

Hamiltonian mechanics

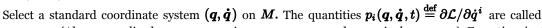
In physics, **Hamiltonian mechanics** is a reformulation of <u>Lagrangian mechanics</u> that emerged in 1833. Introduced by <u>Sir William Rowan Hamilton</u>, [1] Hamiltonian mechanics replaces (generalized) velocities \dot{q}^i used in Lagrangian mechanics with (generalized) *momenta*. Both theories provide interpretations of classical mechanics and describe the same physical phenomena.

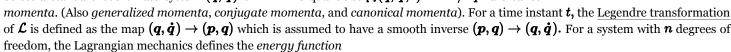
Hamiltonian mechanics has a close relationship with geometry (notably, <u>symplectic geometry</u> and Poisson structures) and serves as a link between classical and quantum mechanics.

Overview

Phase space coordinates (p, q) and Hamiltonian H

Let (M, \mathcal{L}) be a <u>mechanical system</u> with the <u>configuration space</u> M and the smooth <u>Lagrangian</u> \mathcal{L} .





$$E_{\mathcal{L}}(oldsymbol{q},t) \stackrel{ ext{def}}{=} \sum_{i=1}^n \dot{q}^i rac{\partial \mathcal{L}}{\partial \dot{q}^i} - \mathcal{L}.$$

The Legendre transform of \mathcal{L} turns $E_{\mathcal{L}}$ into a function $\mathcal{H}(p,q,t)$ known as the *Hamiltonian*. The Hamiltonian satisfies

$$\mathcal{H}\left(rac{\partial \mathcal{L}}{\partial \dot{m{q}}},m{q},t
ight)=E_{\mathcal{L}}(m{q},\dot{m{q}},t)$$

which implies that

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

where the velocities $\dot{\boldsymbol{q}} = (\dot{q}^1, \dots, \dot{q}^n)$ are found from the (*n*-dimensional) equation $\boldsymbol{p} = \partial \mathcal{L}/\partial \dot{\boldsymbol{q}}$ which, by assumption, is uniquely solvable for $\dot{\boldsymbol{q}}$. The (2*n*-dimensional) pair (*p*, *q*) is called *phase space coordinates*. (Also *canonical coordinates*).

From Euler-Lagrange equation to Hamilton's equations

In phase space coordinates (p, q), the (n-dimensional) Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} = 0$$

becomes Hamilton's equations in **2n** dimensions

$$rac{\mathrm{d}oldsymbol{q}}{\mathrm{d}t} = rac{\partial\mathcal{H}}{\partialoldsymbol{p}}, \quad rac{\mathrm{d}oldsymbol{p}}{\mathrm{d}t} = -rac{\partial\mathcal{H}}{\partialoldsymbol{q}}$$

Proof

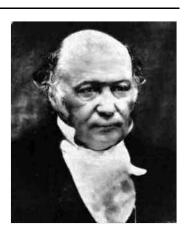
The Hamiltonian $\mathcal{H}(\boldsymbol{p},\boldsymbol{q})$ is the Legendre transform of the Lagrangian $\mathcal{L}(\boldsymbol{q},\boldsymbol{\dot{q}})$, thus one has

$$\mathcal{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + \mathcal{H}(\boldsymbol{p}, \boldsymbol{q}) = \boldsymbol{p}\dot{\boldsymbol{q}}$$

and thus

$$\partial \mathcal{H}/\partial \boldsymbol{p} = \dot{\boldsymbol{q}}$$

 $\partial \mathcal{L}/\partial \boldsymbol{q} = -\partial \mathcal{H}/\partial \boldsymbol{q}$



Sir William Rowan Hamilton

Besides, since $\mathbf{p} = \partial \mathcal{L}/\partial \dot{\mathbf{q}}$ the Euler-Lagrange equations yield $d\mathbf{p}/dt = \partial \mathcal{L}/\partial \mathbf{q} = -\partial \mathcal{H}/\partial \mathbf{q}$.

From stationary action principle to Hamilton's equations

Let $\mathcal{P}(a,b,\boldsymbol{x}_a,\boldsymbol{x}_b)$ be the set of smooth paths $\boldsymbol{q}:[a,b]\to M$ for which $\boldsymbol{q}(a)=\boldsymbol{x}_a$ and $\boldsymbol{q}(b)=\boldsymbol{x}_b$. The action functional $\mathcal{S}:\mathcal{P}(a,b,\boldsymbol{x}_a,\boldsymbol{x}_b)\to\mathbb{R}$ is defined via

$$\mathcal{S}[oldsymbol{q}] = \int_a^b \mathcal{L}(t,oldsymbol{q}(t),\dot{oldsymbol{q}}(t))\,dt = \int_a^b \left(\sum_{i=1}^n p_i \dot{oldsymbol{q}}^i - \mathcal{H}(oldsymbol{p},oldsymbol{q},t)
ight)\,dt,$$

where $\mathbf{q} = \mathbf{q}(t)$, and $\mathbf{p} = \partial \mathcal{L}/\partial \dot{\mathbf{q}}$ (see above). A path $\mathbf{q} \in \mathcal{P}(a, b, \mathbf{x}_a, \mathbf{x}_b)$ is a <u>stationary point</u> of \mathcal{S} (and hence is an equation of motion) if and only if the path $(\mathbf{p}(t), \mathbf{q}(t))$ in phase space coordinates obeys the Hamilton's equations.

Basic physical interpretation

A simple interpretation of Hamiltonian mechanics comes from its application on a one-dimensional system consisting of one nonrelativistic particle of mass m. The value H(p,q) of the Hamiltonian is the total energy of the system, in this case the sum of kinetic and potential energy, traditionally denoted T and V, respectively. Here p is the momentum mv and q is the space coordinate. Then

$$\mathcal{H}=T+V, \qquad T=rac{p^2}{2m}, \qquad V=V(q)$$

T is a function of p alone, while V is a function of q alone (i.e., T and V are scleronomic).

In this example, the time derivative of q is the velocity, and so the first Hamilton equation means that the particle's velocity equals the derivative of its kinetic energy with respect to its momentum. The time derivative of the momentum p equals the *Newtonian force*, and so the second Hamilton equation means that the force equals the negative gradient of potential energy.

Example

A spherical pendulum consists of a <u>mass</u> m moving without <u>friction</u> on the surface of a <u>sphere</u>. The only <u>forces</u> acting on the mass are the <u>reaction</u> from the sphere and <u>gravity</u>. <u>Spherical coordinates</u> are used to describe the position of the mass in terms of (r, θ, φ) , where r is fixed, $r = \ell$.

The Lagrangian for this system is [2]

$$L=rac{1}{2}m\ell^2\left(\dot{ heta}^2+\sin^2 heta\,\dot{arphi}^2
ight)+mg\ell\cos heta.$$

Thus the Hamiltonian is

$$H=P_{ heta}\dot{ heta}+P_{\omega}\dot{arphi}-L$$

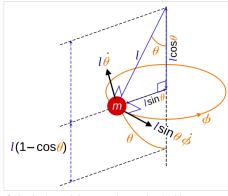
where

$$P_{ heta} = rac{\partial L}{\partial \dot{ heta}} = m \ell^2 \dot{ heta}$$

and

$$P_{arphi} = rac{\partial L}{\partial \dot{\phi}} = m \ell^2 \sin^2\! heta \, \dot{arphi}.$$

In terms of coordinates and momenta, the Hamiltonian reads



Spherical pendulum: angles and velocities.

$$H = \underbrace{\left[rac{1}{2}m\ell^2\dot{ heta}^2 + rac{1}{2}m\ell^2\sin^2 heta\,\dot{arphi}^2
ight]}_{T} + \underbrace{\left[-mg\ell\cos heta
ight]}_{ ilde{V}} = rac{P_ heta^2}{2m\ell^2} + rac{P_arphi^2}{2m\ell^2\sin^2 heta} - mg\ell\cos heta.$$

Hamilton's equations give the time evolution of coordinates and conjugate momenta in four first-order differential equations,

$$egin{aligned} \dot{ heta} &= rac{P_{ heta}}{m\ell^2} \ \dot{arphi} &= rac{P_{arphi}}{m\ell^2\sin^2 heta} \ \dot{P}_{ heta} &= rac{P_{arphi}^2}{m\ell^2\sin^3 heta}\cos heta - mg\ell\sin heta \ \dot{P}_{arphi} &= 0. \end{aligned}$$

Momentum P_{φ} , which corresponds to the vertical component of <u>angular momentum</u> $L_z = \ell \sin \theta \times m \ell \sin \theta \dot{\varphi}$, is a constant of motion. That is a consequence of the rotational symmetry of the system around the vertical axis. Being absent from the Hamiltonian, <u>azimuth</u> φ is a cyclic coordinate, which implies conservation of its conjugate momentum.

Deriving Hamilton's equations

Hamilton's equations can be derived by a calculation with the <u>Lagrangian</u> \mathcal{L} , generalized positions q^i , and generalized velocities \dot{q}^i , where $i = 1, \dots, n^{[3]}$ Here we work <u>off-shell</u>, meaning q^i , \dot{q}^i , t are independent coordinates in phase space, not constrained to follow any equations of motion (in particular, \dot{q}^i is not a derivative of q^i). The total differential of the Lagrangian is:

$$\mathrm{d}\mathcal{L} = \sum_i \left(\frac{\partial \mathcal{L}}{\partial q^i} \mathrm{d}q^i + \frac{\partial \mathcal{L}}{\partial \dot{q}^i} \, \mathrm{d}\dot{q}^i \right) + \frac{\partial \mathcal{L}}{\partial t} \, \mathrm{d}t \; .$$

The generalized momentum coordinates were defined as $p_i = \partial \mathcal{L}/\partial \dot{q}^i$, so we may rewrite the equation as:

$$egin{aligned} \mathrm{d}\mathcal{L} &= \sum_i \left(rac{\partial \mathcal{L}}{\partial q^i} \, \mathrm{d}q^i + p_i \mathrm{d}\dot{q}^i
ight) + rac{\partial \mathcal{L}}{\partial t} \, \mathrm{d}t \ &= \sum_i \left(rac{\partial \mathcal{L}}{\partial q^i} \, \mathrm{d}q^i + \mathrm{d}(p_i \dot{q}^i) - \dot{q}^i \, \mathrm{d}p_i
ight) + rac{\partial \mathcal{L}}{\partial t} \, \mathrm{d}t \,. \end{aligned}$$

After rearranging, one obtains:

$$\mathrm{d}igg(\sum_{i}p_{i}\dot{q}^{i}-\mathcal{L}igg) = \sum_{i}igg(-rac{\partial\mathcal{L}}{\partial q^{i}}\,\mathrm{d}q^{i}+\dot{q}^{i}\mathrm{d}p_{i}igg) - rac{\partial\mathcal{L}}{\partial t}\,\mathrm{d}t\;.$$

The term in parentheses on the left-hand side is just the Hamiltonian $\mathcal{H} = \sum p_i \dot{q}^i - \mathcal{L}$ defined previously, therefore:

$$\mathrm{d}\mathcal{H} = \sum_i \left(-rac{\partial \mathcal{L}}{\partial q^i} \, \mathrm{d}q^i + \dot{q}^i \, \mathrm{d}p_i
ight) - rac{\partial \mathcal{L}}{\partial t} \, \mathrm{d}t \; .$$

One may also calculate the total differential of the Hamiltonian \mathcal{H} with respect to coordinates q^i, p_i, t instead of q^i, \dot{q}^i, t , yielding:

$$\mathrm{d}\mathcal{H} = \sum_i \left(rac{\partial \mathcal{H}}{\partial q^i} \mathrm{d}q^i + rac{\partial \mathcal{H}}{\partial p_i} \mathrm{d}p_i
ight) + rac{\partial \mathcal{H}}{\partial t} \, \mathrm{d}t \; .$$

One may now equate these two expressions for $d\mathcal{H}$, one in terms of \mathcal{L} , the other in terms of \mathcal{H} :

$$\sum_{i} \left(-\frac{\partial \mathcal{L}}{\partial q^{i}} dq^{i} + \dot{q}^{i} dp_{i} \right) - \frac{\partial \mathcal{L}}{\partial t} dt = \sum_{i} \left(\frac{\partial \mathcal{H}}{\partial q^{i}} dq^{i} + \frac{\partial \mathcal{H}}{\partial p_{i}} dp_{i} \right) + \frac{\partial \mathcal{H}}{\partial t} dt.$$

Since these calculations are off-shell, one can equate the respective coefficients of $\mathbf{d}q^i$, $\mathbf{d}p_i$, $\mathbf{d}t$ on the two sides:

$$rac{\partial \mathcal{H}}{\partial q^i} = -rac{\partial \mathcal{L}}{\partial q^i} \quad , \quad rac{\partial \mathcal{H}}{\partial p_i} = \dot{q}^i \quad , \quad rac{\partial \mathcal{H}}{\partial t} = -rac{\partial \mathcal{L}}{\partial t} \; .$$

On-shell, one substitutes parametric functions $q^i = q^i(t)$ which define a trajectory in phase space with velocities $\dot{q}^i = \frac{d}{dt}q^i(t)$, obeying Lagrange's equations:

$$rac{\mathrm{d}}{\mathrm{d}t}rac{\partial \mathcal{L}}{\partial \dot{q}^i} - rac{\partial \mathcal{L}}{\partial q^i} = 0 \; .$$

Rearranging and writing in terms of the on-shell $p_i = p_i(t)$ gives:

$$rac{\partial \mathcal{L}}{\partial q^i} = \dot{p}_i \; .$$

Thus Lagrange's equations are equivalent to Hamilton's equations:

$$rac{\partial \mathcal{H}}{\partial q^i} = -\dot{p}_i \quad , \quad rac{\partial \mathcal{H}}{\partial p_i} = \dot{q}^i \quad , \quad rac{\partial \mathcal{H}}{\partial t} = -rac{\partial \mathcal{L}}{\partial t} \ .$$

In the case of time-independent \mathcal{H} and \mathcal{L} , i.e. $\partial \mathcal{H}/\partial t = -\partial \mathcal{L}/\partial t = 0$, Hamilton's equations consist of 2n first-order <u>differential</u> <u>equations</u>, while Lagrange's equations consist of n second-order equations. Hamilton's equations usually do not reduce the difficulty of finding explicit solutions, but important theoretical results can be derived from them, because coordinates and momenta are independent variables with nearly symmetric roles.

Hamilton's equations have another advantage over Lagrange's equations: if a system has a symmetry, so that some coordinate q_i does not occur in the Hamiltonian (i.e. a *cyclic coordinate*), the corresponding momentum coordinate p_i is conserved along each trajectory, and that coordinate can be reduced to a constant in the other equations of the set. This effectively reduces the problem from n coordinates to (n-1) coordinates: this is the basis of <u>symplectic reduction</u> in geometry. In the Lagrangian framework, the conservation of momentum also follows immediately, however all the generalized velocities \dot{q}_i still occur in the Lagrangian, and a system of equations in n coordinates still has to be solved. [4]

The Lagrangian and Hamiltonian approaches provide the groundwork for deeper results in classical mechanics, and suggest analogous formulations in quantum mechanics: the path integral formulation and the Schrödinger equation.

Properties of the Hamiltonian

- The value of the Hamiltonian \mathcal{H} is the total energy of the system if and only if the energy function $E_{\mathcal{L}}$ has the same property. (See definition of \mathcal{H}).
- $lacksquare rac{d\mathcal{H}}{dt} = rac{\partial \mathcal{H}}{\partial t}$ when $\mathbf{p}(t)$, $\mathbf{q}(t)$ form a solution of Hamilton's equations.

Indeed, $\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial p} \cdot \dot{p} + \frac{\partial \mathcal{H}}{\partial q} \cdot \dot{q} + \frac{\partial \mathcal{H}}{\partial t}$, and everything but the final term cancels out.

- \mathcal{H} does not change under *point transformations*, i.e. smooth changes $\mathbf{q} \leftrightarrow \mathbf{q'}$ of space coordinates. (Follows from the invariance of the energy function $\mathbf{E}_{\mathcal{L}}$ under point transformations. The invariance of $\mathbf{E}_{\mathcal{L}}$ can be established directly).
- $\frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}.$ (See § Deriving Hamilton's equations).
- $-\frac{\partial \mathcal{H}}{\partial q^i} = \dot{p}_i = \frac{\partial \mathcal{L}}{\partial q^i}$. (Compare Hamilton's and Euler-Lagrange equations or see § Deriving Hamilton's equations).

A coordinate for which the last equation holds is called *cyclic* (or *ignorable*). Every cyclic coordinate q^i reduces the number of degrees of freedom by 1, causes the corresponding momentum p_i to be conserved, and makes Hamilton's equations easier to solve.

Hamiltonian as the total system energy

In its application to a given system, the Hamiltonian is often taken to be

$$\mathcal{H} = T + V$$

where T is the kinetic energy and V is the potential energy. Using this relation can be simpler than first calculating the Lagrangian, and then deriving the Hamiltonian from the Lagrangian. However, the relation is not true for all systems.

The relation holds true for nonrelativistic systems when all of the following conditions are satisfied [5][6]

$$\frac{\partial V(\boldsymbol{q},\boldsymbol{\dot{q}},t)}{\partial \dot{q}_{i}}=0\;,\quad\forall i$$

$$rac{\partial T(oldsymbol{q},oldsymbol{\dot{q}},t)}{\partial t}=0$$

$$T(oldsymbol{q},\dot{oldsymbol{q}}) = \sum_{i=1}^n \sum_{j=1}^n \left(c_{ij}(oldsymbol{q}) \dot{q}_i \dot{q}_j
ight)$$

where t is time, n is the number of degrees of freedom of the system, and each $c_{ij}(q)$ is an arbitrary scalar function of q.

In words, this means that the relation $\mathcal{H} = T + V$ holds true if T does not contain time as an explicit variable (it is <u>scleronomic</u>), V does not contain generalised velocity as an explicit variable, and each term of T is quadratic in generalised velocity.

Proof

Preliminary to this proof, it is important to address an ambiguity in the related mathematical notation. While a change of variables can be used to equate $\mathcal{L}(\boldsymbol{p},\boldsymbol{q},t)=\mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}},t)$, it is important to note that $\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}},t)}{\partial \dot{q}_i}\neq \frac{\partial \mathcal{L}(\boldsymbol{p},\boldsymbol{q},t)}{\partial \dot{q}_i}$. In this case, the right hand side always evaluates to o. To perform a change of variables inside of a partial derivative, the multivariable chain rule should be used. Hence, to avoid

Additionally, this proof uses the notation f(a,b,c)=f(a,b) to imply that $\dfrac{\partial f(a,b,c)}{\partial c}=0.$

ambiguity, the function arguments of any term inside of a partial derivative should be stated.

Proof

Starting from definitions of the Hamiltonian, generalized momenta, and Lagrangian for an n degrees of freedom system

$$\mathcal{H} = \sum_{i=1}^n \left(p_i \dot{q}_i
ight) - \mathcal{L}(oldsymbol{q}, \dot{oldsymbol{q}}, t)$$

$$p_i(oldsymbol{q}, \dot{oldsymbol{q}}, t) = rac{\partial \mathcal{L}(oldsymbol{q}, \dot{oldsymbol{q}}, t)}{\partial \dot{oldsymbol{q}}_i}$$

$$\mathcal{L}(oldsymbol{q}, \dot{oldsymbol{q}}, t) = T(oldsymbol{q}, \dot{oldsymbol{q}}, t) - V(oldsymbol{q}, \dot{oldsymbol{q}}, t)$$

Substituting the generalized momenta into the Hamiltonian gives

$$\mathcal{H} = \sum_{i=1}^n \left(rac{\partial \mathcal{L}(oldsymbol{q}, \dot{oldsymbol{q}}, t)}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i
ight) - \mathcal{L}(oldsymbol{q}, \dot{oldsymbol{q}}, t)$$

Substituting the Lagrangian into the result gives

$$\mathcal{H} = \sum_{i=1}^{n} \left(rac{\partial \left(T(oldsymbol{q}, \dot{oldsymbol{q}}, t) - V(oldsymbol{q}, \dot{oldsymbol{q}}, t)
ight)}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i
ight) - \left(T(oldsymbol{q}, \dot{oldsymbol{q}}, t) - V(oldsymbol{q}, \dot{oldsymbol{q}}, t)
ight) \ = \sum_{i=1}^{n} \left(rac{\partial T(oldsymbol{q}, \dot{oldsymbol{q}}, t)}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i - rac{\partial V(oldsymbol{q}, \dot{oldsymbol{q}}, t)}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i
ight) - T(oldsymbol{q}, \dot{oldsymbol{q}}, t) + V(oldsymbol{q}, \dot{oldsymbol{q}}, t)$$

Now assume that

$$rac{\partial V(oldsymbol{q},oldsymbol{\dot{q}},t)}{\partial \dot{oldsymbol{q}}_i}=0\;,\quad orall i$$

and also assume that

$$rac{\partial T(oldsymbol{q},oldsymbol{\dot{q}},t)}{\partial t}=0$$

Applying these assumptions results in

$$egin{aligned} \mathcal{H} &= \sum_{i=1}^n \left(rac{\partial T(oldsymbol{q},\dot{oldsymbol{q}})}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i - rac{\partial V(oldsymbol{q},t)}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i
ight) - T(oldsymbol{q},\dot{oldsymbol{q}}) + V(oldsymbol{q},t) \ &= \sum_{i=1}^n \left(rac{\partial T(oldsymbol{q},\dot{oldsymbol{q}})}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i
ight) - T(oldsymbol{q},\dot{oldsymbol{q}}) + V(oldsymbol{q},t) \end{aligned}$$

Next assume that T is of the form

$$T(oldsymbol{q}, \dot{oldsymbol{q}}) = \sum_{i=1}^n \sum_{j=1}^n \left(c_{ij}(oldsymbol{q}) \dot{q}_i \dot{q}_j
ight)$$

where each $c_{ij}(q)$ is an arbitrary scalar function of q.

Differentiating this with respect to \dot{q}_l , $l \in [1, n]$, gives

$$egin{aligned} rac{\partial T(oldsymbol{q},\dot{oldsymbol{q}})}{\partial \dot{oldsymbol{q}}_l} &= \sum_{i=1}^n \sum_{j=1}^n \left(rac{\partial \left[c_{ij}(oldsymbol{q})\dot{q}_i\dot{q}_j
ight]}{\partial \dot{q}_l}
ight) \ &= \sum_{i=1}^n \sum_{j=1}^n \left(c_{ij}(oldsymbol{q})rac{\partial \left[\dot{q}_i\dot{q}_j
ight]}{\partial \dot{q}_l}
ight) \end{aligned}$$

Splitting the summation, evaluating the partial derivative, and rejoining the summation gives

$$\begin{split} \frac{\partial T(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}_{l}} &= \sum_{i \neq l}^{n} \sum_{j \neq l}^{n} \left(c_{ij}(\boldsymbol{q}) \frac{\partial \left[\dot{q}_{i} \dot{q}_{j} \right]}{\partial \dot{q}_{l}} \right) + \sum_{i \neq l}^{n} \left(c_{il}(\boldsymbol{q}) \frac{\partial \left[\dot{q}_{i} \dot{q}_{l} \right]}{\partial \dot{q}_{l}} \right) + \sum_{j \neq l}^{n} \left(c_{lj}(\boldsymbol{q}) \frac{\partial \left[\dot{q}_{l} \dot{q}_{j} \right]}{\partial \dot{q}_{l}} \right) + c_{ll}(\boldsymbol{q}) \frac{\partial \left[\dot{q}_{l}^{2} \right]}{\partial \dot{q}_{l}} \\ &= \sum_{i \neq l}^{n} \sum_{j \neq l}^{n} \left(0 \right) + \sum_{i \neq l}^{n} \left(c_{il}(\boldsymbol{q}) \dot{q}_{i} \right) + \sum_{j \neq l}^{n} \left(c_{lj}(\boldsymbol{q}) \dot{q}_{j} \right) + 2c_{ll}(\boldsymbol{q}) \dot{q}_{l} \\ &= \sum_{i = 1}^{n} \left(c_{il}(\boldsymbol{q}) \dot{q}_{i} \right) + \sum_{j = 1}^{n} \left(c_{lj}(\boldsymbol{q}) \dot{q}_{j} \right) \end{split}$$

Summing (this multiplied by \dot{q}_l) over l results in

$$\begin{split} \sum_{l=1}^n \left(\frac{\partial T(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{q}_l} \dot{q}_l \right) &= \sum_{l=1}^n \left(\left(\sum_{i=1}^n \left(c_{il}(\boldsymbol{q}) \dot{q}_i \right) + \sum_{j=1}^n \left(c_{lj}(\boldsymbol{q}) \dot{q}_j \right) \right) \dot{q}_l \right) \\ &= \sum_{l=1}^n \sum_{i=1}^n \left(c_{il}(\boldsymbol{q}) \dot{q}_i \dot{q}_l \right) + \sum_{l=1}^n \sum_{j=1}^n \left(c_{lj}(\boldsymbol{q}) \dot{q}_j \dot{q}_l \right) \\ &= \sum_{i=1}^n \sum_{l=1}^n \left(c_{il}(\boldsymbol{q}) \dot{q}_i \dot{q}_l \right) + \sum_{l=1}^n \sum_{j=1}^n \left(c_{lj}(\boldsymbol{q}) \dot{q}_l \dot{q}_j \right) \\ &= T(\boldsymbol{q}, \dot{\boldsymbol{q}}) + T(\boldsymbol{q}, \dot{\boldsymbol{q}}) \\ &= 2T(\boldsymbol{q}, \dot{\boldsymbol{q}}) \end{split}$$

This simplification is a result of <u>Euler's homogeneous function theorem</u>.

Hence, the Hamiltonian becomes

$$egin{aligned} \mathcal{H} &= \sum_{i=1}^n \left(rac{\partial T(oldsymbol{q},\dot{oldsymbol{q}})}{\partial \dot{oldsymbol{q}}_i} \dot{oldsymbol{q}}_i
ight) - T(oldsymbol{q},\dot{oldsymbol{q}}) + V(oldsymbol{q},t) \ &= 2T(oldsymbol{q},\dot{oldsymbol{q}}) - T(oldsymbol{q},\dot{oldsymbol{q}}) + V(oldsymbol{q},t) \ &= T(oldsymbol{q},\dot{oldsymbol{q}}) + V(oldsymbol{q},t) \end{aligned}$$

Application to systems of point masses

For a system of point masses, the requirement for T to be quadratic in generalised velocity is always satisfied for the case where $T(q, \dot{q}, t) = T(q, \dot{q})$, which is a requirement for $\mathcal{H} = T + V$ anyway.

Proof

Consider the kinetic energy for a system of N point masses. If it is assumed that $T(q, \dot{q}, t) = T(q, \dot{q})$, then it can be shown that $\dot{\mathbf{r}}_k(q, \dot{q}, t) = \dot{\mathbf{r}}_k(q, \dot{q})$ (See *Scleronomous § Application*). Therefore, the kinetic energy is

$$T(oldsymbol{q}, \dot{oldsymbol{q}}) = rac{1}{2} \sum_{k=1}^{N} \left(m_k \dot{f r}_k(oldsymbol{q}, \dot{oldsymbol{q}}) \cdot \dot{f r}_k(oldsymbol{q}, \dot{oldsymbol{q}})
ight)$$

The chain rule for many variables can be used to expand the velocity

$$egin{aligned} \dot{\mathbf{r}}_k(oldsymbol{q},\dot{oldsymbol{q}}) &= rac{d\mathbf{r}_k(oldsymbol{q})}{dt} \ &= \sum_{i=1}^n \left(rac{\partial\mathbf{r}_k(oldsymbol{q})}{\partial oldsymbol{q}_i}\dot{oldsymbol{q}}_i
ight) \end{aligned}$$

Resulting in

$$egin{aligned} T(oldsymbol{q},\dot{oldsymbol{q}}) &= rac{1}{2}\sum_{k=1}^{N} \left(m_k \left(\sum_{i=1}^n \left(rac{\partial \mathbf{r}_k(oldsymbol{q})}{\partial q_i}\dot{q}_i
ight) \cdot \sum_{j=1}^n \left(rac{\partial \mathbf{r}_k(oldsymbol{q})}{\partial q_j}\dot{q}_j
ight)
ight)
ight) \ &= \sum_{k=1}^{N}\sum_{i=1}^n \sum_{j=1}^n \left(rac{1}{2}m_k rac{\partial \mathbf{r}_k(oldsymbol{q})}{\partial q_i} \cdot rac{\partial \mathbf{r}_k(oldsymbol{q})}{\partial q_j}\dot{q}_i\dot{q}_j
ight) \ &= \sum_{i=1}^n \sum_{j=1}^n \left(\sum_{k=1}^N \left(rac{1}{2}m_k rac{\partial \mathbf{r}_k(oldsymbol{q})}{\partial q_i} \cdot rac{\partial \mathbf{r}_k(oldsymbol{q})}{\partial q_j}
ight)\dot{q}_i\dot{q}_j
ight) \ &= \sum_{i=1}^n \sum_{j=1}^n \left(c_{ij}(oldsymbol{q})\dot{q}_i\dot{q}_j
ight) \end{aligned}$$

This is of the required form.

Conservation of energy

If the conditions for $\mathcal{H} = T + V$ are satisfied, then conservation of the Hamiltonian implies conservation of energy. This requires the additional condition that V does not contain time as an explicit variable.

$$\frac{\partial V(\boldsymbol{q}, \boldsymbol{\dot{q}}, t)}{\partial t} = 0$$

With respect to the extended Euler-Lagrange formulation (See <u>Lagrangian mechanics § Extensions to include non-conservative forces</u>), the <u>Rayleigh dissipation function</u> represents energy dissipation by nature. Therefore, energy is not conserved when $R \neq 0$. This is similar to the velocity dependent potential.

In summary, the requirements for $\mathcal{H} = T + V = \text{constant}$ of time to be satisfied for a nonrelativistic system are [5][6]

- 1. V = V(q)
- 2. $T = T(q, \dot{q})$
- 3. T is a homogeneous quadratic function in $\dot{\boldsymbol{q}}$

Hamiltonian of a charged particle in an electromagnetic field

A sufficient illustration of Hamiltonian mechanics is given by the Hamiltonian of a charged particle in an <u>electromagnetic field</u>. In <u>Cartesian coordinates the Lagrangian of a non-relativistic classical particle in an electromagnetic field is (in SI Units):</u>

$$\mathcal{L} = \sum_i rac{1}{2} m \dot{x}_i^2 + \sum_i q \dot{x}_i A_i - q arphi,$$

where q is the <u>electric charge</u> of the particle, φ is the <u>electric scalar potential</u>, and the A_i are the components of the <u>magnetic vector</u> potential that may all explicitly depend on x_i and t.

This Lagrangian, combined with Euler-Lagrange equation, produces the Lorentz force law

$$m\ddot{\mathbf{x}} = q\mathbf{E} + q\dot{\mathbf{x}} \times \mathbf{B}$$

and is called minimal coupling.

The canonical momenta are given by:

$$p_i = rac{\partial \mathcal{L}}{\partial \dot{x}_i} = m \dot{x}_i + q A_i.$$

The Hamiltonian, as the Legendre transformation of the Lagrangian, is therefore:

$$\mathcal{H} = \sum_i \dot{x}_i p_i - \mathcal{L} = \sum_i rac{(p_i - qA_i)^2}{2m} + q arphi.$$

This equation is used frequently in quantum mechanics.

Under gauge transformation:

$$\mathbf{A} \to \mathbf{A} + \nabla f$$
, $\varphi \to \varphi - \dot{f}$,

where $f(\mathbf{r}, t)$ is any scalar function of space and time. The aforementioned Lagrangian, the canonical momenta, and the Hamiltonian transform like:

$$L
ightarrow L' = L + q rac{df}{dt} \,, \quad {f p}
ightarrow {f p}' = {f p} + q
abla f \,, \quad H
ightarrow H' = H - q rac{\partial f}{\partial t} \,,$$

which still produces the same Hamilton's equation:

$$\begin{split} \frac{\partial H'}{\partial x_i} \bigg|_{p_i'} &= \frac{\partial}{\partial x_i} \bigg|_{p_i'} (\dot{x}_i p_i' - L') = -\frac{\partial L'}{\partial x_i} \bigg|_{p_i'} \\ &= -\frac{\partial L}{\partial x_i} \bigg|_{p_i'} - q \frac{\partial}{\partial x_i} \bigg|_{p_i'} \frac{df}{dt} \\ &= -\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_i} \bigg|_{p_i'} + q \frac{\partial f}{\partial x_i} \bigg|_{p_i'} \right) \\ &= -\dot{p}_i' \end{split}$$

In quantum mechanics, the <u>wave function</u> will also undergo a <u>local</u> $\underline{U(1)}$ group transformation during the Gauge Transformation, which implies that all physical results must be invariant under local $\underline{U(1)}$ transformations.

Relativistic charged particle in an electromagnetic field

The relativistic Lagrangian for a particle (rest mass m and charge q) is given by:

$$\mathcal{L}(t) = -mc^2\sqrt{1-rac{\dot{\mathbf{x}}(t)^2}{c^2}} + q\dot{\mathbf{x}}(t)\cdot\mathbf{A}\left(\mathbf{x}(t),t
ight) - qarphi\left(\mathbf{x}(t),t
ight)$$

Thus the particle's canonical momentum is

$$\mathbf{p}(t) = rac{\partial \mathcal{L}}{\partial \dot{\mathbf{x}}} = rac{m \dot{\mathbf{x}}}{\sqrt{1 - rac{\dot{\mathbf{x}}^2}{c^2}}} + q \mathbf{A}$$

that is, the sum of the kinetic momentum and the potential momentum.

Solving for the velocity, we get

$$\dot{\mathbf{x}}(t) = rac{\mathbf{p} - q\mathbf{A}}{\sqrt{m^2 + rac{1}{c^2}(\mathbf{p} - q\mathbf{A})^2}}$$

So the Hamiltonian is

$$\mathcal{H}(t) = \dot{\mathbf{x}} \cdot \mathbf{p} - \mathcal{L} = c \sqrt{m^2 c^2 + (\mathbf{p} - q \mathbf{A})^2} + q arphi$$

This results in the force equation (equivalent to the Euler-Lagrange equation)

$$\dot{\mathbf{p}} = -rac{\partial \mathcal{H}}{\partial \mathbf{x}} = q\dot{\mathbf{x}}\cdot(\mathbf{\nabla}\mathbf{A}) - q\mathbf{\nabla}\varphi = q\mathbf{\nabla}(\dot{\mathbf{x}}\cdot\mathbf{A}) - q\mathbf{\nabla}\varphi$$

from which one can derive

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{m\dot{\mathbf{x}}}{\sqrt{1 - \frac{\dot{\mathbf{x}}^2}{c^2}}} \right) = \frac{\mathrm{d}}{\mathrm{d}t} (\mathbf{p} - q\mathbf{A}) = \dot{\mathbf{p}} - q \frac{\partial \mathbf{A}}{\partial t} - q(\dot{\mathbf{x}} \cdot \nabla) \mathbf{A}$$
$$= q \nabla (\dot{\mathbf{x}} \cdot \mathbf{A}) - q \nabla \varphi - q \frac{\partial \mathbf{A}}{\partial t} - q(\dot{\mathbf{x}} \cdot \nabla) \mathbf{A}$$
$$= q \mathbf{E} + q \dot{\mathbf{x}} \times \mathbf{B}$$

The above derivation makes use of the vector calculus identity:

$$\frac{1}{2}\nabla (\mathbf{A} \cdot \mathbf{A}) = \mathbf{A} \cdot \mathbf{J}_{\mathbf{A}} = \mathbf{A} \cdot (\nabla \mathbf{A}) = (\mathbf{A} \cdot \nabla)\mathbf{A} + \mathbf{A} \times (\nabla \times \mathbf{A}).$$

An equivalent expression for the Hamiltonian as function of the relativistic (kinetic) momentum, $\mathbf{P} = \gamma m \dot{\mathbf{x}}(t) = \mathbf{p} - q \mathbf{A}$, is

$$\mathcal{H}(t) = \dot{\mathbf{x}}(t) \cdot \mathbf{P}(t) + rac{mc^2}{\gamma} + q arphi(\mathbf{x}(t),t) = \gamma mc^2 + q arphi(\mathbf{x}(t),t) = E + V$$

This has the advantage that kinetic momentum \mathbf{P} can be measured experimentally whereas canonical momentum \mathbf{p} cannot. Notice that the Hamiltonian (<u>total energy</u>) can be viewed as the sum of the <u>relativistic energy</u> (<u>kinetic+rest</u>), $E = \gamma mc^2$, plus the <u>potential energy</u>, $V = q\varphi$.

From symplectic geometry to Hamilton's equations

Geometry of Hamiltonian systems

The Hamiltonian can induce a <u>symplectic structure</u> on a <u>smooth even-dimensional manifold</u> M^{2n} in several equivalent ways, the best known being the following: [8]

As a <u>closed nondegenerate symplectic</u> <u>2-form</u> ω . According to the <u>Darboux's theorem</u>, in a small neighbourhood around any point on M there exist suitable local coordinates $p_1, \dots, p_n, q_1, \dots, q_n$ (<u>canonical</u> or <u>symplectic</u> coordinates) in which the <u>symplectic form</u> becomes:

$$\omega = \sum_{i=1}^n dp_i \wedge dq_i \ .$$

The form ω induces a <u>natural isomorphism</u> of the <u>tangent space</u> with the <u>cotangent space</u>: $T_xM \cong T_x^*M$. This is done by mapping a vector $\xi \in T_xM$ to the 1-form $\omega_{\xi} \in T_x^*M$, where $\omega_{\xi}(\eta) = \omega(\eta, \xi)$ for all $\eta \in T_xM$. Due to the <u>bilinearity</u> and non-degeneracy of ω , and the fact that $\dim T_xM = \dim T_x^*M$, the mapping $\xi \to \omega_{\xi}$ is indeed a <u>linear isomorphism</u>. This isomorphism is *natural* in that it does not change with change of coordinates on M. Repeating over all $x \in M$, we end up with an isomorphism $J^{-1} : \operatorname{Vect}(M) \to \Omega^1(M)$ between the infinite-dimensional space of smooth vector fields and that of smooth 1-forms. For every $f, g \in C^{\infty}(M, \mathbb{R})$ and $\xi, \eta \in \operatorname{Vect}(M)$,

$$J^{-1}(f\xi+g\eta)=fJ^{-1}(\xi)+gJ^{-1}(\eta).$$

(In algebraic terms, one would say that the $C^{\infty}(M,\mathbb{R})$ -modules $\mathrm{Vect}(M)$ and $\Omega^1(M)$ are isomorphic). If $H \in C^{\infty}(M \times \mathbb{R}_t, \mathbb{R})$, then, for every fixed $t \in \mathbb{R}_t$, $dH \in \Omega^1(M)$, and $J(dH) \in \mathrm{Vect}(M)$. J(dH) is known as a Hamiltonian vector field. The respective differential equation on M

$$\dot{x} = J(dH)(x)$$

is called Hamilton's equation. Here x = x(t) and $J(dH)(x) \in T_xM$ is the (time-dependent) value of the vector field J(dH) at $x \in M$.

A Hamiltonian system may be understood as a <u>fiber bundle</u> E over $\underline{\text{time}} R$, with the $\underline{\text{fiber}} E_t$ being the position space at time $t \in R$. The Lagrangian is thus a function on the <u>jet bundle</u> J over E; taking the fiberwise <u>Legendre transform</u> of the Lagrangian produces a function on the dual bundle over time whose fiber at t is the cotangent space T^*E_t , which comes equipped with a natural symplectic form, and this

latter function is the Hamiltonian. The correspondence between Lagrangian and Hamiltonian mechanics is achieved with the $\underline{\text{tautological}}$ one-form.

Any smooth real-valued function \mathcal{H} on a symplectic manifold can be used to define a Hamiltonian system. The function \mathcal{H} is known as "the Hamiltonian" or "the energy function." The symplectic manifold is then called the phase space. The Hamiltonian induces a special vector field on the symplectic manifold, known as the Hamiltonian vector field.

The Hamiltonian vector field induces a <u>Hamiltonian flow</u> on the manifold. This is a one-parameter family of transformations of the manifold (the parameter of the curves is commonly called "the time"); in other words, an <u>isotopy</u> of <u>symplectomorphisms</u>, starting with the identity. By <u>Liouville's theorem</u>, each symplectomorphism preserves the <u>volume form</u> on the <u>phase space</u>. The collection of symplectomorphisms induced by the Hamiltonian flow is commonly called "the Hamiltonian mechanics" of the Hamiltonian system.

The symplectic structure induces a <u>Poisson bracket</u>. The Poisson bracket gives the space of functions on the manifold the structure of a Lie algebra.

If F and G are smooth functions on M then the smooth function $\omega(J(dF), J(dG))$ is properly defined; it is called a *Poisson bracket* of functions F and G and is denoted $\{F, G\}$. The Poisson bracket has the following properties:

- 1. bilinearity
- 2. antisymmetry
- 3. Leibniz rule: $\{F_1 \cdot F_2, G\} = F_1\{F_2, G\} + F_2\{F_1, G\}$
- 4. Jacobi identity: $\{\{H,F\},G\}+\{\{F,G\},H\}+\{\{G,H\},F\}\equiv 0$
- 5. non-degeneracy: if the point x on M is not critical for F then a smooth function G exists such that $\{F, G\}(x) \neq 0$.

Given a function f

$$\frac{\mathrm{d}}{\mathrm{d}t}f = \frac{\partial}{\partial t}f + \{f,\mathcal{H}\}\,,$$

if there is a <u>probability distribution</u> ρ , then (since the phase space velocity (\dot{p}_i, \dot{q}_i) has zero divergence and probability is conserved) its convective derivative can be shown to be zero and so

$$\frac{\partial}{\partial t}
ho = -\left\{
ho, \mathcal{H}
ight\}$$

This is called <u>Liouville's theorem</u>. Every <u>smooth function</u> G over the <u>symplectic manifold</u> generates a one-parameter family of symplectomorphisms and if $\{G, H\} = 0$, then G is conserved and the symplectomorphisms are symmetry transformations.

A Hamiltonian may have multiple conserved quantities G_i . If the symplectic manifold has dimension 2n and there are n functionally independent conserved quantities G_i which are in involution (i.e., $\{G_i, G_j\} = 0$), then the Hamiltonian is Liouville integrable. The Liouville—Arnold theorem says that, locally, any Liouville integrable Hamiltonian can be transformed via a symplectomorphism into a new Hamiltonian with the conserved quantities G_i as coordinates; the new coordinates are called *action-angle coordinates*. The transformed Hamiltonian depends only on the G_i , and hence the equations of motion have the simple form

$$\dot{G}_i = 0$$
 , $\dot{\varphi}_i = F_i(G)$

for some function F. [9] There is an entire field focusing on small deviations from integrable systems governed by the KAM theorem.

The integrability of Hamiltonian vector fields is an open question. In general, Hamiltonian systems are <u>chaotic</u>; concepts of measure, completeness, integrability and stability are poorly defined.

Riemannian manifolds

An important special case consists of those Hamiltonians that are quadratic forms, that is, Hamiltonians that can be written as

$$\mathcal{H}(q,p)=rac{1}{2}\langle p,p
angle_q$$

where $\langle \; , \; \rangle_q$ is a smoothly varying <u>inner product</u> on the <u>fibers</u> $T_q^* \mathcal{Q}$, the <u>cotangent space</u> to the point q in the <u>configuration space</u>, sometimes called a cometric. This Hamiltonian consists entirely of the <u>kinetic term</u>.

If one considers a <u>Riemannian manifold</u> or a pseudo-Riemannian <u>manifold</u>, the <u>Riemannian metric</u> induces a linear isomorphism between the tangent and cotangent bundles. (See <u>Musical isomorphism</u>). Using this isomorphism, one can define a cometric. (In coordinates, the matrix defining the cometric is the inverse of the matrix defining the metric.) The solutions to the Hamilton–Jacobi

equations for this Hamiltonian are then the same as the geodesics on the manifold. In particular, the <u>Hamiltonian flow</u> in this case is the same thing as the <u>geodesic flow</u>. The existence of such solutions, and the completeness of the set of solutions, are discussed in detail in the article on geodesics. See also *Geodesics as Hamiltonian flows*.

Sub-Riemannian manifolds

When the cometric is degenerate, then it is not invertible. In this case, one does not have a Riemannian manifold, as one does not have a metric. However, the Hamiltonian still exists. In the case where the cometric is degenerate at every point q of the configuration space manifold Q, so that the rank of the cometric is less than the dimension of the manifold Q, one has a sub-Riemannian manifold.

The Hamiltonian in this case is known as a **sub-Riemannian Hamiltonian**. Every such Hamiltonian uniquely determines the cometric, and vice versa. This implies that every <u>sub-Riemannian manifold</u> is uniquely determined by its sub-Riemannian Hamiltonian, and that the converse is true: every sub-Riemannian manifold has a unique sub-Riemannian Hamiltonian. The existence of sub-Riemannian geodesics is given by the Chow–Rashevskii theorem.

The continuous, real-valued <u>Heisenberg group</u> provides a simple example of a sub-Riemannian manifold. For the Heisenberg group, the Hamiltonian is given by

$$\mathcal{H}\left(x,y,z,p_{x},p_{y},p_{z}
ight)=rac{1}{2}\left(p_{x}^{2}+p_{y}^{2}
ight).$$

 p_z is not involved in the Hamiltonian.

Poisson algebras

Hamiltonian systems can be generalized in various ways. Instead of simply looking at the <u>algebra</u> of <u>smooth functions</u> over a <u>symplectic</u> manifold, Hamiltonian mechanics can be formulated on general <u>commutative unital real Poisson algebras</u>. A <u>state</u> is a <u>continuous linear functional</u> on the Poisson algebra (equipped with some suitable <u>topology</u>) such that for any element A of the algebra, A^2 maps to a nonnegative real number.

A further generalization is given by Nambu dynamics.

Generalization to quantum mechanics through Poisson bracket

Hamilton's equations above work well for <u>classical mechanics</u>, but not for <u>quantum mechanics</u>, since the differential equations discussed assume that one can specify the exact position and momentum of the particle simultaneously at any point in time. However, the equations can be further generalized to then be extended to apply to quantum mechanics as well as to classical mechanics, through the deformation of the Poisson algebra over p and q to the algebra of Moyal brackets.

Specifically, the more general form of the Hamilton's equation reads

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \{f, \mathcal{H}\} + \frac{\partial f}{\partial t},$$

where f is some function of p and q, and H is the Hamiltonian. To find out the rules for evaluating a <u>Poisson bracket</u> without resorting to differential equations, see <u>Lie algebra</u>; a Poisson bracket is the name for the Lie bracket in a <u>Poisson algebra</u>. These Poisson brackets can then be extended to Moyal brackets comporting to an inequivalent Lie algebra, as proven by Hilbrand J. Groenewold, and thereby

describe quantum mechanical diffusion in phase space (See <u>Phase space formulation</u> and <u>Wigner-Weyl transform</u>). This more algebraic approach not only permits ultimately extending <u>probability distributions</u> in <u>phase space</u> to <u>Wigner quasi-probability distributions</u>, but, at the mere Poisson bracket classical setting, also provides more power in helping analyze the relevant conserved quantities in a system.

See also

- Canonical transformation
- Classical field theory
- Hamiltonian field theory
- Covariant Hamiltonian field theory
- Classical mechanics
- Dynamical systems theory
- Hamiltonian system
- Hamilton–Jacobi equation
- Hamilton-Jacobi-Einstein equation
- Lagrangian mechanics
- Maxwell's equations

- Hamiltonian (quantum mechanics)
- Quantum Hamilton's equations
- Quantum field theory
- Hamiltonian optics
- De Donder-Weyl theory
- Geometric mechanics
- Routhian mechanics
- Nambu mechanics
- Hamiltonian fluid mechanics
- Hamiltonian vector field

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