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A short coverage of equilibrium statistical physics.

$F = ma$, Lagrangian mechanics, Hamiltonian mechanics, statistical ensemble (系, 综,) Liouville theorem, equilibrium distribution PDF.

statistical independence for macroscopic systems. Gibbs ensemble. Boltzmann distribution. Markov chain, Importance sampling M.C. method.

Classical mechanics.

$F = ma$.

Lagrangian $\quad \mathcal{L} = \mathcal{L}(q_i, \dot{q}_i)$

q : generalized coordinates

$\dot{q}$: generalized velocities. $\quad \dot{q}_i = \frac{d}{dt} q_i$

$$\mathcal{L} = \sum_{i=1}^{s} \frac{1}{2} m \dot{q}_i^2 - U(q_i)$$

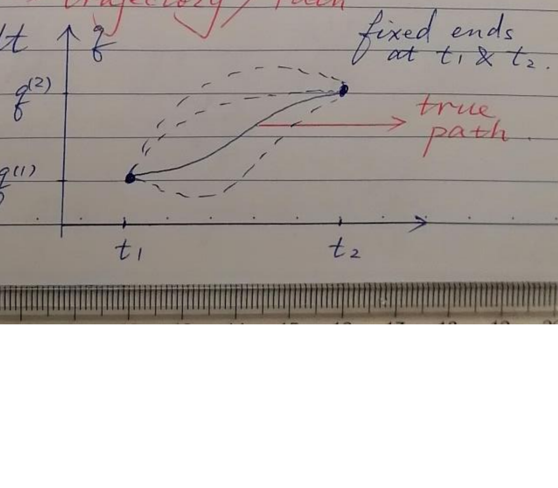
$= K - U$ Kinetic energy − Potential energy.

$s=3$ for a particle in 3D space

Variational principle

$S[q(t)]$ $\quad$ $S[q(t)]$ ↳ trajectory / Path

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



Least Action Principle

$\delta S = 0$

true path → min of S.

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Actual path / true path :

$$\frac{\delta S}{\delta q} = 0 \quad \text{stationary condition.}$$

$$\frac{\delta}{\delta q}\int_{t_1}^{t_2} \mathcal{L}(q, \dot{q})\, dt = 0$$

δS : variation of S w.r.t. q.

$$\sum_i \int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial q_i}\delta q_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\delta \dot{q} \quad dt$$

$$\hookrightarrow \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\frac{d}{dt}\delta q_i$$

Integration by parts

$$\sum_i \int_{t_1}^{t_2}\left[\frac{\partial \mathcal{L}}{\partial q_i}\delta q_i - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right)\delta q_i\right] dt$$

$$+ \cancel{\sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\delta q_i}\Big|_{t_1}^{t_2} \quad \text{fixed ends.}$$

$\hookrightarrow 0$ $\quad \delta q_i$ at t_1 & $t_2 = 0$.

$$\delta S = \sum_i \int_{t_1}^{t_2}\left(\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right)\delta q_i \, dt$$

δq_i is arbitrary. $\quad \delta S = 0 \rightarrow \frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = 0$.

for each i.

Euler-Lagrange eq.

Lagrange eq of motion $\quad \frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = 0$

$$\mathcal{L} = \frac{1}{2}m\dot{q}^2 - U(q)$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial q}, \quad \frac{d}{dt}(m\dot{q}) = -\frac{\partial U}{\partial q}$$

$$m\ddot{q} = -\frac{dU}{dq}$$

$F = ma$ $\quad \downarrow ma \quad \downarrow$ force $-\frac{dU}{dq}$.

Lagrangian mechanics derived from Least Action Principle
最小作用量原理

Change of variables

generalized momentum (动量)

$p_i = \partial \mathcal{L} / \partial \dot{q}_i$, conjugate to q_i.

$$\delta \mathcal{L} = \sum_i \frac{\partial \mathcal{L}}{\partial q_i} \delta q_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \delta \dot{q}_i$$

$$= \sum_i \frac{\partial \mathcal{L}}{\partial q_i} \delta q_i + p_i \delta \dot{q}_i$$

$$= \sum_i \dot{p}_i \delta q_i + p_i \delta \dot{q}_i$$

$\delta \mathcal{L}$ at actual path.

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

Actual path.

$$\frac{d}{dt} p_i = \dot{p}_i = \frac{\partial \mathcal{L}}{\partial q_i}$$

Define Hamiltonian

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

q: all q_i; p: all p_i; $p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$

$\mathcal{H}$ is a function of q, p.

$$\mathcal{L} = \frac{1}{2} m \dot{q}^2 - U(q)$$

$$p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = m\dot{q} , \quad \dot{q} = \frac{p}{m}$$

$$\mathcal{H} = p\dot{q} - \frac{1}{2} m \dot{q}^2 + U(q) = \frac{p^2}{m} - \frac{m}{2}\left(\frac{p}{m}\right)^2 + U(q)$$

Total energy.

$$= \underbrace{\frac{1}{2}\frac{p^2}{m}}_{K} + \underbrace{U(q)}_{U}$$

$$\delta \mathcal{H} = \sum_i \Big[\cancel{p_i \delta \dot{q}_i} + \delta p_i \dot{q}_i - \underbrace{(\dot{p}_i \delta q_i + \cancel{p_i \delta \dot{q}_i})}_{\delta \mathcal{L} \text{ at actual path}} \Big]$$

$$= \sum_i \dot{q}_i \delta p_i - \dot{p}_i \delta q_i$$

$$\delta H = \sum_i \dot{q}_i \,\delta p_i - \dot{p}_i \,\delta q_i$$ at the actual path.

$$= \sum_i \frac{\partial H}{\partial p_i}\delta p_i + \frac{\partial H}{\partial q_i}\delta q_i$$

At actual path, $\frac{\partial H}{\partial p_i} = \dot{q}_i$

$\frac{\partial H}{\partial q_i} = -\dot{p}_i$

正则运动方程

$\dot{q}_i = \partial H / \partial p_i$, $\dot{p}_i = - \partial H / \partial q_i$ Canonical equations

in Lagrangian description, s 2nd-order equations.

in Hamiltonian description, $2s$ 1st-order equations.

Language to use for statistical physics

Review of Classical Mechanics done!

Invariants (Conserved quantities)

$Q(q,p)$: any mechanical quantity

$Q(t) = Q(q(t), p(t))$

$$\frac{d}{dt}Q(t) = \sum_i \frac{\partial Q}{\partial q_i}\dot{q}_i + \frac{\partial Q}{\partial p_i}\dot{p}_i$$ Chain rule.

$$= \sum_i \frac{\partial Q}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial Q}{\partial p_i}\frac{\partial H}{\partial q_i}$$

$= \{Q, H\}$ Poisson's 泊松 bracket.

$\frac{d}{dt}H = \{H, H\} = 0$, H is conserved mechanical invariant.

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$$\mathcal{H} = \frac{p^2}{2m} + U(q) = K + U$$

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}, \qquad \dot{p} = -\frac{\partial H}{\partial q} = -\frac{\partial U}{\partial q}$$

$$p = m\dot{q} \qquad m\ddot{q} = -\partial U/\partial q, \quad ma = F$$

$$\ddot{q} \qquad -\partial U/\partial q.$$

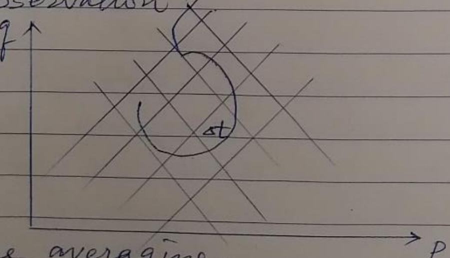
In Hamiltonian dynamics, we have $q(t)$ & $p(t)$.

Phase space spanned by $\{q_i, p_i\}$
相空间.

Trajectory of a system is $\{q_i(t), p_i(t)\}$, the phase trajectory.
A curve developed in time in phase space.

A system of N particles. 3N degrees of freedom 自由度.
$i = 1, \cdots, 3N$, $s = 3N$.
q_i, p_i developing in time.
Time evolution of the microscopic state $(q_i, p_i) \rightarrow$ phase trajectory

Observation



time averaging.

In the course of time, every phase region will be visited by the system.

$$\frac{\Delta t}{T} \longrightarrow \Delta W$$

probability for the system in that small region.

~~$\Delta W \to dW = \int f(q,p)\, dq\, dp$~~

$\Delta W \to dW = \underbrace{f(q,p)}_{\text{pdf at that region}} \underbrace{dq\, dp}_{\text{phase volume of a small region}}$

$$\int f(q,p)\, dq\, dp = \int dW = 1 = \frac{\sum \Delta t}{T} = 1$$

normalization

A statistical distribution
from one single system over a long time.

$$\langle Q(q,p) \rangle = \frac{1}{T}\int_0^T Q(q(t), p(t))\, dt$$ time average

$\frac{dt}{T} = dW = f(q,p)\, dq\, dp$

$$= \int Q(q,p)\, dW$$

$$= \int Q(q,p)\, f(q,p)\, dq\, dp.$$

Practically, not feasible

$f(q,p)$? Cannot follow the trajectory.
Two many degrees of freedom

$10^{23} \sim s$.

How to generate $f(q,p)$ when $s \sim 10^{23}$

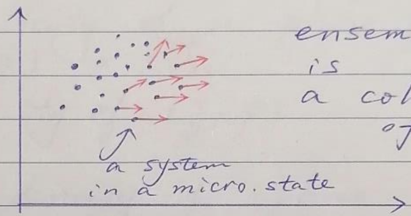
Statistical ensemble. (Conceptual)
A conceptual collection of many many systems that are macroscopically identical, but microscopically different.
$\longrightarrow$ A distribution (instantaneously)

The microscopic state is described by $\{q_i, p_i\}$, a phase point in phase space

(q, p) in the space of q and p.

In an ensemble, every system is represented by a phase point that moves in the phase space.

At time t.



ensemble is a collection of phase points.

Density of these phase points in phase space.
These points form a continuum
连续体.

Dots $\rightarrow$ A continuum

$$\int f(q, p, t)\, dq\, dp = 1$$

Normalized density of phase points in phase space at time t.
PDF of an ensemble.

In the course of time, each point moves, and hence $f(q, p, t)$ evolves.

We know the motion of each point.
$\dot{q} = \partial H / \partial p, \quad \dot{p} = -\partial H / \partial q.$ Canonical eqs.

$\hookrightarrow$ evolution of $f(q, p, t)$

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

Phase space is 2s-dimensional.

$i = 1, \cdots, s.$ $\{ \underset{s}{q_i}, \underset{s}{p_i} \}$

In this 2s-dim space,

a velocity vector $\vec{V}_{2s} = (\dot{q}_i, \dot{p}_i)$

velocity of a phase point.

(q, p) point , $(\dot{q}, \dot{p}) = \vec{V}_{2s}$. velocity of (q, p)

$f(q, p, t)$, a density of phase points.

Continuity eq for f in the 2s-dimensional space.

$$\frac{\partial f}{\partial t} + \vec{\nabla}_{2s} \cdot (f \vec{V}_{2s}) = 0$$

$\uparrow$ current density in phase space.

$$\frac{\partial f}{\partial t} + \sum_i \frac{\partial}{\partial q_i}(f \dot{q}_i) + \frac{\partial}{\partial p_i}(f \dot{p}_i) = 0$$

$$\frac{\partial f}{\partial t} + \sum_i \dot{q}_i \frac{\partial f}{\partial q_i} + \cancel{f \frac{\partial \dot{q}_i}{\partial q_i}} + \cancel{f \frac{\partial \dot{p}_i}{\partial p}} + \dot{p}_i \frac{\partial f}{\partial p_i} = 0$$

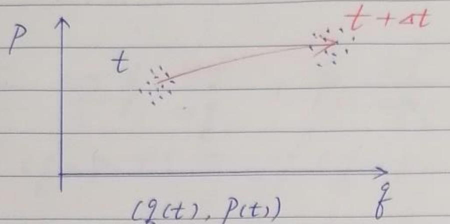
$$\sum_i \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} = \sum_i \frac{\partial}{\partial q_i} \frac{\partial H}{\partial p_i} + \frac{\partial}{\partial p_i}\left(-\frac{\partial H}{\partial q_i}\right)$$

$$= \sum_i \frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} = 0$$

$$\frac{\partial f}{\partial t} + \sum_i \dot{q}_i \frac{\partial f}{\partial q_i} + \dot{p}_i \frac{\partial f}{\partial p_i} = 0, \quad \frac{\partial f}{\partial t} + \vec{V}_{2s} \cdot \vec{\nabla}_{2s} f = 0$$

$$\begin{cases} \vec{V}_{2s} = (\dot{q}_i, \dot{p}_i) \\ \nabla_{2s} = \left(\frac{\partial}{\partial q_i}, \frac{\partial}{\partial p_i}\right) \end{cases}$$

$$\frac{\partial f}{\partial t} + \vec{V}_{2s} \cdot \nabla_{2s} f = 0$$



following the phase trajectory, a constant density.

$(q(t), p(t))$ to $(q(t+\Delta t), p(t+\Delta t))$, f is not changed.

Liouville's theorem.

$$f(q(t+\Delta t), p(t+\Delta t), t+\Delta t) - f(q(t), p(t), t) = 0$$

$$\Delta t \frac{\partial f}{\partial t} + (q(t+\Delta t) - q(t)) \frac{\partial f}{\partial q} + (p(t+\Delta t) - p(t)) \frac{\partial f}{\partial p} = 0$$

$$\frac{\partial f}{\partial t} + \dot{q} \frac{\partial f}{\partial q} + \dot{p} \frac{\partial f}{\partial p} = 0$$

$$\frac{\partial f}{\partial t} + \vec{V}_{2s} \cdot \nabla_{2s} f = 0 .$$

Bold move → equilibrium ensemble.

An equilibrium ensemble is a PDF, which can be used to compute the average quantities for a system in equilibrium.

Ensemble average ⟶ Time average for a system.

special PDF.

What feature is demanded for an equilibrium ensemble?

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A stationary solution to Liouville's eq.

$$\frac{\partial f}{\partial t} + \sum_i \dot{q}_i \frac{\partial f}{\partial q_i} + \dot{p}_i \frac{\partial f}{\partial p_i} = 0$$

$f(q,p,t) = f(q,p)$ no explicit time dependence.

Under certain distribution of phase points, although each point moves, the density does not change in time.

$f(q,p)$ satisfies $\dot{q}\frac{\partial f}{\partial q} + \dot{p}\frac{\partial f}{\partial p} = 0$.

$$\frac{\partial H}{\partial p}\frac{\partial f}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial f}{\partial p} = 0 \qquad \{f, H\} = 0.$$

f, the stationary solution, $f = f(q,p)$ is itself a conserved quantity.

$f(q,p)$: a distribution in (q,p) space. a PDF.

$\{f, H\} = 0$, $f(q,p)$ is a mechanical invariant

$$\frac{df}{dt} \equiv \dot{q}\frac{\partial f}{\partial q} + \dot{p}\frac{\partial f}{\partial p} = 0.$$

$H(q,p)$ is a mech. invariant.

$f(q,p)$ is a function of q, p through $H(q,p)$.

f depends on q, p via $H(q,p)$.

$$f = g(H(q,p)), \quad \frac{df}{dt} = g' \frac{dH}{dt} = 0$$

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$F=ma$, $\longrightarrow$ $f(q,p) \propto e^{-\beta H(q,p)}$

Boltzmann distribution.

Stationary solution $f(q,p)$, Statistical independence. $\}$ $\log f \sim \alpha - \beta H$

Markov chain, Importance Sampling MC method.