Hamiltonian mechanics in the "extended" phase space

Jürgen Struckmeier

j.struckmeier@gsi.de

GSI Accelerator Seminar

Darmstadt, 03 July 2003

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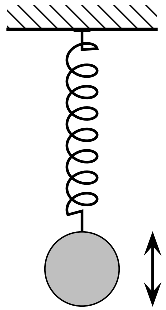

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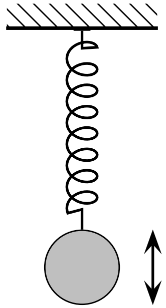

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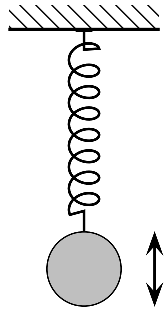

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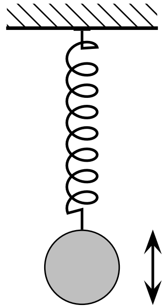

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- Solution strategy: canonical mapping into the time-independent harmonic oscillator $H'(q',p')$, back transformation of its solution into the original time-dependent system. $H'(q,p,t)$ is an invariant!
- Problem: a conventional generating function $f_2(q,p',t)$ that defines such a mapping does not exist.
- Necessary: (re-)formulation of the canonical transformation theory in the "extended" phase space.

Outline

- Principle of least action and its general formulation
- Extended form of the canonical equations
- Canonical transformations in the extended phase space
- Example 1: time-dependent harmonic oscillator
- Example 2: general time-dependent potential
- Conclusions and outlook

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A *path* γ in the $2n$ dimensional phase space with the time t the independent variable is defined by

$$\gamma : \left\{ \left(\vec{q}, \vec{p}\right) \in \mathbb{R}^{2n} \,\middle|\, \vec{q} = \vec{q}(t), \vec{p} = \vec{p}(t), t_0 \leq t \leq t_1 \right\} \, .$$

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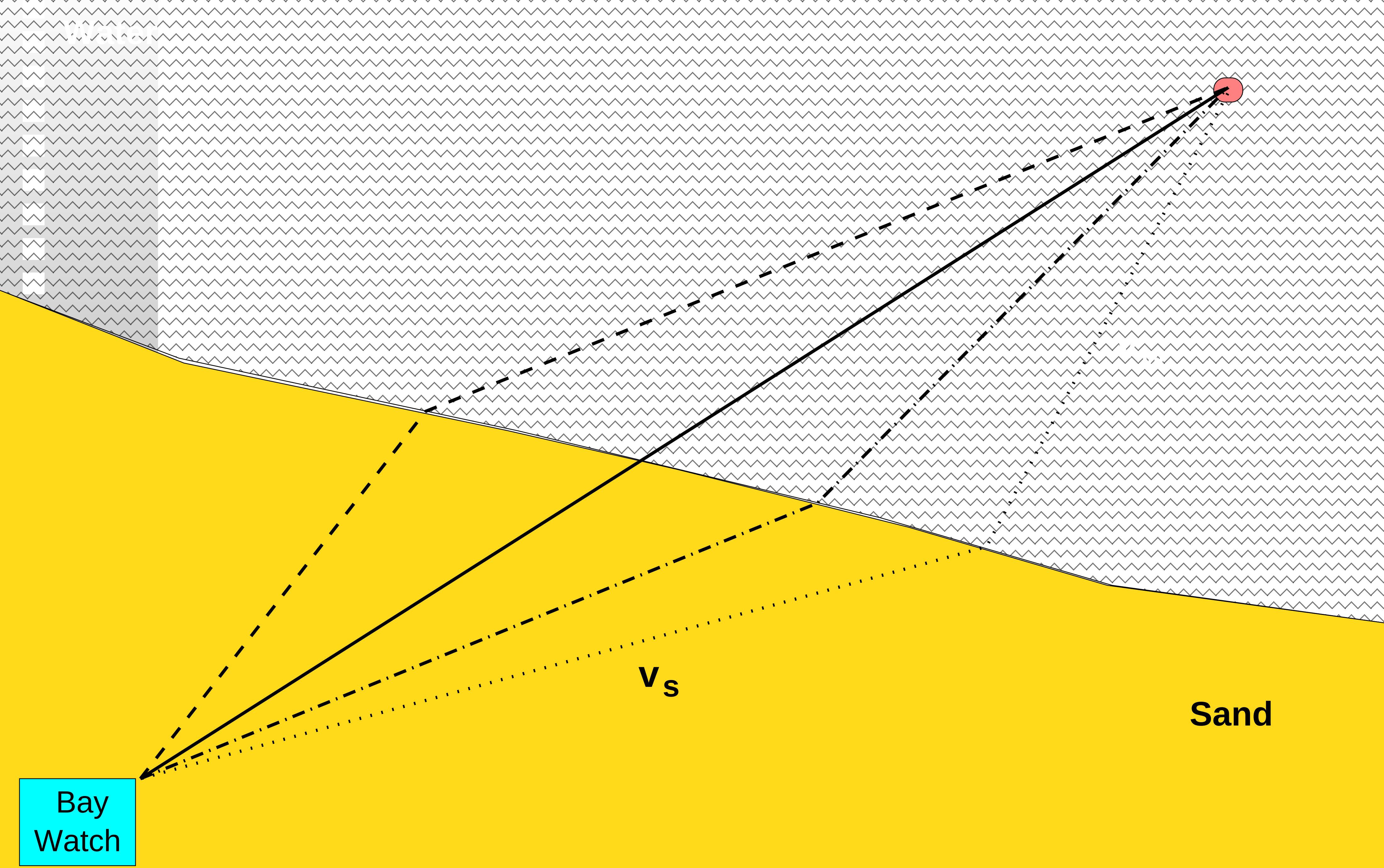
We formulate the principle of least action via a *functional* Φ, hence with a mapping of the set of paths γ into $\mathbb{R}$

$$\Phi(\gamma) = \int_{t_0}^{t_1} \left[\vec{p}(t) \frac{d\vec{q}(t)}{dt} - H\left(\vec{q}(t), \vec{p}(t), t\right) \right] dt .$$

The function $H : \mathbb{R}^{2n} \times \mathbb{R} \to \mathbb{R}$ denotes the Hamiltonian.



Example of a functional $\Phi : \gamma \mapsto \Delta t \in \mathbb{R}$.

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Among all thinkable paths γ, a dynamical system "chooses" exactly that one γ_{ext}, where $\Phi(\gamma_{\mathrm{ext}})$ takes on a minimum.

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Calculus of variations: the functional $\Phi(\gamma)$ takes on a minimum ($\delta\Phi(\gamma) = 0$), exactly if the phase-space path $\big(\vec{q}(t), \vec{p}(t)\big)$ satisfies the "canonical equations"

$$\frac{d\vec{q}}{dt} = \frac{\partial H}{\partial \vec{p}}\,, \qquad \frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{q}}\,.$$

Let us look back to the variational problem $\delta\Phi(\gamma) \stackrel{!}{=} 0$

$$\delta\Phi(\gamma) = \delta \int_{t_0}^{t_1} \left[\vec{p}(t)\frac{d\vec{q}(t)}{dt} - H\big(\vec{q}(t), \vec{p}(t), t\big)\right] dt \stackrel{!}{=} 0\,.$$

We observe: the time t plays a *twofold* role, namely that of the formal *integration variable* and that of an *external parameter* in the argument list of the Hamiltonian.

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$\leadsto$ Not the most general formulation of the principle of least action!

$\leadsto$ We must *separate* the explicit t-dependence of the Hamiltonian from the formal integration variable.

A more general form of the variational problem is obtained substituting $t = t(s)$, with s the new integration variable

$$\Phi(\gamma) = \int_{s_0}^{s_1} \left[\vec{p}(s)\, \frac{d\vec{q}(s)}{ds} - H\big(\vec{q}(s), \vec{p}(s), t(s)\big) \frac{dt(s)}{ds} \right] \, ds \, .$$

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The symmetric form of the integrand suggests to define the $2n+2$ dimensional “extended” phase space, introducing

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$\leadsto$ $\mathcal{H} = \mathcal{H}(s) \in \mathbb{R}$ must be understood as the *value* of the Hamiltonian $H(\vec{q}, \vec{p}, t)$, hence as the system’s “instantaneous energy”

$$\mathcal{H}(s) = H(\vec{q}(s), \vec{p}(s), t(s))\,.$$

Defining the extended vectors $\vec{q}_1 = (\vec{q}, t)$ and $\vec{p}_1 = (\vec{p}, -\mathcal{H})$, the variational integral can be cast into the familiar form

$$\delta \int_{s_0}^{s_1} \left[\vec{p}_1(s) \, \frac{d\vec{q}_1(s)}{ds} - H_1\big(\vec{q}_1(s), \vec{p}_1(s)\big) \right] ds \stackrel{!}{=} 0 \,,$$

with the extended Hamiltonian $H_1 = 0$ as the *implicit function*

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$\rightsquigarrow$ The variation of the functional vanishes again if the *extended phase-space path* $\big(\vec{q}_1(s), \vec{p}_1(s)\big)$ satisfies the *extended set of canonical equations*

$$\frac{d\vec{q}_1}{ds} = \frac{\partial H_1}{\partial \vec{p}_1} \, , \qquad \frac{d\vec{p}_1}{ds} = -\frac{\partial H_1}{\partial \vec{q}_1} \, .$$

In terms of the conv. quantities $\vec{q}$, $\vec{p}$, t, $\mathcal{H}$ and H, this means

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- The principle of least action is equally satisfied for *all* differentiable parameterizations of time $t = t(s)$.
- Exactly this freedom to appropriately adapt $t = t(s)$ allows to define more general canonical transformations in the extended phase space.

Canonical transformations

General condition for canonical transformations:

The variational principle must be maintained.

This means in the *conventional* description

$$\delta \int_{t_0}^{t_1} \left[\vec{p}\,\dot{\vec{q}} - H\big(\vec{q}, \vec{p}, t\big)\right] dt = \delta \int_{t_0}^{t_1} \left[\vec{p}\,'\dot{\vec{q}}\,' - H'\big(\vec{q}\,', \vec{p}\,', t\big)\right] dt\,.$$

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$\leadsto$ Only a CT in the extended phase space can do that job

$$H(\vec{q},\vec{p},t) \xrightarrow{\text{CT in the extended PhSp}} H'(\vec{q}^{\,\prime},\vec{p}^{\,\prime},t')\,.$$

The general condition for transformations to be canonical writes analogously in the *extended phase-space description*

$$\delta \int_{s_1}^{s_2} \left[\vec{p}_1 \frac{d\vec{q}_1}{ds} - H_1\big(\vec{q}_1, \vec{p}_1\big) \right] ds = \delta \int_{s_1}^{s_2} \left[\vec{p}_1^{\,\prime} \frac{d\vec{q}_1^{\,\prime}}{ds} - H_1^{\prime}\big(\vec{q}_1^{\,\prime}, \vec{p}_1^{\,\prime}\big) \right] ds \, .$$

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If we require the extended Hamiltonian H_1 to be conserved

$$H_1(\vec{q}_1, \vec{p}_1) \equiv H_1'(\vec{q}_1', \vec{p}_1') \,,$$

this yields the general condition

$$\vec{p}_1 \, d\vec{q}_1 = \vec{p}_1' \, d\vec{q}_1' + dF_1\big(\vec{q}_1, \vec{q}_1'\big) \,,$$

with

$$dF_1 = \frac{\partial F_1}{\partial \vec{q}_1} d\vec{q}_1 + \frac{\partial F_1}{\partial \vec{q}_1'} d\vec{q}_1' \,.$$

Comparing the coefficients, we find the transformation rules

$$\vec{p}_1 = \frac{\partial F_1}{\partial \vec{q}_1}\,, \qquad \vec{p}_1^{\,\prime} = -\frac{\partial F_1}{\partial \vec{q}_1^{\,\prime}}\,,$$

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or, equivalently, in terms of the quantities $\vec{q}$, $\vec{p}$, t and $\mathcal{H}$

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Accordingly, we refer to $F_1(\vec{q}, t, \vec{q}\,', t')$ as the *generating function* of the extended canonical transformation.

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By means of a *Legendre* transformation

$$F_2\big(\vec{q}_1, \vec{p}_1^{\,\prime}\big) = F_1\big(\vec{q}_1, \vec{q}_1^{\,\prime}\big) + \vec{q}_1^{\,\prime}\,\vec{p}_1^{\,\prime}\,,$$

the generating function F_1 can be converted into a generating function of type F_2.

The transformation rules associated with $F_2(\vec{q}, \vec{p}', t, \mathcal{H}')$ are

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The "conventional" CTs, generated by $f_2(\vec{q}, \vec{p}', t)$, constitute a *subset* of CTs in the extended phase space. Defining

$$F_2(\vec{q}, \vec{p}', t, \mathcal{H}') = f_2(\vec{q}, \vec{p}', t) - t\,\mathcal{H}'\,,$$

we find the well-known conventional transformation rules

$$\vec{p} = \frac{\partial f_2}{\partial \vec{q}}\,, \quad \vec{q}\,' = \frac{\partial f_2}{\partial \vec{p}\,'}\,, \quad H' = H + \frac{\partial f_2}{\partial t}\,, \quad t' = t\,,$$

substituting finally $\mathcal{H} = H$ and $\mathcal{H}' = H'$.

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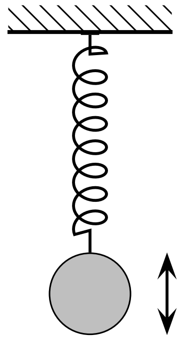
$$\vec{p} = \frac{\partial f_2}{\partial \vec{q}}\,, \quad \vec{q}\,' = \frac{\partial f_2}{\partial \vec{p}\,'}\,, \quad H' = H + \frac{\partial f_2}{\partial t}\,, \quad t' = t\,,$$

substituting finally $\mathcal{H} = H$ and $\mathcal{H}' = H'$.

$\leadsto$ The extended transformation rules allow more general relations of $H \leftrightarrow H'$ and $t \leftrightarrow t'$ than the conventional ones.

Example 1: harmonic oscillator

We consider the time-dependent 1-D Hamiltonian system



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

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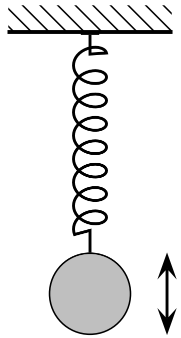

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We want to transform this system into a time-<u>in</u>dependent system of the *same form*

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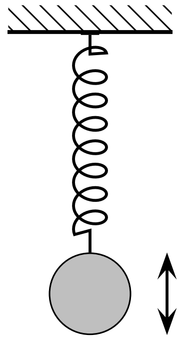

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The generating function F_2 that does the job has been found to be

$$F_2\big(q,p',t,\mathcal{H}'\big) = \frac{q\,p'}{\sqrt{\xi(t)}} + \frac{\dot{\xi}(t)}{4\xi(t)}\,q^2 - \mathcal{H}'\int_0^t \frac{d\tau}{\xi(\tau)}\,.$$

$\xi(t)$ denotes a yet undetermined differentiable function of time.

For this particular F_2, the transformation rules follow as

$$\begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} 1/\sqrt{\xi} & 0 \\ -\frac{1}{2}\dot{\xi}/\sqrt{\xi} & \sqrt{\xi} \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \,,$$

$$t' = \int_0^t \frac{d\tau}{\xi(\tau)} \,, \qquad \mathcal{H}' = \xi\,\mathcal{H} - \tfrac{1}{2}\dot{\xi}\,q\,p + \tfrac{1}{4}\ddot{\xi}\,q^{\,2}\,.$$

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Replacing $\mathcal{H}'$ and $\mathcal{H}$ by H' and H, and eliminating the unprimed variables, the requested Hamiltonian H' emerges

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

with

$$\omega_0^2 = \tfrac{1}{2}\xi\ddot{\xi} - \tfrac{1}{4}\dot{\xi}^2 + \omega^2(t) \, \xi^2 \, .$$

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Due to $\omega_0^2 \stackrel{!}{=}$ const., the function $\xi(t)$ is now *determined*. With this $\xi(t)$, the value $\mathcal{H}'$ of H' embodies an invariant I

$$H' \equiv I(q, p, t) = \xi H - \tfrac{1}{2}\dot{\xi}\,q\,p + \tfrac{1}{4}\ddot{\xi}\,q^2 .$$

Question: what is the physical meaning of $\xi(t)$? We easily verify that

$$\xi(t) = q^{2}(t)$$

satisfies $\frac{1}{2}\xi\ddot{\xi} - \frac{1}{4}\dot{\xi}^2 + \omega^2(t)\,\xi^2 =$ const., provided that $q(t)$ is a solution of the equation of motion of the time-dependent harmonic oscillator

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With $\xi(t) = \bar{q}^{\,2}(t)$, $\bar{q}(t)$ denoting a *second* solution of the equation of motion, the invariant takes on the form

$$I = \tfrac{1}{2}(p\,\bar{q} - q\,\bar{p})^2\,.$$

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$\leadsto$ The invariant of the time-dependent harmonic oscillator has the form of a conservation law of the angular momentum in central force fields.

$\leadsto$ Accelerator physics: I is referred to as “rms emittance”.

Example 2: time-dependent potential

We now consider the general n-dimensional non-linear time-dependent Hamiltonian system

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

Again, we want to transform it into a time-<u>in</u>dependent Hamiltonian system *of the same form*

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The most general function F_2 generating the transformation that maintains the form of H is given by

$$F_2(\vec{q}, \vec{p}\,', t, \mathcal{H}') = \frac{\vec{q}\,\vec{p}\,'}{\sqrt{\xi(t)}} + \frac{\dot{\xi}(t)}{4\xi(t)}\,\vec{q}^{\,2} - \mathcal{H}' \int_0^t \frac{d\tau}{\xi(\tau)}\,.$$

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$$\begin{pmatrix} \vec{q}\,' \\ \vec{p}\,' \end{pmatrix} = \begin{pmatrix} 1/\sqrt{\xi} & 0 \\ -\frac{1}{2}\dot{\xi}/\sqrt{\xi} & \sqrt{\xi} \end{pmatrix} \begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix} ,$$

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$$V'(\vec{q}\,', t') = \tfrac{1}{4}\vec{q}\,'^{\,2}\left(\xi\ddot{\xi} - \tfrac{1}{2}\dot{\xi}^2\right) + \xi\, V\left(\sqrt{\xi}\,\vec{q}\,', t\right).$$

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We now make use of the freedom to choose $\xi(t)$ by requiring

$$\frac{\partial V'}{\partial t'} \stackrel{!}{=} 0\,.$$

Hereby, we determine transformation of time $t'(t)$.

The value $\mathcal{H}'$ of H' then constitutes a constant of motion.

This leads to a *linear, homogeneous* third-order system

$$\frac{d}{dt}\begin{pmatrix}\xi\\ \dot{\xi}\\ \ddot{\xi}\end{pmatrix} = \begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ -f_1(\vec{q}(t),t) & -f_2(\vec{q}(t),t) & 0\end{pmatrix}\begin{pmatrix}\xi\\ \dot{\xi}\\ \ddot{\xi}\end{pmatrix}$$

For *known* $\vec{q} = \vec{q}\,(t)$, the coefficients are functions of time only

$$f_1(\vec{q}\,(t),t) = \frac{4}{\vec{q}^{\,2}}\frac{\partial V}{\partial t}\,, \qquad f_2(\vec{q}\,(t),t) = \frac{4}{\vec{q}^{\,2}}\left[V(\vec{q},t) + \tfrac{1}{2}\vec{q}\,\frac{\partial V}{\partial \vec{q}}\right]\,.$$

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- The trace of the system matrix is zero. $\leadsto$ The Wronski determinant of any solution matrix $\Xi(t)$ is constant. $\leadsto$ With $\Xi(0) = E$, we get $\det \Xi(t) \equiv 1$.

The transformed Hamiltonian

$$H'\big(\vec{q}\,',\vec{p}\,'\big) = \tfrac{1}{2}\vec{p}\,'^{\,2} + V'\big(\vec{q}\,'\big) = \text{const.}$$

can be expressed in terms of the original coordinates

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With the 3×3 solution matrix $\Xi(t)$ of the third-order system ($\Xi(0)=E$), this writes in terms of the transpose matrix $\Xi^T(t)$

$$\begin{pmatrix} H_0 \\ -\frac{1}{2}\vec{q}_0\,\vec{p}_0 \\ \frac{1}{4}\vec{q}_0^{\,2} \end{pmatrix} = \begin{pmatrix} \xi_1 & \dot{\xi}_1 & \ddot{\xi}_1 \\ \xi_2 & \dot{\xi}_2 & \ddot{\xi}_2 \\ \xi_3 & \dot{\xi}_3 & \ddot{\xi}_3 \end{pmatrix} \begin{pmatrix} H \\ -\frac{1}{2}\vec{q}\,\vec{p} \\ \frac{1}{4}\vec{q}^{\,2} \end{pmatrix}, \qquad \det\Xi = 1\,.$$

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We find: the vector $\big(H, -\frac{1}{2}\vec{q}\,\vec{p}, \frac{1}{4}\vec{q}^{\,2}\big)$ has *always* a *linear correlation to its initial state*.

For $\partial V/\partial t \equiv 0$, a solution $\xi_1(t)\equiv 1$ exists $\rightsquigarrow$ $H = H_0$.

Finally, we consider the transformation of the 3-form $dH\, d(\vec{q}\,\vec{p})\, d(\vec{q}^{\,2})$:

$$dH_0\, d(\vec{q}_0\, \vec{p}_0\,)\, d(\vec{q}_0^{\,2}) = \frac{\partial\,(H_0, \vec{q}_0\, \vec{p}_0, \vec{q}_0^{\,2})}{\partial\,(H, \vec{q}\,\vec{p}, \vec{q}^{\,2})}\; dH\, d(\vec{q}\,\vec{p})\, d(\vec{q}^{\,2})\,.$$

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Because of $\det\Xi = 1$ conclude that

$$\boxed{J = dH\, d(\vec{q}\,\vec{p})\, d(\vec{q}^{\,2}) = \text{const.}}$$

$\rightsquigarrow$ The 3-form J is invariant with regard to the time evolution of the general Hamiltonian system

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

Conclusions and outlook

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- To investigate: what does a chaotic evolution of $\Xi(t)$ tell us about the evolution of the system as a whole?
- To investigate: physical meaning of the invariant 3-form

$$J = d\mathcal{H}\, d(\vec{q}\,\vec{p})\, d(\vec{q}^{\,2}) = \text{const.}$$

Publications

- Phys. Rev. Lett. **85**, 3830 (2000)
- Phys. Rev. E **64**, 026503 (2001)
- Phys. Rev. E **66**, 066605 (2002)
- Ann. Phys. (Leipzig) **11**, 15 (2002)
- Habilitation thesis (GSI Report 2002-06)
- This talk may be downloaded from "http://www.gsi.de/˜struck"