

(Non) equilibrium dynamics: a (broken) symmetry

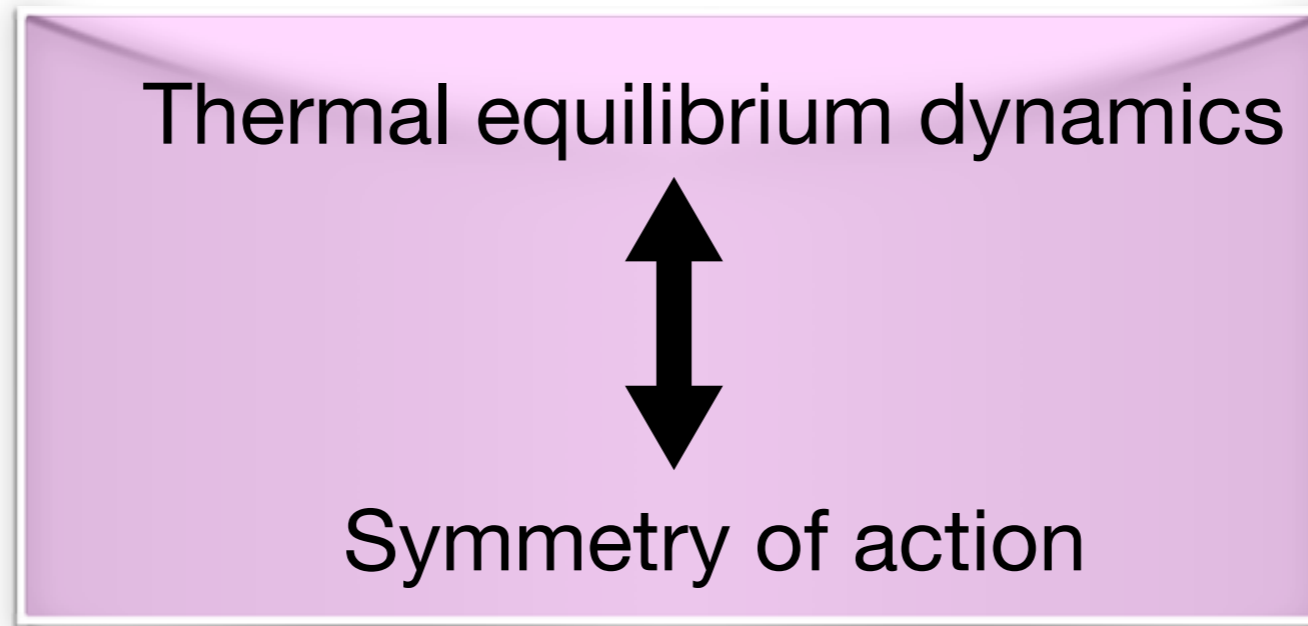
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Spoiler



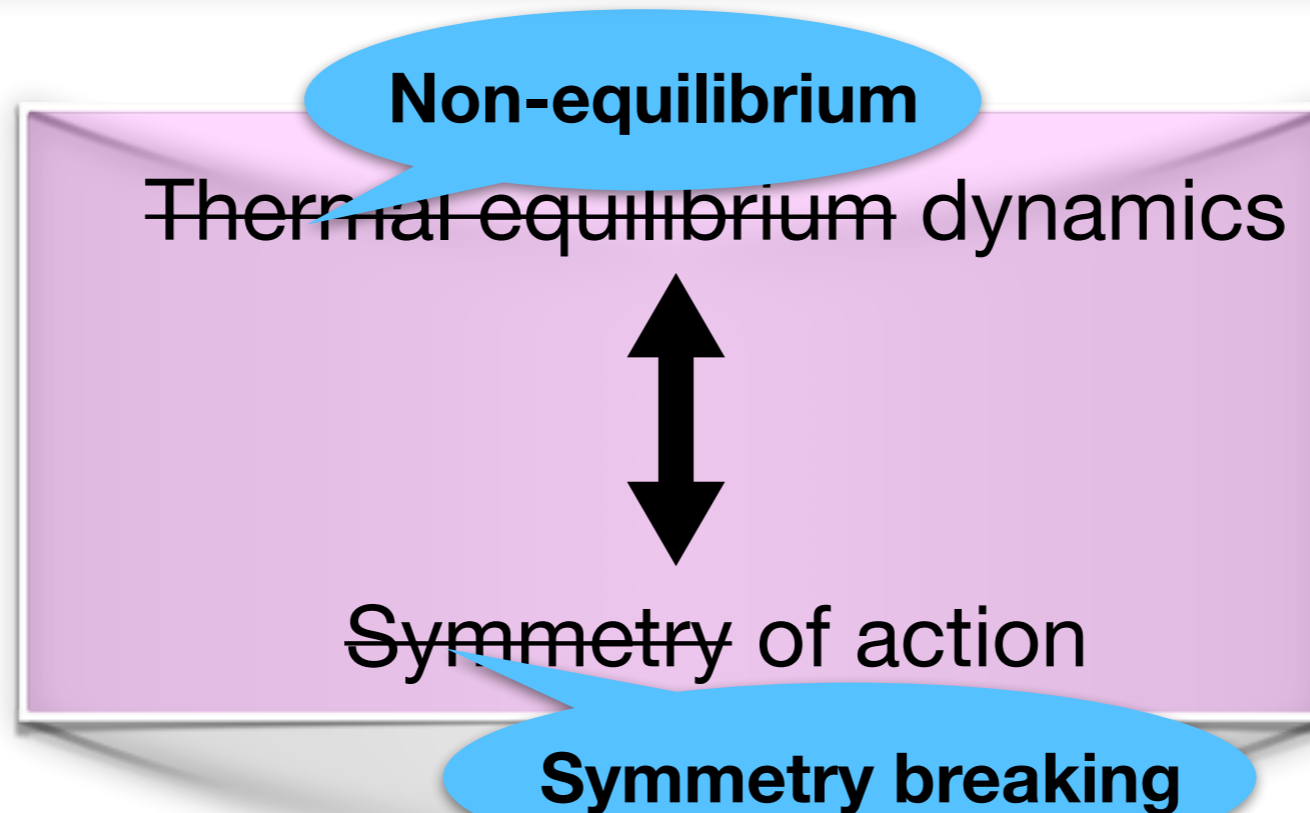
$$\psi \mapsto \mathcal{T}_\beta[\psi]$$

$$S[\psi] = \int dx \mathcal{L}(\psi(x), \partial_\mu \psi(x); x) \mapsto S[\psi]$$

Ward-Takahashi identities

$$\langle \mathcal{O}[\psi(x)] \dots \mathcal{O}[\psi(x')] \rangle = \langle \mathcal{O}[\mathcal{T}_\beta \psi(x)] \dots \mathcal{O}[\mathcal{T}_\beta \psi(x')] \rangle$$

Spoiler



$$\psi \mapsto \mathcal{T}_\beta[\psi]$$

$$S[\psi] = \int dx \mathcal{L}(\psi(x), \partial_\mu \psi(x); x) \mapsto S[\psi] + \Delta S[\psi]$$

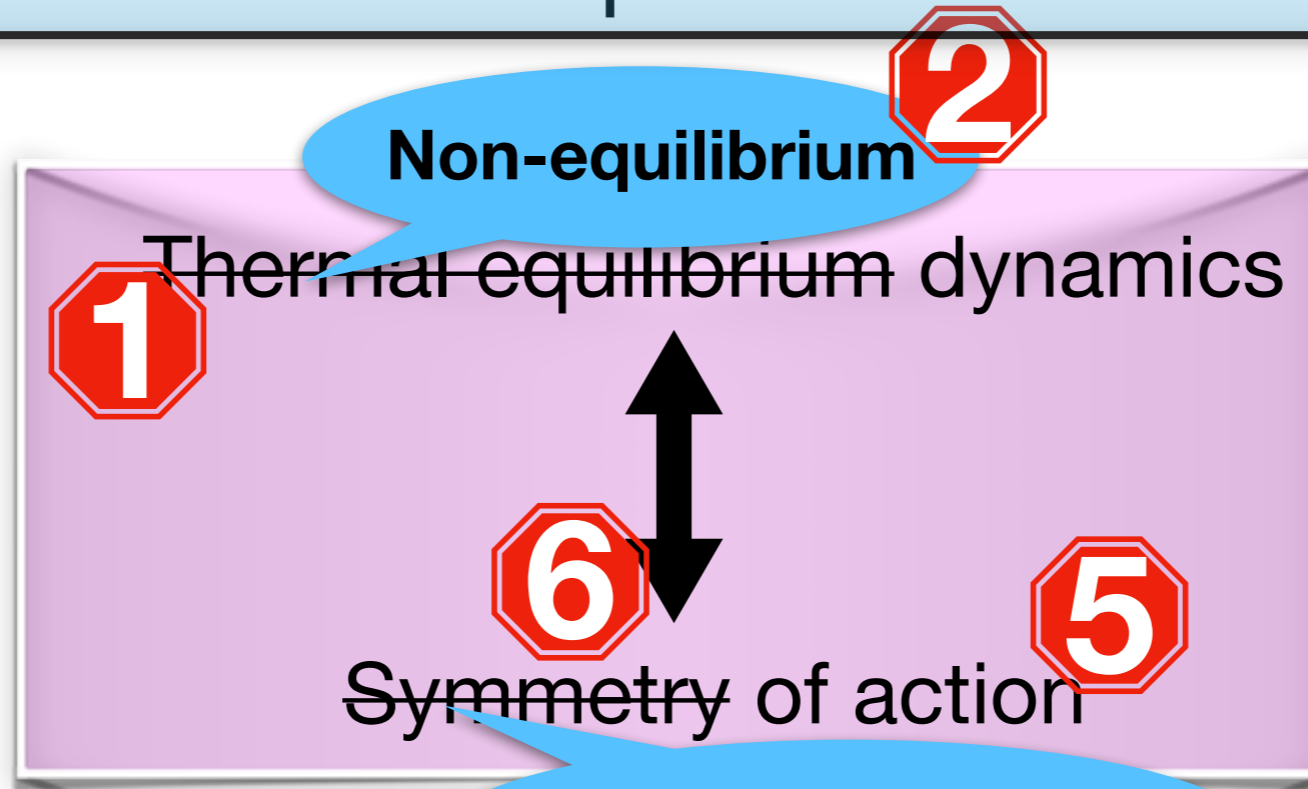
Fluctuation theorems

Entropy production

~~Ward-Takahashi identities~~

$$\langle \mathcal{O}[\psi(x)] \dots \mathcal{O}[\psi(x')] \rangle = \langle \mathcal{O}[\mathcal{T}_\beta \psi(x)] \dots \mathcal{O}[\mathcal{T}_\beta \psi(x')] e^{\Delta S} \rangle$$

Spoiler



Symmetry breaking

$$\psi \mapsto \mathcal{T}_\beta[\psi]$$

$$S[\psi] = \int dx \mathcal{L}(\psi(x), \partial_\mu \psi(x); x) \mapsto S[\psi] + \Delta S[\psi]$$

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Fluctuation theorems

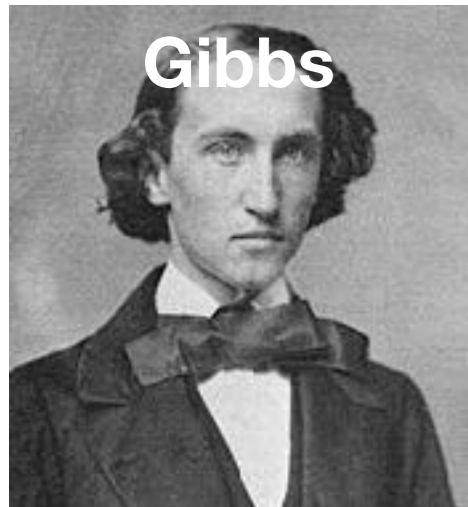
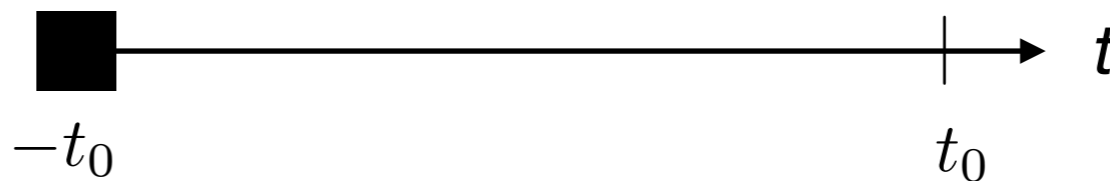
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Entropy production

~~Ward-Takahashi identities~~

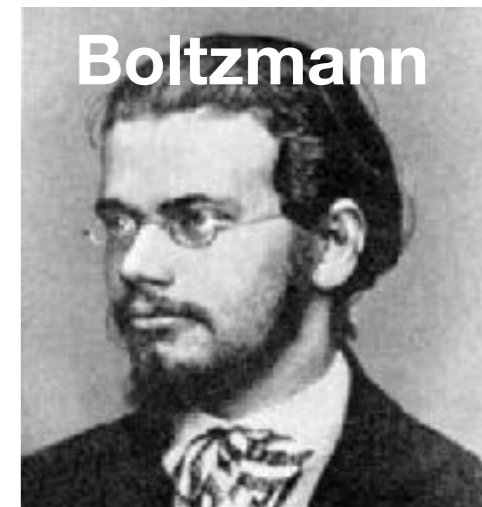
$$\langle \mathcal{O}[\psi(x)] \dots \mathcal{O}[\psi(x')] \rangle = \langle \mathcal{O}[\mathcal{T}_\beta \psi(x)] \dots \mathcal{O}[\mathcal{T}_\beta \psi(x')] e^{\Delta S} \rangle$$

Equilibrium dynamics



Gibbs

	preparation	evolution
Classical	$P_{\text{GB}}(x, \dot{x})$ $\sim e^{-\beta \mathcal{E}(x, \dot{x})}$	$m\ddot{x} = -V'(x)$
Quantum	$\hat{\rho}_{\text{GB}} \sim e^{-\beta \hat{H}}$	$\hat{O}_{\text{H}}(t) = e^{i\hat{H}t} \hat{O} e^{-i\hat{H}t}$



Boltzmann

Equilibrium conditions

- prepare in equilibrium at temperature β^{-1} wrt \hat{H}
- evolve with same \hat{H}
- (coupled to bath at β^{-1})

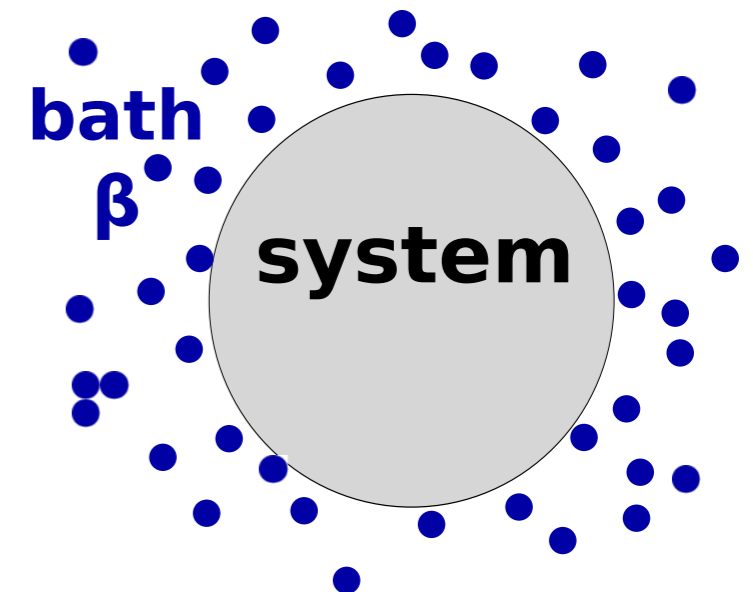
Prepare

- With thermostat

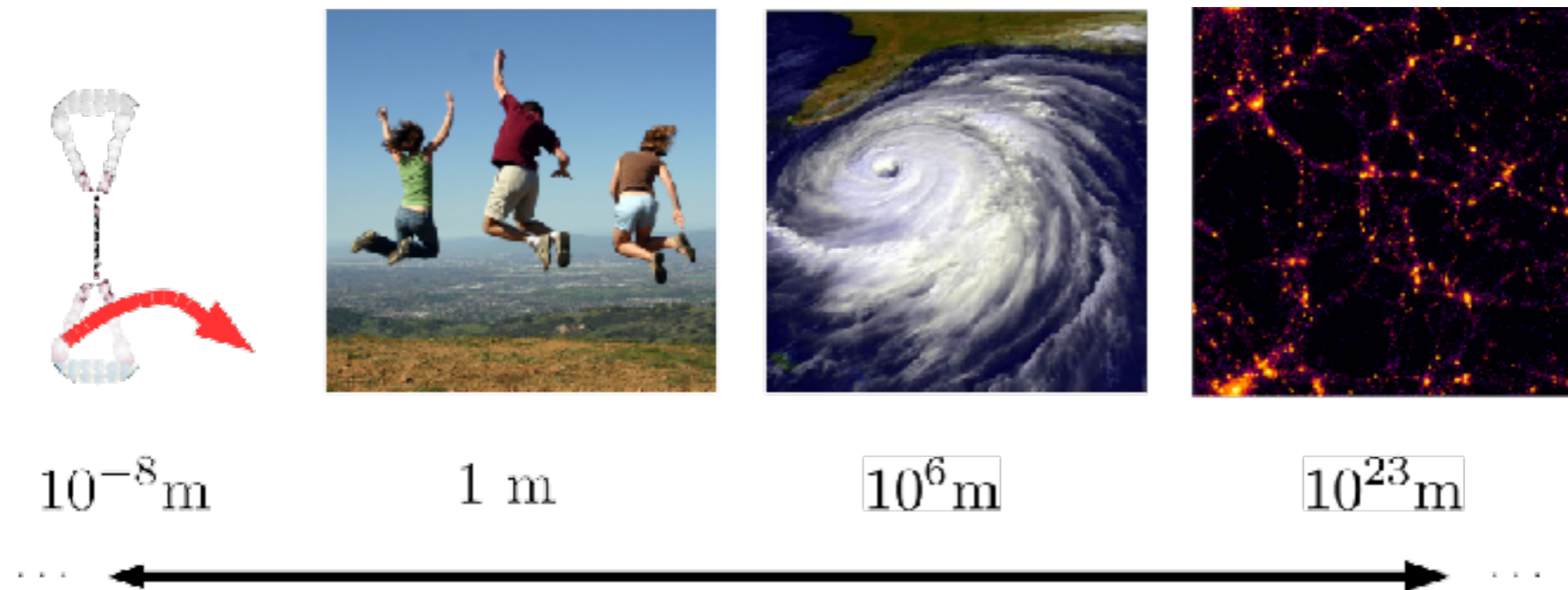
$$\text{ex: } m\ddot{x} = -V'(x) - \eta\dot{x} + \xi(t)$$

$$\langle \xi(t)\xi(t') \rangle = 2\eta\beta^{-1} \delta(t - t')$$

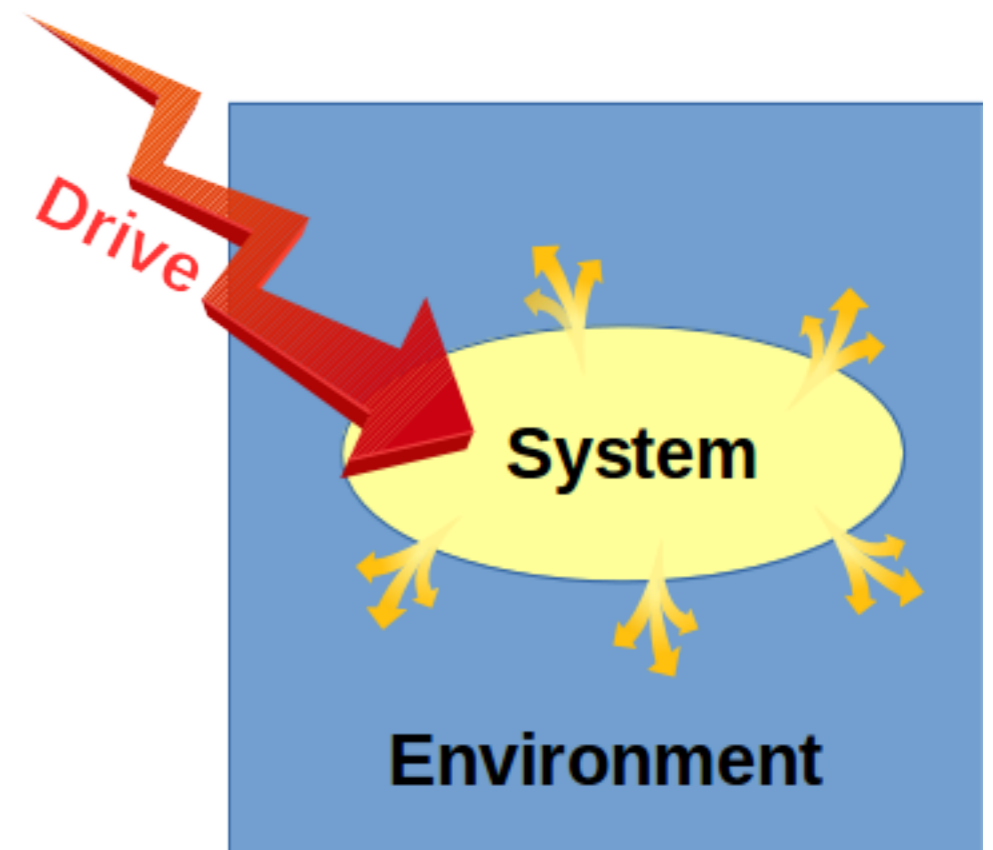
- Isolated (thermalization)

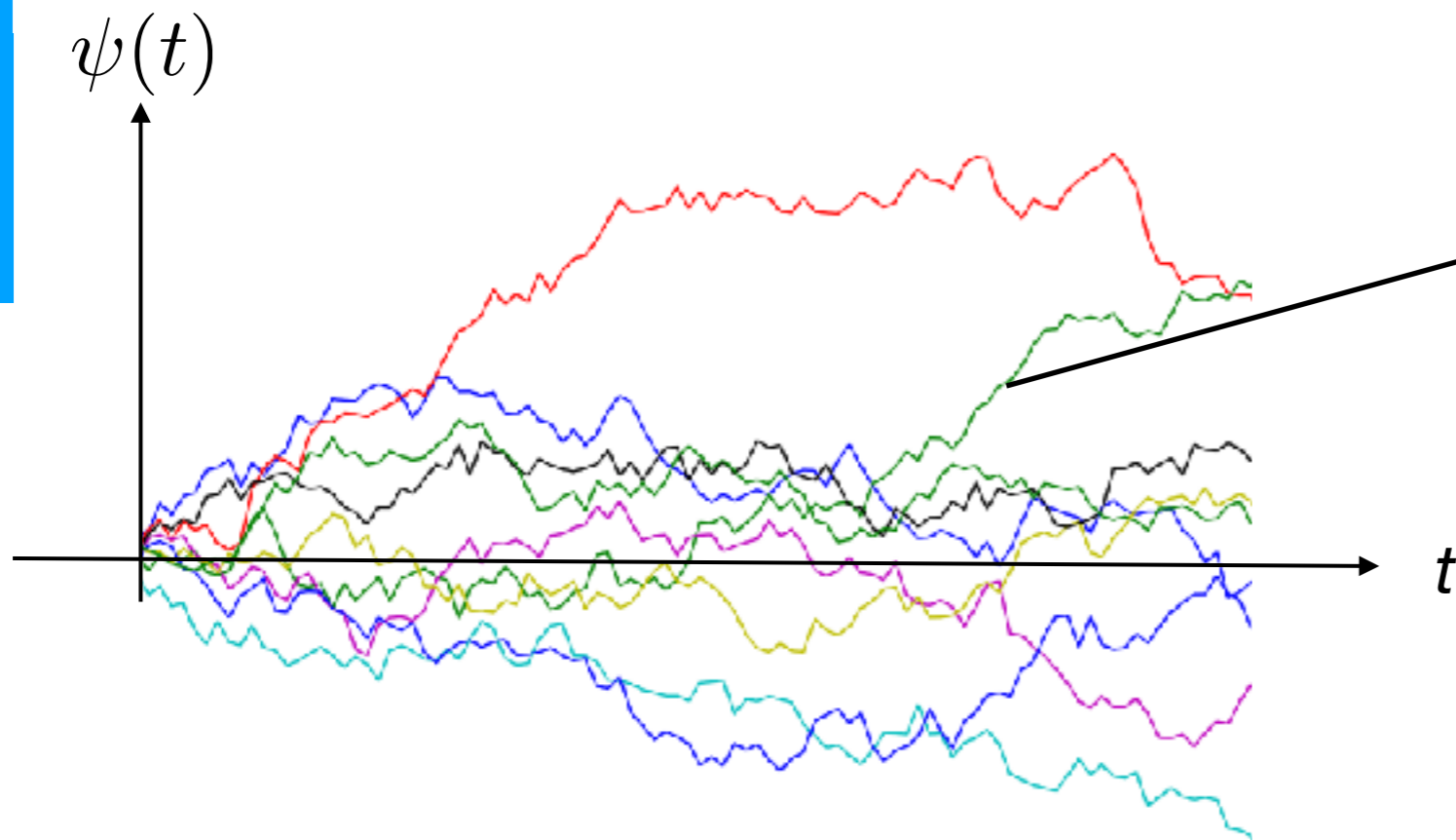


Non-equilibrium dynamics



- relaxation dynamics: quench $\hat{H}_0 \mapsto \hat{H}$
- non-equilibrium drive:
 - time-dependent $\hat{H}(t)$ (work)
 - environment (currents)
- non-equilibrium “engineering”





single trajectory

- work $\mathcal{W}[\psi]$
- heat $\mathcal{Q}[\psi]$
- entropy $\mathcal{S}[\psi]$

First law

$$\Delta\mathcal{E} = \mathcal{W}[\psi] + \mathcal{Q}[\psi]$$

Second law

$$\Delta\mathcal{S} = \beta\mathcal{Q}[\psi] + \underbrace{\mathcal{S}^{\text{irr}}[\psi]}$$

in average $\langle \mathcal{S}^{\text{irr}}[\psi] \rangle \geq 0$

Fluctuation Theorem

$$P(\mathcal{S}^{\text{irr}}) = P_r(-\mathcal{S}^{\text{irr}}) e^{\mathcal{S}^{\text{irr}}}$$

Gallavoti Cohen (1995)

Fluctuation theorems

classical

Work fluctuation theorem

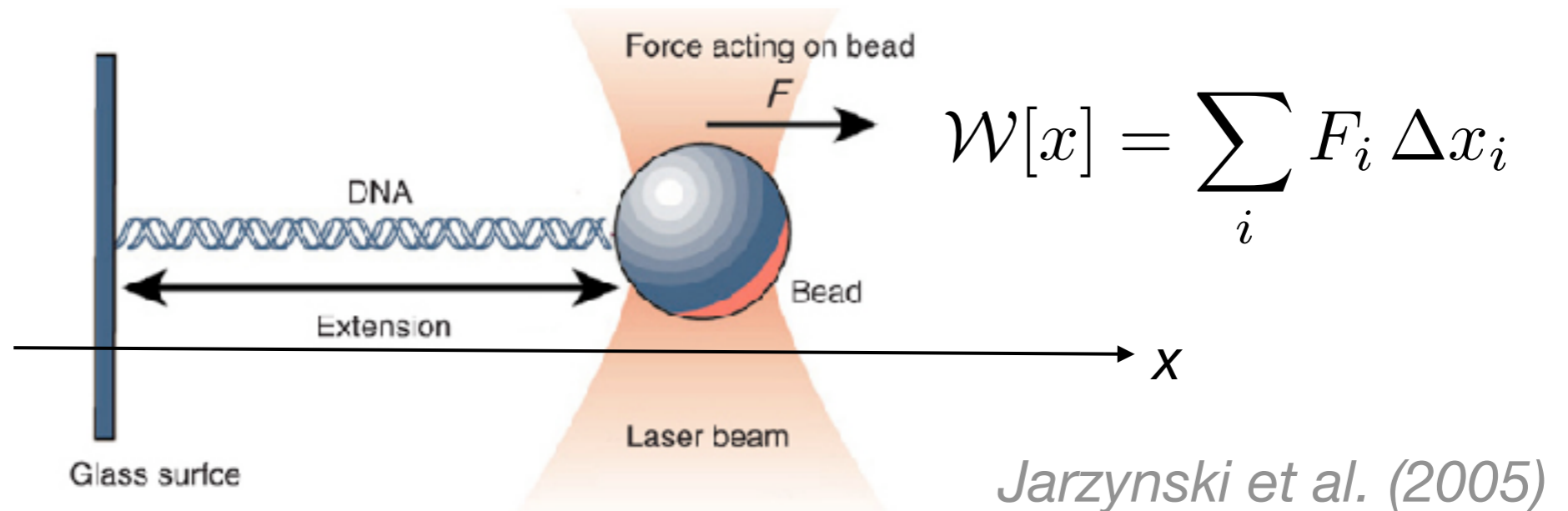
$$P(\mathcal{W}) = P_r(-\mathcal{W}) e^{\beta(\mathcal{W} - \Delta\mathcal{F})}$$

Crooks (1999)

nature LETTERS

Verification of the Crooks fluctuation theorem and recovery of RNA folding free energies

D. Collin¹, F. Ritort^{2*}, C. Jarzynski³, S. B. Smith¹, I. Tinoco Jr¹ & C. Bustamante^{1,4}

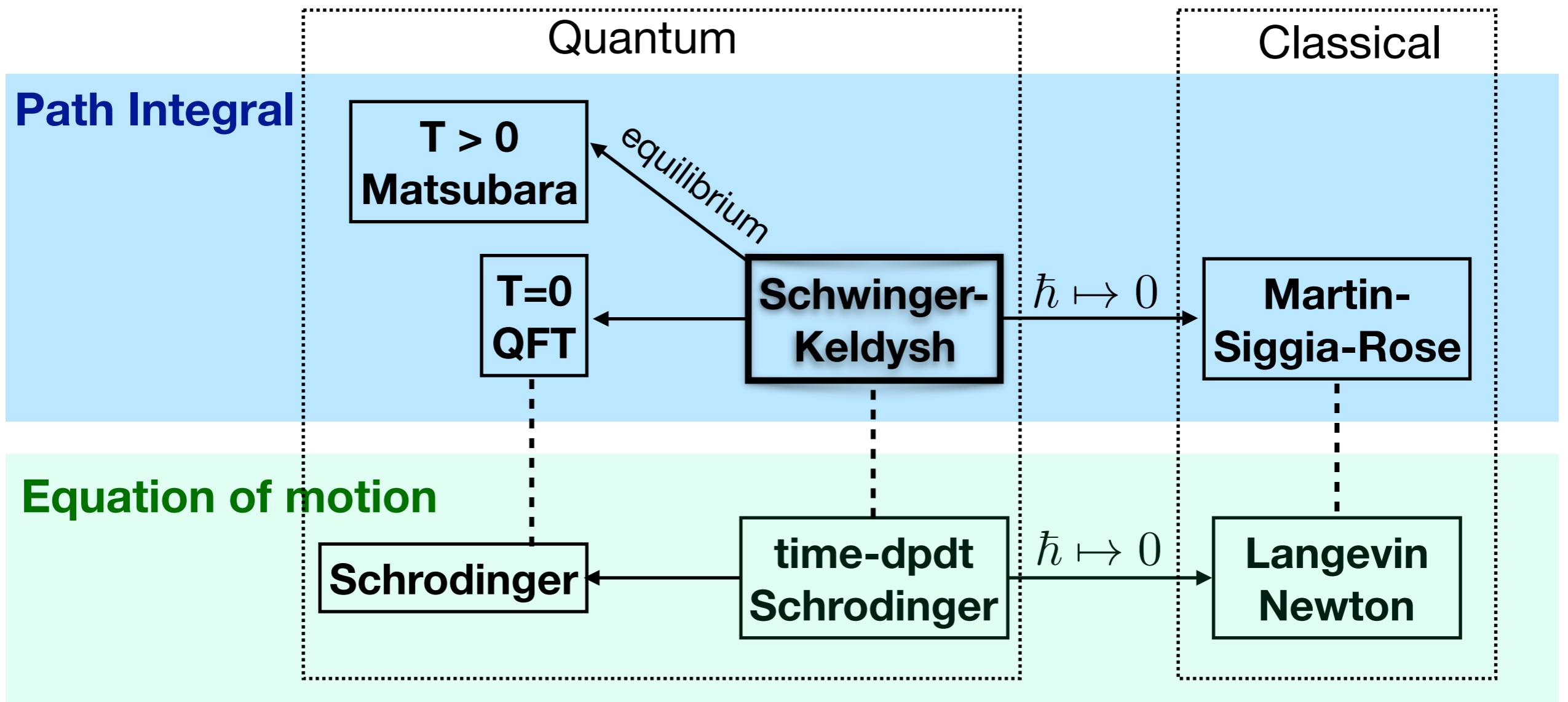


Quantum trajectories

- Work fluctuation theorem (*Kurchan 2000*)
- Entropy production ?
- Entropy fluctuation theorem ?

quantum

Formalisms

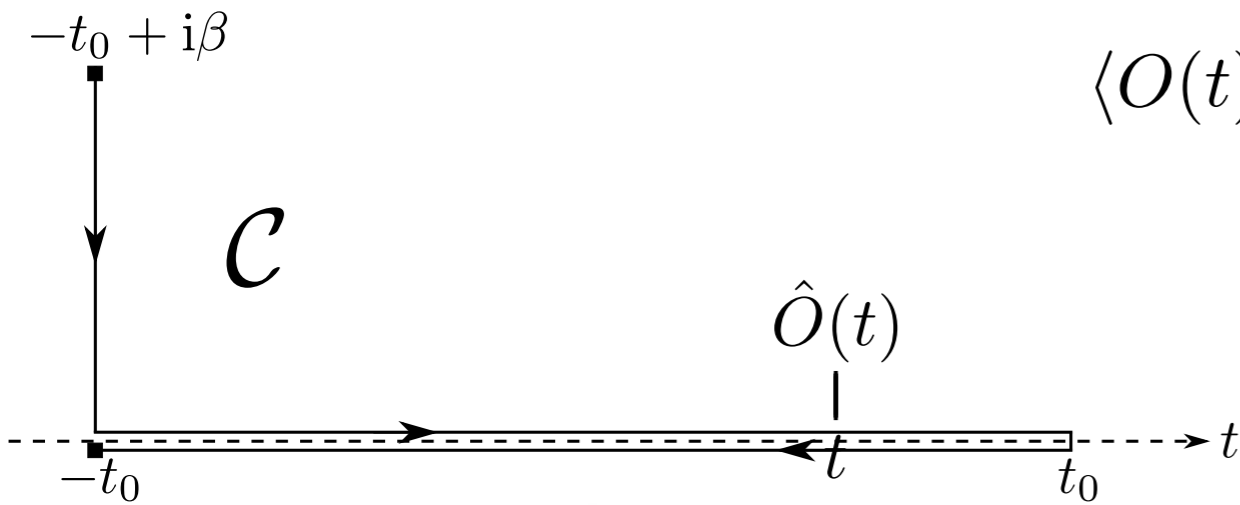


non-relativistic real scalar field $\psi(t)$

$$\begin{array}{c}
 \hat{H}(-t_0) \\
 \beta \blacksquare \\
 -t_0
 \end{array}
 \xrightarrow{\hat{H}(t)}
 \begin{array}{c}
 t_0 \\
 t
 \end{array}$$

ex: $\hat{H}(t) = \frac{\pi^2}{2m} + V(\psi; t)$

Schwinger-Keldysh formalism



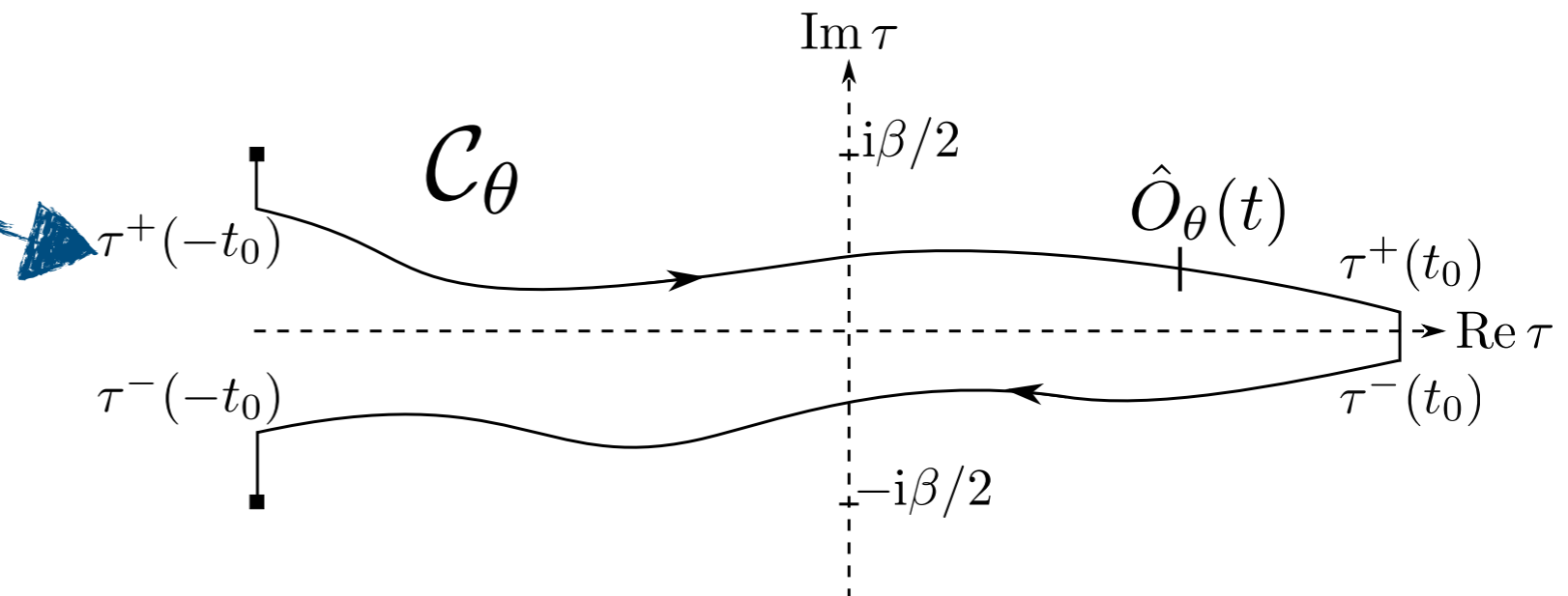
$$\begin{aligned} \langle O(t) \rangle &= \mathcal{Z}^{-1} \text{Tr} [e^{i\hat{H}t} \hat{O}(t) e^{-i\hat{H}t} e^{-\beta\hat{H}}] \\ &= \mathcal{Z}^{-1} \text{Tr} [\mathbf{T}_C e^{i \int_C d\tau \hat{H}} \hat{O}(t)] \\ &= \mathcal{Z}^{-1} \int \mathcal{D}[\psi] e^{i \int_C d\tau \mathcal{L}[\psi(\tau)]} \langle \psi(t) | \hat{O}(t) | \psi(t) \rangle \end{aligned}$$

Novel formal degree of freedom

$$t \mapsto \tau = t + \theta(t) \quad \psi(t) \mapsto \psi(\tau)$$

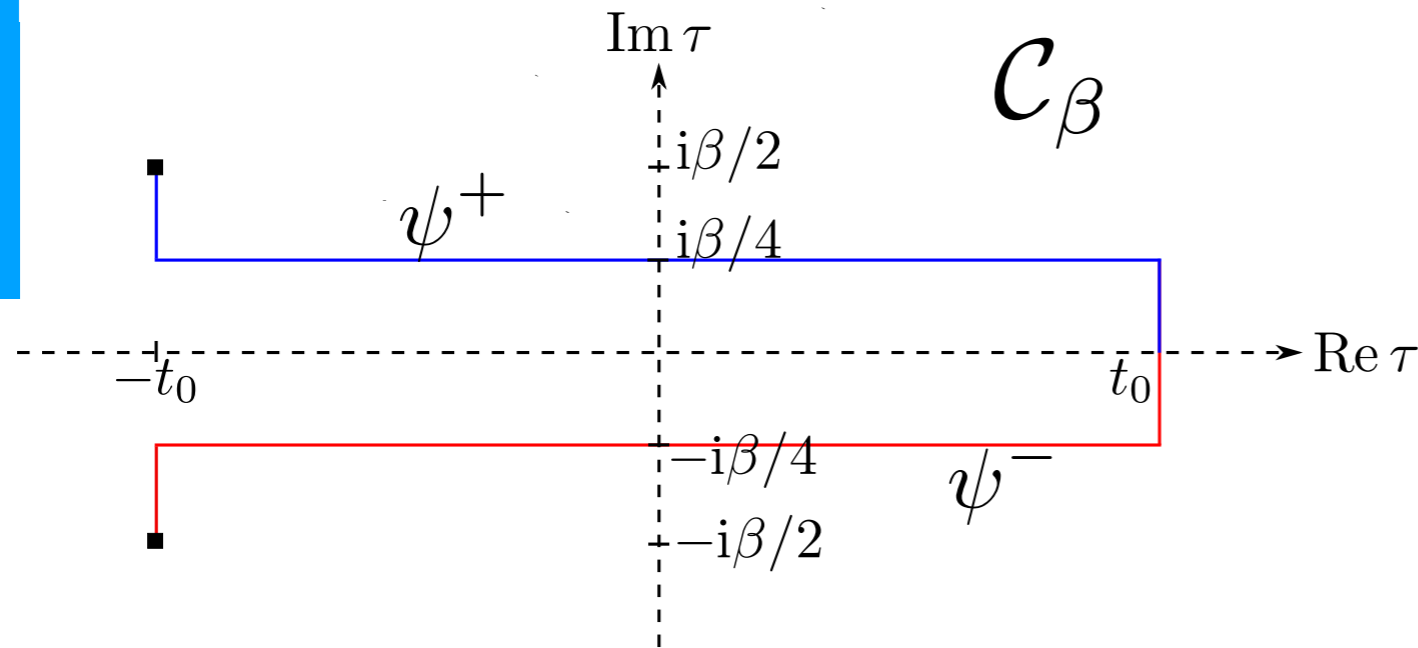
$$\mathbb{I} = \int d\psi(t) e^{+i\theta(t)\hat{H}} |\psi(t)\rangle \langle \psi(t)| e^{-i\theta(t)\hat{H}}$$

$$\hat{O} \mapsto \hat{O}_\theta(t) \equiv e^{-i\theta(t)\hat{H}} \hat{O} e^{i\theta(t)\hat{H}}$$



Symmetry of equilibrium

equilibrium



$$\hat{H} = \text{const.}$$

$$S[\psi] = \int_{\mathcal{C}_\beta} d\tau \mathcal{L}[\psi(\tau)]$$

Field transformation

$$\mathcal{T}_\beta : \psi^\pm(\tau) \mapsto \psi^\pm(-\tau \pm i\beta/2)$$

$$\mathcal{T}_\beta \circ \mathcal{T}_\beta = \text{Id}$$

Invariance of the action

$$\beta\mathcal{F}(-t_0) + iS[\psi] \xrightarrow{\mathcal{T}_\beta} \beta\mathcal{F}(-t_0) + iS[\psi]$$

Ward-Takahashi identities

$$\langle \psi^a(\tau) \psi^b(\tau') \dots \rangle_{\mathcal{S}_\beta} = \langle \mathcal{T}_\beta \psi^a(\tau) \mathcal{T}_\beta \psi^b(\tau') \dots \rangle_{\mathcal{S}_\beta}$$

Keldysh Green's functions

$$iG^{ab}(t, t') = \langle \psi^a(t) \psi^b(t') \rangle \quad a, b = +, -$$

Fluctuation-dissipation theorem

$$G^{-+}(t, t') \stackrel{\mathcal{T}_\beta}{=} e^{i\beta/2(\partial_t - \partial_{t'})} G^{+-}(-t', -t)$$

Classical limit

$$\left. \frac{\delta \langle \psi(t) \rangle}{\delta f(t')} \right|_{f=0} = -\beta \partial_t \langle \psi(t) \psi(t') \rangle \quad \text{if } t > t'$$
$$= 0 \quad \text{if } t < t'$$

Symmetry breaking

non-equilibrium

Time-dependent drive: $\hat{H} \mapsto \hat{H}(t)$

$$S[\psi] = \int_{\mathcal{C}_\beta} d\tau \mathcal{L}[\psi(\tau); t(\tau)] + \int_{\mathcal{C}_\beta} dt \tilde{\mathcal{L}}[\psi(\tau); t(\tau)]$$

New!

Variation of the action

$$\beta\mathcal{F}(-t_0) + iS[\psi] \xrightarrow{\mathcal{T}_\beta} \beta\mathcal{F}_r(-t_0) + iS_r[\psi] + \beta\Delta\mathcal{F}_r - \Sigma_r[\psi]$$

New!

$\mathcal{S}_r^{\text{irr}}[\psi]$

with

$$\Sigma[\psi] = \int_{\mathcal{C}} dt \langle \psi(t) | e^{\beta/4 \hat{H}(t)} \left[\frac{d}{dt} e^{-\beta/2 \hat{H}(t)} \right] e^{\beta/4 \hat{H}(t)} | \psi(t) \rangle$$

$\hbar \mapsto 0$

$$\beta\mathcal{W}[\psi]$$

Symmetry breaking

non-
equilibrium

Measure of irreversibility

$$\mathcal{S}^{\text{irr}}[\psi] = \beta \Delta \mathcal{F} - \Sigma[\psi]$$

$$\Sigma[\psi] = \int_c dt \langle \psi(t) | e^{\beta/4 \hat{H}(t)} \left[\frac{d}{dt} e^{-\beta/2 \hat{H}(t)} \right] e^{\beta/4 \hat{H}(t)} | \psi(t) \rangle$$

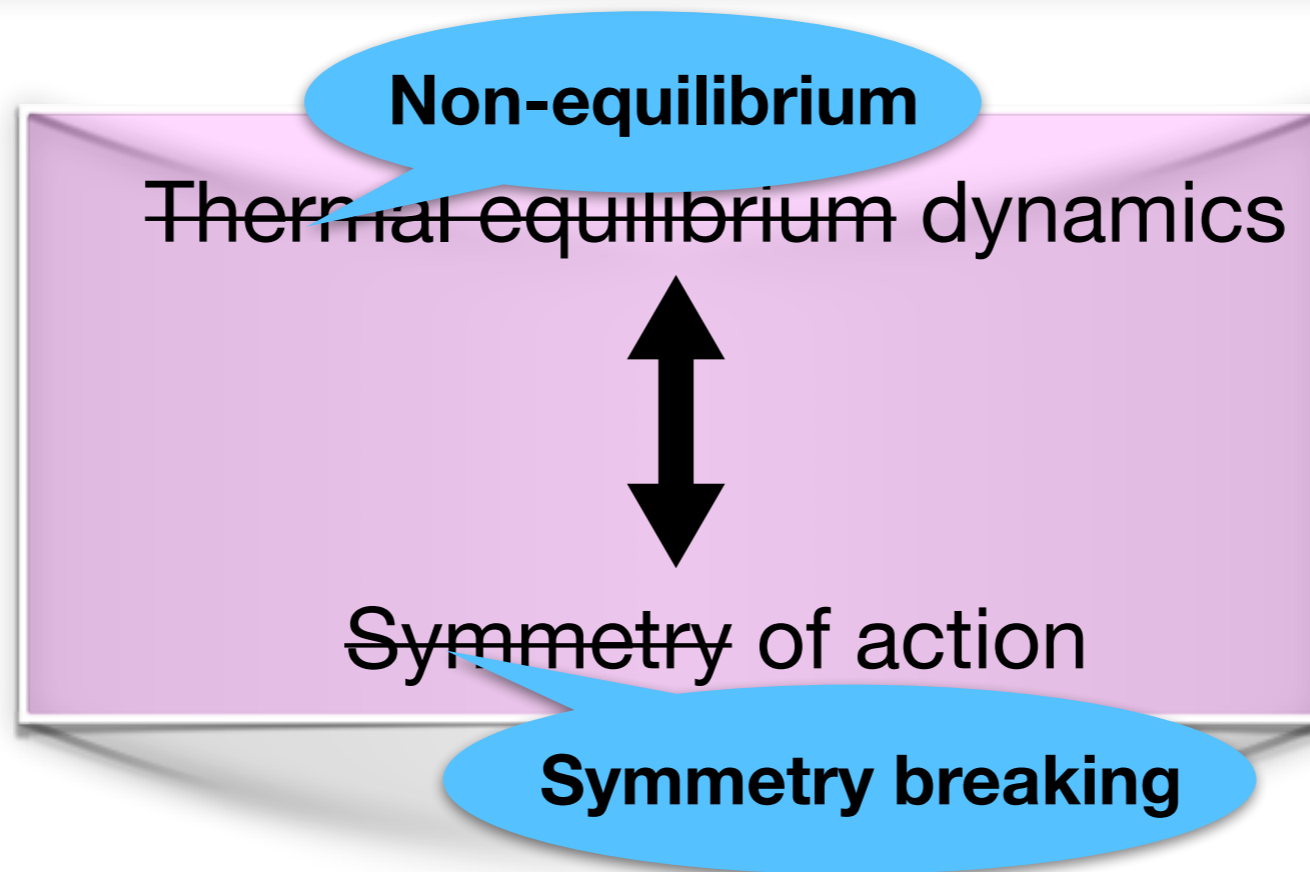
- ☑ $\langle \mathcal{S}^{\text{irr}}[\psi] \rangle \geq 0$
- ☑ Classical limit
- ☑ Reversible process

☑ Fluctuation Theorem

$$P(\mathcal{S}^{\text{irr}}) = P_r(-\mathcal{S}^{\text{irr}}) e^{\mathcal{S}^{\text{irr}}}$$

Entropy production operator ?

Recap



$$S[\psi] \xrightarrow{\mathcal{T}_\beta} S[\psi] + \mathcal{S}^{\text{irr}}[\psi]$$

Fluctuation theorems

Entropy production

~~Ward-Takahashi identities~~

$$\langle \mathcal{O}[\psi(\tau)] \dots \mathcal{O}[\psi(\tau')] \rangle = \langle \mathcal{O}[\mathcal{T}_\beta \psi(\tau)] \dots \mathcal{O}[\mathcal{T}_\beta \psi(\tau')] e^{\mathcal{S}_r^{\text{irr}}[\psi]} \rangle_r$$