi.de/˜struck"