Newtonian dynamics
flow!Hamiltonian
degree of freedom

Chapter 5

Newtonian dynamics

You might think that the strangeness of contracting flows, flows such as the Rössler flow of figure 2.3 is of concern only to chemists; real physicists do Hamiltonians, right? Not at all - while it is easier to visualize aperiodic dynamics when a flow is contracting onto a lower-dimensional attracting set, there are plenty examples of chaotic flows that do preserve the full symplectic invariance of Hamiltonian dynamics. The truth is, the whole story started with Poincaré's restricted 3-body problem, a realization that chaos rules also in general (non-Hamiltonian) flows came much later.

Here we briefly review parts of classical dynamics that we will need later on; symplectic invariance, canononical transformations, and stability of Hamiltonian flows. We discuss billiard dynamics in some detail in chapter 6.

5.1 Hamiltonian flows

(P. Cvitanović and L.V. Vela-Arevalo)

An important class of flows are Hamiltonian flows, given by a Hamiltonian $H(q,p)$ together with the Hamilton's equations of motion

☞ appendix D

revert to (q,p) order throughtout

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \tag{5.1}$$

with the $2D$ phase space coordinates x split into the configuration space coordinates and the conjugate momenta of a Hamiltonian system with D degrees of freedom (dof):

☞ sect. 31.1.1

$$x = (\mathbf{q}, \mathbf{p}), \qquad \mathbf{q} = (q_1, q_2, \ldots, q_D), \qquad \mathbf{p} = (p_1, p_2, \ldots, p_D). \tag{5.2}$$

The energy, or the value of the Hamiltonian function at the phase space

level set
Duffing!undamped
integrable system
helium!collinear

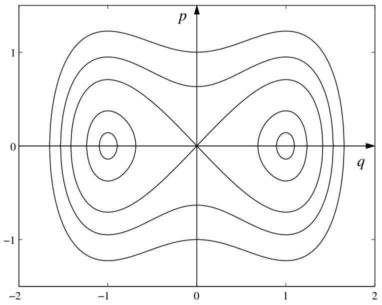


Figure 5.1: Phase plane of the unforced, undamped Duffing oscillator. The trajectories lie on level sets of the Hamiltonian (5.4).

point $x = (\mathbf{q}, \mathbf{p})$ is constant along the trajectory $x(t)$,

$$\begin{aligned} \frac{d}{dt} H(\mathbf{q}(t), \mathbf{p}(t)) &= \frac{\partial H}{\partial q_i} \dot{q}_i(t) + \frac{\partial H}{\partial p_i} \dot{p}_i(t) \\ &= \frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} = 0 \,, \end{aligned} \tag{5.3}$$

so the trajectories lie on surfaces of constant energy, or *level sets* of the Hamiltonian $\{(q,p) : H(q,p) = E\}$. For 1-dof Hamiltonian systems this is basically the whole story.

Example 5.1 Unforced undamped Duffing oscillator: *When the damping term is removed from the Duffing oscillator (2.6), the system can be written in Hamiltonian form with the Hamiltonian*

$$H(q,p) = \frac{p^2}{2} - \frac{q^2}{2} + \frac{q^4}{4} . \tag{5.4}$$

This is a 1-dof Hamiltonian system, with a 2-dimensional phase space, the plane (q,p). The Hamilton's equations (5.1) are

$$\dot{q} = p \,, \qquad \dot{p} = q - q^3 \,. \tag{5.5}$$

For 1-dof systems, the "surfaces" of constant energy (5.3) are simply curves in the phase plane (q,p), and the dynamics is very simple: the curves of constant energy are *the trajectories, as shown in figure 5.1.*

trajectories need arrows, label font too small in figure 5.1

Thus all 1-dof systems are *integrable*, in the sense that the entire phase plane is foliated by curves of constant energy, either periodic – as is the case for the harmonic oscillator (a "bound state") – or open (a "scattering trajectory"). Add one more degree of freedom, and chaos breaks loose.

☞ example 7.1

Example 5.2 Collinear helium: *In chapter 38, we shall apply the periodic orbit theory to the quantization of helium. In particular, we will study* collinear helium, *a doubly charged nucleus with two electrons arranged on a line, an electron on each side of the nucleus. The Hamiltonian for this system is* [1]

☞ chapter 38

$$H = \frac{1}{2} p_1^2 + \frac{1}{2} p_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_1 + r_2} \,. \tag{5.6}$$

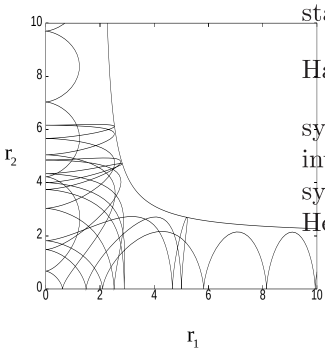


Figure 5.2: A typical collinear helium trajectory in the $r_1 - r_2$ plane; the trajectory enters along the r_1-axis and then, like almost every other trajectory, after a few bounces escapes to infinity, in this case along the r_2-axis.

stability!Hamiltonian flows
Hamiltonian!flows, stability
symplectic!invariance
invariance!symplectic
symplectic!form
Hessian matrix

Collinear helium has 2 dof, and thus a 4-dimensional phase space $\mathcal{M}$, which energy conservation reduces to 3 dimensions. The dynamics can be projected onto the 2-dimensional configuration plane, the (r_1, r_2), $r_i \geq 0$ quadrant, figure 5.2. It looks messy, and, indeed, it will turn out to be no less chaotic than a pinball bouncing between three disks. As always, a Poincaré section will be more informative than this rather arbitrary projection of the flow.

5.2 Stability of Hamiltonian flows

Hamiltonian flows offer an illustration of the ways in which an invariance of equations of motion can affect the dynamics. In the case at hand, the *symplectic invariance* will reduce the number of independent stability eigenvalues by a factor of 2 or 4.

5.2.1 Canonical transformations

The equations of motion for a time-independent, D-dof Hamiltonian (5.1) can be written

$$\dot{x}_i = \omega_{ij} H_j(x) , \qquad \omega = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix} , \quad H_j(x) = \frac{\partial}{\partial x_j} H(x) , \qquad (5.7)$$

use O de Almeida book argument here?

where $x = (\mathbf{q}, \mathbf{p}) \in \mathcal{M}$ is a phase space point, $H_k = \partial_k H$ is the column vector of partial derivatives of H, $\mathbf{I}$ is the $[D \times D]$ unit matrix, and ω the $[2D \times 2D]$ *symplectic* the form

$$\omega^T = -\omega , \qquad \omega^2 = -\mathbf{1} . \qquad (5.8)$$

The linearized motion in the vicinity $x + \delta x$ of a phase space trajectory $x(t) = (\mathbf{q}(t), \mathbf{p}(t))$ is described by the Jacobian matrix (4.23). For Hamiltonian flows the matrix of variations (4.32) takes form

$$\frac{d}{dt}\mathbf{J}^t(x) = A(x)\mathbf{J}^t(x) , \qquad A_{ij}(x) = \omega_{ik} H_{kj}(x) , \qquad (5.9)$$

[1]Mason: mention briefly "transition state"

symplectic!transformation
canonical!transformation
Lie group!orthogonal
orthogonal!Lie group
symplectic!Lie algebra
Lie algebra!symplectic
canonical transformation
symplectic!map
conservation!phase space volume
Liouville!theorem

where the matrix of second derivatives $H_{kn} = \partial_k \partial_n H$ is called the *Hessian matrix*. From the symmetry of H_{kn} it follows that

$$A^T \omega + \omega A = 0 \,. \tag{5.10}$$

This is the defining property for infinitesimal generators of *symplectic* (or canonical) transformations, transformations which leave the symplectic form ω invariant.

More explicitely: just as the rotation group $O(d)$ is the Lie group of all matrix transformations which preserve a bilinear symmetric invariant $x^2 = x_i \delta_{ij} x_j$, that is, the length squared, the symplectic group $Sp(2D)$ is defined as the Lie group of all matrix transformations $x' = \mathbf{J}x$ which preserve a bilinear *antisymmetric* invariant $x_i \omega_{ij} y_j$. The symplectic Lie algebra $sp(2D)$ follows by writing $\mathbf{J} = \exp(\delta t A)$ and linearizing $\mathbf{J} = 1 + \delta t A$. This yields (5.10) as the defining property of infinitesimal symplectic transformations.

Consider now a smooth nonlinear change of variables of form $y = h(x)$, and the Hamiltonian as the function of the new phase space variables, $K(x) = H(h(x))$. Rewriting (5.7) as a function of y and employing the chain rule we find

$$\begin{aligned} \partial K(x) &= (\partial h)^T \partial H(h(x)) = (\partial h)^T (-\omega \, \dot{y}) \\ &= -(\partial h)^T \omega \, (\partial h) \, \dot{x} \,, \end{aligned} \tag{5.11}$$

where $(\partial h)_{kn} = \partial h_k / \partial x_n$. Consider the case that ∂h, the linearization of h, is a symplectic transformation, that is, a map that preserves the symplectic form,

$$(\partial h)^T \omega \, (\partial h) = \omega \,. \tag{5.12}$$

In that case $K(x)$ also induces a Hamiltonian flow $\dot{x}_i = \omega_{ij} K_j(x)$, and h is called a *canonical transformation*. We care about canonical transformations for two reasons. First (and this is a dark art), if the canonical transformation h is very cleverly chosen, the flow in new coordinates might be considerably simpler than the original flow. Second, Hamiltonian flows themselves are a prime example of canonical transformations.

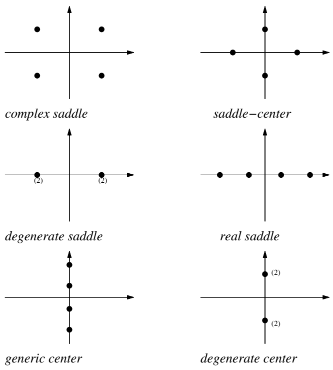
☞ example 7.1

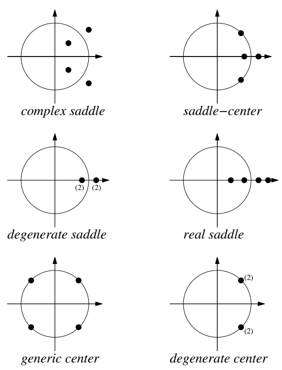
Example 5.3 Hamiltonian flows are canonical: *For Hamiltonian flows it follows from (5.10) that* $\frac{d}{dt}\left(\mathbf{J}^T \omega \mathbf{J}\right) = 0$, *and since at the initial time* $\mathbf{J}^0(x_0) = \mathbf{1}$, $\mathbf{J}$ *is a symplectic transformation* $\mathbf{J}^T \omega \mathbf{J} = \omega$. *This equality is valid for all times, so a Hamiltonian flow* $f^t(x)$ *is a canonical transformation, with the linearization* $\partial_x f^t(x)$ *a symplectic transformation (5.12):*

$$\mathbf{J}^T \omega \mathbf{J} = \omega \,. \tag{5.13}$$

For notational brevity here we have suppressed the dependence on time and the initial point, $\mathbf{J} = \mathbf{J}^t(x_0)$. *By elementary properties of determinants it follows from (5.13) that Hamiltonian flows are phase space volume preserving:*

$$\det \mathbf{J} = 1 \,. \tag{5.14}$$





ity!exponent

Figure 5.3: (a) Stability exponents of a Hamiltonian equilibrium point, 2-dof. (b) Stability of a symplectic map in $\mathbb{R}^4$.

5.2.2 Stability of equilibria of Hamiltonian flows

sect. 4.3.1

For an equilibrium point x_q the matrix of variations A is constant. Its eigenvalues describe the linear stability of the equilibrium point. In the case of Hamiltonian flows, from (5.10) it follows that the characteristic polynomial of A for an equilibrium x_q satisfies

$$\begin{aligned} \det(A - \lambda\mathbf{1}) &= \det(\omega^{-1}(A - \lambda\mathbf{1})\omega) = \det(-\omega A\omega - \lambda\mathbf{1}) \\ &= -\det(A^T + \lambda\mathbf{1}) = -\det(A + \lambda\mathbf{1}) . \end{aligned} \tag{5.15}$$

A is the matrix (5.10) with real matrix elements, so its eigenvalues (the stability exponents of (4.25)) are either real or come in complex pairs. Symplectic invariance implies in addition that if λ is an eigenvalue, then $-\lambda$, λ^* and $-\lambda^*$ are also eigenvalues. Distinct symmetry classes of the stability exponents of an equilibrium point in a 2-dof system are displayed in figure 5.3(a). It is worth noting that while the linear stability of equilibria in a Hamiltonian system always respects this symmetry, the nonlinear stability can be completely different.

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need to replace figure 4.2(a) by edited version of figure 5.3(a)

Luz, give references in a remark

5.3 Symplectic maps

A stability eigenvalue $\Lambda = \Lambda(x_0, t)$ associated to a trajectory is an eigenvalue of the Jacobian matrix $\mathbf{J}$. The transpose $\mathbf{J}^T$ and the inverse $\mathbf{J}^{-1}$ are related by

$$\mathbf{J}^{-1} = -\omega\mathbf{J}^T\omega\,, \tag{5.16}$$

so the characteristic polynomial satisfies

$$\begin{aligned} \det(\mathbf{J} - \Lambda\mathbf{1}) &= \det(\mathbf{J}^T - \Lambda\mathbf{1}) = \det(-\omega\mathbf{J}^T\omega - \Lambda\mathbf{1}) \\ &= \det(\mathbf{J}^{-1} - \Lambda\mathbf{1}) = \det(\mathbf{J}^{-1})\det(\mathbf{1} - \Lambda\mathbf{J}) \\ &= \Lambda^{2D}\det(\mathbf{J} - \Lambda^{-1}\mathbf{1}) . \end{aligned} \tag{5.17}$$

loxodromic
conservation!phase space volume
Liouville!theorem
elliptic!stability
residue!stability
stability!residue
hyperbolic!flow
flow!hyperbolic
inverse!hyperbolic flow
flow!inverse hyperbolic
Henon@Hénon!map!Hamiltonian
map!Hénon!Hamiltonian
map!Hamiltonian!Hénon
Hamiltonian!Hénon map
symplectic!Hénon map
area preserving!Hénon map
Henon@Hénon!map
conservation!phase space volume
Liouville!theorem

this is not needed, so I dropped it: (we used that $\det(\mathbf{J}) = \det(\mathbf{J}^{-1}) = 1$, which is true for all symplectic maps).

6.8 page 100

Hence if Λ is an eigenvalue of $\mathbf{J}$, so are $1/\Lambda$, Λ^* and $1/\Lambda^*$. Real (non-marginal, $|\Lambda| \neq 1$) eigenvalues always come paired as Λ, $1/\Lambda$. The Liouville conservation of phase space volumes (5.14) is an immediate consequence of this pairing up of eigenvalues. The complex eigenvalues come in pairs Λ, Λ^*, $|\Lambda| = 1$, or in loxodromic quartets Λ, $1/\Lambda$, Λ^* and $1/\Lambda^*$. These possibilities are illustrated in figure 5.3(b).

Example 5.4 2-dimensional symplectic maps: *In the 2-dimensional case the eigenvalues (8.2) depend only on* $\mathrm{tr}\,\mathbf{J}^t$

$$\Lambda_{1,2} = \frac{1}{2}\left(\mathrm{tr}\,\mathbf{J}^t \pm \sqrt{(\mathrm{tr}\,\mathbf{J}^t - 2)(\mathrm{tr}\,\mathbf{J}^t + 2)}\right) . \tag{5.18}$$

The trajectory is elliptic if the residue $|\mathrm{tr}\,\mathbf{J}^t| - 2 \leq 0$, *with complex eigenvalues* $\Lambda_1 = e^{i\theta t}$, $\Lambda_2 = \Lambda_1^* = e^{-i\theta t}$. *If* $|\mathrm{tr}\,\mathbf{J}^t| - 2 > 0$, λ *is real, and the trajectory is either*

$$\text{hyperbolic} \qquad \Lambda_1 = e^{\lambda t} , \quad \Lambda_2 = e^{-\lambda t} , \text{ or} \tag{5.19}$$

$$\text{inverse hyperbolic} \qquad \Lambda_1 = -e^{\lambda t} , \quad \Lambda_2 = -e^{-\lambda t} . \tag{5.20}$$

Example 5.5 Hamiltonian Hénon map, reversibility: *By (4.37) the Hénon map (3.12) for $b = -1$ value is the simplest 2-d orientation preserving area-preserving map, often studied to better understand topology and symmetries of Poincaré sections of 2 dof Hamiltonian flows. We find it convenient to multiply (3.13) by a and absorb the a factor into x in order to bring the Hénon map for the $b = -1$ parameter value into the form*

$$x_{i+1} + x_{i-1} = a - x_i^2 , \quad i = 1, ..., n_p , \tag{5.21}$$

The 2-dimensional Hénon map *for $b = -1$ parameter value*

$$\begin{aligned} x_{n+1} &= a - x_n^2 - y_n \\ y_{n+1} &= x_n . \end{aligned} \tag{5.22}$$

is Hamiltonian (symplectic) in the sense that it preserves area in the $[x, y]$ plane.

For definitiveness, in numerical calculations in examples to follow we shall fix (arbitrarily) the stretching parameter value to $a = 6$, a value large enough to guarantee that all roots of $0 = f^n(x) - x$ (periodic points) are real.

link to next exer

5.3.1 Poincaré invariants

Let C a region in the phase space and $V(0)$ its volume. Denoting the flow of the Hamiltonian system by $f^t(x)$, the volume of C after a time t is $V(t) = f^t(C)$, and using (5.14) we derive the *Liouville theorem*:

$$\begin{aligned} V(t) &= \int_{f^t(C)} dx = \int_C \left\| \frac{\partial f^t(x')}{\partial x} \right\| dx' \\ & \int_C \det(\mathbf{J}) dx' = \int_C dx' = V(0) , \end{aligned} \tag{5.23}$$

Hamiltonian flows preserve phase-space volumes.

Poincar“'e!invariants
Stokes theorem
Henon@Hénon!map!reversible
map!reversible!Hénon
reversible!Hénon map

The symplectic structure of Hamilton's equations buys us much more than the "incompressibility," or the phase space volume conservation. Consider the symplectic product of two infinitesimal vectors

$$
\begin{aligned}
(\delta x, \delta \hat{x}) &= \delta x^T \omega \delta \hat{x} = \delta p_i \delta \hat{q}_i - \delta q_i \delta \hat{p}_i \\
&= \sum_{i=1}^{D} \{\text{oriented area in the } (q_i, p_i) \text{ plane}\} \,. \qquad (5.24)
\end{aligned}
$$

Time t later we have

$$
(\delta x', \delta \hat{x}') = \delta x^T \mathbf{J}^T \omega \mathbf{J} \delta \hat{x} = \delta x^T \omega \delta \hat{x} \,.
$$

This has the following geometrical meaning. We imagine there is a reference phase space point. We then define two other points infinitesimally close so that the vectors δx and $\delta \hat{x}$ describe their displacements relative to the reference point. Under the dynamics, the three points are mapped to three new points which are still infinitesimally close to one another. The meaning of the above expression is that the area of the parallelopiped spanned by the three final points is the same as that spanned by the inital points. The integral (Stokes theorem) version of this infinitesimal area invariance states that for Hamiltonian flows the D oriented areas $\mathcal{V}_i$ bounded by D loops $\Omega\mathcal{V}_i$, one per each (q_i, p_i) plane, are separately conserved:

$$
\int_{\mathcal{V}} dp \wedge dq = \oint_{\Omega\mathcal{V}} p \cdot dq = \text{invariant} \,. \qquad (5.25)
$$

Morally a Hamiltonian flow is really D-dimensional, even though its phase space is $2D$-dimensional. Hence for Hamiltonian flows one emphasizes D, the number of the degrees of freedom.

in depth:
appendix D.1, p. 797

⇓PRIVATE

5.4 Reversibility

Example 5.6 Hamiltonian Hénon map, reversibility: *The Hénon map (5.22) is reversible, with its inverse interchanging the roles of x and y:*

$$
\begin{aligned}
x_{n-1} &= y_n \\
y_{n-1} &= a - y_n^2 - x_n \,, \qquad (5.26)
\end{aligned}
$$

hence the dynamics is symmetric in the $[x, y]$ plane: a trajectory maps into a trajectory under the flip across the $x = y$ diagonal

$$
\begin{pmatrix} y \\ x \end{pmatrix} = R \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \qquad (5.27)
$$

residue!stability
stability!residue
symplectic!invariance
invariance!symplectic

and time reversal. The reversor R is orientation reversing, $\det[\partial R] = -1$, and is an involution, $R^2 = \mathbb{1}$. In other words, the Hamiltonian Hénon map is conjugate to its inverse $f \circ R = R \circ f^{-1}$, and can be factored into a pair of orientation reversing involutions, $f = (fR) \circ R = T \circ R$, with

$$T\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ a - x^2 - y \end{pmatrix} . \tag{5.28}$$

⇓PRELIMINARY

Equivalently, writing $f = S \circ (Sf) = S \circ U$, the reversor

$$U\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} a - y^2 - x \\ y \end{pmatrix} \tag{5.29}$$

factorizes the Hénon map as $f = ST$.

⇑PRELIMINARY
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Commentary

In theory there is no difference between theory and practice. In practice there is.
Yogi Berra

Remark 5.1 Hamiltonian dynamics literature.

If you are reading this book, in theory you already know everything that is in this chapter. In practice you do not. Try this: Put your right hand on your heart and say: "I understand why nature preferes symplectic geometry". Honest? We make an attempt in sect. 31.1. Out there there are about 2 centuries of accumulated literature on Hamilton, Lagrange, Jacobi etc. formulation of mechanics, some of it excellent. In context of what we will need here, we make a very subjective recommendation - we enjoyed reading Percival and Richards [7.10] and Ozorio de Almeida [7.11].

Remark 5.2 Symplectic. The term symplectic - Greek for twining or plaiting together - was introduced into mathematics by Hermann Weyl. "Canonical" lineage is church-doctrinal: Greek "kanon", referring to a reed used for measurement, came to mean in Latin a rule or a standard.

perhaps move remark A.4 here, as it reformulates Bohr-Somm. (A.4)

Remark 5.3 The sign convention of ω. The overall sign of ω, the symplectic invariant in (5.7), is set by the convention that the Hamilton's principal function (for energy conserving flows) is given by $R(q, q', t) = \int_q^{q'} p_i dq_i - Et$. With this sign convention the action along a classical path is minimal, and the kinetic energy of a free particle is positive.

Remark 5.4 Symmetries of the symbol square. For a more detailed discussion of symmetry lines see refs. [17.4, 3.5, 12.46]. In discussion of example 5.6, we have followed refs. [5.3, 5.4, 5.5].

improve references

⇓PRELIMINARY

Remark 5.5 Stability residue. Stability residue was introduced by Greene [5.7].

Résumé

Hamiltonian flow $\dot{x}_i = \omega_{ij} H_j(x)$, $\omega_{mn} = -\omega_{nm}$ is canonical in the sense that $x' = f^t(x)$ is a transformation whose Jacobian matrix $\mathbf{J} = \partial x'/\partial x$ preserves the symplectic invariant $\mathbf{J}^T \omega \mathbf{J} = \omega$. Infinitesimal symplectic transformations are generated by $A_{ij} = \omega_{ik} H_{kj}$ satisfying $A^T \omega + \omega A = 0$. This implies that A are elements of the symplectic algebra $sp(2D)$, and that the $2D$-dimensional flow preserves D oriented infinitesimal areas $\delta x^T \omega \delta \hat{x} = \delta p_i \delta \hat{q}_i - \delta q_i \delta \hat{p}_i$. The Liouville phase space volume conservation is a consequences of this general invariance.

⇑PRELIMINARY

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complete ref. [5.2]

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