Classical Mechanics

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History

- 300 BC, Aristotelian physics: general principles of change that govern all natural bodies. "continuation of motion depends on continued action of a force".
- 6^{th}-14^{th} centuries, The theory of impetus. Intellectual precursor to the concepts of inertia, momentum and acceleration in classical mechanics.
- 17^{th} century Isaac Newton: The three laws of motion " Philosophiae Naturalis Principia Mathematica".
- 17^{th} century Isaac Newton and Gottfried Leibniz: Calculus.
- 18^{th} century, Leonhard Euler: Rigid Body Motion.
- 18^{th} century, Joseph Louis Lagrange: Lagrangian Mechanics.
- 19^{th} century, William Rowan Hamilton: Hamiltonian Mechanics.
- 20^{th} century, Relativity and Quantum Mechanics. Classical physics defines the non-relativistic, non-quantum mechanical limit for massive particles.

Some nomenclature

- $\mathbf{r}(t) = (x(t), y(t), z(t))$ position vector
- $\mathbf{v}(t) = \frac{d\mathbf{r}(t)}{dt}$ velocity vector
- $\mathbf{p}(t) = m\frac{d\mathbf{r}(t)}{dt}$ momentum vector
- $\mathbf{a}(t) = \frac{d\mathbf{v}(t)}{dt}$ or $\frac{d^2\mathbf{r}}{dt^2}$ acceleration vector
- $\mathbf{F} =$ Force vector.
- $\mathbf{v}(t) = \dot{\mathbf{r}}(t)$, $\mathbf{a}(t) = \ddot{\mathbf{r}}(t)$ over dot notation
- $\mathcal{V}, \mathcal{U} =$ Potential Energy or capacity to do work.
- $\mathcal{K} = \frac{1}{2}m\mathbf{v}^2 or \frac{\mathbf{p}^2}{2m}$ Kinetic Energy.

The Newton Laws

- 1st Law: No external forces: $\mathbf{v} = C$, $\frac{d\mathbf{v}}{dt} = 0$ Inertia.
- 2nd Law: $\mathbf{F} = ma$, where $\mathbf{a} = \frac{d\mathbf{v}}{dT}$.
- $\mathbf{F}_{AB} = -\mathbf{F}_{BA}$ Action and Reaction.

Some comments:

- These laws assume that the response to a force is instantaneous (no lag).
- Measurement does not affect system and uncertainty principle does not apply. No QM
- Time and space lie outside physical existence and are absolute. Different observers can always measure the same time and space. No relativity.

Newton's second Law can be restated:

$$\ddot{\mathbf{r}}(t) = \frac{\mathbf{F}}{m} \tag{1}$$

Equation (1) is a 2nd order differential equation, thus two initial conditions need to be specified.

$$\mathbf{r}(t) = \int \int \frac{\mathbf{F}}{m} dt \tag{2}$$

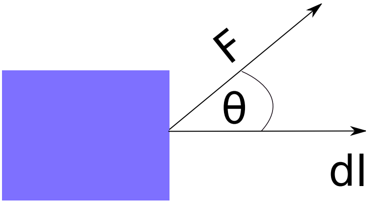
For a constant force:

$$\mathbf{r}(t) = \frac{\mathbf{F}}{m} \Delta t^2 + C_1 \Delta t + C_2 \tag{3}$$

$C_1 =$ Initial Velocity and $C_2 =$Initial position. Equation (3) uniquely specifies the motion of an object in time.

Basic Concepts: Mechanical work

$$W_{A\rightarrow B}(\text{path}) \equiv \int_A^B \mathbf{F} \cdot dL \tag{4}$$



*Dot product $\mathbf{F} \cdot dL \equiv |\mathbf{F}||\mathbf{L}| \cos\theta$ or $\sum F_i \cdot L_i$. It is the projection of a vector into another.

Basic Concepts: Conservative Forces

Conservative forces are defined as vector quantities that are derivable from a scalar function $V(r1, ..., rN)$, known as a potential energy function, via

$$\mathbf{F}(\mathbf{r}_1, ..., \mathbf{r}_N) = -\nabla_i V(\mathbf{r}_1, ...\mathbf{r}_N) \tag{5}$$

where $\nabla_i = \partial/\partial r_i$. Consider the work done by the force $\mathbf{F}_i$ in moving particle i from points A to B along a particular path. The work done is:

$$W_{A\to B} = \int_A^B \mathbf{F}_i \cdot dL = \int_A^B -\nabla_i V \cdot dL = \Delta V_{B\to A} \tag{6}$$

Thus, we conclude that the work done by conservative forces is independent of the path taken between A and B. It follows, therefore, that along a closed path:

$$\oint \mathbf{F}_i \cdot L = 0 \tag{7}$$

Basic Concepts: Newton's Laws for many particle systems

Classical mechanics in the microscopic world, deals with a large number of particles that are the constituent of matter. It is assumed that the laws of classical physics can be applied at the molecular level:

$$\mathbf{F}_i = \mathbf{F}_i(\mathbf{r}_1 \ldots.., \mathbf{r}_n, \dot{r}_i) \tag{8}$$

$\mathbf{F}_i$ depends on the positions of the rest of the particles plus a friction term. Now if the force only depends on the individual terms we say that is pairwise additive:

$$\mathbf{F}_i(\mathbf{r}_1 \ldots.., \mathbf{r}_n, \dot{r}_i) = \sum_{j \neq i} \mathbf{F}_{i,j}(r_i - r_j) + \mathbf{F}^{ext}(r_i, \dot{r}_j) \tag{9}$$

Newton's second law:

$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i(\mathbf{r}_1 \ldots.., \mathbf{r}_n, \dot{\mathbf{r}}_i) \tag{10}$$

Basic Concepts: Phase Space

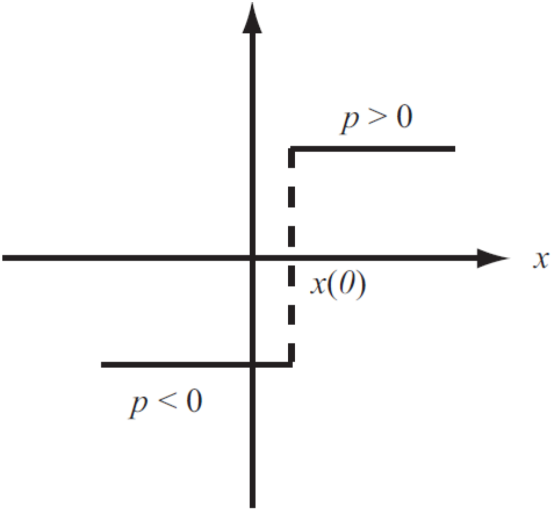
-6N dimensional space, each point compromises the 3N positions + the 3N momentum

$$\mathbf{X} = (r_1......r_{3N}, p_1.......p_{3N}) \rightarrow \text{phase space vector} \tag{11}$$

- All information required to propagate the system in time is contained in the phase space vector.
- Classical motion can be visualized a the motion of a phase-space point in time.
- For $N \sim 10^{23}$ it is a enormous element.

Basic Concepts: Phase Space Examples

-1D free particle:



Basic Concepts: Phase Space Examples

-1D Harmonic oscillator:

$$\ddot{x} = -\frac{k}{m}x \tag{12}$$

$$V(x) = -\int -kx = \frac{1}{2}kx^2 \tag{13}$$

Let's propose $x(t) = e^{i\omega t}$

$$\frac{\partial}{\partial t}\frac{\partial e^{i\omega t}}{\partial t} = i^2\omega^2 e^{i\omega t} = -\frac{k}{m}x(t) \tag{14}$$

with $\omega = \sqrt{k/m}$ and employing euler's identity $e^{ikx} = \cos kx + i \sin kx$ and subject to two initial conditions:

$$x(t) = A\cos(\omega t + \phi) \tag{15}$$

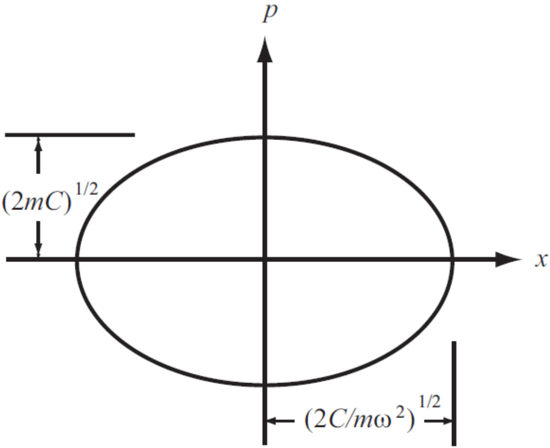
or

$$x(t) = x(0)\cos(\omega t) + \frac{p(0)}{\omega m}\sin(\omega t) \tag{16}$$

$$p(t) = p(0)cos(\omega t) - m\omega x(0)\sin(\omega t) \tag{17}$$

Assuming energy conservation:

$$\frac{p(t)^2}{2m} + \frac{1}{2}m\omega^2 x(t)^2 = C \tag{18}$$



p
x
(2mC)^{1/2}
(2C/mω^2)^{1/2}

Conserved Quantities from Newton's equations

Let's assume N particles in 2D:
$E_T = \mathcal{K}(v) + \mathcal{V}(x)$
$\mathcal{K} = \frac{1}{2} m_1 (v_{x_1}^2 + v_{y_1}^2) + ...$ and $\dot{\mathcal{K}} = \sum \frac{1}{2} 2 v_{i_1} \dot{v}_{i_1} = \sum m v_{i_1} a_{i_1} + ...$
$\dot{\mathcal{V}} = \frac{dU}{dx_1} \dot{x}_1 + \frac{dU}{dy_1} \dot{y}_1 + ... = \sum -m_i v_{i_1} a_{i_1} + ...$

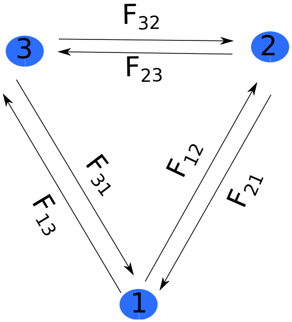
$$\dot{E}_t = \dot{\mathcal{V}} + \dot{\mathcal{K}} = \sum m_i v_{i_1} a_{i_1} + ... + \sum -m_i v_{i_1} a_{i_1} + ... = 0 \qquad (19)$$

Total Energy is conserved!!!!

Conserved Quantities from Newton's equations

Let's assume 3 particles in 3D:

- $\mathbf{F}_i = \frac{d}{dt}(m_i v_i) = \dot{\mathbf{p}}_i$
- $\mathbf{F}_1 = \mathbf{F}_{21} + \mathbf{F}_{31}$
- $\mathbf{F}_2 = \mathbf{F}_{12} + \mathbf{F}_{32}$
- $\mathbf{F}_3 = \mathbf{F}_{13} + \mathbf{F}_{23}$



Given that Newton's 3rd law implies $\mathbf{F}_{ij} = \mathbf{F}_{ji}$

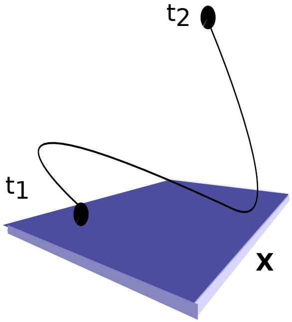
$$\dot{p}_t = \sum \dot{p}_i = \sum \mathbf{F}_i = 0 \tag{20}$$

Total momentum is conserved!!!

Lagrangian Mechanics

- Newton's equations are a local approach, *i.e.* derivatives, in other words local equations along a trajectory.
- A global approach only looks at the end-points. There is a unique trajectory that connects both end-points.
- There is a quantity that is minimized along the trajectory.

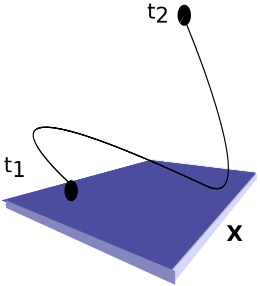
- What to minimize?
- Trajectory is a multivariate function.



Lagrangian Mechanics: The Action

$$A = \int_{t_1}^{t_2} dt\mathcal{K}(\dot{q}) - \mathcal{V}(q_1....q_n) \tag{21}$$

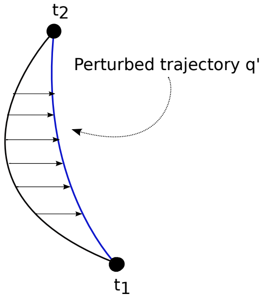
- Generalized coordinates q_i: cartesian, polar, orientation etc...
- What to minimize? The action.
- The integrand in equation (21) is called the **Lagrangian** $\mathcal{L}(\dot{q}, q)$.



$$A = \int_{t_1}^{t_2} dt\mathcal{L}(\dot{q}, q) \tag{22}$$

Lagrangian Mechanics: Calculus of variations

- Small first order variation on the trajectory
- $q_1(t)......q_n(t) \rightarrow q_i(t) + \alpha f_i(t) = q_i'(t)$
- α is any number.
- and $f_i(t)$ vanishes at the end-points.
- We postulate that the action is minimized in $q'(t)$



$$\frac{\partial A(\alpha)}{\partial \alpha} = 0 \tag{23}$$

$\frac{\partial q_i'(t)}{\partial \alpha} = f_i(t)$, $\frac{\partial \dot{q}_i'(t)}{\partial \alpha} = \dot{f}_i(t)$

$$\frac{\partial A}{\partial \alpha} = \int_{t_1}^{t_2} dt \sum_{i=1}^{n} \left[\frac{\partial \mathcal{L}}{\partial q_i} \cdot f_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \cdot \dot{f}_i \right] = 0 \tag{24}$$

Integrating by parts the second term and using the fact that f_i vanishes at the end-points:

$$\frac{\partial A}{\partial \alpha} = \int_{t_1}^{t_2} dt \sum_{i=1}^{n} f_i \left[\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right] = 0 \tag{25}$$

Given that dt is not zero and f_i only vanishes at the end-points, it implies:

$$\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} = 0 \tag{26}$$

Equation (26) is known as the **Euler-Lagrange equation**. There are n equation for each q_i generalized coordinate.

Euler-Lagrange equation

- $\Pi_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} =$ The conjugate momentum to q_i.
- $\frac{\partial \mathcal{L}}{\partial q_i} =$ The generalized force.

Example: Single particle 1D

$\mathcal{L} = \frac{p_i^2}{2m} - \mathcal{V}(x_i)$
$\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = p_i$
$\frac{\partial \mathcal{L}}{\partial x_i} = -\frac{\partial \mathcal{V}}{\partial x_i}$
$\dot{p}_i = -\frac{\partial \mathcal{V}}{\partial x_i} = f_i = m_i a_i$
Thus we recover Newton's 2nd law.

Lagrangian and Conservation Laws

-Multiple Particle system in Cartesian coordinates:

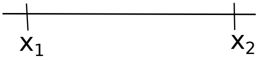
$$\mathcal{L} = \sum_{i=1}^{n} \frac{{p_i}^2}{2m_i} - \mathcal{V}(x_1.....x_n)^* \tag{27}$$

* Inter-particle potential.

Example: Two particle system in 1D.

- $\mathcal{L} = \sum_{i=1}^{2} \frac{p_i^2}{2m} - \mathcal{V}(x_1 - x_2)$
- $\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}_i} = \frac{\partial \mathcal{L}}{\partial x_i}$
- $\dot{p}_1 = -\frac{\partial \mathcal{V}(x_1 - x_2)}{\partial x_1}$,

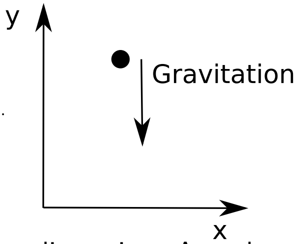
  $\dot{p}_2 = -\frac{\partial \mathcal{V}(x_1 - x_2)}{\partial x_2} = \dot{p}_1 + \dot{p}_2 = 0$



Total momentum is conserved. If we translate the system the Lagrangian does not change ($\mathcal{V}$ only depends on distance. Momentum is conserved due to translational symmetry. Relation between symmetries and conservation laws.

-1 Particle in 2D under gravitation:

- $\mathcal{V} = mgy$
- $\mathcal{L} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} - mgy$
- $\dot{p}_x = \frac{\partial \mathcal{L}}{\partial x} = 0$
- $\dot{p}_y = \frac{\partial \mathcal{L}}{\partial y} = -mg$



Gravitation breaks translational symmetry in the y dimension. Any change in the y direction changes the Lagrangian.

-Symmetries and conservations laws are related to operations that do not alter the Action.
- $F(\alpha)$, $dF = \sum \frac{\partial F}{\partial \alpha_i} d\alpha_i = 0$
-Small variations in the trajectory, first order.
$q_i \to q_i + \epsilon \cdot f_i(q)$, $dq_i = \epsilon f_i(q)$
The variation in the action is:

$$dA = \int_{t_1}^{t_2} dt \sum_{i=1}^{n} \left[\frac{\partial \mathcal{L}}{\partial q_i} dq_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} d\dot{q}_i \right] = 0 \tag{28}$$

Integrating by parts equation (28):

$$dA = \int_{t_1}^{t_2} dt \sum_{i=1}^{n} dq_i \left[\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q_i} \right] + \frac{\partial \mathcal{L}}{\partial \dot{q}} dq_i \Big|_{t_1}^{t_2} \tag{29}$$

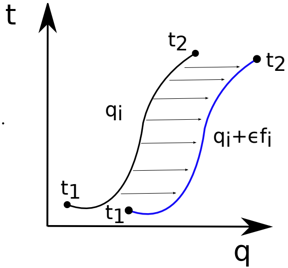
Now, the end-point contributions $\sum_{i=1}^{n} \frac{\partial \mathcal{L}}{\partial \dot{q}} dq_i|_{t_1}^{t_2}$ do not vanish and by virtue of the Euler-Lagrange equation and the condition of null variation of the action $dA = 0$ the following expression is obtained:

$$\sum_{i=1}^{n} \frac{\partial \mathcal{L}}{\partial \dot{q}} dq_i|_{t_1}^{t_2} = \sum_{i=1}^{n} \Pi_i \epsilon f_i|_{t_1}^{t_2} = 0 \tag{30}$$

In other words the quantity $\sum_{i=1}^{n} \Pi_i f_i$ is conserved when performing a variation ϵf_i that does not alter the Action. $\sum_{i=1}^{n} \Pi_i f_i$ is know as **Noether charge.**

Example: Translate all particles by ϵ in the x direction:

- $dx_i = \epsilon,\ f_x = 1$
- $dx_i = 0,\ f_y = 0$
- $dz_i = 0,\ f_z = 0$

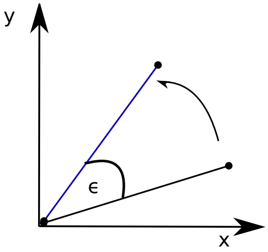


$$\sum \Pi_i f_i = \sum p_{ix} = C \tag{31}$$

Momentum is conserved due to translational invariance.

Example: Rotate all particles by ϵ in the x-y plane:

- $dx = -\epsilon y$, $f_x = -y$
- $dy = \epsilon x$, $f_y = x$

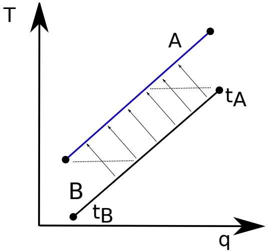


$$\sum \Pi_i f_i = \sum -p_x y + p_y x = L = \text{Angular momentum} \tag{32}$$

Angular momentum is conserved due to rotational invariance.

Example: Move forward in time by ϵ :

- $q(t) \to q(t-\epsilon)$
- $dq(t) = -\frac{dq}{dt}\epsilon = -\dot{q}\epsilon$



What is the Variation in the Action:

$$dA = \int_{t_B}^{t_A} dt \sum_{i=1}^{n} \left[\frac{\partial \mathcal{L}}{\partial q_i} dq_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} d\dot{q}_i \right] + A - B = 0 \tag{33}$$

Integrating by parts equation (33):

$$dA = \int_{t_B}^{t_A} dt \sum_{i=1}^{n} dq_i \left[\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right] + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} dq_i |_{t_B}^{t_A} + A - B = 0 \qquad (34)$$

Applying the Euler-Lagrange equation:

$$\sum_{i=1}^{n} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} dq_i |_{t_1}^{t_2} + A - B = 0 \qquad (35)$$

And given than ϵ is small, A and B can be approximated by $\mathcal{L}(t_A) * \epsilon$ and $\mathcal{L}(t_B) * \epsilon$ respectively.

$$\sum_{i=1}^{n} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} dq_i |_{t_B}^{t_A} + \epsilon [\mathcal{L}(t_A) - \mathcal{L}(t_B)] = 0 \qquad (36)$$

$$\epsilon \left[\sum_{i=1}^{n} - \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \dot{q}_i + \mathcal{L} \right] |_{t_B}^{t_A} = 0 \qquad (37)$$

Thus the quantity $\sum_{i=1}^{n} -\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\dot{q}_i + \mathcal{L}$ is conserved due to **time-translational symmetry** and it is defined as $-\mathcal{H}$. $\mathcal{H}$ is known as the hamiltonian.

$$\mathcal{H} = \sum \dot{q}\Pi_i - \mathcal{L}(q, \dot{q}) \tag{38}$$

Example: 1D Particle in a Potential.

- $\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \mathcal{V}(x)$
- $\Pi = m\dot{x}$
- $\Pi\dot{x} = m\dot{x}^2$
- $\mathcal{H} = m\dot{x}^2 - [\frac{1}{2}m\dot{x}^2 - \mathcal{V}(x)]$

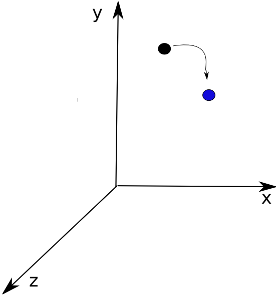
$$\mathcal{H} = \frac{1}{2}m\dot{x}^2 + \mathcal{V}(x) \tag{39}$$

Thus **the total Energy** is the quantity that is conserved due to time-translational symmetry. This is the most general definition of energy.

Hamiltonian Mechanics

Laws of mechanics:

- Subject to conservation Laws.
- Information is conserved.
- Nothing disappear or appears.
- For each degree of freedom we need to know "where we are" and "where we are going"

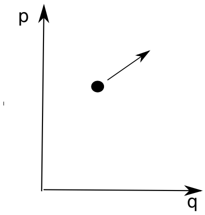


- Lagrangian : 2^{nd}-order differential equation.
  $m\frac{d^2x_i}{dt^2} = F_i$

-Mathematically it is trivial to convert a 2^{nd} order differential equation in to two first-order differential equations:

- $m\frac{dx_i}{dt} = p_i$
- $m\frac{dp_i}{dt} = F_i$

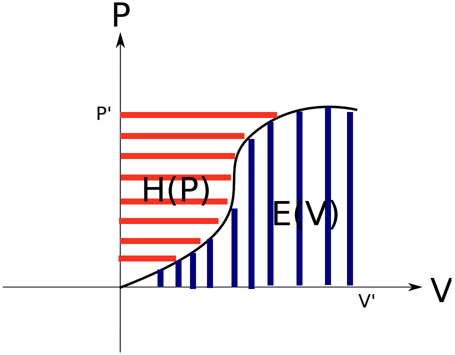
Thus we need position and momentum for each degree of freedom.



The Legendre transform

Consider a function $E(V)$ of one variable. The Legendre transform allows to replace the independent variable V by the derivative $\frac{\partial E}{\partial V}$.

- $\frac{\partial E(V)}{\partial V} = P(V)$
- $\frac{\partial H(P)}{\partial P} = V(P)$
- $E(V) = \int_0^{V'} P(V) dV$
- $H(P) = \int_0^{P'} V(P) dP$
- $H(P) + E(V) = P'V'$



The Legendre transform II

We define the Legendre transform of the function $E(V)$ as

$$H(P) = PV - E(V) \tag{40}$$

Thus for any function $f(x(y))$ the Legendre transform $f^*(y(x))$ is defined as:

The Legendre Transform

$$f^*(y(x)) = \frac{\partial f(x(y))}{\partial x} x(y) - f(x(y)) \tag{41}$$

or

$$-f^*(y(x)) = f(x(y)) - \frac{\partial f(x(y))}{\partial x} x(y) \tag{42}$$

Hamiltonian Mechanics and Legendre transforms

Based on the definition of the Hamiltonian $\mathcal{H} = \sum \dot{q}\Pi_i - \mathcal{L}(q, \dot{q})$ it is evident that it has the form of a legendre transform of the Lagrangian. Let's compute the variation in $\mathcal{H}$:

$$d\mathcal{H} = \sum \dot{q}_i dp_i + \sum p_i d\dot{q}_i - \sum \frac{\partial \mathcal{L}}{dq_i} dq_i - \sum \frac{\partial \mathcal{L}}{d\dot{q}_i} d\dot{q}_i \tag{43}$$

$$d\mathcal{H} = \sum \dot{q}_i dp_i - \sum \frac{\partial \mathcal{L}}{dq_i} dq_i \tag{44}$$

Thus $\mathcal{H}$ is function of the p_i's and q_i's. $\mathcal{H}(q, p)$

Derivating with respect to each q_i and p_i equation (44) while keeping the rest of variables fixed we obtain:

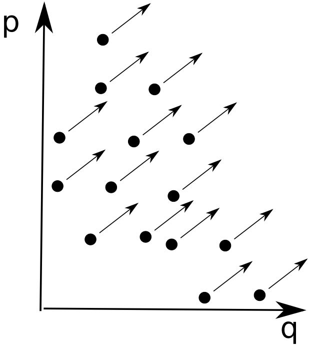
$$\left(\frac{\partial \mathcal{H}}{\partial p_i}\right)_{qi} = \dot{q}_i \tag{45}$$

and

$$-\left(\frac{\partial \mathcal{H}}{\partial q_i}\right)_{pi} = \dot{p}_i \tag{46}$$

Equations (45) and (46) are know as the **Hamilton equation of motion**.

- $\left(\frac{\partial \mathcal{H}}{\partial p_i}\right)_{qi} = \dot{q}_i$. Velocity of positions.
- $\left(\frac{-\partial \mathcal{H}}{\partial q_i}\right)_{pi} = \dot{p}_i$. Velocity of momentums



A pair of equations for each degree of freedom that define a **flux** in phase-space.

-Energy Conservation

$$\frac{d\mathcal{H}}{dt} = \sum \left[\frac{\partial \mathcal{H}}{\partial p} \dot{p} + \frac{\partial \mathcal{H}}{\partial q} \dot{q} \right] \tag{47}$$

$$\frac{d\mathcal{H}}{dt} = \sum \left[-\frac{\partial \mathcal{H}}{\partial p} \frac{\partial \mathcal{H}}{\partial q} + \frac{\partial \mathcal{H}}{\partial q} \frac{\partial \mathcal{H}}{\partial p} \right] = 0 \tag{48}$$

The hamiltonian is conserved!!!

General form of conservation Laws

Any property of a system of particles is a function of the phase-space variable p and q.

- $\frac{dA(p,q)}{dt} = \sum \left[\frac{\partial A}{\partial p} \dot{p} + \frac{\partial A}{\partial q} \dot{q} \right]$
- $\frac{dA}{dt} = \sum \left[\frac{\partial A}{\partial q} \frac{\partial \mathcal{H}}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial \mathcal{H}}{\partial q} \right] = \{A, \mathcal{H}\}$
- Poisson Bracket $= \{A, B\} = \sum \left[\frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q} \right]$

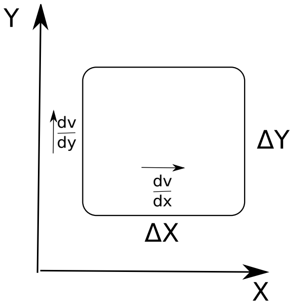
$$\frac{d\mathcal{H}}{dt} = \sum \left[-\frac{\partial \mathcal{H}}{\partial p} \frac{\partial \mathcal{H}}{\partial q} + \frac{\partial \mathcal{H}}{\partial q} \frac{\partial \mathcal{H}}{\partial p} \right] = 0 \tag{49}$$

-Hamiltonian generates time-depedence

- $\dot{q} = \{q, \mathcal{H}\} = \sum \left[\frac{\partial q}{\partial q} \frac{\partial \mathcal{H}}{\partial p} - \frac{\partial q}{\partial p} \frac{\partial \mathcal{H}}{\partial q} \right] = \dot{q}$
- $\dot{p} = \{p, \mathcal{H}\} = \sum \left[\frac{\partial p}{\partial q} \frac{\partial \mathcal{H}}{\partial p} - \frac{\partial p}{\partial p} \frac{\partial \mathcal{H}}{\partial q} \right] = \dot{p}$

Phase-Space incompressibility

- Flow in x-y plane
- All fluid moves with the same velocity
- no gradient of velocity
- Number of points that enter or leave are the same.
- $\frac{\partial V}{\partial x}\Delta y + \frac{\partial V}{\partial y}\Delta x = 0$
- $\left[\frac{\partial V}{\partial x} + \frac{\partial V}{\partial y}\right] = \nabla_{x_i} \cdot F(x_1 \ldots x_n) = 0$



$\nabla_{x_i} \cdot F(x_1 \ldots x_n)$ is defined as the divergence operator. When the fluid velocity (flux) has zero divergence it is called an incompressible fluid.

$\dot{\mathbf{X}} = \rho(\mathbf{X})$ Phase-space velocity vector

$$\nabla \cdot \dot{\mathbf{X}} = \sum \frac{\partial \dot{p}_i}{\partial p_i} + \frac{\partial \dot{q}_i}{\partial q_i} = \sum -\frac{\partial}{\partial p_i}\frac{\mathcal{H}}{\partial q_i} + \frac{\partial}{\partial q_i}\frac{\mathcal{H}}{\partial p_i} = 0 \tag{50}$$

The divergence of phase-space flow is incompressible!!!!!!

The ensemble distribution function

The trajectory approach involves the knowledge with a infinite precision of all p and q in phase-space, in this way is an idealization specially for microscopic systems. We can tackle with employing an statistical approach:

- Phase Space : All possible microstates available to a system of N particles.
- Ensemble: Contains all microstates consistent with a set of macroscopic variables *e.g* Total energy, Volume and number of particles.

Thus it is:

- A Strict subset of all possible phase-space points or
- Clustered more densely in certain regions of phase-space and less densely in other.

The objective is to find the precise mathematical form of how these systems are distributed in phase-space at any point in time.

Let's define $\rho(\mathbf{X}, t)$ as the ensemble distribution function:

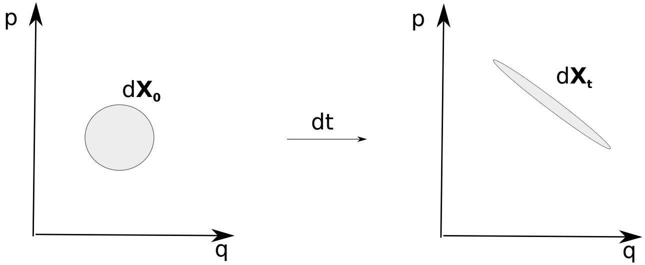
The ensemble distribution function: properties

$$\rho(\mathbf{X}, t) \geq 0 \tag{51}$$

$$\int_V d\mathbf{X}\rho(\mathbf{X}, t) = 1 \tag{52}$$

It is a density function !!!

- Bundle of trajectories in a volume element $d\mathbf{X}_t$ centered around a trajectory X_t
- All evolving at the same according to Hamilton equations of motion.
- How this bundle is distributed in time t?



We will derive an equation for the time-evolution of $\rho(\mathbf{X}, t)$

- Phase-space incompressibility.
- No sources or sinks for any volume element.
- Members (bundle) remain constant.

The latter implies that in any volume element Ω in phase-space with a surface S, the rate of decrease (or increase) of ensemble members in Ω must equal the rate at which ensemble members leave (or enter) Ω through the surface S.

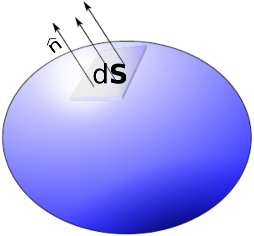
Fraction of phase-space points in volume of phase-space Ω at time t

$$\int_{\Omega} d\mathbf{X}_t \rho(\mathbf{X}, t) \tag{53}$$

Rate of decrease of phase-space points:

$$-\frac{d}{dt}\int_{\Omega} d\mathbf{X}_t \rho(\mathbf{X}, t) = -\int_{\Omega} d\mathbf{X}_t \frac{\partial}{\partial t}\rho(\mathbf{X}, t) \tag{54}$$

The flux of phase-space points through a surface **S**. This is the number of ensemble members per unit area, per unit time passing through the surface **S**.



$$\int_S d\mathbf{S}\dot{\mathbf{X}}_\mathbf{t} \cdot \hat{\mathbf{n}}\rho(\mathbf{X}_t, t) = \int_\Omega d\mathbf{X}_t \nabla_{\mathbf{X}_t} \cdot \dot{\mathbf{X}}_\mathbf{t}\rho(\mathbf{X}_t, t) \tag{55}$$

The flux is expressed as a fraction of ensemble members. The right side follows from the divergence theorem.

Now equating both equations:

$$-\int_\Omega d\mathbf{X}_t \frac{\partial}{\partial t}\rho(\mathbf{X},t) = \int_\Omega d\mathbf{X}_t \nabla_{\mathbf{X}_t} \cdot \dot{\mathbf{X}}_\mathbf{t} \rho(\mathbf{X}_t, t) \tag{56}$$

The choice of the volume element Ω is arbitrary, thus we can equate both integrands and after rearrangement :

$$\frac{\partial}{\partial t}\rho(\mathbf{X},t) + \nabla_{\mathbf{X}_t} \cdot \dot{\mathbf{X}}_\mathbf{t} \rho(\mathbf{X}_t, t) = 0 \tag{57}$$

now:

$$\nabla_{\mathbf{X}_t} \cdot \dot{\mathbf{X}}_{\mathbf{t}} \rho(\mathbf{X}_t, t) = \dot{\mathbf{X}}_{\mathbf{t}} \cdot \nabla_{\mathbf{X}_t} \rho(\mathbf{X}_t, t) + \rho(\mathbf{X}_t, t) \nabla_{\mathbf{X}_t} \cdot \dot{\mathbf{X}}_{\mathbf{t}} \tag{58}$$

and from Hamilton equations:

$$\nabla_{\mathbf{X}_t} \cdot \dot{\mathbf{X}}_{\mathbf{t}} = 0 \tag{59}$$

Finally we get :

$$\frac{\partial}{\partial t} \rho(\mathbf{X}_t, t) + \dot{\mathbf{X}}_{\mathbf{t}} \cdot \nabla_{\mathbf{X}_t} \rho(\mathbf{X}_t, t) = 0 \tag{60}$$

The last equations defines a total time derivative and it named Liouville's equation

The Liouville equation

$$\frac{d\rho(\mathbf{X}_t, t)}{dt} = \frac{\partial}{\partial t}\rho(\mathbf{X}_t, t) + \dot{\mathbf{X}}_\mathbf{t} \cdot \nabla_{\mathbf{X}_t}\rho(\mathbf{X}_t, t) = 0 \tag{61}$$

Some comments:

- $\rho(\mathbf{X}, t)$ is a conserved quantity, from LE.
- Volume in phase-space is conserved from HE

Thus:

$$\rho(\mathbf{X}_0, 0)d\mathbf{X}_\mathbf{0} = \rho(\mathbf{X}_t, t)d\mathbf{X}_\mathbf{t} \tag{62}$$

The fraction of member in any volume element $d\mathbf{X}$ is conserved, and ensures that we can perform ensembles averages at any point in time.

Now we can rewrite the LE, remembering that the Hamiltonian generates the time dependence for any function of p's and q's and employing the poisson brackets formalism :

$$\dot{\mathbf{X}}_{\mathbf{t}} \cdot \nabla_{\mathbf{X}_t} \rho(\mathbf{X}_t, t) = \{\rho(\mathbf{X}_t, t), \mathcal{H}(\mathbf{X}, t)\} \tag{63}$$

The Liouville equation: poisson bracket formulation

$$\frac{d\rho(\mathbf{X}, t)}{dt} = \frac{\partial}{\partial t}\rho(\mathbf{X}_t, t) + \{\rho(\mathbf{X}_t, t), \mathcal{H}(\mathbf{X}_t, t)\} \tag{64}$$

Equilibrium solution of the Liouville equation

$$A = \langle a(\mathbf{X}) \rangle = \int d\mathbf{X} \rho(\mathbf{X}, t) a(\mathbf{X}) \tag{65}$$

no external driving forces:

- $\mathcal{H}(\mathbf{X}, t) \rightarrow \mathcal{H}(\mathbf{X})$
- $\mathbf{X}_t(\mathbf{X}, t) \rightarrow \mathbf{X}_t(\mathbf{X})$

At equilibrium, A has not time dependence, thus $\langle a(\mathbf{X}) \rangle$ has no time dependence, if so $\rho(\mathbf{X}, t)$ has not explicit time dependence

$$\frac{\partial \rho(\mathbf{X}, t)}{\partial t} = 0 \tag{66}$$

By the LE we get :

$$\{\rho(\mathbf{X}), \mathcal{H}(\mathbf{X})\} = 0 \tag{67}$$

Thus the solution for $\rho\mathbf{X}$ is any function of $\mathcal{H}(\mathbf{X})$!!!!

$$\rho(\mathbf{X}) \propto \varrho(\mathbf{X}) \tag{68}$$

and to ensure normalization:

$$\rho(\mathbf{X}) = \frac{\varrho(\mathbf{X})}{\mathcal{Z}(\mathbf{X})} \tag{69}$$

where $\mathcal{Z}(\mathbf{X})$ is defined:

$$\mathcal{Z}(\mathbf{X}) = \int d\mathbf{X}\rho(\mathbf{X}) \tag{70}$$

$\mathcal{Z}(\mathbf{X})$ is the partition function, and it is the essential quantity in equilibrium statistical mechanics. It measures the number of accessible microstates.

$$A = \langle a(\mathbf{X})\rangle = \frac{1}{\mathcal{Z}(\mathbf{X})}\int d\mathbf{X}\varrho(\mathbf{X})a(\mathbf{X}) \tag{71}$$

Summary

- Classical equations of motion from Newton's laws.
  - Concepts of Mechanical work
  - Classical equations of motion for many-particle systems.
  - Phase space concept.
  - Conserved quantities from Newton's laws.
- Lagrangian form of classical mechanics.
  - Action, Lagrangian and generalized coordinates.
  - Symmetries and conserved quantities.
    - Translational Invariance: Momentum is conserved.
    - Rotational Invariance: angular momentum is conserved.
    - Time invariance: Energy is conserved.
- Hamiltonian form of classical mechanics.
  - Legendre transform of Lagrangian.
  - Hamiltonian equations of motion.
  - Flux in phase space.
  - Liouville's equation.
  - Foundation of statistical mechanics.

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