Thermodynamics and embedding
of non-Markovian Langevin dynamics

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in collaboration with Kiyoshi Kanazawa (*Kyoto University*)

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KYOTO UNIVERSITY

Stochastic thermodynamics and non-Markovian dynamics

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▶ probability of $\boldsymbol{x}(t)$ given prior observations $\boldsymbol{x}(t-t_1), \boldsymbol{x}(t-t_2), \ldots$ $(t_1 < t_2 < \ldots)$

dynamics Markovian $\quad \Leftrightarrow \quad P(\boldsymbol{x}(t)|\boldsymbol{x}(t-t_1), \boldsymbol{x}(t-t_2), \ldots) = P(\boldsymbol{x}(t)|\boldsymbol{x}(t-t_1))$

Non-Markovian stochastic thermodynamics

▶ in thermodynamics: system interacting with an environment

▶ Markovian dynamics of system only in specific limits: "Markov approximation"

  • size of environment $\gg$ size of system
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- however: many results in stochastic thermodynamics restricted to Markovian dynamics
  - TUR, speed limits, power-efficiency trade-off, . . .
  - stochastic entropy production $\hat{\Sigma} = \ln \frac{\mathbb{P}(\hat{\boldsymbol{x}})}{\mathbb{P}^{\dagger}(\hat{\boldsymbol{x}}^{\dagger})}$: $\mathbb{P}^{\dagger}(\hat{\boldsymbol{x}}^{\dagger})$ time-reversed dynamics
    meaning of time-reversal in non-Markovian dynamics?

Time-reversal for non-Markovian dynamics

▶ simple example of non-Markovian dynamics: generalized Langevin equation

$$\int_0^t dt' \ \boldsymbol{M}(t-t')\dot{\boldsymbol{x}}(t') = \boldsymbol{f}_{\boldsymbol{\lambda}(t)}(\boldsymbol{x}(t)) + \boldsymbol{\eta}(t)$$

▶ control protocol $\boldsymbol{\lambda}(t)$, $t \in [0, \tau]$; initial probability $p_0(\boldsymbol{x}_0)$

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▶ for all definitions: "stochastic entropy" $\hat{\Sigma} = \ln \frac{\mathbb{P}(\hat{\boldsymbol{x}})}{\mathbb{P}^\dagger(\hat{\boldsymbol{x}}^\dagger)}$ satisfies

$$\left\langle \hat{\Sigma} \right\rangle \geq 0 \qquad \left\langle e^{-\hat{\Sigma}} \right\rangle = 1$$

Non-Markovian stochastic thermodynamics via Markov embedding

► assumption: non-Markovian dynamics = effective model of underlying Markovian dynamics

► underlying Markovian dynamics should fix time-reversal of non-Markovian dynamics

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  - Markovian dynamics on larger state space with same dynamics for $x(t)$
  - compute entropy production Σ^{M} of embedded Markovian dynamics
  - want to assign $\Sigma^{\mathsf{M}} = \Sigma$

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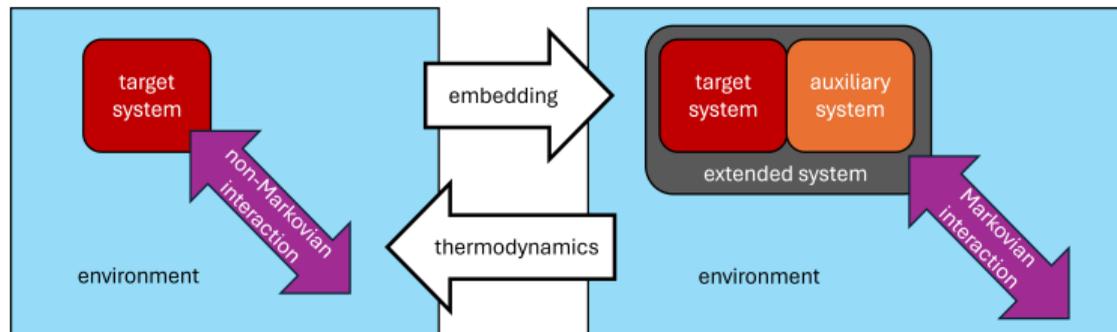
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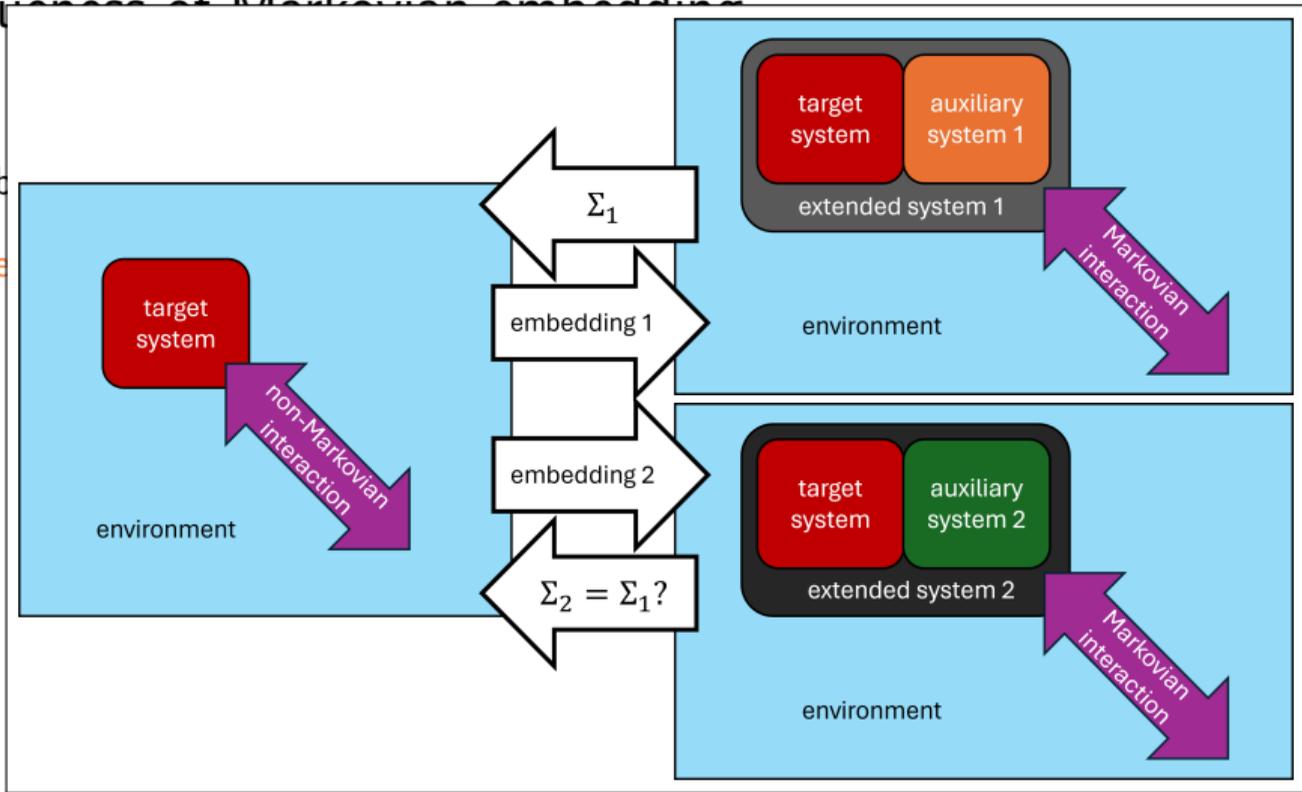
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- ▶ different extended Markovian systems result in same dynamics for $x(t)$
- ▶ thermodynamic quantities (entropy production) in general not invariant
- ▶ ambiguity of non-Markovian time reversal $\rightarrow$ ambiguity of Markovian embedding

Embedding and thermodynamic reversibility

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▶ here: generalized Langevin equations

(Semi)-linear generalized Langevin equation

Generalized Langevin equation

▶ "semi-linear" generalized Langevin equation for system s: $x^{\mathfrak{s}} \in \mathbb{R}^{d^{\mathfrak{s}}}$

$$\int_0^t dt' \, \boldsymbol{M}(t,t') \dot{\boldsymbol{x}}^{\mathfrak{s}}(t') = \boldsymbol{f}_{\boldsymbol{\lambda}(t)}^{\mathfrak{s}}(\boldsymbol{x}^{\mathfrak{s}}(t)) + \boldsymbol{\eta}(t) \qquad \text{(GLE)}$$

- force $\boldsymbol{f}_{\boldsymbol{\lambda}}^{\mathfrak{s}}(\boldsymbol{x}^{\mathfrak{s}})$ depends on control parameters $\boldsymbol{\lambda}$: can be non-linear
- linear memory kernel $\boldsymbol{M}(t,t')$
- colored noise $\left\langle \boldsymbol{\eta}(t)\boldsymbol{\eta}^{\mathsf{T}}(t') \right\rangle = \boldsymbol{N}(t,t')$

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▶ questions
- what types of GLEs can be obtained from "mesoscopic" models?
- what are the possible Markovian representations of (GLE)?
- what are their thermodynamic properties?
- can we identify a unique Markovian entropy production Σ^{M} associated with (GLE)?

Mesoscopic model: interacting Langevin equations

▶ start from Markovian description of target system x^{s} and auxiliary system x^{a}

$$\gamma^{\mathsf{s}}\dot{x}^{\mathsf{s}} = f_{\lambda}^{\mathsf{s}}(x^{\mathsf{s}}) - K^{\mathsf{s}}(x^{\mathsf{s}} - \mathcal{K}^{\mathsf{sa}}x^{\mathsf{a}}) + \sqrt{2\gamma^{\mathsf{s}}T}\xi^{\mathsf{s}}$$
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Mesoscopic model: interacting Langevin equations

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▶ assumptions

- only target system force depends on control parameters
- linear dynamics of auxiliary degrees of freedom
- target and auxiliary system in contact with equilibrium environment T
- independent noises acting on target and auxiliary system "bipartite"

Mesoscopic model: interacting dynamics...

▶ start from Markov ... ... system $\boldsymbol{x}^{\mathsf{a}}$

$\boldsymbol{\xi}^{\mathsf{s}}$

▶ assumptions
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- target and aux... T
- independent n...

$\lambda(t)$

target system x^s

auxiliary system x^a

Markovian environment T

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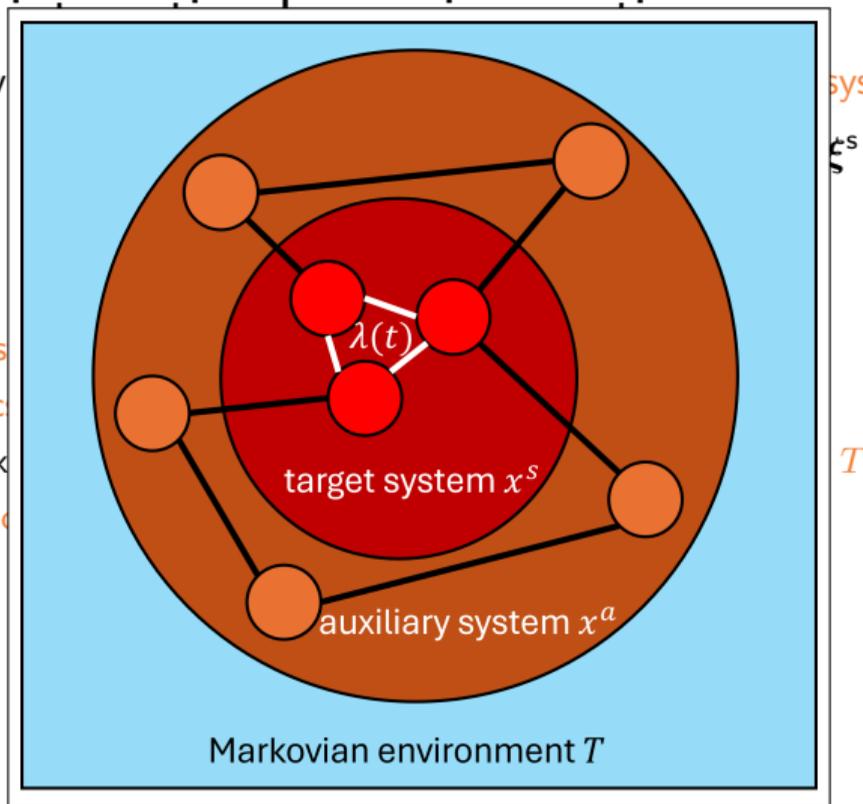
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▶ coarse-graining: eliminate $\boldsymbol{x}^{\text{a}} \Rightarrow$ effective dynamics for $\boldsymbol{x}^{\text{s}}$

Mesoscopic model:

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                                                                            $\boldsymbol{\xi}^{\mathsf{s}}$

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$\lambda(t)$

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non-Markovian environment

Semi-linear generalized Langevin equation

▶ non-Markovian generalized Langevin equation for target system

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$$\boldsymbol{M}(t) = \boldsymbol{K}^{\mathsf{s}}\boldsymbol{\mathcal{K}}^{\mathsf{sa}}e^{-(\boldsymbol{\gamma}^{\mathsf{a}})^{-1}\boldsymbol{K}^{\mathsf{a}}t}\boldsymbol{\mathcal{K}}^{\mathsf{as}}, \qquad \langle\boldsymbol{\chi}(t)\boldsymbol{\chi}^{\mathsf{T}}(t')\rangle = T\boldsymbol{N}(t,t')$$

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▶ formally exact, but fundamental problems

- noise correlations non-stationary $\boldsymbol{N}(t,t') \neq \boldsymbol{N}^{\mathsf{st}}(t-t')$ even for initial steady state
- equation depends on $\boldsymbol{x}^{\mathsf{s}}(0)$ and $\boldsymbol{x}^{\mathsf{a}}(0)$ via $\boldsymbol{\chi}(t)$ and $\langle \boldsymbol{u}_0(t)\rangle$

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▶ in general: GLE is not a closed equation for target system

Stationary GLE

▶ under what conditions is GLE driven by stationary noise and independent of $x^s(0)$?

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▶ scenario 0: time-scale separation
  - auxiliary system conditionally stationary $p_0^{\mathsf{a}}(x^{\mathsf{a}}|x^{\mathsf{s}}) = p_{x^{\mathsf{s}} \text{ fixed}}^{\mathsf{a,st}}(x^{\mathsf{a}})$
  - requires $\tau^{\mathsf{a,rel}} \ll \min(\tau^{\mathsf{s,rel}}, \tau^{\mathsf{prot}})$

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- ▶ in this limit: target system Markovian $\rightarrow$ auxiliary system renormalizes friction coefficient

Stationary GLE in equilibrium

▶ scenario 1: equilibrium
- conservative forces: $\boldsymbol{f}^{\mathsf{s}}_{\boldsymbol{\lambda}}(\boldsymbol{x}^{\mathsf{s}}) = -\boldsymbol{\nabla}_{x^{\mathsf{s}}} U^{\mathsf{s}}_{\boldsymbol{\lambda}}(\boldsymbol{x}^{\mathsf{s}})$, $\boldsymbol{K} = \boldsymbol{K}^{\mathsf{T}}$
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- ▶ initial state equilibrium for $\boldsymbol{\lambda}(0)$
  - stationary noise $\boldsymbol{N}(t, t') = \boldsymbol{M}(|t - t'|)$ fluctuation-dissipation theorem
  - GLE closed if target system in equilibrium at $t = 0$

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Stationary GLE out of equilibrium

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  - linear forces: $f_{\lambda}^{\text{s}}(x^{\text{s}}) = -\mathcal{K}_{\lambda}^{\text{s}}(x^{\text{s}} - a_{\lambda})$
  - steady state $\Leftrightarrow$ covariance matrix Ξ_{λ} and irreversible circulation $C_{\lambda} = -C_{\lambda}^{\mathsf{T}}$

- ▶ if initial state is steady state for $\lambda(0)$ and $C_{\lambda(0)} = \begin{pmatrix} C^{\text{s}} & 0 \\ 0 & C^{\text{a}} \end{pmatrix}$
  - stationary noise $N(t, t') = N^{\text{st}}(t - t')$
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- stationary noise $\boldsymbol{N}(t, t') = \boldsymbol{N}^{\mathsf{st}}(t - t')$
- GLE closed if target system in steady state at $t = 0$

▶ no constraints on protocol: time-dependent driving for $t > 0$

Irreversible circulation and entropy production

▶ write Langevin equations as

$$\begin{pmatrix} \dot{\boldsymbol{x}}^{\mathsf{s}} \\ \dot{\boldsymbol{x}}^{\mathsf{a}} \end{pmatrix} = - \begin{pmatrix} \boldsymbol{A}^{\mathsf{aa}} & \boldsymbol{A}^{\mathsf{as}} \\ \boldsymbol{A}^{\mathsf{sa}} & \boldsymbol{A}^{\mathsf{aa}} \end{pmatrix} \begin{pmatrix} \boldsymbol{x}^{\mathsf{s}} \\ \boldsymbol{x}^{\mathsf{a}} \end{pmatrix} + \sqrt{2T} \begin{pmatrix} \boldsymbol{\xi}^{\mathsf{s}} \\ \boldsymbol{\xi}^{\mathsf{a}} \end{pmatrix}$$

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▶ steady state covariance $\boldsymbol{\Xi}$ from Lyapunov equation $\boldsymbol{A}\boldsymbol{\Xi} + \boldsymbol{\Xi}\boldsymbol{A}^{\mathsf{T}} = 2T\boldsymbol{I}$

$$\boldsymbol{C} = \frac{1}{2T}\big(\boldsymbol{A}\boldsymbol{\Xi} - \boldsymbol{\Xi}\boldsymbol{A}^{\mathsf{T}}\big) \quad \Leftrightarrow \quad \boldsymbol{A} = T(\boldsymbol{I} + \boldsymbol{C})\boldsymbol{\Xi}^{-1}$$

▶ intuitively: $\boldsymbol{C}$ quantifies steady-state currents

$$\sigma = \frac{1}{T}\mathsf{tr}\big(\boldsymbol{C}\boldsymbol{\Xi}^{-1}\boldsymbol{C}^{\mathsf{T}}\big)$$

Irreversible circulation and entropy production

▶ write Langevin equations as

$$\begin{pmatrix} \dot{\boldsymbol{x}}^{\mathsf{s}} \\ \dot{\boldsymbol{x}}^{\mathsf{a}} \end{pmatrix} = - \begin{pmatrix} \boldsymbol{A}^{\mathsf{aa}} & \boldsymbol{A}^{\mathsf{as}} \\ \boldsymbol{A}^{\mathsf{sa}} & \boldsymbol{A}^{\mathsf{aa}} \end{pmatrix} \begin{pmatrix} \boldsymbol{x}^{\mathsf{s}} \\ \boldsymbol{x}^{\mathsf{a}} \end{pmatrix} + \sqrt{2T} \begin{pmatrix} \boldsymbol{\xi}^{\mathsf{s}} \\ \boldsymbol{\xi}^{\mathsf{a}} \end{pmatrix}$$

▶ steady state covariance $\boldsymbol{\Xi}$ from Lyapunov equation $\boldsymbol{A}\boldsymbol{\Xi} + \boldsymbol{\Xi}\boldsymbol{A}^{\mathsf{T}} = 2T\boldsymbol{I}$

$$\boldsymbol{C} = \frac{1}{2T}\big(\boldsymbol{A}\boldsymbol{\Xi} - \boldsymbol{\Xi}\boldsymbol{A}^{\mathsf{T}}\big) \quad \Leftrightarrow \quad \boldsymbol{A} = T\big(\boldsymbol{I} + \boldsymbol{C}\big)\boldsymbol{\Xi}^{-1}$$

▶ intuitively: $\boldsymbol{C}$ quantifies steady-state currents

$$\sigma = \frac{1}{T}\mathsf{tr}\big(\boldsymbol{C}\boldsymbol{\Xi}^{-1}\boldsymbol{C}^{\mathsf{T}}\big)$$

▶ introduce partial entropy production $\sigma = \sigma^{\mathsf{s}} + \sigma^{\mathsf{a}}$

$$\boldsymbol{C} = \begin{pmatrix} \boldsymbol{C}^{\mathsf{s}} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{C}^{\mathsf{a}} \end{pmatrix} \quad \Rightarrow \quad \sigma^{\mathsf{s}} = \frac{1}{T}\mathsf{tr}\big(\boldsymbol{C}^{\mathsf{s}}(\boldsymbol{\Xi}^{-1})^{\mathsf{ss}}\boldsymbol{C}^{\mathsf{s},\mathsf{T}}\big), \quad \sigma^{\mathsf{a}} = \frac{1}{T}\mathsf{tr}\big(\boldsymbol{C}^{\mathsf{a}}(\boldsymbol{\Xi}^{-1})^{\mathsf{aa}}\boldsymbol{C}^{\mathsf{a},\mathsf{T}}\big)$$

▶ no currents between target and auxiliary system

Equilibrium and non-equilibrium noise

- $C^{\mathsf{a}} = 0$ and $C^{\mathsf{s}} \neq 0$: target system out of equilibrium

$$\sigma^{\mathsf{a}} = 0 \quad \text{and} \quad \boldsymbol{N}^{\mathsf{st}}(t) = \boldsymbol{N}^{\mathsf{st}}(-t)$$
$$\text{but} \quad \sigma^{\mathsf{s}} > 0 \quad \text{and} \quad \boldsymbol{N}^{\mathsf{st}}(t) \neq \boldsymbol{M}(t)$$

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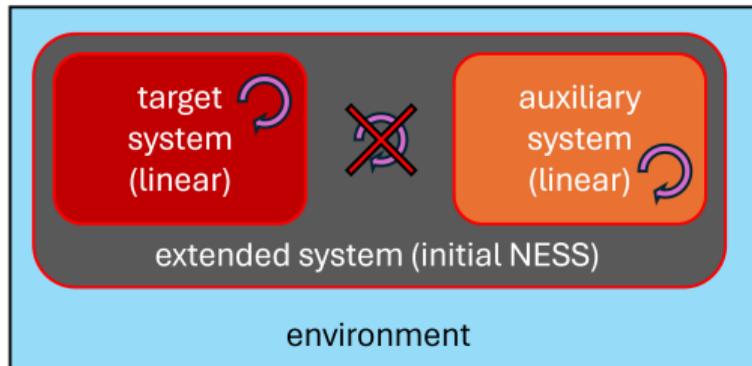$$\sigma^{\mathsf{s}} = 0 \quad \text{and} \quad N^{\mathsf{st}}(t) = M(t)\Theta(t) + M^{\mathsf{T}}(-t)\Theta(-t)$$
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▶ thermodynamic infererence: $\sigma^{\mathsf{a}} > 0$ can be detected from finite-time correlations of x^{s}

Conditions for stationary generalized Langevin equation
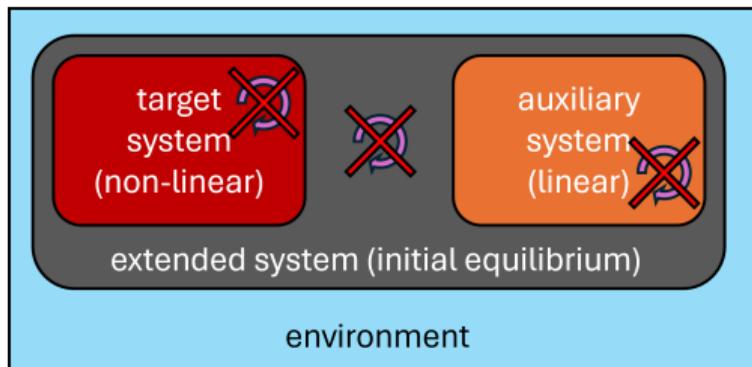
$$\boldsymbol{\gamma}^{\mathsf{s}}\dot{\boldsymbol{x}}^{\mathsf{s}}(t) - \sqrt{2\boldsymbol{\gamma}^{\mathsf{s}}T}\boldsymbol{\xi}^{\mathsf{s}}(t)$$

$$+ \int_0^t dt' \ \boldsymbol{M}(t - t')\dot{\boldsymbol{x}}^{\mathsf{s}}(t') - \boldsymbol{\chi}(t)$$

$$= \boldsymbol{f}^{\mathsf{s}}_{\boldsymbol{\lambda}(t)}(\boldsymbol{x}^{\mathsf{s}}(t)) - \boldsymbol{\mathcal{A}}^{\mathsf{s}}\boldsymbol{x}^{\mathsf{s}}(t)$$

with $\quad \left\langle \boldsymbol{\chi}(t)\boldsymbol{\chi}^{\mathsf{T}}(t') \right\rangle = T\boldsymbol{N}^{\mathsf{st}}(t - t')$

Embbeding and Markovian entropy production

Embedding problem

▶ coarse-graining: Langevin equation → derive GLE ("easy")

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- ▶ possible form of memory kernel

$$\boldsymbol{N}^{\mathsf{st}}(t) = \boldsymbol{M}(t) = \sum_k \boldsymbol{b}_k \boldsymbol{b}_k^{\mathsf{T}} e^{-\alpha_k t}, \qquad \alpha_k > 0$$

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▶ reconstruct candidate Langevin equation

$$\{\alpha_k, \boldsymbol{b}_k\} \qquad \Rightarrow \qquad \{\boldsymbol{K}^{\mathsf{s}}, \boldsymbol{K}^{\mathsf{a}}, \boldsymbol{\mathcal{K}}^{\mathsf{sa}}, \boldsymbol{\mathcal{K}}^{\mathsf{as}}\}$$

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  • invertible variable transformations $x^{\mathsf{a}} \to Q x^{\mathsf{a}}$
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- ▶ both transformations leave entropy production invariant
- ▶ linear GLE in equilibrium $\to$ unique Markovian entropy production

Markovian entropy production

▶ given: non-Markovian evolution of target system

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▶ Σ^{M} is entropy production of Markovian Langevin equation

$$\Sigma^{\mathsf{M}} = \left\langle \ln\frac{\mathbb{P}(\hat{\boldsymbol{x}}^{\mathsf{s}}, \hat{\boldsymbol{x}}^{\mathsf{a}})}{\mathbb{P}^{\dagger}(\hat{\boldsymbol{x}}^{\mathsf{s}\dagger}, \hat{\boldsymbol{x}}^{\mathsf{a}\dagger})}\right\rangle \geq \left\langle \ln\frac{\mathbb{P}(\hat{\boldsymbol{x}}^{\mathsf{s}})}{\mathbb{P}^{\dagger}(\hat{\boldsymbol{x}}^{\mathsf{s}\dagger})}\right\rangle = \Sigma^{\mathsf{NM}}$$

Markovian time-reversed process

- ▶ time-reversal $\mathbb{P}^\dagger(\hat{\boldsymbol{x}}^{\mathsf{s}\dagger}, \hat{\boldsymbol{x}}^{\mathsf{a}\dagger})$ in Markovian Langevin equation
  - reverse trajectory $(\hat{\boldsymbol{x}}^{\mathsf{s}\dagger}, \hat{\boldsymbol{x}}^{\mathsf{a}\dagger}) = (\boldsymbol{x}^{\mathsf{s}}(\tau - t), \boldsymbol{x}^{\mathsf{a}}(\tau - t))_{t \in [0,\tau]}$
  - reverse protocol $\boldsymbol{\lambda}^\dagger(t) = \boldsymbol{\lambda}(\tau - t)$
  - start from final state $p_0^\dagger(\boldsymbol{x}^{\mathsf{s}}, \boldsymbol{x}^{\mathsf{a}}) = p_\tau(\boldsymbol{x}^{\mathsf{s}}, \boldsymbol{x}^{\mathsf{a}})$

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- ▶ GLE for time-reversed process has same memory but non-stationary noise!
- ▶ more general notion of time-reversal may be necessary for non-Markovian systems

Uniqueness of entropy production

▶ more generally: arbitrary conservative interactions with energy separation

$$U_{\boldsymbol{\lambda}}(\boldsymbol{x}^{\mathsf{s}}, \boldsymbol{x}^{\mathsf{a}}) = \underbrace{U_{\boldsymbol{\lambda}}^{\mathsf{s}}(\boldsymbol{x}^{\mathsf{s}})}_{\text{controllable}} + \underbrace{U^{\mathsf{int}}(\boldsymbol{x}^{\mathsf{s}}, \boldsymbol{x}^{\mathsf{a}})}_{\text{uncontrollable}}$$

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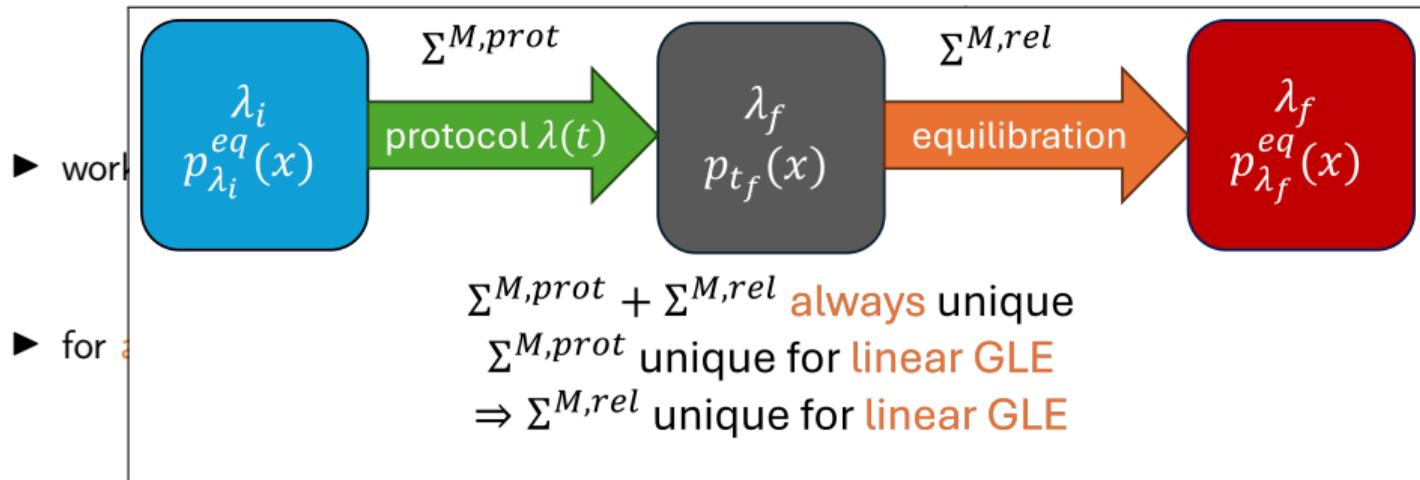$$W = W^{\mathsf{s}} \qquad \Delta F = \Delta F^{\mathsf{s}}$$

▶ for any embedding that results in the correct dynamics of $\boldsymbol{x}^{\mathsf{s}}$

$$W^{\mathsf{s}} = \Delta F^{\mathsf{s}} + T\Sigma^{\mathsf{M}} \quad \text{if initial and final state in equilibrium}$$

▶ Σ^{M} is unique for equilibrium-to-equilibrium processes

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▶ work

$$\Sigma^{M,prot} + \Sigma^{M,rel} \text{ always unique}$$
$$\Sigma^{M,prot} \text{ unique for linear GLE}$$
$$\Rightarrow \Sigma^{M,rel} \text{ unique for linear GLE}$$

▶ for

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Non-uniqueness of embedding out of equilibrium

▶ explicitly construct embedding of equilibrium GLE using non-conservative forces

▶ entropy production different from conservative embedding

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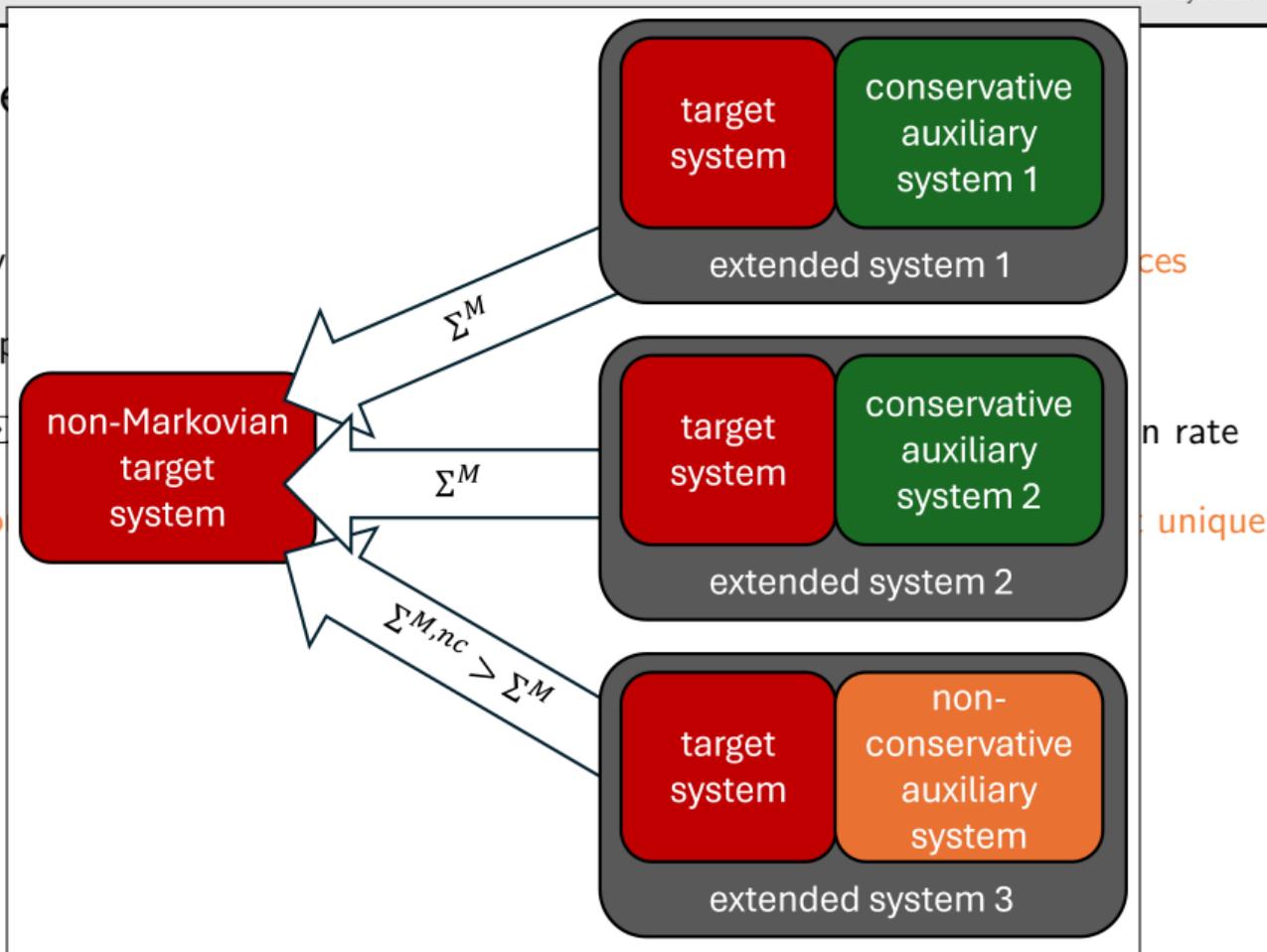
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Underdamped generalized Langevin equation

Underdamped Langevin equations

▶ start from underdamped equations

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▶ satisfies fluctuation-dissipation relation

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  - gauge invariance of entropy production ↔ excess/housekeeping decomposition

Thank you for your attention!