Stochastic Differential Equation for a System Coupled to a Thermostatic Bath via an Arbitrary Interaction Hamiltonian

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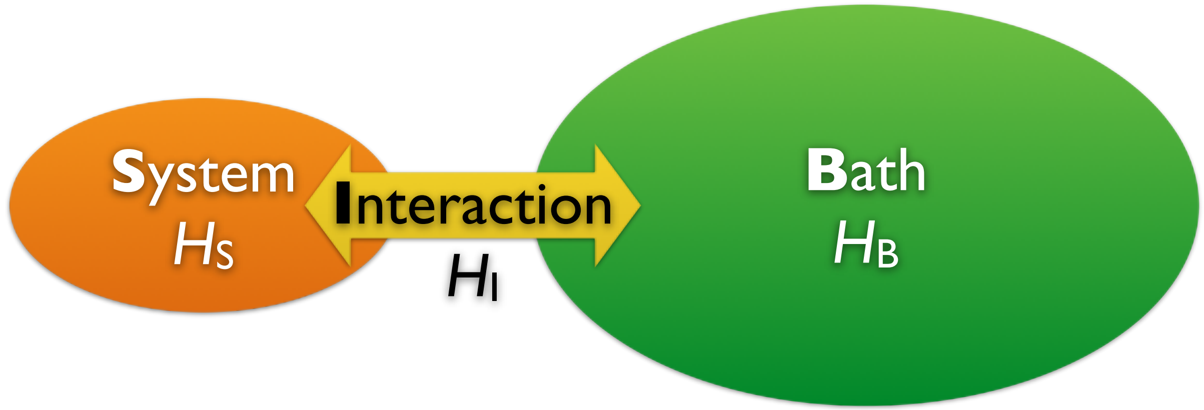
Thermodynamics: Study of Open systems

Total Hamiltonian

$$H_{\mathrm{tot}} = H_{\mathrm{S}} + H_{\mathrm{I}} + H_{\mathrm{B}}$$



- System dynamics depend on System-Bath (SB) interaction.

- Full H_{tot} info is needed for accurate description of system dynamics.

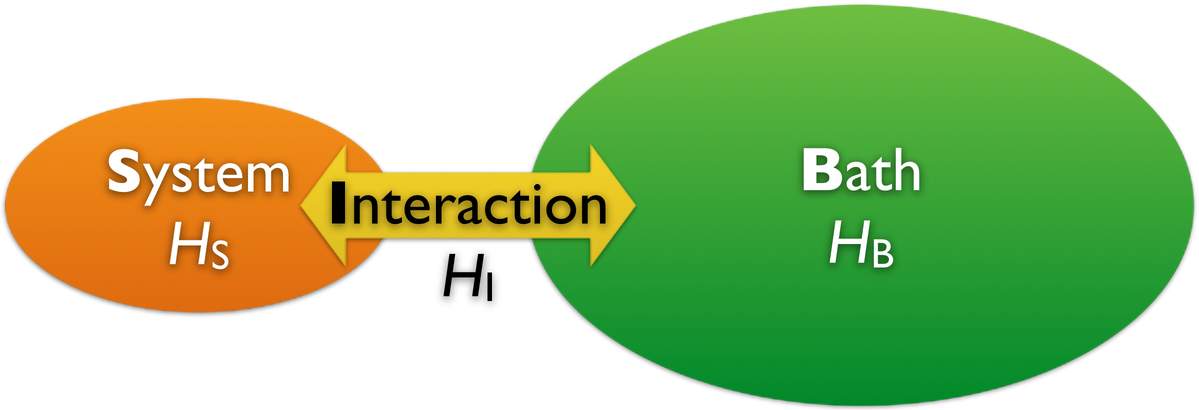
- Bath has huge degrees of freedom (not feasible to consider all).

- Effective description is necessary.

Effective Description of SB interaction

Total Hamiltonian

$$H_{\mathrm{tot}} = H_{\mathrm{S}} + H_{\mathrm{I}} + H_{\mathrm{B}}$$



- master equation: $\dot{\mathbf{P}} = \mathbb{R}\mathbf{P}$
  (discrete states)

$\mathbf{P}$: probability vector

$\mathbb{R}$: transition rate matrix

- **S**tochastic **D**ifferential **E**quation (SDE) (continuous states)

: $m\dot{v} = -\partial_x U(x) \underbrace{-\gamma v + \xi}_{\text{effective description of bath influence}}$ (Langevin eq.) $\langle \xi(t)\xi(t') \rangle = 2k_{\mathrm{B}}\gamma T\delta(t-t')$

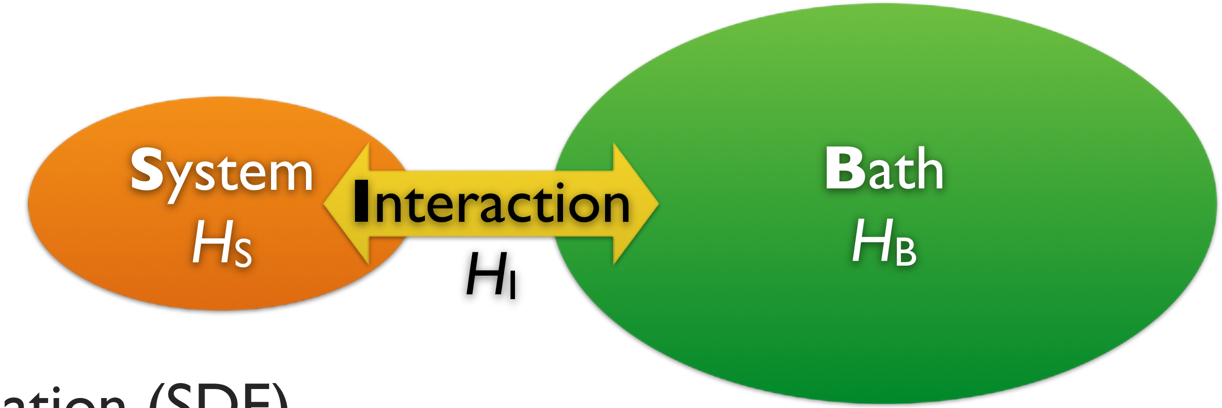
- enable to build stochastic thermodynamics and crucial relations

: fluctuation theorems, TURs, speed limits…

Weak vs. Strong Coupling

Total Hamiltonian

$$H_{\text{tot}} = H_{\text{S}} + H_{\text{I}} + H_{\text{B}}$$



- **S**tochastic **D**ifferential **E**quation (SDE)

: $m\dot{v} = -\partial_x U(x) \underline{-\gamma v + \xi}$ (Langevin eq.) $\langle \xi(t)\xi(t') \rangle = 2k_{\text{B}}\gamma T\delta(t-t')$

effective description of bath influence

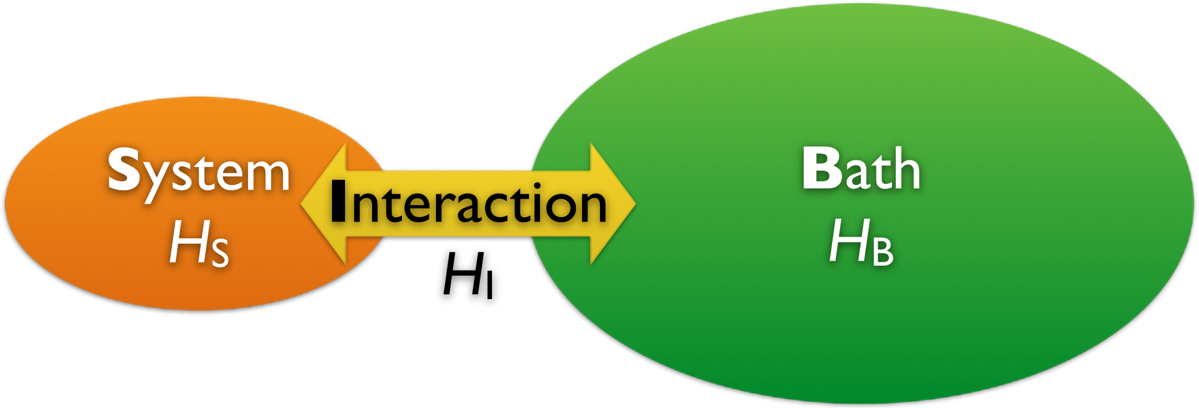
→ simple, but no information on H_{I}

- equilibrium state (Langevin eq.): $\rho^{\text{eq}} = \dfrac{e^{-\beta H_{\text{S}}}}{Z_{\text{S}}}$ (H_{S} only) $Z_{\text{S}} = \int dS\ e^{-\beta H_{\text{S}}}$

Weak vs. Strong Coupling

Total Hamiltonian

$$H_{\rm tot} = H_{\rm S} + H_{\rm I} + H_{\rm B}$$



- equilibrium state (Langevin eq.): $\rho^{\rm eq} = \dfrac{e^{-\beta H_{\rm S}}}{Z_{\rm S}}$ (H_S only) $Z_{\rm S} = \int dS\, e^{-\beta H_{\rm S}}$

- equilibrium state for S+B: $p_{\rm tot}^{\rm eq} = \dfrac{e^{-\beta H_{\rm tot}}}{Z_{\rm tot}}$ $Z_{\rm tot} = \int dS dB\, e^{-\beta H_{\rm tot}}$

- equilibrium state for S: $p_{\rm S}^{\rm eq} = \int dB\, p_{\rm tot}^{\rm eq} = \dfrac{e^{-\beta H_{\rm S}} \int dB\, e^{-\beta H_{\rm I}} e^{-\beta H_{\rm B}}/Z_{\rm B}}{Z_{\rm tot}/Z_{\rm B}} = \dfrac{e^{-\beta \mathscr{H}_{\rm eff}}}{Z_{\mathscr{H}_{\rm eff}}}$

$$Z_{\rm B} = \int dB\, e^{-\beta H_{\rm B}}$$

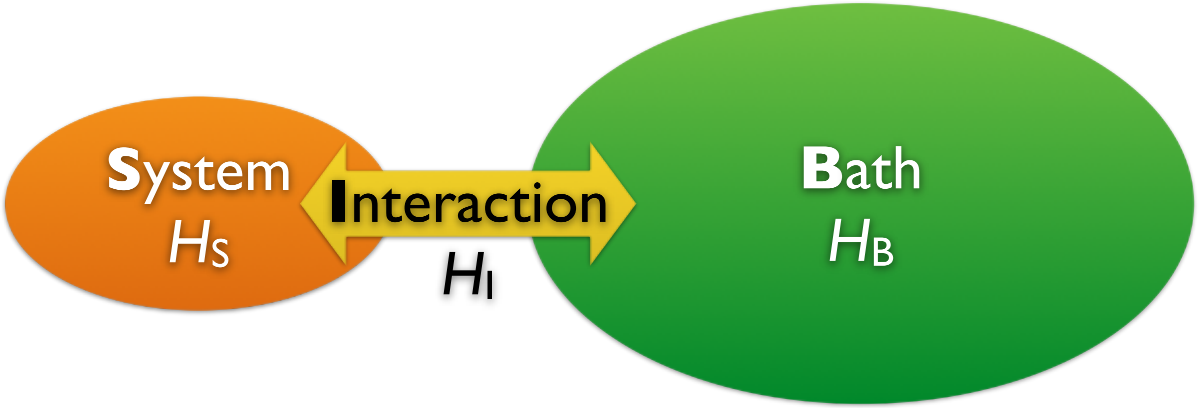
mean-force Hamiltonian: $\mathscr{H}_{\rm eff} \equiv H_{\rm S} + \Delta$ $\Delta \equiv -\beta^{-1} \ln \langle e^{-\beta H_{\rm I}} \rangle_{\rm B}$

$$Z_{\mathscr{H}_{\rm eff}} \equiv \int dS\, e^{-\beta \mathscr{H}_{\rm eff}} = Z_{\rm tot}/Z_{\rm B} \qquad \langle \cdots \rangle_{\rm B} = \int dB \cdots e^{-\beta H_{\rm B}}/Z_{\rm B}$$

Weak vs. Strong Coupling

Total Hamiltonian

$$H_{\rm tot} = H_{\rm S} + H_{\rm I} + H_{\rm B}$$



- equilibrium state (Langevin eq.): $\rho^{\rm eq} = \dfrac{e^{-\beta H_{\rm S}}}{Z_{\rm S}}$ ($H_{\rm S}$ only) $Z_{\rm S} = \int dS\; e^{-\beta H_{\rm S}}$

- equilibrium state for S+B: $p^{\rm eq}_{\rm tot} = \dfrac{e^{-\beta H_{\rm tot}}}{Z_{\rm tot}}$ $Z_{\rm tot} = \int dSdB\; e^{-\beta H_{\rm tot}}$

- equilibrium state for S: $p^{\rm eq}_{\rm S} = \int dB\; p^{\rm eq}_{\rm tot} = \dfrac{e^{-\beta H_{\rm S}} \int dB\; e^{-\beta H_{\rm I}} e^{-\beta H_{\rm B}} / Z_{\rm B}}{Z_{\rm tot}/Z_{\rm B}} = \dfrac{e^{-\beta \mathscr{H}_{\rm eff}}}{Z_{\mathscr{H}_{\rm eff}}}$

mean-force Hamiltonian: $\mathscr{H}_{\rm eff} \equiv H_{\rm S} + \Delta$ $\Delta \equiv -\beta^{-1} \ln \langle e^{-\beta H_{\rm I}} \rangle_{\rm B}$

mean-force potential: coupling effect

- weak-coupling limit: $\lim_{|H_{\rm I}| \to 0} p^{\rm eq}_{\rm S} = \rho^{\rm eq}$ $\longrightarrow$ Langevin eq. regarded as weak-coupling description

Main Questions and Results of This Study

- Conventional Langevin equation

  : $m\dot{v} = -\partial_x U(x) - \gamma v + \xi$

  $\rightarrow$ not proper to investigate strong coupling systems

  $\rightarrow$ major obstacle to explore and establish stochastic thermodynamics for strong-coupling systems

1. Is there an SDE to capture the nature of S-B interaction?

   $\rightarrow$ we develop the SDE for arbitrary H_I under the assumption of time-scale separation (bath relaxes much faster than system)

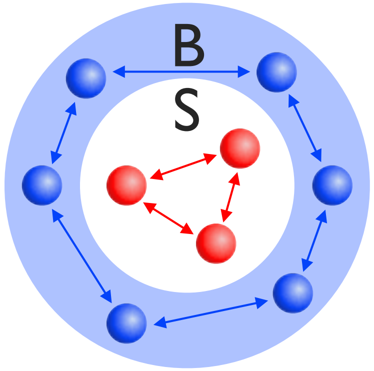
   : $m\dot{v} = -\partial_x U(x) - \partial_x \Delta(x) - G(x)v + \xi$ $\quad \langle \xi(t)\xi(t')\rangle = 2k_\mathrm{B} G(x) T\delta(t-t')$

2. Is the conventional Langevin equation weak-coupling description?

   - derivation from Caldeira-Leggett model: not weak-coupling limit

   $\rightarrow$ two conditions leading to conventional Langevin derived from our SDE

Setup



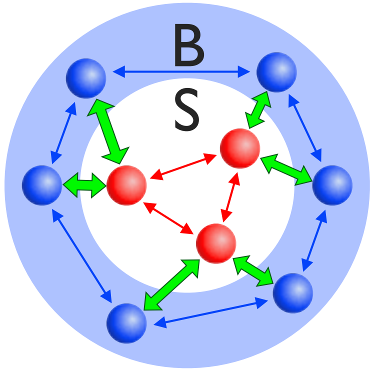
$$\mathsf{S} : \boldsymbol{v}(t) = \dot{\boldsymbol{x}}(t) \qquad \boldsymbol{x} = (x_1, x_2, \cdots, x_N)$$

$$m\dot{\boldsymbol{v}}(t) = \underbrace{\boldsymbol{f}(\boldsymbol{x}(t), t)}_{\text{interaction btw S + external force}}$$

$$\mathsf{B} : \tilde{\boldsymbol{v}}(t) = \dot{\tilde{\boldsymbol{x}}}(t) \qquad \tilde{\boldsymbol{x}} = (\tilde{x}_1, \tilde{x}_2, \cdots, \tilde{x}_{\tilde{N}})$$

$$\tilde{m}\dot{\tilde{\boldsymbol{v}}}(t) = \underbrace{-\nabla_{\tilde{\boldsymbol{x}}}\tilde{\Phi}_{\mathrm{I}}(\tilde{\boldsymbol{x}}(t))}_{\text{interaction btw B}}$$

Setup



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B : $\tilde{\boldsymbol{v}}(t) = \dot{\tilde{\boldsymbol{x}}}(t)$ $\quad\quad$ $\tilde{\boldsymbol{x}} = (\tilde{x}_1, \tilde{x}_2, \cdots, \tilde{x}_{\tilde{N}})$

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$$V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \equiv H_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) + \tilde{\Phi}(\tilde{\boldsymbol{x}})$$

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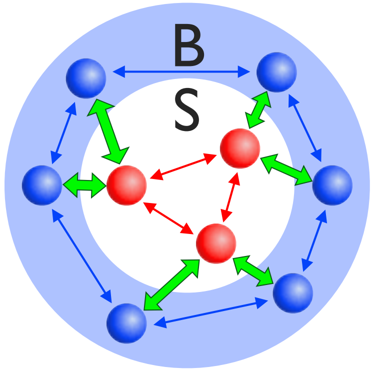

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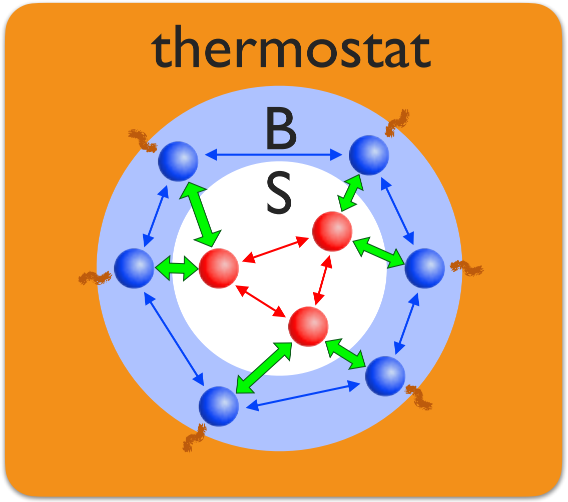

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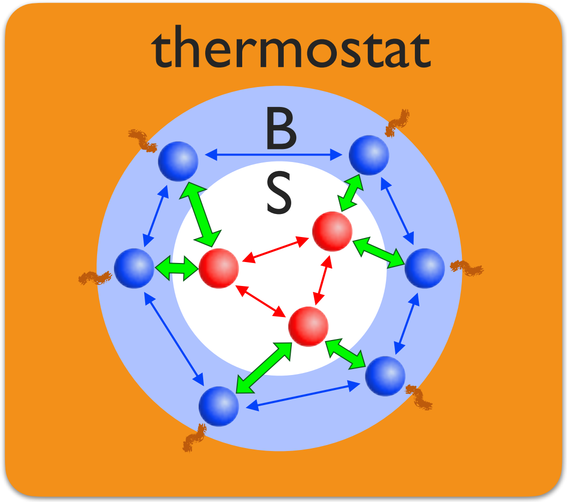
Derivation of SDE for System: Time-Scale Separation



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1. $\tilde{v}$ relaxes much faster than $\tilde{x}$ (small $\tilde{m}/\tilde{\gamma}$)

: underdamped eq. of B $\rightarrow$ overdamped eq. of B

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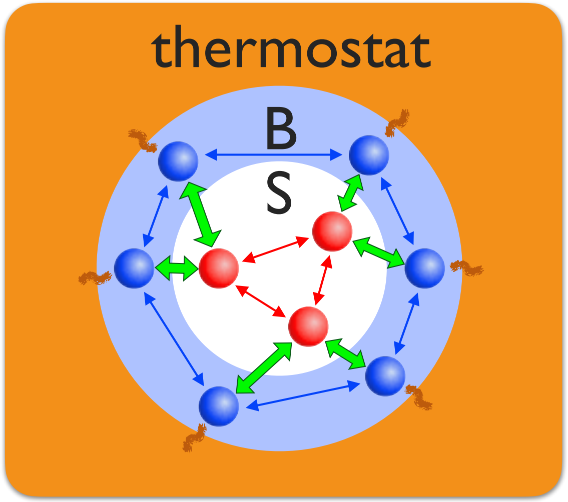

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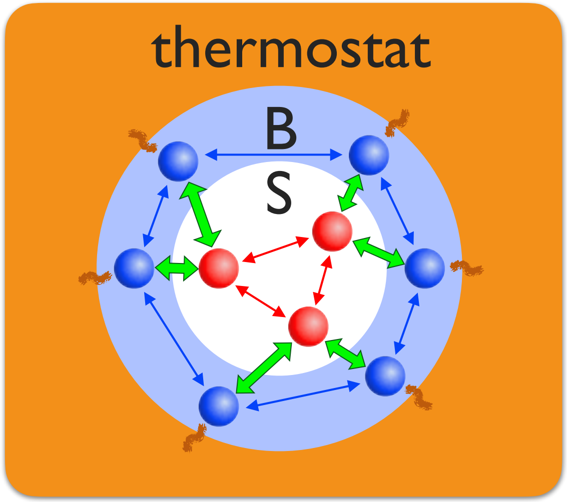

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$$V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \equiv H_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) + \tilde{\Phi}(\tilde{\boldsymbol{x}})$$

2. $\tilde{x}$ relaxes much faster than v, x (small $\tilde{\gamma}$ limit) : adiabatic elimination of $\tilde{x}$

$$\dot{P}(\boldsymbol{x}, \boldsymbol{v}, \tilde{\boldsymbol{x}}, t) = \left(\mathscr{L} + \frac{1}{\tilde{\gamma}}\tilde{\mathscr{L}}\right) P(\boldsymbol{x}, \boldsymbol{v}, \tilde{\boldsymbol{x}}, t)$$

$$\mathscr{L} = -\nabla_x^{\mathrm{T}} \boldsymbol{v} - \frac{1}{m}\nabla_v^{\mathrm{T}}\left[\boldsymbol{f}(\boldsymbol{x}, t) - \{\nabla_x V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}})\}\right]$$

$$\tilde{\mathscr{L}} = \nabla_{\tilde{x}}^{\mathrm{T}}\left[\{\nabla_{\tilde{x}} V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}})\} + T\nabla_{\tilde{x}}\right]$$

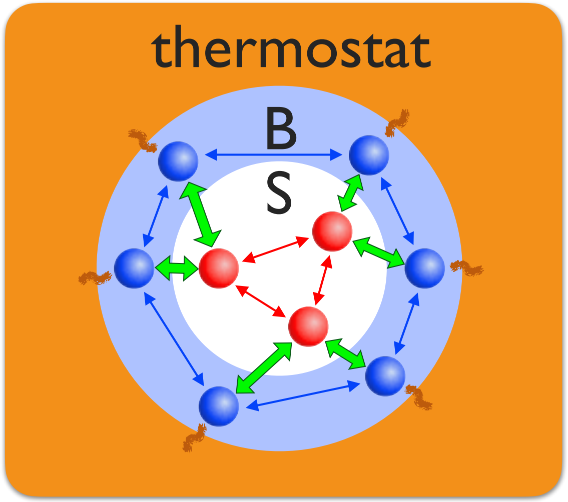
$\rightarrow$ small $\tilde{\gamma}$ expansion and keeping up to $\tilde{\gamma}$ order

$$P(\boldsymbol{x}, \boldsymbol{v}, \tilde{\boldsymbol{x}}, t) = \sum_k C_k(\boldsymbol{x}, \boldsymbol{v}, t)\varphi_k(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x})$$

$$\tilde{\mathscr{L}}\underbrace{\varphi_k(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x})}_{\text{eigenfunction}} = -\underbrace{\lambda_k}_{\text{eigenvalue}}\varphi_k(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x})$$

$$\varphi_0(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x}) = \frac{e^{-\beta V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}})}}{Z_{\mathrm{I}}(\boldsymbol{x})} \qquad \lambda_0 = 0$$

Derivation of SDE for System: Time-Scale Separation



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$$\dot{C}_0(\boldsymbol{x}, \boldsymbol{v}, t) = \Big(\mathscr{F}_{0,0} + \tilde{\gamma}\sum_{k\geq 1} \frac{\mathscr{F}_{0,k}\mathscr{F}_{k,0}}{\lambda_k}\Big) C_0(\boldsymbol{x}, \boldsymbol{v}, t) \qquad C_0(\boldsymbol{x}, \boldsymbol{v}, t) = \int d\tilde{\boldsymbol{x}} P(\boldsymbol{x}, \boldsymbol{v}, \tilde{\boldsymbol{x}}, t)$$

marginal distribution

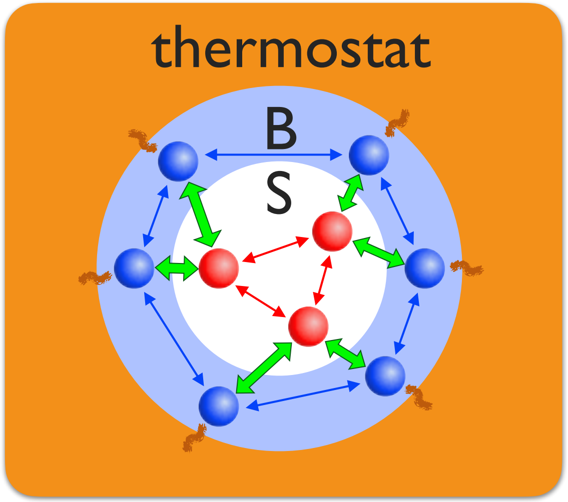
→ small $\tilde{\gamma}$ expansion and keeping up to $\tilde{\gamma}$ order

$$P(\boldsymbol{x}, \boldsymbol{v}, \tilde{\boldsymbol{x}}, t) = \sum_k C_k(\boldsymbol{x}, \boldsymbol{v}, t)\varphi_k(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x}) \qquad \tilde{\mathscr{L}}\varphi_k(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x}) = -\lambda_k \varphi_k(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x})$$

eigenfunction eigenvalue

$$\varphi_0(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x}) = \frac{e^{-\beta V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}})}}{Z_{\mathrm{I}}(\boldsymbol{x})} \qquad \lambda_0 = 0$$

Derivation of SDE for System: Time-Scale Separation



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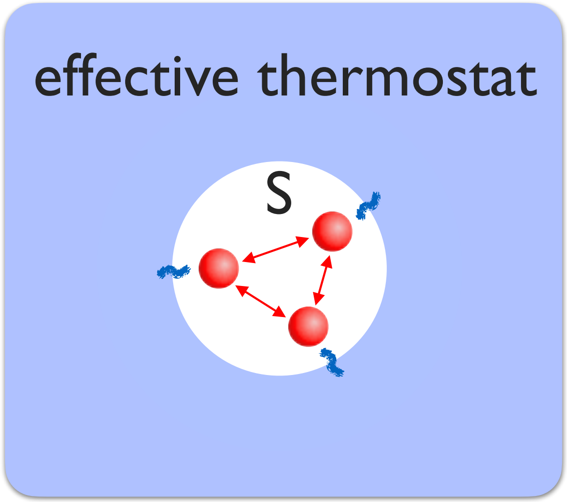
$$= \Bigg[\underbrace{-\nabla_x^{\mathrm{T}} \boldsymbol{v} - \frac{1}{m}\nabla_v^{\mathrm{T}}\big[\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{v}, t) - \{\nabla_x \Delta(\boldsymbol{x})\}\big]}_{\text{deterministic part}} + \underbrace{\frac{1}{m}\nabla_v^{\mathrm{T}} \mathrm{G}(\boldsymbol{x})\Big(\boldsymbol{v} + \frac{T}{m}\nabla_v\Big)}_{\text{effective bath influence}}\Bigg] C_0(\boldsymbol{x}, \boldsymbol{v}, t)$$

effective SDE

$$: \boldsymbol{v}(t) = \dot{\boldsymbol{x}}(t) \qquad m\dot{\boldsymbol{v}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), t) - \nabla_x \Delta(\boldsymbol{x}(t)) - \mathrm{G}(\boldsymbol{x}(t))\, \boldsymbol{v}(t) + \boldsymbol{\xi}(t)$$

$$\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^{\mathrm{T}}(t')\rangle = 2T\mathrm{G}(\boldsymbol{x}(t))\delta(t - t')$$

Derivation of SDE for System: Time-Scale Separation



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1. SDE for a system with arbitrary interaction (T unchanged)

2. Mean force is included in SDE.

$$\Delta(\boldsymbol{x}) = -T \ln \int d\tilde{\boldsymbol{x}}\ e^{-\beta V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}})} + T \ln Z_{\tilde{\Phi}} \qquad Z_{\tilde{\Phi}} = \int d\tilde{\boldsymbol{x}} e^{-\beta \tilde{\Phi}(\tilde{\boldsymbol{x}})}$$

when $\boldsymbol{f}(\boldsymbol{x}, t) = -\nabla_{\boldsymbol{x}} U(\boldsymbol{x}) \to$ steady state: $p_{\mathrm{S}}^{\mathrm{eq}}(\boldsymbol{x}, \boldsymbol{v}) = \dfrac{e^{-\beta \mathscr{H}_{\mathrm{eff}}}}{Z_{\mathscr{H}_{\mathrm{eff}}}}$

$$\mathscr{H}_{\mathrm{eff}} = H_{\mathrm{S}} + \Delta$$

$$H_{\mathrm{S}} = U(\boldsymbol{x}) + \frac{1}{2} m \boldsymbol{v}^2$$

3. Dissipation matrix $\mathsf{G}(\boldsymbol{x})$

$$\mathsf{G}_{n,m}(\boldsymbol{x}) = \frac{1}{T} \int_0^\infty dt\ C_{\partial_{x_n} V_{\mathrm{I}}, \partial_{x_m} V_{\mathrm{I}}}(t \,|\, \boldsymbol{x})$$

$$C_{h,g}(t \,|\, \boldsymbol{x}) \equiv \langle \delta h(\boldsymbol{x}, \tilde{\boldsymbol{x}}(t)) \delta g(\boldsymbol{x}, \tilde{\boldsymbol{x}}(0)) \rangle_{\mathrm{b}}^{\mathrm{eq}}$$

$$\delta h(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = h(\boldsymbol{x}, \tilde{\boldsymbol{x}}) - \langle h(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \rangle_{\mathrm{b}}^{\mathrm{eq}}$$

$$\langle \cdots \rangle_{\mathrm{b}}^{\mathrm{eq}} = \int d\tilde{\boldsymbol{x}} \cdots \varphi_0(\tilde{\boldsymbol{x}} \,|\, \boldsymbol{x})$$

Main Questions and Results of This Study

1. Is there an SDE to capture the nature of S-B interaction?

$: \boldsymbol{v}(t) = \dot{\boldsymbol{x}}(t) \qquad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^{\mathrm{T}}(t') \rangle = 2T\mathsf{G}(\boldsymbol{x}(t))\delta(t-t')$

$$m\dot{\boldsymbol{v}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), t) - \nabla_{\boldsymbol{x}}\Delta(\boldsymbol{x}(t)) - \mathsf{G}(\boldsymbol{x}(t))\,\boldsymbol{v}(t) + \boldsymbol{\xi}(t)$$

$$\boxed{\Delta(\boldsymbol{x}) = -T\ln\int d\tilde{\boldsymbol{x}}\; e^{-\beta V_{\mathrm{I}}(\boldsymbol{x},\tilde{\boldsymbol{x}})} + T\ln Z_{\tilde{\Phi}} \qquad \mathsf{G}_{n,m}(\boldsymbol{x}) = \frac{1}{T}\int_0^\infty dt\; C_{\partial_{x_n}V_{\mathrm{I}},\partial_{x_m}V_{\mathrm{I}}}(t\,|\,\boldsymbol{x})}$$

→ Information on S-B interaction is included in $\Delta(\boldsymbol{x})$ and $\mathsf{G}(\boldsymbol{x})$.

2. Is the conventional Langevin equation weak-coupling description?

conventional Langevin: $m\dot{\boldsymbol{v}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), t) - \mathsf{G}\boldsymbol{v}(t) + \boldsymbol{\xi}(t)$

$$\lim_{|H_{\mathrm{I}}|\to 0} \Delta(\boldsymbol{x}) = 0 \qquad \lim_{|H_{\mathrm{I}}|\to 0} \mathsf{G}_{n,m}(\boldsymbol{x}) = 0 \quad \Rightarrow \quad \cancel{\Rightarrow}\; m\dot{\boldsymbol{v}}(t) = \boldsymbol{f}(\boldsymbol{x}(t), t)$$

(isolation, deterministic)

$\nabla_{\boldsymbol{x}}\Delta(\boldsymbol{x}) = 0$: mean-force vanishes

$\mathsf{G}_{n,m}(\boldsymbol{x}) = \gamma_n\delta_{n,m}$: independet of V_{I}

Main Questions and Results of This Study

1. Is there an SDE to capture the nature of S-B interaction?

$$: \boldsymbol{v}(t) = \dot{\boldsymbol{x}}(t) \qquad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^{\mathrm{T}}(t')\rangle = 2T\mathsf{G}(\boldsymbol{x}(t))\delta(t-t')$$

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$$\lim_{|H_{\mathrm{I}}|\to 0} \Delta(\boldsymbol{x}) = 0 \qquad \lim_{|H_{\mathrm{I}}|\to 0} \mathsf{G}_{n,m}(\boldsymbol{x}) = 0 \quad \Rightarrow \quad \cancel{\neq}\; m\dot{\boldsymbol{v}}(t) = \boldsymbol{f}(\boldsymbol{x}(t),t)$$

(isolation, deterministic)

→ Conventional Langevin is not a weak-coupling description.

- Many experiments are well described by conventional Langevin.

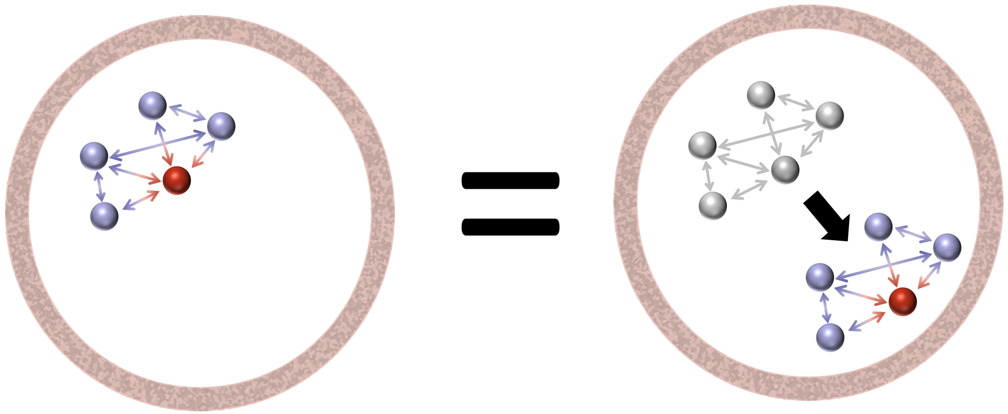
- there exists another mechanism leading to conventional Langevin.

Two Conditions for Conventional Langevin Equation

1. Translational invariance of interaction potential

$$V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \equiv H_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) + \tilde{\Phi}(\tilde{\boldsymbol{x}})$$

$$= V_{\mathrm{I}}(x_1, \cdots, x_N, \tilde{x}_1, \cdots, \tilde{x}_{\tilde{N}}) = V_{\mathrm{I}}(x_1 + a, \cdots, x_N + a, \tilde{x}_1 + a, \cdots, \tilde{x}_{\tilde{N}} + a)$$

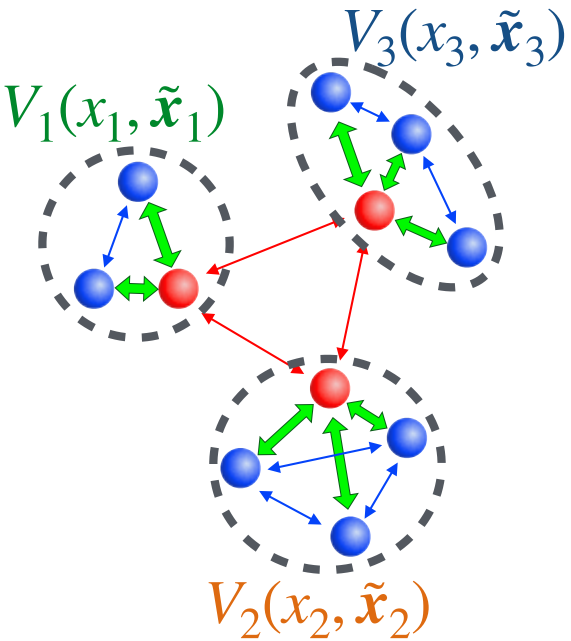


: valid for experiments implemented in the bulk region (far from boundary) of their environment

Two Conditions for Conventional Langevin Equation

2. Mutual independence of baths

(*N* system particles)



1) entire bath can be partitioned into *N* mutually independent subbaths

- no direct interaction between different subbaths

2) each subbath exclusively interacts with one of the system particles

- each bath particle cannot interact with multiple system particles simultaneously)

$\rightarrow$ each system particle has its own subbath.

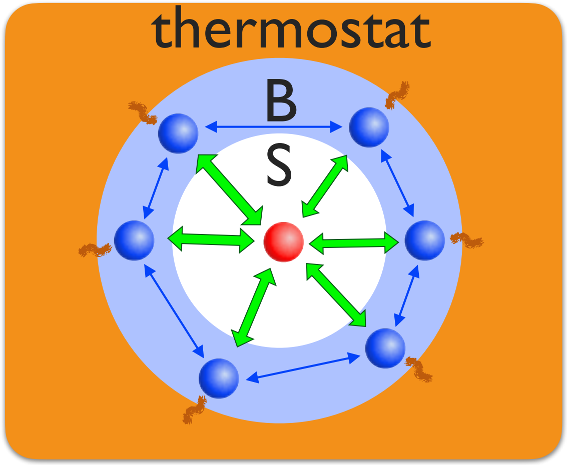
- mathematical expression for mutual independence

$$V_{\mathrm{I}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \sum_{n=1}^{N} V_n(x_n, \tilde{\boldsymbol{x}}_n)$$

- always hold for one-particle system

- but not for multiparticle system

Two Conditions for Conventional Langevin Equation



Example 1. One-particle system

1) Mutual independence is satisfied.

2) Assume translational invariance.

$$V_{\rm I}(\boldsymbol{x},\tilde{\boldsymbol{x}}) \equiv H_{\rm I}(\boldsymbol{x},\tilde{\boldsymbol{x}}) + \tilde{\Phi}(\tilde{\boldsymbol{x}})$$

$$= V_{\rm I}(x_1,\tilde{x}_1,\cdots,\tilde{x}_{\tilde{N}}) = V_{\rm I}(x_1+a,\tilde{x}_1+a,\cdots,\tilde{x}_{\tilde{N}}+a) \qquad (a = -x_1)$$

$$= V_{\rm I}(0,\tilde{X}_1,\cdots,\tilde{X}_{\tilde{N}}) \qquad (\tilde{X}_i \equiv \tilde{x}_i - x_1)$$

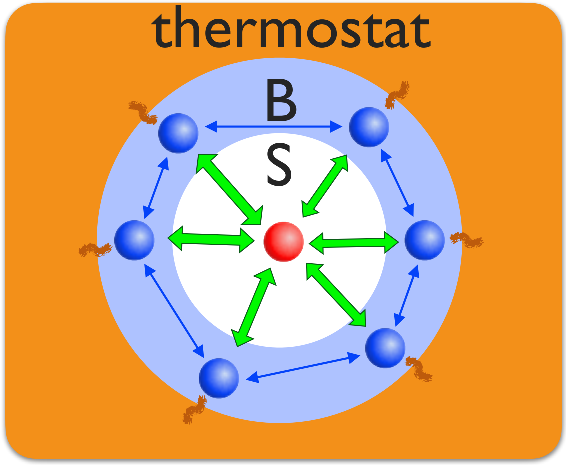
- mean-force term

$$\Delta(x_1) = -T\ln\int d\tilde{\boldsymbol{x}}\ e^{-\beta V_{\rm I}(x_1,\tilde{\boldsymbol{x}})} + T\ln Z_{\tilde{\Phi}} \qquad Z_{\tilde{\Phi}} = \int d\tilde{\boldsymbol{x}} e^{-\beta\tilde{\Phi}(\tilde{\boldsymbol{x}})}$$

$$= -T\ln\int d\tilde{\boldsymbol{X}}\ e^{-\beta V_{\rm I}(0,\tilde{X})} + T\ln Z_{\tilde{\Phi}} \ \rightarrow\ \text{independent of } x_1$$

$\partial_{x_1}\Delta(\boldsymbol{x}) = 0$: mean-force term vanishes

Two Conditions for Conventional Langevin Equation



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$$= V_{\rm I}(0,\tilde{X}_1,\cdots,\tilde{X}_{\tilde{N}}) \qquad (\tilde{X}_i \equiv \tilde{x}_i - x_1)$$

- mean-force term $\partial_{x_1}\Delta(\boldsymbol{x}) = 0$

- G matrix

$$\mathrm{G}_{1,1}(x_1) = \frac{1}{T}\int_0^\infty dt\ C_{\partial_{x_1}V_{\rm I},\partial_{x_1}V_{\rm I}}(t\,|\,x_1)$$

$$= \frac{1}{T}\sum_{\tilde{n},\tilde{m}}\int_0^\infty dt\ C_{\partial_{\tilde{x}_{\tilde{n}}}V_{\rm I},\partial_{\tilde{x}_{\tilde{m}}}V_{\rm I}}(t\,|\,x_1)$$

$$= \tilde{N}\tilde{\gamma} \equiv \gamma \ \text{: independent of } V_{\rm I}$$

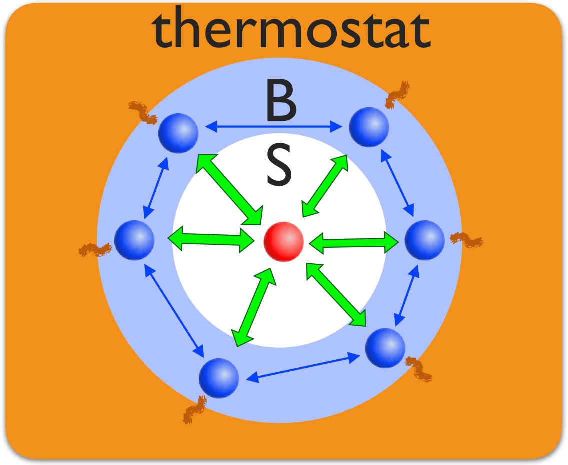
action-reaction law:

$$-\partial_{x_1}V_{\rm I}(x_1,\tilde{\boldsymbol{x}}) - \sum_{\tilde{n}}\partial_{\tilde{x}_{\tilde{n}}}V_{\rm I}(x_1,\tilde{\boldsymbol{x}}) = 0$$

generalized Green-Kubo:

$$\int_0^\infty dt C_{\partial_{\tilde{x}_{\tilde{n}}}V_{\rm I},\partial_{\tilde{x}_{\tilde{m}}}V_{\rm I}}(t\,|\,x_1) = \tilde{\gamma}T\delta_{\tilde{n},\tilde{m}}$$

Two Conditions for Conventional Langevin Equation



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$$= V_{\mathrm{I}}(0,\tilde{X}_1,\cdots,\tilde{X}_{\tilde{N}}) \qquad (\tilde{X}_i \equiv \tilde{x}_i - x_1)$$

- mean-force term $\partial_{x_1}\Delta(\boldsymbol{x}) = 0$

- G matrix γ : independent of V_{I}

$$m\dot{v}_1 = f(x_1,t) - \partial_{x_1}\Delta(x_1) - \mathrm{G}(x_1)v_1 + \xi \qquad \langle \xi(t)\xi^{\mathrm{T}}(t')\rangle = 2T\mathrm{G}(x_1)\delta(t-t')$$

$$\to m\dot{v}_1 = f(x_1,t) - \gamma v_1 + \xi \qquad \langle \xi(t)\xi^{\mathrm{T}}(t')\rangle = 2T\gamma\delta(t-t')$$

Information on V_{I} dissapears (conventional Langevin equation).

→ the reason why one-particle experiment is well fitted by Langevin.

Two Conditions for Conventional Langevin Equation

Example 2. Multi-particle system

1) Assume mutual independence of bath.

2) Assume translational invariance.

- mean-force term : $\Delta = -T \sum_n \ln \int d\tilde{X}_n \, e^{-\beta V_n(\mathbf{0}, \tilde{X}_n)} + T \ln Z_{\tilde{\Phi}} \quad \to \nabla_{\boldsymbol{x}} \Delta = 0$

- G matrix : $\mathrm{G}_{n,m} = \frac{1}{T} \sum_{\tilde{n}_n=1}^{\tilde{N}_n} \sum_{\tilde{n}_m=1}^{\tilde{N}_m} \int_0^\infty dt \; C_{\partial_{\tilde{x}_{\tilde{n}_n}} V_n, \partial_{\tilde{x}_{\tilde{n}_m}} V_m}(t \,|\, x_1) \; = \gamma_n \delta_{n,m} \qquad (\gamma_n \equiv \tilde{N}_n \tilde{\gamma})$

$\to$ diagonal matrix without V_{I} dependence

$$m\dot{\boldsymbol{v}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{v}, t) - \nabla_x \Delta(\boldsymbol{x}) - \mathrm{G}(\boldsymbol{x}) \cdot \boldsymbol{v} + \boldsymbol{\xi} \qquad \langle \boldsymbol{\xi}(t) \boldsymbol{\xi}^{\mathrm{T}}(t') \rangle = 2T\mathrm{G}(\boldsymbol{x}(t))\delta(t - t')$$

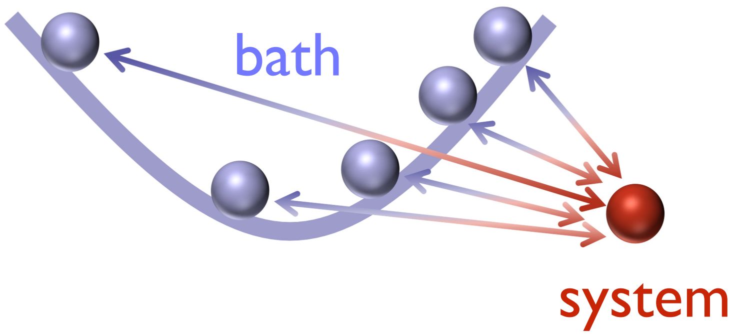
$$\to m\dot{v}_n = f(\boldsymbol{x}, t) - \gamma_n v_n + \xi_n \qquad \langle \xi_n(t) \xi_m^{\mathrm{T}}(t') \rangle = 2T\gamma_n \delta_{nm} \delta(t - t')$$

Information on V_{I} dissapears (conventional Langevin equation).

Numerical Confirmation

ex) Single particle without translational invariance (mutual independence O)

Setup



$$H_{\mathrm{I}}(x_1, \tilde{\boldsymbol{x}}) = \sum_{\tilde{n}} \frac{1}{2} k_{\mathrm{I}} (x_1 - \tilde{x}_{\tilde{n}})^2, \quad \tilde{\Phi}(\tilde{\boldsymbol{x}}) = \frac{1}{2} \tilde{k} \tilde{\boldsymbol{x}}^{\mathrm{T}} \tilde{\boldsymbol{x}}$$

$V_{\mathrm{I}} = H_{\mathrm{I}} + \tilde{\Phi}$: translational invariance is broken

$\tilde{k} = 0$: translational invariance is recovered

SDE: $m\dot{v}_1 = f(x_1, t) - \partial_{x_1} \Delta(x_1) - \mathrm{G}(x_1) v_1 + \xi \qquad \langle \xi(t) \xi^{\mathrm{T}}(t') \rangle = 2T\mathrm{G}(x_1)\delta(t - t')$

$$f(x_1, t) = 0$$

$\partial_{x_1} \Delta(x_1) = k x_1 \qquad k \equiv \tilde{N} k_{\mathrm{I}} \tilde{k} / (k_{\mathrm{I}} + \tilde{k})$

$\mathrm{G}(x_1) = \gamma \qquad \gamma = \tilde{N} \tilde{\gamma} \left[k_{\mathrm{I}} / (k_{\mathrm{I}} + \tilde{k}) \right]^2$

$\xrightarrow{\tilde{k} = 0}$

$\partial_{x_1} \Delta(x_1) = 0$

$\mathrm{G}(x_1) = \tilde{N} \tilde{\gamma}$

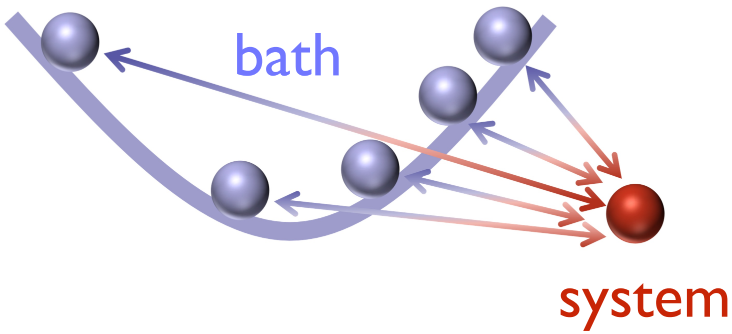
$\rightarrow m\dot{v}_1 = -k x_1 - \gamma v_1 + \sqrt{2\gamma T} \xi_1$

Information on V_{I} dissapears.

Numerical Confirmation

ex) Single particle without translational invariance (mutual independence O)

Setup



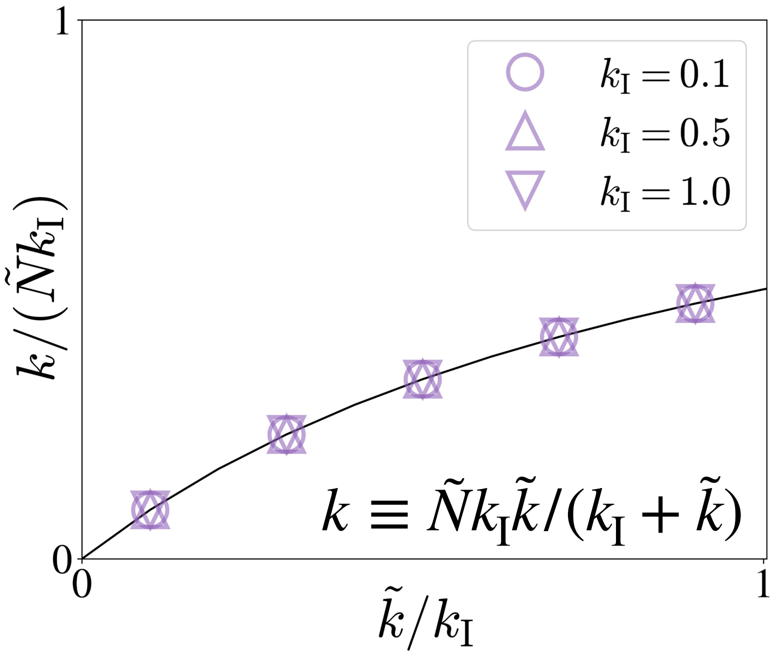
$$H_{\mathrm{I}}(x_1, \tilde{\boldsymbol{x}}) = \sum_{\tilde{n}} \frac{1}{2} k_{\mathrm{I}} (x_1 - \tilde{x}_{\tilde{n}})^2, \quad \tilde{\Phi}(\tilde{\boldsymbol{x}}) = \frac{1}{2} \tilde{k} \tilde{\boldsymbol{x}}^{\mathrm{T}} \tilde{\boldsymbol{x}}$$

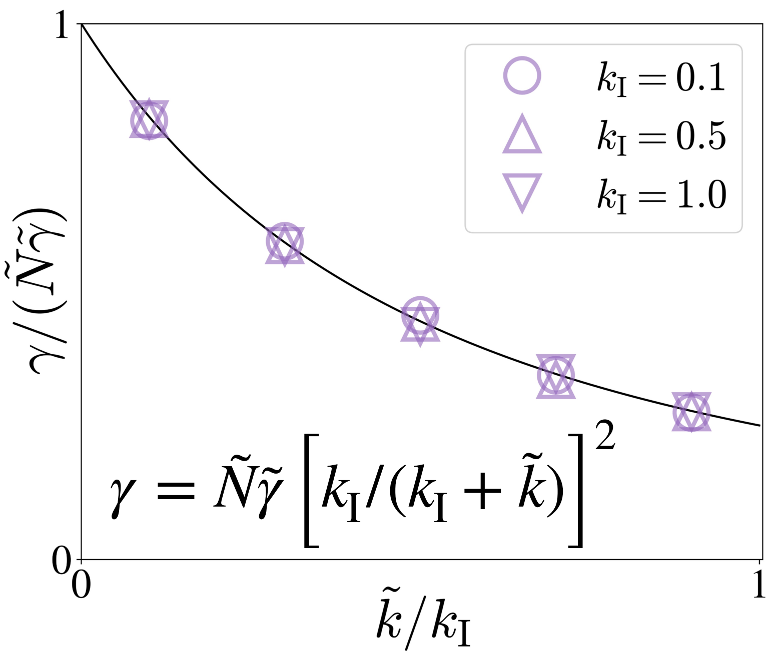
$V_{\mathrm{I}} = H_{\mathrm{I}} + \tilde{\Phi}$: translational invariance is broken

$\tilde{k} = 0$: translational invariance is recovered

SDE: $\rightarrow m\dot{v}_1 = -kx_1 - \gamma v_1 + \sqrt{2\gamma T}\xi_1$

$\tilde{N} = 10^4$, $\tilde{\gamma} = 10^{-2}$, $\tilde{m} = 10^{-4}$, and $m = T = 1$

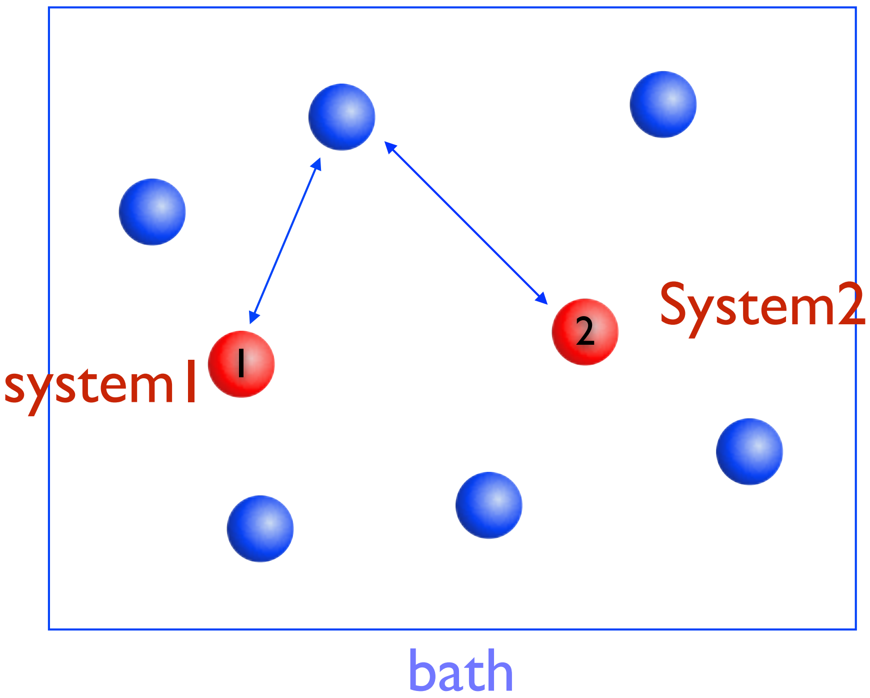




Numerical Confirmation

Effective mutual independence of baths

Real experimental setup: multi-particle system in a single bath



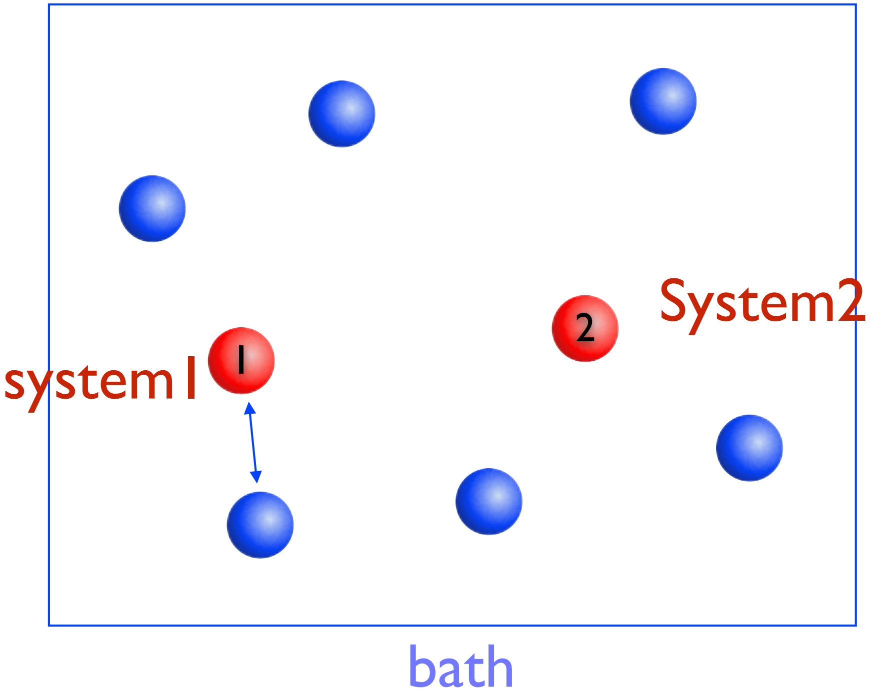
No clear division for mutually independent subbaths

- One bath particle can interact with several system particles simultaneously.

Numerical Confirmation

Effective mutual independence of baths

Real experimental setup: multi-particle system in a single bath



$t = t_1$

No clear division for mutually independent subbaths

- One bath particle can interact with several system particles simultaneously.

- Interaction partner may change over time.

Numerical Confirmation

Effective mutual independence of baths

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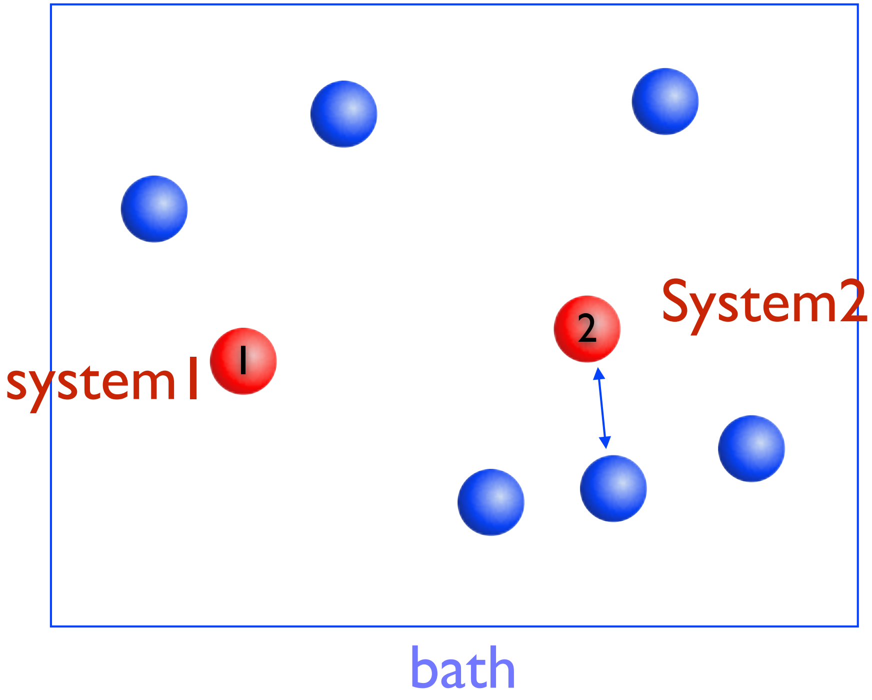


$t = t_2$

No clear division for mutually independent subbaths

- One bath particle can interact with several system particles simultaneously.

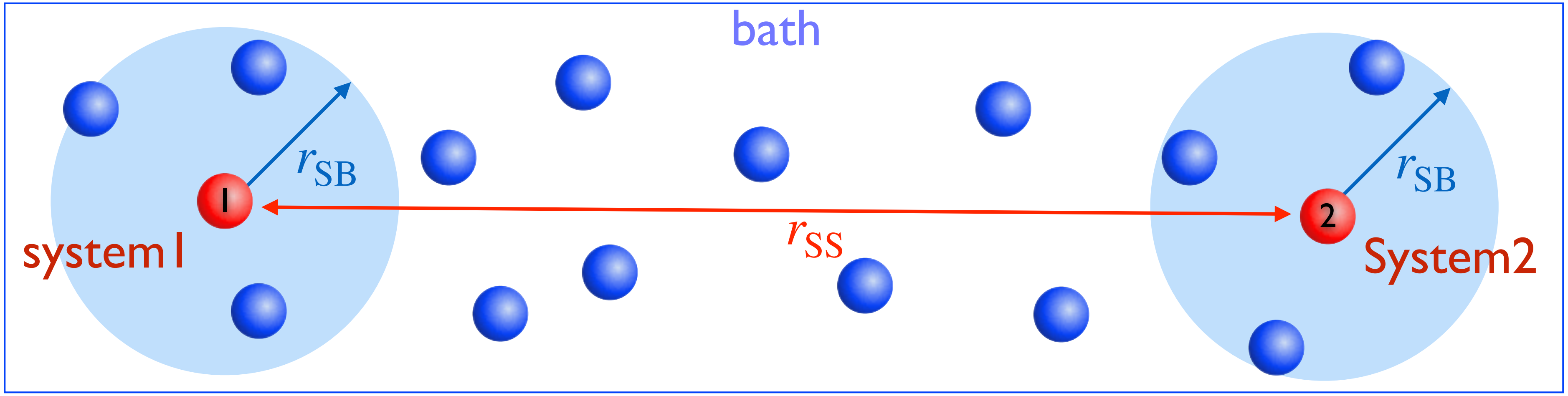
- Interaction partner may change over time.

→ effective mutual independence, instead of strict one

Numerical Confirmation

Effective mutual independence of baths

Effective mutual independence



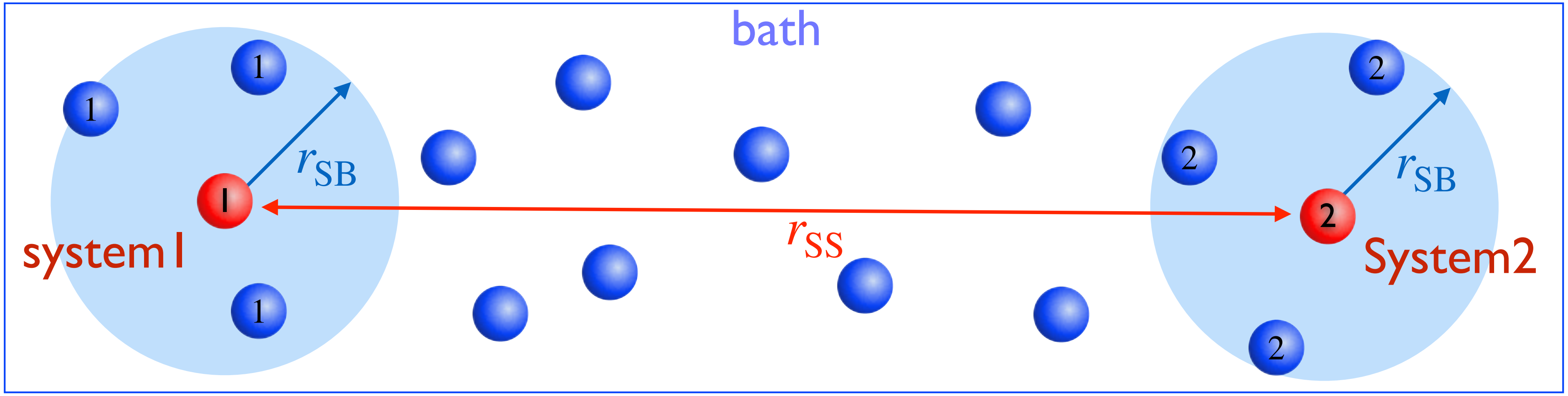
$r_{\rm SB}$: S-B interaction range

$r_{\rm SS}$: S-S distance

Numerical Confirmation

Effective mutual independence of baths

Effective mutual independence



r_{SB} : S-B interaction range

$r_{\mathrm{SB}} \ll r_{\mathrm{SS}}$

r_{SS} : S-S distance

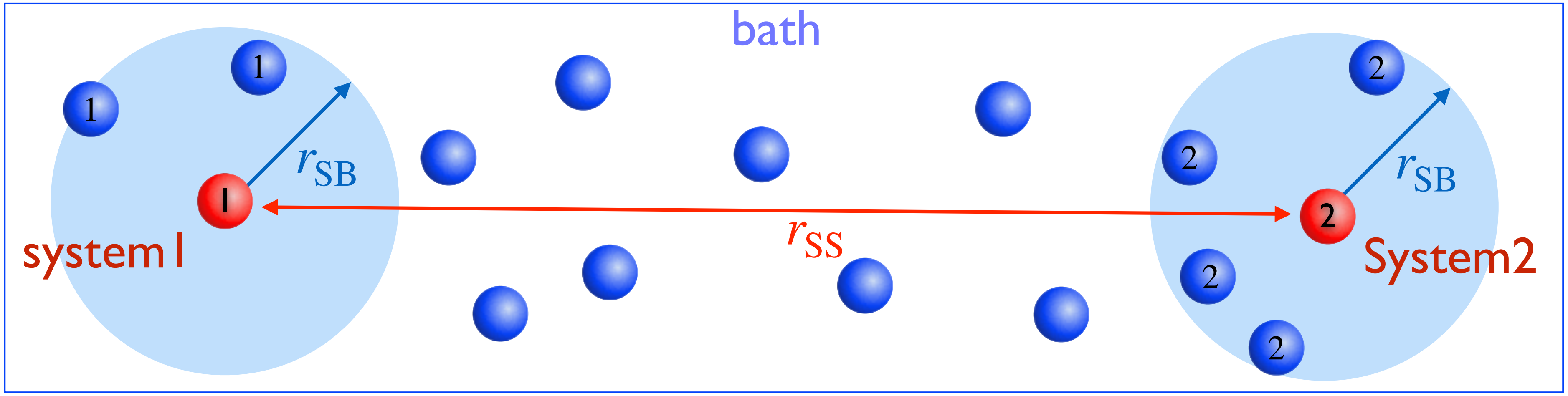
We can construct mutually independent subbaths.

- one bath particle interacts with a single system particle.

Numerical Confirmation

Effective mutual independence of baths

Effective mutual independence



r_{SB} : S-B interaction range

$r_{SB} \ll r_{SS}$

r_{SS} : S-S distance

We can construct mutually independent sabbaths.
- one bath particle interacts with a single system particle.

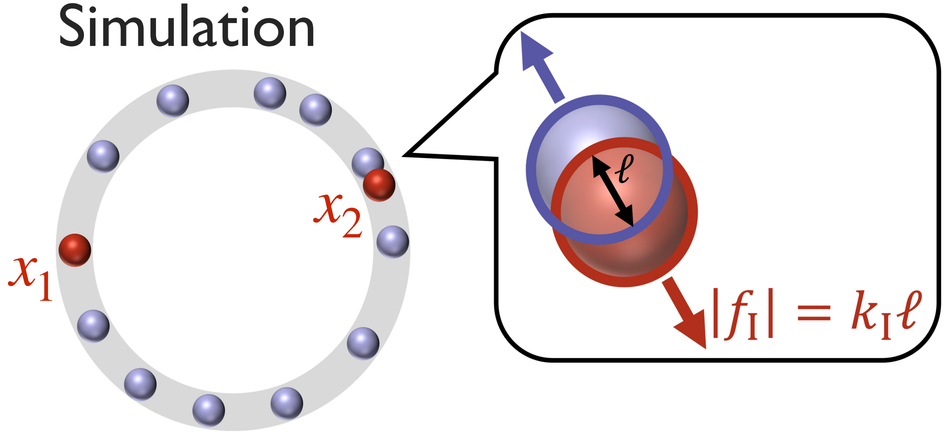
- Though the interaction partner may change over time, memory of past interactions is dissipated and does not affect subsequent S-B interactions.

$\rightarrow$ Effective mutual independence of baths

Numerical Confirmation

Effective mutual independence of baths

Simulation

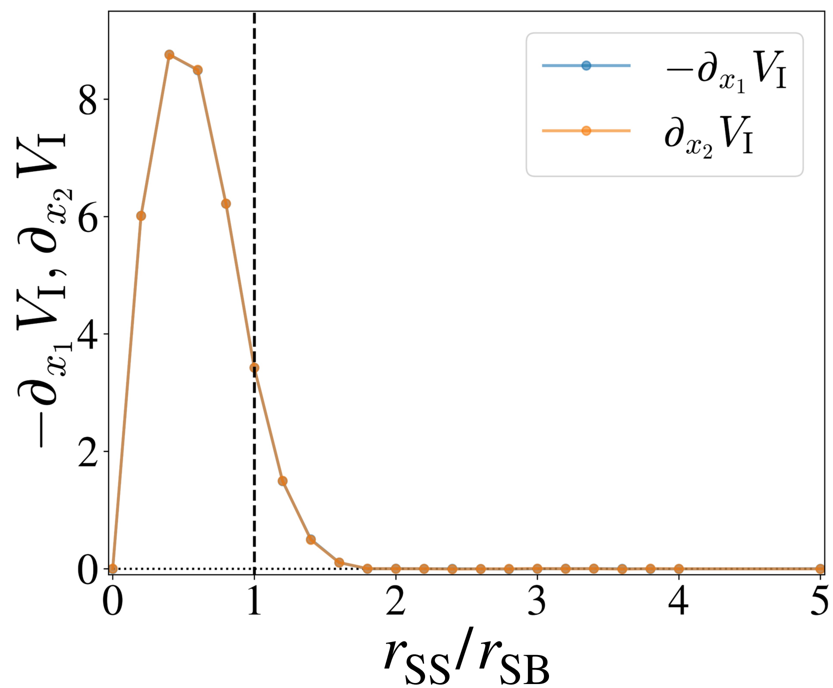


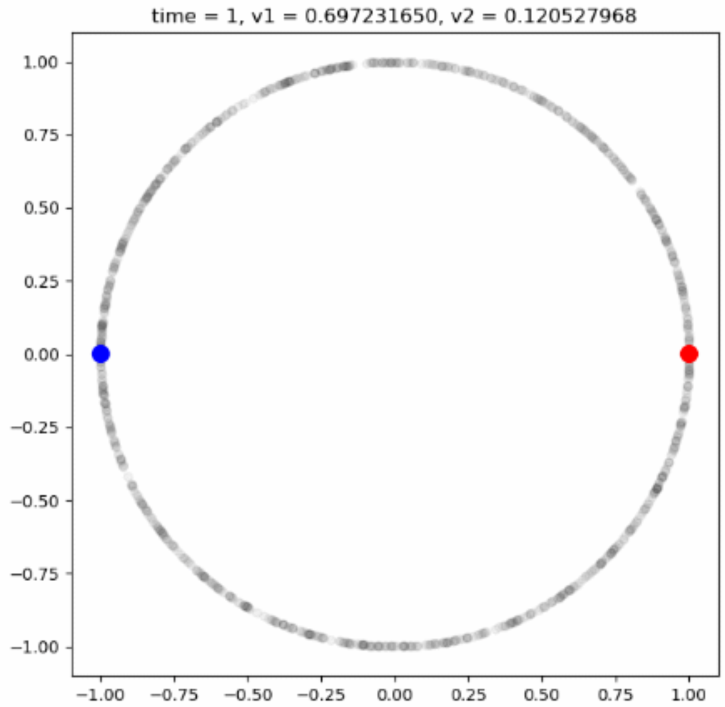
- Two-system particles in 1D ring
- No other potentials exist except for S-B interaction
- S-B overlapping (repulsive) force: $k_\mathrm{I}\ell$

d : particle diameter = r_{SB}

$\tilde{N} = 10^3,\ \tilde{\gamma} = 10^{-2},\ m = 10^{-2},\ T = 10,\ k_\mathrm{I} = 10,\ d = 1,\ L = 100$

mean force





Numerical Confirmation

Effective mutual independence of baths

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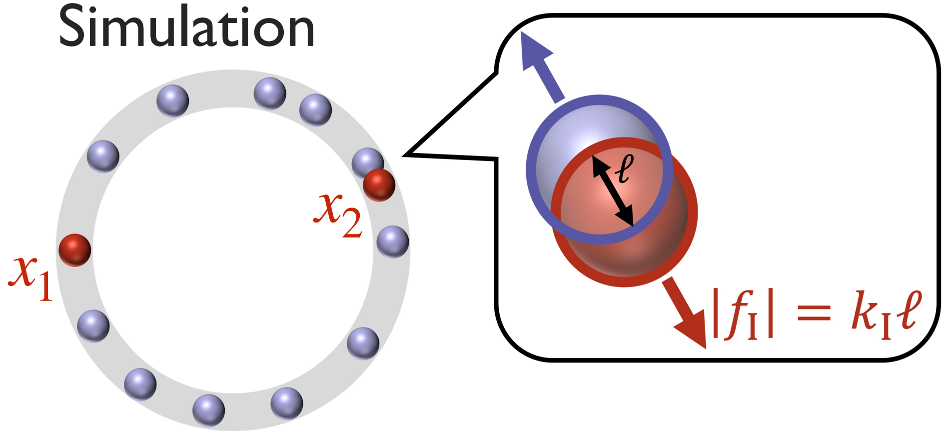

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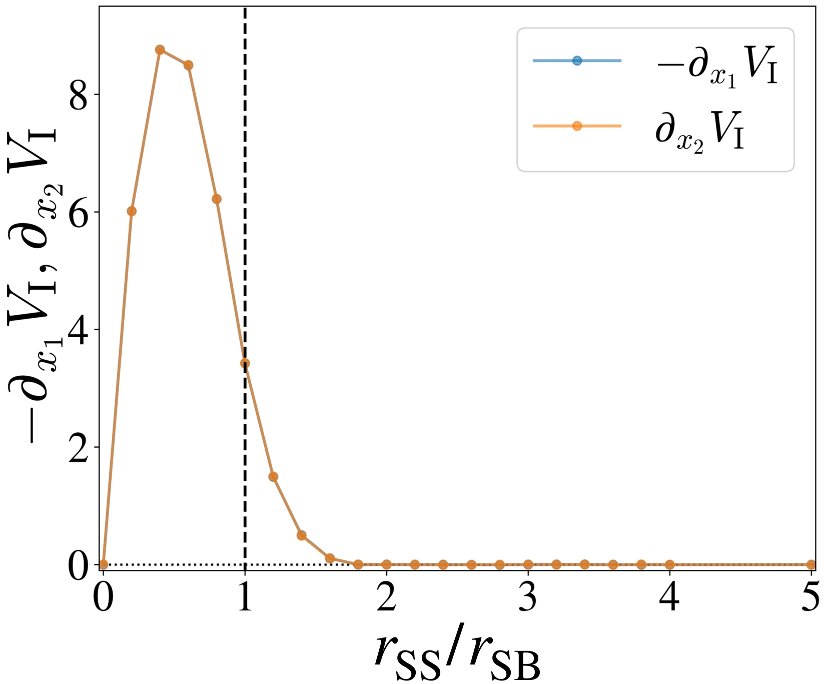
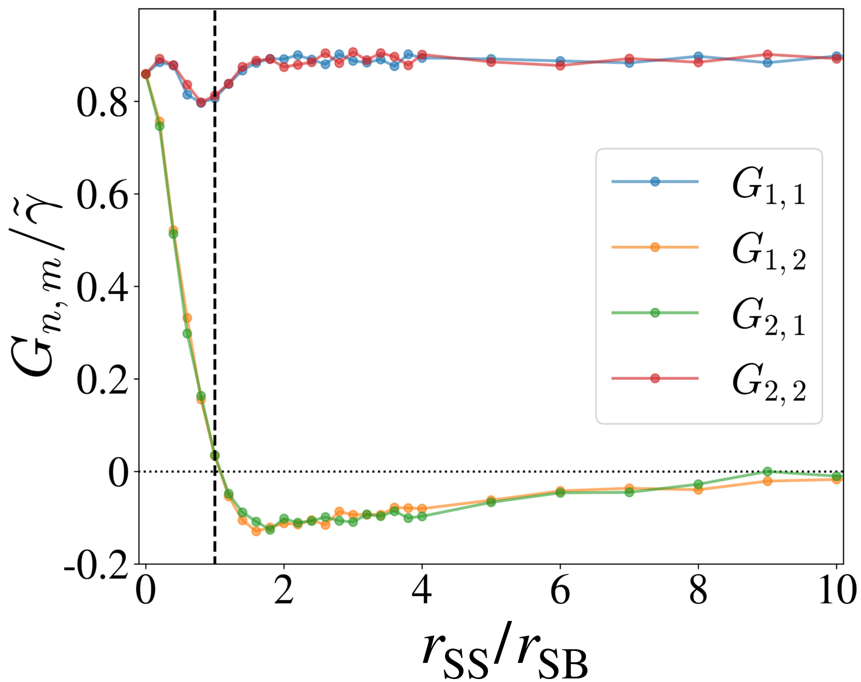


G matrix



Numerical Confirmation

Effective mutual independence of baths

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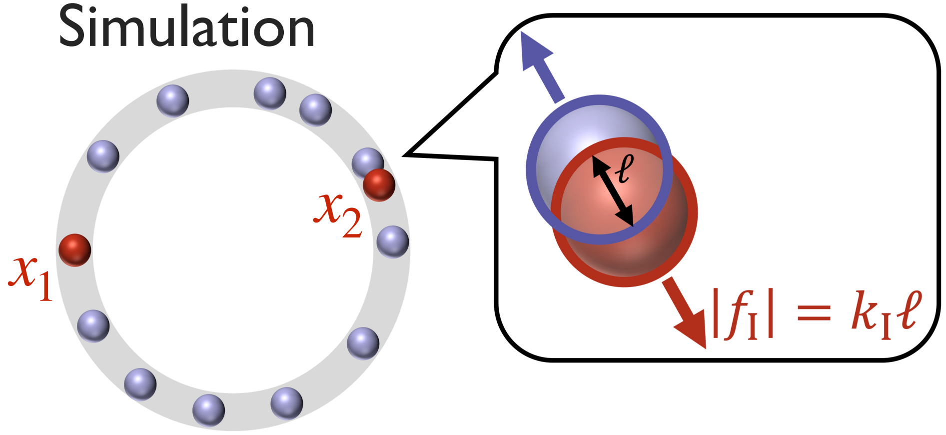

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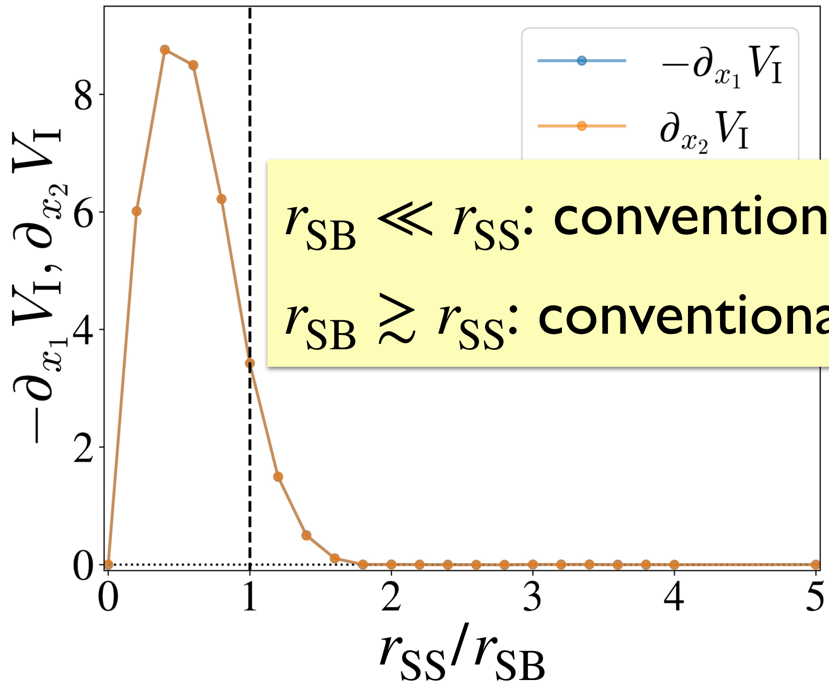

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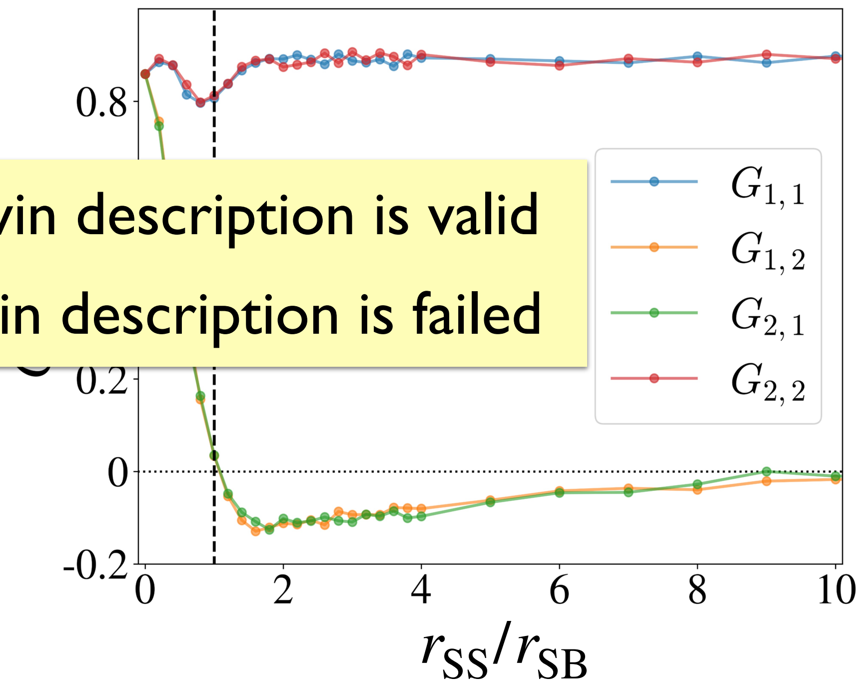

$r_\mathrm{SB} \ll r_\mathrm{SS}$: conventional Langevin description is valid

$r_\mathrm{SB} \gtrsim r_\mathrm{SS}$: conventional Langevin description is failed

Conclusions

1. We developed an SDE to capture the nature of SB interaction, applicable to a system coupled to a bath via arbitrary SB Hamiltonian.

2. Information of SB interaction are included in two terms

   - mean-force term

   - G matrix (damping matrix)

3. We found two physical conditions that can lead to the vanishing of SB interaction effects, even in the case of strong coupling.

   - translational invariance of interaction potential

   - mutual independence of baths

4. With these conditions, our SDE is reduced to conventional Langevin.

5. "Mutual independence" can be effectively satisfied when $r_{\rm SB} \ll r_{\rm SS}$

6. Preprint: arXiv:2311.01098, to appear soon in PRE

in collaboration with Hyunggyu Park (KIAS)

Jong-Min Park (APCTP)