Non-equilibrium fluctuations via symmetry breaking

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Preview

Thermal equilibrium dynamics

⬍

Symmetry of action

$$S[\psi] = \int \mathrm{d}x\, \mathcal{L}(\psi(x), \partial_\mu \psi(x); x) \xrightarrow{\psi \mapsto \mathcal{T}_\beta[\psi]} S[\psi]$$

Ward-Takahashi identies = KMS x time reversal

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

Preview

Non-equilibrium

~~Thermal equilibrium~~ dynamics

↕

~~Symmetry~~ of action

Symmetry breaking

$$S[\psi] = \int \mathrm{d}x \; \mathcal{L}(\psi(x), \partial_u \psi(x); x) \longrightarrow S[\psi] + \Delta S$$

~~Ward-Takahashi identies =~~

Fluctuation theorems

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

Entropy production

Preview

Thermal equilibrium dynamics

⇕

Symmetry of action

$\hbar = 0$

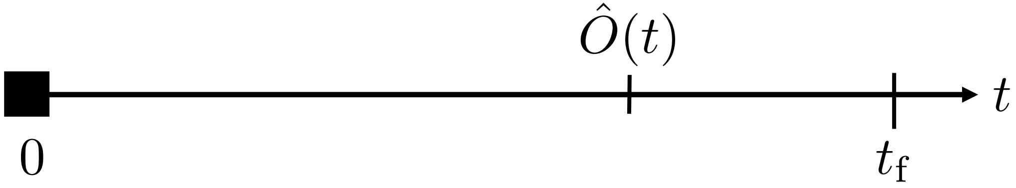
- Stochastic Field Theory
  - SUSY
  - MSR
- Quantum hydrodynamics (EFT)
- Quantum microscopics

$\hbar = 1$

Janssen (1976)
Parisi Sourlas (1982)
Aron Biroli Cugliandolo (2010)
...
Crossley Gloriosio Liu (2015)
Haehl Loganayagam Rangamani (2015)
Jensen Pinzani-Fokeeva Yarom (2017)
...
Sieberer Chiocchehetta Gambassi Tauber Diehl (2015)
Aron Biroli Cugliandolo (2018)
Yeo (2019)

Real-time dynamics

Finite-time experiment

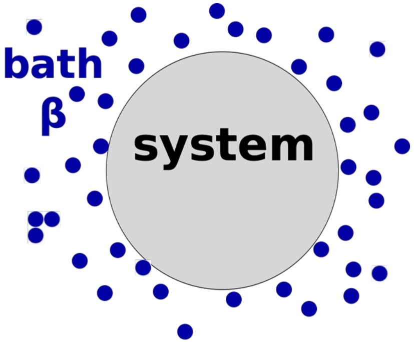


Ex: non-relativistic real scalar in 0+1 dim

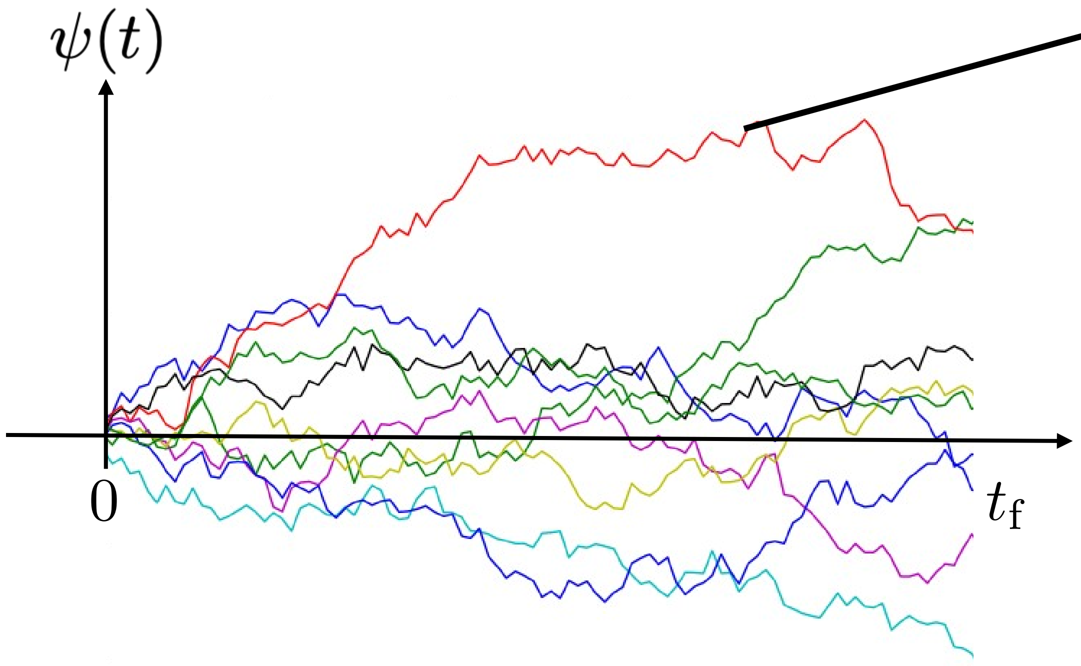
$$H(t) = \frac{\pi^2}{2m} + V(\psi, \lambda(t))$$

Equilibrium conditions

- prepare Gibbs-Boltzmann statistics $\rho_0 = \mathrm{e}^{-\beta H}/\mathcal{Z}_0$
  - isolated: wait (thermalization)
  - or couple thermostat bath
- evolve with
  - same $H = \text{const.}$
  - same bath, β



Stochastic thermodynamics



$$m\partial_t^2\psi = -V'(\psi,\lambda(t)) - \eta\partial_t\psi + \xi(t)$$

single trajectory

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

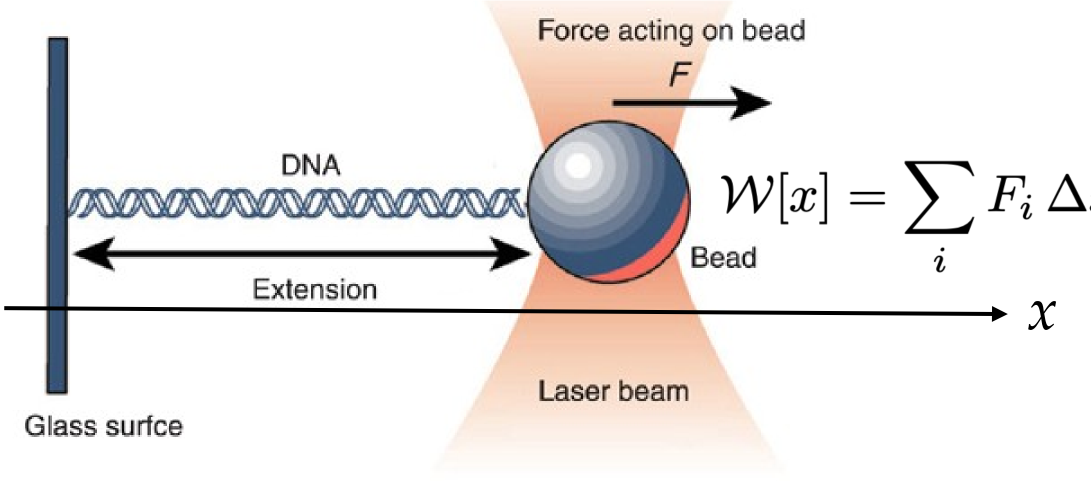
- First law
$$\Delta\mathcal{E} = \mathcal{W}[\psi] + \mathcal{Q}[\psi]$$
- Second law
$$\Delta S = \beta\mathcal{Q}[\psi] + \underbrace{\mathcal{S}^{\mathrm{irr}}[\psi]}_{\text{on average } \langle\mathcal{S}^{\mathrm{irr}}[\psi]\rangle \geq 0}$$
- Isolated system: Clausius inequality
$$\mathcal{W}^{\mathrm{irr}} := \langle\mathcal{W}[\psi]\rangle - \Delta\mathcal{F} \geq 0$$

Stochastic thermodynamics

nature

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

D. Collin[1]*, F. Ritort[2]*, C. Jarzynski[3], S. B. Smith[4], I. Tinoco Jr[5] & C. Bustamante[4,6]



$$\mathcal{W}[x] = \sum_i F_i \, \Delta x_i$$

Fluctuation Theorems

$$P(\mathcal{S}^{\mathrm{irr}}) = P_{\mathrm{r}}(-\mathcal{S}^{\mathrm{irr}})\, \mathrm{e}^{\mathcal{S}^{\mathrm{irr}}}$$

Gallavoti Cohen (1995)

Work fluctuation theorems

$$P(\mathcal{W}) = P_{\mathrm{r}}(-\mathcal{W})\, \mathrm{e}^{\beta(\mathcal{W}-\Delta\mathcal{F})}$$

Crooks (1999)

$$\mathrm{e}^{-\beta\Delta\mathcal{F}} = \langle \mathrm{e}^{-\beta\mathcal{W}[\psi]} \rangle$$

Jarzynski (1997)

exp. review: Ciliberto (2017)

Quantum stochastic thermodynamics

How about quantum fluctuations?

2-point projective measurement

$$\mathcal{W}_{ij} = E_i(t_\mathrm{f}) - E_j(0)$$

Quantum jump trajectories

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

Mukamel, Esposito

Work fluctuation theorem

$$P(\mathcal{W}) = P_\mathrm{r}(-\mathcal{W})\,\mathrm{e}^{\beta(\mathcal{W}-\Delta\mathcal{F})}$$

Kurchan (2000)

cQED: Murch, Lutz et al.

Stochastic equilibrium dynamics

Model B

Martin-Siggia-Rose-Janssen-de Dominicis

$$Z[J,\hat{J}] = \int \mathcal{D}[\psi,\hat{\psi}]\, \mathrm{e}^{-S[\psi,\hat{\psi}] + \int \mathrm{d}t\, \hat{J}\psi + J\mathrm{i}\hat{\psi}}$$

$$S = S_{\text{closed}} + S_{\text{dissip}}$$

$$S_{\text{closed}} = \int \mathrm{d}t\, \mathrm{i}\hat{\psi}\left[m\partial_t\psi + V'(\psi)\right] + \underbrace{\beta\left(\frac{1}{2}m(\partial_t\psi(0))^2 + V(\psi(0))\right) - \beta\mathcal{F}_0}_{\text{- log(initial probability)}}$$

$$S_{\text{dissip}} = \eta \int \mathrm{d}t\, \mathrm{i}\hat{\psi}\left[\partial_t\psi - T\mathrm{i}\hat{\psi}\right]$$

Equilibrium symmetry

Time-reversed fields: $\psi_{\mathrm{r}}(t) := \psi(t_{\mathrm{f}} - t)$

Field transformation

$$\mathcal{T}_\beta : \begin{cases} \psi(t) & \mapsto \psi_{\mathrm{r}}(t) \\ \mathrm{i}\hat{\psi}(t) & \mapsto \mathrm{i}\hat{\psi}_{\mathrm{r}}(t) + \beta \partial_t \psi_{\mathrm{r}}(t) \end{cases}$$

Invariance of the action

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

Chatelain (2003)
Aron Biroli Cugliandolo (2010)
Aron Barci Cugliandolo G-Arenas Lozano (2014)
Aron ... Lozano (2016)

Follow the sources

$$\int \mathrm{d}t\ \hat{J}\psi + J\mathrm{i}\hat{\psi} \overset{\mathcal{T}_\beta}{\mapsto} \int \mathrm{d}t\ \hat{J}_{\mathrm{r}}\psi + J_{\mathrm{r}}[\mathrm{i}\hat{\psi} - \beta\partial_t\psi]$$

$$Z[J, \hat{J}] \overset{\mathcal{T}_\beta}{=} Z[J_{\mathrm{r}}, \hat{J}_{\mathrm{r}} + \beta\partial_t J_{\mathrm{r}}]$$

→ Fluctuation-dissipation theorems

$$R(t,t') = R(t_{\mathrm{f}} - t, t_{\mathrm{f}} - t') + \beta\partial_{t'} C(t_{\mathrm{f}} - t, t_{\mathrm{f}} - t')$$

$$C(t,t') = \langle \psi(t)\psi(t') \rangle$$
$$R(t,t') = \langle \psi(t)\mathrm{i}\hat{\psi}(t') \rangle$$

Symmetry breaking out of equilibrium

Time-dependent non-equilibrium drive: $V(\psi) \to V(\psi, \lambda)$

Variation of the action under $\mathcal{T}_\beta$

Measure of irreversibility

$$S_{\text{closed}}[\psi, \lambda] \overset{\mathcal{T}_\beta}{\mapsto} S_{\text{closed}}[\psi, \lambda_{\text{r}}] + \beta \int \mathrm{d}t\, \dot{\lambda}_{\text{r}} \partial_\lambda V(\psi, \lambda_{\text{r}}) - \beta \Delta \mathcal{F}_{\text{r}} \qquad \lambda_{\text{r}}(t) := \lambda(t_{\text{f}} - t)$$

$$S_{\text{dissip}}[\psi] \overset{\mathcal{T}_\beta}{\mapsto} S_{\text{dissip}}[\psi]$$

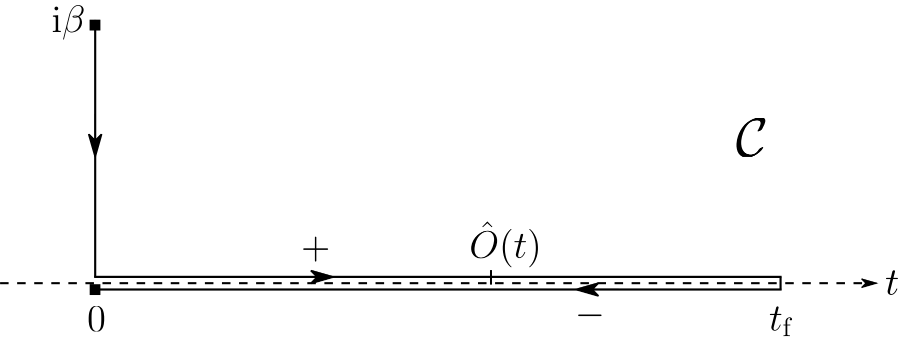
Broken Ward identities

$$\langle O(\psi(t)) \rangle = \langle O(\psi_{\text{r}}(t))\, \mathrm{e}^{-\beta(\mathcal{W}_{\text{r}}[\psi] - \Delta \mathcal{F}_{\text{r}})} \rangle_{\text{r}}$$

→ Work fluctuation theorems

$$\frac{P(\mathcal{W})}{P_{\text{r}}(-\mathcal{W})} = \mathrm{e}^{\beta(\mathcal{W}[\psi] - \Delta \mathcal{F})}$$

Quantum equilibrium dynamics



ex: $H = \frac{\pi^2}{2m} + V(\psi)$ $\qquad [H, \Theta] = 0$

Kadanoff-Baym contour

$$Z[J^+, J^-] = \int \mathcal{D}[\psi^+, \psi^-]\, \mathrm{e}^{\mathrm{i}S[\psi] + \int \mathrm{d}t\, J^+\psi^+ - J^-\psi^-} \times \mathcal{Z}_0^{-1} \langle \psi^+(0)|\mathrm{e}^{-\beta H}|\psi^-(0)\rangle \, \langle \psi^-(t_\mathrm{f})|\psi^+(t_\mathrm{f})\rangle$$

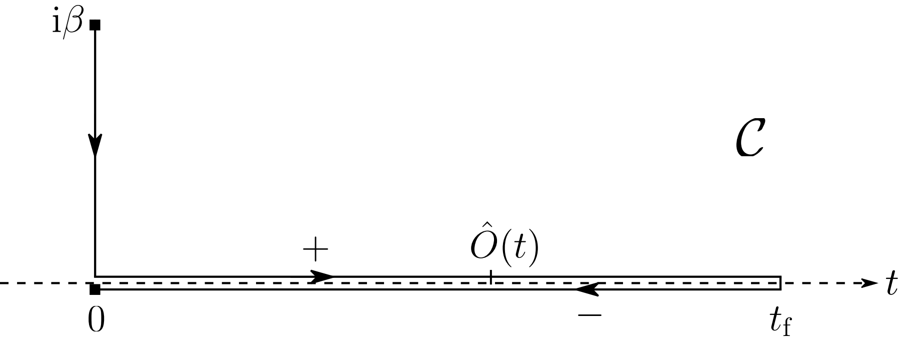
$$S[\psi] = \int \mathrm{d}t\, \mathcal{L}[\psi^+(t)] - \int \mathrm{d}t\, \mathcal{L}[\psi^-(t)]$$

Tentative symmetry transformation

$$\psi^\pm(t) \mapsto \psi^\pm(t_\mathrm{f} - t \pm \mathrm{i}\beta/2)$$

manifestly not symmetric

Complex-time reparametrization



change of frame: R_θ

$$|\psi(t)\rangle \mapsto e^{\mathrm{i}\theta(t)H(t)}|\psi(t)\rangle \qquad \theta(t)\in\mathbb{C}$$

$$\Updownarrow$$

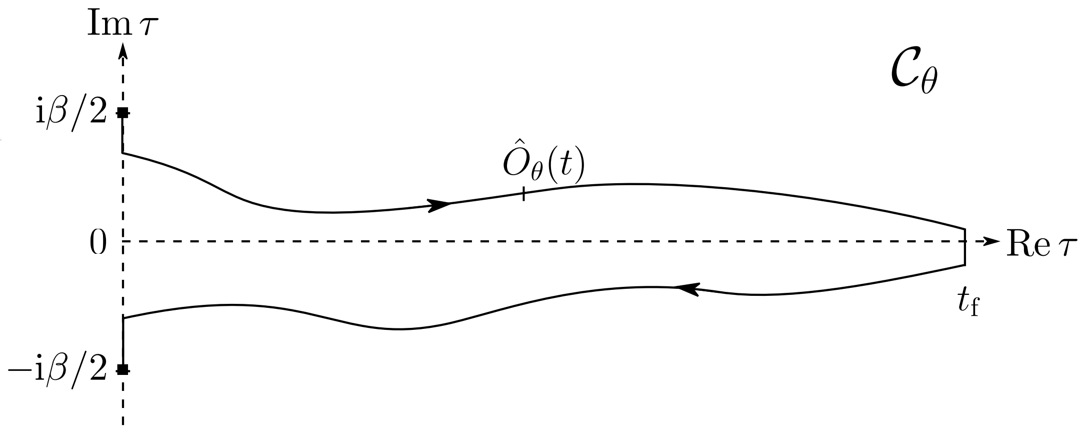
$$\mathbf{I} = \int \mathrm{d}\psi(t)\, e^{+\mathrm{i}\theta(t)H(t)}|\psi(t)\rangle\langle\psi(t)|e^{-\mathrm{i}\theta(t)H(t)}$$

$$\Updownarrow$$

$$H(t) \mapsto e^{-\mathrm{i}\theta(t)H(t)}\,[H(t)-\mathrm{i}\partial_t]\,e^{+\mathrm{i}\theta(t)H(t)}$$

new close-time contour

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



Follow the sources

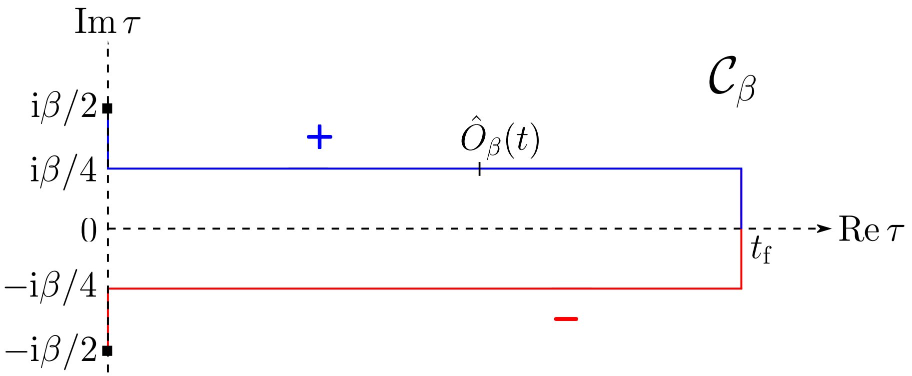
ex: $\int \mathrm{d}t\, J^+\psi^+ \overset{\mathcal{R}_\theta}{\mapsto} \int \mathrm{d}t\, J^+ e^{-\mathrm{i}\theta H}\psi^+ e^{+\mathrm{i}\theta H}$

Symmetry of equilibrum

Equilibrium conditions: $\hat{H} = \text{const}, \ \hat{\rho}_0 = \mathrm{e}^{\beta(\mathcal{F}-\hat{H})}$

Choice of frame/contour: $\theta(t) = \pm \mathrm{i}\beta/4$

Action: $\mathrm{i}S[\psi] = \mathrm{i}\int_{\mathcal{C}_\beta} \mathrm{d}\tau\, \mathcal{L}[\psi(\tau)] + \beta\mathcal{F}_0$



Field transformation

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

Invariance of the action

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

KMS symmetry

$$Z[J^+(t), J^-(t)] \overset{\mathcal{R}_\beta^{-1}\circ\mathcal{T}_\beta\circ\mathcal{R}_\beta}{=} Z[J^+(t_\mathrm{f} - t + \mathrm{i}\beta/2), J^-(t_\mathrm{f} - t - \mathrm{i}\beta/2)]$$

Fluctuation-dissipation theorem

$$G^{-+}(t,t') \overset{\mathcal{R}_\beta^{-1}\circ\mathcal{T}_\beta\circ\mathcal{R}_\beta}{=} G^{+-}(t_\mathrm{f} - t' + \mathrm{i}\beta/2, t_\mathrm{f} - t - \mathrm{i}\beta/2)$$

Symmetry of equilibrum

Open quantum systems

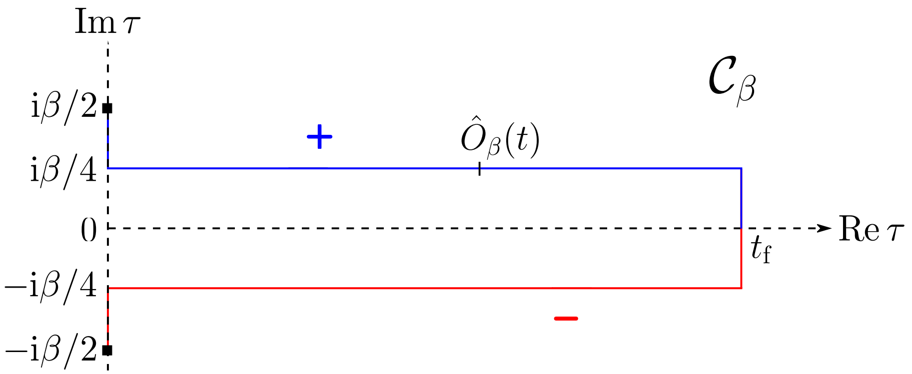
Caldeira-Leggett bath

$$H = H_{\mathrm{S}} + H_{\mathrm{SB}} + H_{\mathrm{B}}$$

$$H_{\mathrm{S}} = \frac{\pi^2}{2m} + V(\psi)$$

$$H_{\mathrm{B}} = \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2} m\omega_i^2 q_i^2$$

$$H_{\mathrm{SB}} = \frac{1}{2}\sum_i c_i (q_i - \psi)^2$$



$$\begin{aligned} S_{\mathrm{dissip}} = & \int_{\mathcal{C}_\beta} \mathrm{d}\tau \int^{\tau} \mathrm{d}\tau' \, \psi^+(\tau) K(\tau - \tau') \psi^+(\tau') \\ & + \int \mathrm{d}\tau \int^{\tau} \mathrm{d}\tau' \, \psi^-(\tau) K(\tau - \tau') \psi^-(\tau') \\ & + \int \mathrm{d}\tau \int \mathrm{d}\tau' \, \psi^+(\tau) K(\tau - \tau') \psi^-(\tau') \end{aligned}$$

$$K(\tau) := \int \mathrm{d}\epsilon \, J(\epsilon) \left[\coth(\beta\epsilon/2) \cosh(\mathrm{i}\epsilon\tau) - \sinh(\mathrm{i}\epsilon\tau)\right]$$

Field transformation

$$T_\beta : \; \psi^\pm(\tau) \mapsto \psi^\pm(t_{\mathrm{f}} - \tau \pm \mathrm{i}\beta/2)$$

Invariance of the action

$$S_{\mathrm{dissip}}[\psi] \overset{T_\beta}{\mapsto} S_{\mathrm{dissip}}[\psi]$$

Yeo (2019)

Symmetry breaking out of equilibrium

Non-equilibrium time-dependent drive: $H \mapsto H(t)$

ex: $H(t) = \dfrac{\pi^2}{2m} + V(\psi, \lambda(t))$ $\qquad H(t) = \displaystyle\int \mathrm{d}x\, h(x) + \lambda(t) O_0$

R_β

Thermal frame: non-Hermitian evolution

$$H \mapsto \begin{cases} H^+ = H - \mathrm{e}^{\beta H/4}\, \mathrm{i}\partial_t \mathrm{e}^{-\beta H/4} \\ H^- = (H^+)^\dagger \end{cases}$$

T_β

$H \mapsto H_\mathrm{r} = \dfrac{\pi^2}{2m} + V(\psi, \lambda_\mathrm{r})$ $\qquad \lambda_\mathrm{r}(t) := \lambda(t_\mathrm{f} - t)$

R_β^{-1} $\qquad \bullet \; \bullet \; \bullet$

Variation of the Kadanoff-Baym action under $\mathcal{R}_\beta^{-1} \circ \mathcal{T}_\beta \circ \mathcal{R}_\beta$

$$\mathrm{i}S[\psi] \mapsto \mathrm{i}S_\mathrm{r}[\psi] + \beta(\Delta\mathcal{F}_\mathrm{r} - \Omega_\mathrm{r}[\psi])$$

Measure of irreversibility

with $\beta\,\Omega_\mathrm{r}[\psi] := \displaystyle\int \mathrm{d}t\, \langle \psi^+(t) | \dot{\sigma} | \psi^+(t) \rangle + \int \mathrm{d}t\, \langle \psi^-(t) | \dot{\sigma} | \psi^-(t) \rangle$

$\psi \in \mathbb{R}$

Symmetry breaking out of equilibrium

$$\dot{\sigma} := -\mathrm{e}^{\beta H/2}\left[\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-\beta H}\right]\mathrm{e}^{\beta H/2}$$

- Semiclassical expansion

$$\dot{\sigma} \simeq \beta\partial_t H + \frac{1}{3!}(\beta/2)^2[H, H, [\beta\partial_t H]] + \dots$$

- Spatially extended

$$\xi \lesssim v_{\mathrm{LR}} \times \beta\hbar$$

- Non-locality in time

$$\langle\dot{\sigma}\rangle = \int_{-\beta\hbar/2}^{\beta\hbar/2} \mathrm{d}\tau\, \mathrm{Tr}[\partial_t H\, \rho(t + \mathrm{i}\tau)] \longrightarrow \tau \sim \beta\hbar$$

- Weak Clausius-like inequality

$$\int \mathrm{d}t\langle\dot{\sigma}\rangle \geq \beta\int \mathrm{d}t\, \langle\partial_t H\rangle \geq \beta\Delta\mathcal{F}$$

Symmetry breaking out of equilibrium

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ex: $H(t) = \frac{\pi^2}{2m} + V(\psi, \lambda(t))$ $\qquad H(t) = \int \mathrm{d}x\, h(x) + \lambda(t) O_0$

$\mathcal{R}_\beta$

Thermal frame: non-Hermitian evolution

$$H \mapsto \begin{cases} H^+ = H - \mathrm{e}^{\beta H/4}\, \mathrm{i}\partial_t \mathrm{e}^{-\beta H/4} \\ H^- = (H^+)^\dagger \end{cases}$$

$\mathcal{T}_\beta$

$$H \mapsto H_\mathrm{r} = \frac{\pi^2}{2m} + V(\psi, \lambda_\mathrm{r}) \qquad \lambda_\mathrm{r}(t) := \lambda(t_\mathrm{f} - t)$$

$\mathcal{R}_\beta$

• • •

Work fluctuation theorem

$$P(\mathcal{W}) = P_\mathrm{r}(-\mathcal{W})\, \mathrm{e}^{\beta(\mathcal{W} - \Delta\mathcal{F})}$$

with $\mathcal{W}_{ij} = E_i(t_\mathrm{f}) - E_j(0)$

Recap

finite-time fluctuations: care for boundaries

	classical thermal	quantum
Equilibrium symmetry	MSR $S[\psi] \overset{\mathcal{T}_\beta}{\mapsto} S[\psi]$	Kadanoff-Baym $\mathcal{R}_\beta \downarrow \quad \uparrow \mathcal{R}_\beta^{-1}$ \`Thermal' frame $\mathrm{S}[\psi] \overset{\mathcal{T}_\beta}{\mapsto} S[\psi]$
	Fluctuation-Dissipation Theorems	Fluctuation-Dissipation Theorems
Non-equilibrium symmetry breaking	$S[\psi] \mapsto S_\mathrm{r}[\psi] - \beta(\Delta\mathcal{F}_\mathrm{r} - \mathcal{W}_\mathrm{r}[\psi])$ work Fluctuation Theorems	$\mathrm{i}S[\psi] \mapsto \mathrm{i}S_\mathrm{r}[\psi] + \beta(\Delta\mathcal{F}_\mathrm{r} - \Omega_\mathrm{r}[\psi])$ non-Hermitian dynamics work Fluctuation Theorems