Particle motion in Hamiltonian Formalism I

Or how to derive and solve equations of motion

Yannis PAPAPHILIPPOU

Accelerator and Beam Physics group

Beams Department

CERN

CERN Accelerator School

Introduction to Accelerator Physics

Everness Hotel, Chavannes de Bogis, Switzerland

September 25th – October 8th, 2021

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Purpose

- The key point is how to derive **equations of motion** and how to **solve** (**integrate**) them
- Introduce **formalism** of **theoretical mechanics** for analysing particle motion in general (linear or non-linear) **dynamical systems**, including **particle accelerators**
- Connect this **formalism** with **concepts** already studied in the introductory school (matrices, synchrotron motion, invariants,…)
- Prepare the **ground** for the approaches followed for **studying non-linear particle motion** in accelerators (in the advanced course)

Equations of motion

Reminder: Newton's law

- The motion of a "classical" particle in a force field is described by **Newton's law**:

$$m\frac{d^2u(t)}{dt^2} = \frac{dp_u(t)}{dt} = F(u) = -\frac{\partial V(u)}{\partial u}$$

with u the position

p_u the momentum

$F(u)$ the force

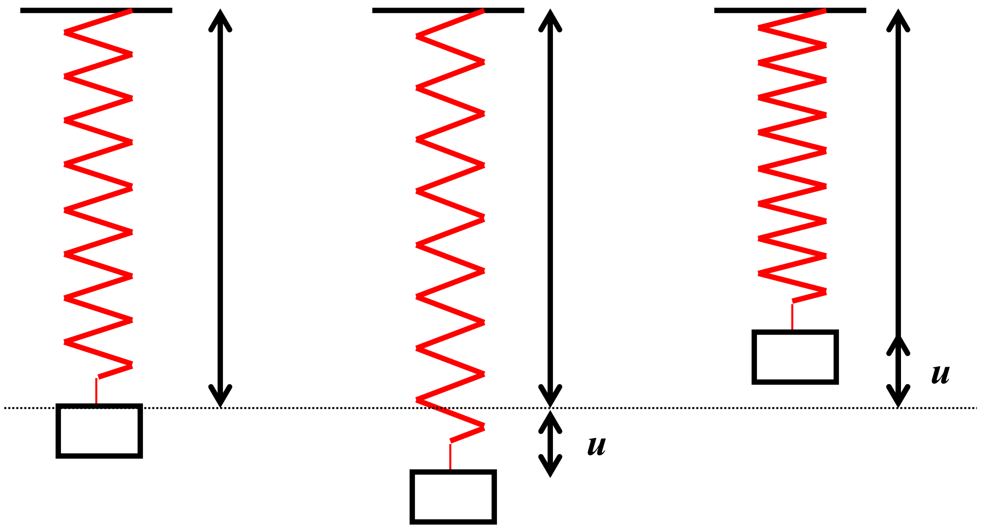
$V(u)$ the corresponding potential

- It is essential to solve (**integrate**) the differential equation for understanding the evolution of the physical (dynamical) system

Reminder: Harmonic oscillator

- A linear restoring force (**Harmonic oscillator**) is described by

$$\frac{d^2u(t)}{dt^2} + \omega_0^2 u(t) = 0 \quad \text{with} \quad \omega_0 = \sqrt{\frac{k}{m}}$$



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- The solution obtained by the **substitution** $u(t) = e^{\lambda t}$

and the solutions of the **characteristic polynomial** are

$\lambda^2 + \omega_0^2 = 0 \Rightarrow \lambda_{\pm} = \pm i\omega_0$, which yields the **general solution**

$$u(t) = ce^{i\omega_0 t} + c^* e^{-i\omega_0 t} = C_1 \cos(\omega_0 t) + C_2 \sin(\omega_0 t) = A \sin(\omega_0 t + \phi)$$

with the "**velocity**"

$$\frac{du(t)}{dt} = -C_1\omega_0 \sin(\omega_0 t) + C_2\omega_0 \cos(\omega_0 t) = A\omega_0 \cos(\omega_0 t + \phi)$$

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- Note that a **negative sign** in the differential equation provides a solution described by **hyperbolic sine/cosine** functions
- Note also that for **no restoring force** $\omega_0 = 0$, the motion is **unbounded**

Matrix solution

- The **amplitude** and **phase** depend on the **initial conditions**

$$u(0) = u_0 = C_1 \ , \ \frac{du(0)}{dt} = u_0' = C_2\omega_0 \ , \ A = \frac{\left(u_0'^{\,2} + \omega_0^2 u_0^2\right)^{1/2}}{\omega_0} \ , \ \tan(\phi) = \frac{u_0'}{\omega_0 u_0}$$

- The solutions can be re-written thus as

$$u(t) = u_0 \cos(\omega_0 t) + \frac{u_0'}{\omega_0} \sin(\omega_0 t)$$
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or in **matrix form**

$$\begin{pmatrix} u(t) \\ u'(t) \end{pmatrix} = \begin{pmatrix} \cos(\omega_0 t) & \frac{1}{\omega_0}\sin(\omega_0 t) \\ -\omega_0 \sin(\omega_0 t) & \cos(\omega_0 t) \end{pmatrix} \begin{pmatrix} u_0 \\ u_0' \end{pmatrix}$$

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- By replacing $\omega_0 \rightarrow \sqrt{k_0}$ and $t \longrightarrow s$, this becomes the solution of a **quadrupole** (see **Transverse Linear Beam Dynamics** lectures)

Matrix formalism

- General **transfer matrix** from s_0 to s

$$\begin{pmatrix} u \\ u' \end{pmatrix}_s = \mathcal{M}(s|s_0) \begin{pmatrix} u \\ u' \end{pmatrix}_{s_0} = \begin{pmatrix} C(s|s_0) & S(s|s_0) \\ C'(s|s_0) & S'(s|s_0) \end{pmatrix} \begin{pmatrix} u \\ u' \end{pmatrix}_{s_0}$$

- Note that $\det(\mathcal{M}(s|s_0)) = C(s|s_0)S'(s|s_0) - S(s|s_0)C'(s|s_0) = 1$ which is always true for **conservative systems ("energy" is constant)**
- Note also that $\mathcal{M}(s_0|s_0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathcal{I}$

(see **Transverse Linear Beam Dynamics lectures**)

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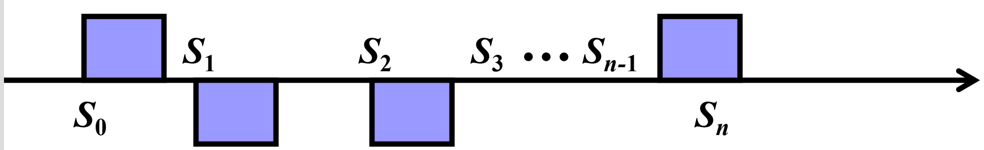
- Note also that $\mathcal{M}(s_0|s_0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathcal{I}$
- The **general solution** can be build by a series of matrix multiplications

$$\mathcal{M}(s_n|s_0) = \mathcal{M}(s_n|s_{n-1}) \ldots \mathcal{M}(s_3|s_2) \cdot \mathcal{M}(s_2|s_1) \cdot \mathcal{M}(s_1|s_0)$$



from s_0 to s_1

from s_0 to s_2

from s_0 to s_3

from s_0 to s_n

(see **Transverse Linear Beam Dynamics lectures**)

Integral of motion

- Rewrite the differential equation of the harmonic oscillator as a pair of coupled 1st order equations

$$\begin{aligned} \frac{du(t)}{dt} &= p_u(t) \\ \frac{dp_u(t)}{dt} &= -\omega_0^2 u(t) \end{aligned}$$

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$$\frac{du(t)}{dt} = p_u(t)$$
$$\frac{dp_u(t)}{dt} = -\omega_0^2 u(t)$$

which can be combined to provide

$$\frac{dp_u}{dt}p_u + \omega_0^2 u\frac{du}{dt} = \frac{1}{2}\frac{d}{dt}\left(p_u^2 + \omega_0^2 u^2\right) = 0$$

or

$\frac{1}{2}\left(p_u^2 + \omega_0^2 u^2\right) = I_1$ with I_1 an **integral of motion**

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- Solving the previous equation for p_u, the system can be reduced to a first order equation

$$\frac{du}{dt} = \sqrt{2I_1 - \omega_0^2 u^2}$$

Integration by quadrature

- The last equation can be solved as an explicit integral or **"quadrature"**

$$\int dt = \int \frac{du}{\sqrt{2I_1 - \omega_0^2 u^2}}\,,\ \text{yielding}\ \ t + I_2 = \frac{1}{\omega_0}\arcsin\left(\frac{u\omega_0}{\sqrt{2I_1}}\right)$$

or the well-known solution $u(t) = \dfrac{\sqrt{2I_1}}{\omega_0}\sin(\omega_0 t + \omega_0 I_2)$

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- **Note**: Although the previous route may seem complicated, it becomes more natural when **non-linear** terms appear, where an **ansatz** of the type $u(t) = e^{\lambda t}$ is **not applicable**
- The ability to integrate a differential equation is not just a nice mathematical feature, but deeply characterizes the **dynamical behavior** of the system described by the equation

Frequency of motion

- The **period** of the harmonic oscillator is calculated through the previous integral after integration between two extrema (when the velocity $\frac{du}{dt} = \sqrt{2I_1 - \omega_0^2 u^2}$ vanishes), i.e. $u_{\rm ext} = \pm \frac{\sqrt{2I_1}}{\omega_0}$:

$$T = 2\int_{-\frac{\sqrt{2I_1}}{\omega_0}}^{\frac{\sqrt{2I_1}}{\omega_0}} \frac{du}{\sqrt{2I_1 - \omega_0^2 u^2}} = \frac{2\pi}{\omega_0}$$

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- The **period** (or the **frequency**) of linear systems is **independent** of the **integral of motion** (energy)
- Note that this is not true for non-linear systems, e.g. for an oscillator with a **non-linear restoring force** $\frac{d^2u}{dt^2} + k\ u(t)^3 = 0$
- The integral of motion is $I_1 = \frac{1}{2}p_u^2 + \frac{1}{4}k\ u^4$ and the integration yields $T = 2\int_{-(4I_1/k)^{1/4}}^{(4I_1/k)^{1/4}} \frac{du}{\sqrt{2I_1 - \frac{1}{2}k\ u^4}} = \sqrt{\frac{1}{2\pi}}\Gamma^2(\frac{1}{4})\,(I_1\ k)^{-1/4}$
- This means that the **period** (frequency) **depends** on the **integral of motion** (energy) i.e. the maximum "amplitude"

The pendulum

- An important non-linear equation which can be integrated is the one of the **pendulum**, for a string of length L and gravitational constant g

$$\frac{d^2\phi}{dt^2} + \frac{g}{L}\sin\phi = 0$$

- For small displacements it reduces to a **harmonic oscillator** with frequency $\omega_0 = \sqrt{\frac{g}{L}}$
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- By appropriate substitutions, this becomes the equation of **synchrotron motion** (**see Longitudinal BD lectures**)
- The **integral of motion** (scaled energy) is

$$\frac{1}{2}\left(\frac{d\phi}{dt}\right)^2 - \frac{g}{L}\cos\phi = I_1 = E'$$

and the quadrature is written as $t = \int \frac{d\phi}{\sqrt{2(I_1 + \frac{g}{L}\cos\phi)}}$

assuming that for $t = 0\,,\quad \phi_0 = \phi(0) = 0$

Solution for the pendulum

- Using the substitutions $\cos\phi = 1 - 2k^2\sin^2\theta$ with $k = \sqrt{1/2(1 + I_1 L/g)}$, the integral is

$$t = \sqrt{\frac{L}{g}}\int_0^\theta \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}$$ and can be solved using

Jacobi elliptic functions: $\phi(t) = 2\arcsin\left[k\ \mathrm{sn}\left(t\sqrt{\frac{g}{L}}, k\right)\right]$

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- For the **period**, the integration is performed between the two extrema, i.e. $\phi = 0$ and $\phi = \arccos(-I_1 L/g)$, corresponding to $\theta = 0$ and $\theta = \pi/2$, for which

$$T = 4\sqrt{\frac{L}{g}}\int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} = 4\sqrt{\frac{L}{g}}\mathcal{F}(\pi/2, k) \quad ,$$

i.e. the complete elliptic integral (whose argument **depends** on the **integral of motion**) multiplied by four times the period of the harmonic oscillator

Langrangian and Hamiltonian

Lagrangian formalism

- Describe motion of particles in q_n coordinates (***n* degrees of freedom)** from time t_1 to time t_2
- It can be achieved by the **Lagrangian function** $L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n, t)$ with $(q_1, \ldots, q_n)$ the **generalized coordinates** and $(\dot{q}_1, \ldots, \dot{q}_n)$ the **generalized velocities**

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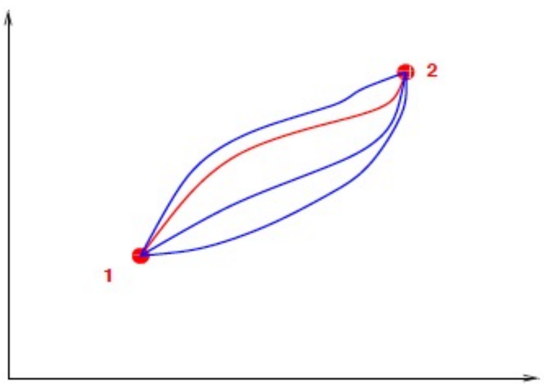
- The Lagrangian is defined as $L = T - V$, i.e. difference between **kinetic** and **potential** energy
- The integral $W = \int L(q_i,\dot{q}_i,t)dt$ defines the **action**
- **Hamilton's principle**: system evolves so as the action becomes extremum (principle of **stationary action**)



Euler- Lagrange equations

- By using **Hamilton's principle,** i.e. $\delta W = 0$, over some time interval t_1 and t_2 for two stationary points $\delta q(t_1) = \delta q(t_2) = 0$ (see appendix), the following differential equations for each degree of freedom are obtained, the **Euler-Lagrange equations**

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

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- In other words, by knowing the form of the Lagrangian, the **equations of motion** can be **derived**

Lagrangian mechanics

- For a simple **force law** contained in a potential function, governing motion among interacting particles, the Lagrangian is (or as Landau-Lifshitz put it "experience has shown that…")

$$L = T - V = \sum_{i=1}^{n} \frac{1}{2} m_i q_i^2 - V(q_1, \ldots, q_n)$$

- For velocity independent potentials, Lagrange equations become

$$m_i \ddot{q}_i = -\frac{\partial V}{\partial q_i} \ ,$$

i.e. **Newton's equations.**

From Lagrangian to Hamiltonian

- Some **disadvantages** of the Lagrangian formalism:
  - **No uniqueness**: different Lagrangians can lead to same equations
  - **Physical significance** not straightforward (even its basic form given more by “experience” and the fact that it actually works that way!)

From Lagrangian to Hamiltonian

- Some **disadvantages** of the Lagrangian formalism:
  - **No uniqueness**: different Lagrangians can lead to same equations
  - **Physical significance** not straightforward (even its basic form given more by "experience" and the fact that it actually works that way!)
- Lagrangian function provides in general n second order differential equations (**coordinate space**)
- We already observed the advantage to move to a system of $2n$ first order differential equations, which are more straightforward to solve (**phase space**)
- These equations can be derived by the **Hamiltonian** of the system

Hamiltonian formalism

- The **Hamiltonian** of the system is defined as the **Legendre transformation** of the Lagrangian

$$H(\mathbf{q},\mathbf{p},t) = \sum_i \dot{q}_i p_i - L(\mathbf{q},\dot{\mathbf{q}},t)$$

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- The **generalised velocities** can be expressed as a function of the **generalised momenta** if the previous equation is invertible, and thereby define the Hamiltonian of the system
- **Example**: consider $L(\mathbf{q},\dot{\mathbf{q}}) = \frac{1}{2}\sum_i m_i \dot{q}_i^2 - V(q_1,\ldots,q_n)$
- From this, the momentum can be determined as $p_i = \frac{\partial L}{\partial \dot{q}_i} = m\dot{q}_i$

which can be trivially inverted to provide the Hamiltonian

$$H(\mathbf{q},\mathbf{p}) = \sum_i \frac{p_i^2}{2m_i} + V(q_1,\ldots,q_n)$$

Hamilton's equations

- The **equations of motion** can be derived from the Hamiltonian following the same variational principle as for the Lagrangian ("stationary" action) but also by simply taking the differential of the Hamiltonian (see appendix)

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \ , \quad \dot{p}_i = -\frac{\partial H}{\partial q} \ , \quad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}$$

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- These are indeed $2n + 2$ equations describing the motion in the **"extended" phase space** $(q_i, \ldots, q_n, p_1, \ldots, p_n, t, -H)$

Properties of Hamiltonian flow

- The variables $(q_i, \ldots, q_n, p_1, \ldots, p_n, t, -H)$ are called **canonically conjugate** (or canonical) and define the evolution of the system in **phase space**
- These variables have the special property that they preserve volume in phase space, i.e. satisfy the well-known **Liouville's theorem**
- The variables used in the **Lagrangian do not necessarily have** this **property**

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- The variables used in the **Lagrangian do not necessarily have** this **property**
- Hamilton's equations can be written in **vector form** $\dot{\mathbf{z}} = \mathbf{J} \cdot \nabla H(\mathbf{z})$ with $\mathbf{z} = (q_i, \ldots, q_n, p_1, \ldots, p_n)$ and $\nabla = (\partial q_i, \ldots, \partial q_n, \partial p_1, \ldots, \partial p_n)$
- The $2n \times 2n$ matrix $\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix}$ is called the **symplectic** matrix

Poisson brackets

- Crucial step in study of Hamiltonian systems is identification of **integrals of motion**
- Consider a **time dependent function** of phase space. Its time evolution is given by

$$\frac{d}{dt}f(\mathbf{p},\mathbf{q},t) = \sum_{i=1}^{n}\left(\frac{dq_i}{dt}\frac{\partial f}{\partial q_i} + \frac{dp_i}{dt}\frac{\partial f}{\partial p_i}\right) + \frac{\partial f}{\partial t}$$

$$= \sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i}\right) + \frac{\partial f}{\partial t} = [H,f] + \frac{\partial f}{\partial t}$$

where $[H,f]$ is the **Poisson bracket** of f with H

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- Consider a **time dependent function** of phase space. Its time evolution is given by

$$\frac{d}{dt}f(\mathbf{p},\mathbf{q},t) = \sum_{i=1}^{n}\left(\frac{dq_i}{dt}\frac{\partial f}{\partial q_i} + \frac{dp_i}{dt}\frac{\partial f}{\partial p_i}\right) + \frac{\partial f}{\partial t}$$

$$= \sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i}\right) + \frac{\partial f}{\partial t} = [H,f] + \frac{\partial f}{\partial t}$$

where $[H,f]$ is the **Poisson bracket** of f with H

- If a quantity is explicitly **time-independent** and its Poisson bracket with the Hamiltonian vanishes (i.e. **commutes** with the H), it is a **constant** (or **integral**) of motion (as an **autonomous** Hamiltonian itself)

Appendix

Derivation of Lagrange equations

- The variation of the action can be written as

$$\delta W = \int_{t_1}^{t_2} \left(L(q+\delta q, \dot{q}+\delta\dot{q}, t) - L(q,\dot{q},t) \right) dt = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta\dot{q} \right) dt$$

- Taking into account that $\delta\dot{q} = \frac{d\delta q}{dt}$, the 2nd part of the integral can be integrated by parts giving

$$\delta W = \left| \frac{\partial L}{\partial \dot{q}}\delta q \right|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}} \right) \right) \delta q dt = 0$$

- The first term is zero because $\delta q(t_1) = \delta q(t_2) = 0$ so the second integrant should also vanish, providing the following differential equations for each degree of freedom, the **Lagrange equations**

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

Derivation of Hamilton's equations

- The **equations of motion** can be derived from the Hamiltonian following the same variational principle as for the Lagrangian ("least" action) but also by simply taking the differential of the Hamiltonian

$$dH = \sum_i p_i d\dot{q}_i + \dot{q}_i dp_i - \underbrace{\frac{\partial L}{\partial \dot{q}_i}}_{p_i} d\dot{q}_i - \underbrace{\frac{\partial L}{\partial q_i}}_{\dot{p}_i} dq_i - \frac{\partial L}{\partial t} dt$$

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or

$$dH(q,p,t) = \sum_i \dot{q}_i dp_i - \dot{p}_i dq_i - \frac{\partial L}{\partial t} dt = \sum_i \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial t} dt$$

- By equating terms, **Hamilton's equations** are derived

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q}, \quad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}$$

- These are indeed $2n+2$ equations describing the motion in the **"extended" phase space** $(q_i, \ldots, q_n, p_1, \ldots, p_n, t, -H)$

Poisson brackets' properties

- The Poisson brackets between two functions of a set of canonical variables can be defined by the differential **operator**

$$[f, g] = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial p_i} \frac{\partial f}{\partial q_i} \right)$$

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- From this definition, and for any three given functions, the following **properties** can be shown

$$[af + bg, h] = a[f, h] + b[g, h] \ , a, b \in \mathbb{R}$$ **bilinearity**

$$[f, g] = -[g, f]$$ **anticommutativity**

$$[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = 0$$ **Jacobi's identity**

$$[f, gh] = [f, g]h + g[f, h]$$ **Leibniz's rule**

- Poisson brackets operation satisfies a **Lie algebra**