Part 0 Introduction

What is nonequilibrium statistical mechanics?

The approach in the present lecture

The outline of the course

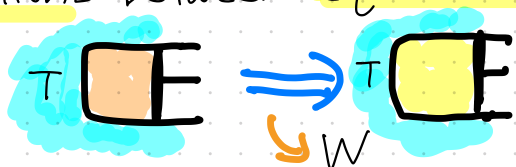
⟨Introduction⟩

§ What is nonequilibrium statistical mechanics?

(equilibrium) thermodynamics

a macroscopic theory that places strong constraints on

- properties of equilibrium states and thermodynamic functions
- transitions between equilibrium states



$$W \leq F_{init} - F_{fin}$$

← maximum work principle

(equilibrium) statistical mechanics

a universal framework for determining properties of equilibrium states and thermodynamic functions of macroscopic systems based on microscopic mechanics → classical or quantum

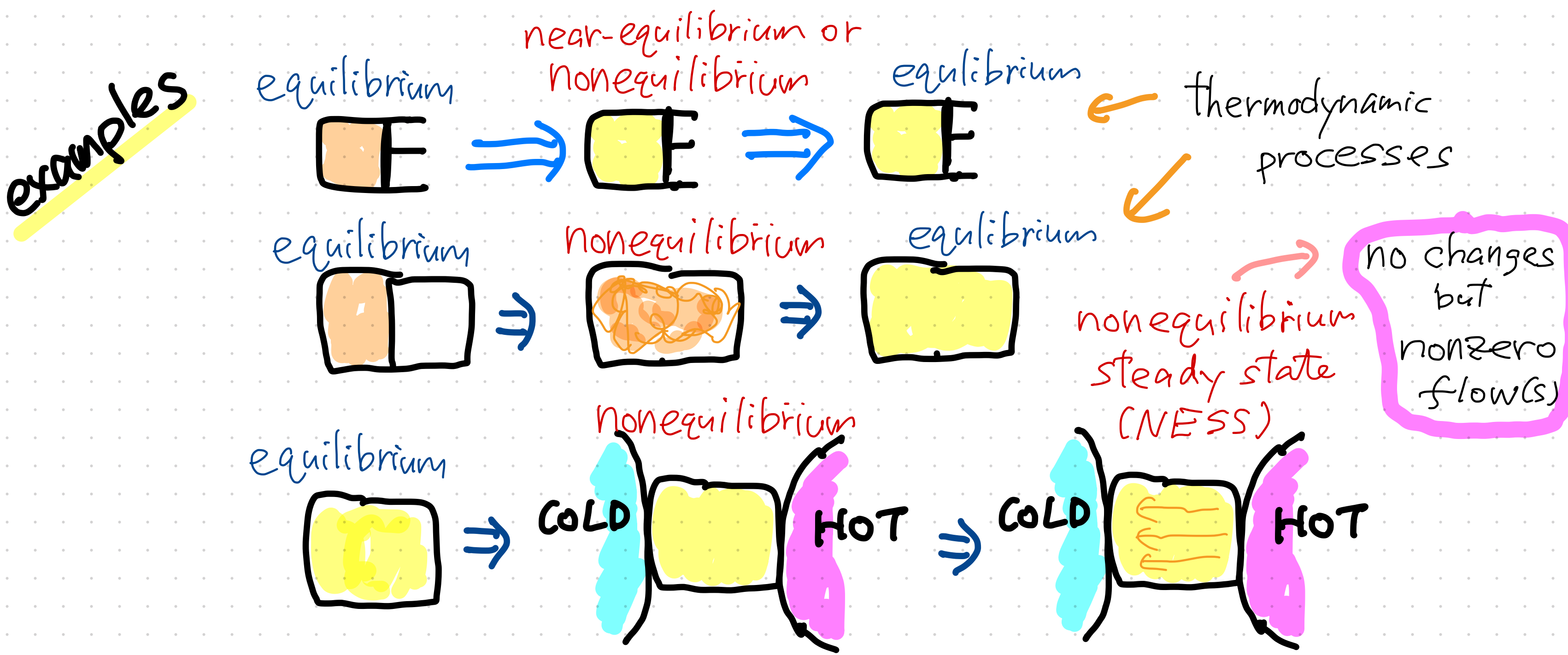
$$S = k \log \Omega, \quad F = -\frac{1}{\beta} \log \sum_j e^{-\beta E_j}$$

nonequilibrium states and processes

equilibrium state a state with no macroscopically observable changes OR flows

nonequilibrium state any state that is NOT an equilibrium state

nonequilibrium process any process that involves nonequilibrium states



nonequilibrium statistical mechanics

? a universal framework for determining properties of nonequilibrium states and processes based on microscopic mechanics

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we still do not have such a theory

no principles like the principle of equal weights.

basically we can only use: equilibrium statistical mechanics + mechanics

remark: there is a priori no guarantee that this is allowed

describe the initial state by an equilibrium distribution

$$P(X) = \frac{e^{-\beta H(X)}}{Z}$$

Solve Newton's equation for all particles

$$m_j \frac{d^2}{dt^2} \boldsymbol{r}_j(t) = -\mathrm{grad}_j V(\boldsymbol{r}_1, \dots, \boldsymbol{r}_N)\Big|_{\boldsymbol{r}_k = \boldsymbol{r}_k(t)}$$

then we can describe the resulting nonequlibrium state....

this is impossible!!

nonequilibrium statistical mechanics (not yet complete)

equilibrium statistical mechanics + mechanics

→ { • concrete computations
• useful new quantities
• general relations } in { • general setting
• some restricted setting }

Useful new quantities:
- entropy production
- entropy production rate
- excess heat
- ⋮

General relations:
- reciprocal relations
- fluctuation-dissipation relation
- linear response relation
- approach to equilibrium
- the 2nd law of thermodynamics
- (detailed) fluctuation theorem
- various trade-off relations
- thermodynamic uncertainty principles
- ⋮

Some restricted setting:
- close to equilibrium
- only a small part of the system is out of equilibrium

§ The approach in the present lecture

equilibrium statistical mechanics + classical mechanics

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fluctuation theorem ≃ detailed balance condition

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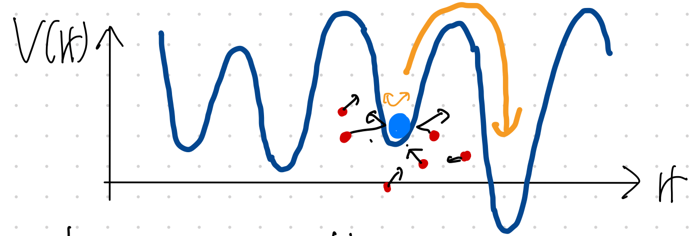
effective stochastic processes (Markov jump processes) → classical system with almost stable (discrete) states in touch with larger system(s) (= bath(s))

large or small



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some general results for nonequlibrium proceses and states

- suitable approach for discussing general results
- not very suitable for practical applications

Part 1 Foundation

What do we get from mechanics and equilibrium statistical mechanics?

Classical Hamiltonian mechanics

Jarzynski equality

Fluctuation theorem

Detailed balance condition

Part 2 Abstract theory

Probability

Entropy

Stochastic matrix and basic convergence theorem

Markov jump process

Part 3 Nonequilibrium processes in an equilibrium environment

Relaxation process in an equilibrium environment

Approach to thermal equilibrium

Fluctuation theorem

Operations in an equilibrium environment

Jarzynski equality and the second law of thermodynamics

No pumping theorem

Part 4 Nonequilibrium states and processes in nonequilibrium environments

Nonequilibrium steady states (NESS)

Relaxation to NESS

Linear response relations

Reciprocal relations

Inequality between current and dissipation

Improved Shiraishi-Saito inequality

No free-pumping theorem

Trade-off relation between power and efficiency in a heat engine

Part 5 The theory of Brownian motion

Typical experiment

Basic symmetry and the transition probability

Kramers equation

Langevin equation

Einstein's theory of Brownian motion