Unveiling the Invisible System-Bath Coupling Dependence in Microscopic System

Jong-Min Park[1] , Hyunggyu Park[2], and Jae Sung Lee[3]

[1]Asia Pacific Center for Theoretical Physics (APCTP)

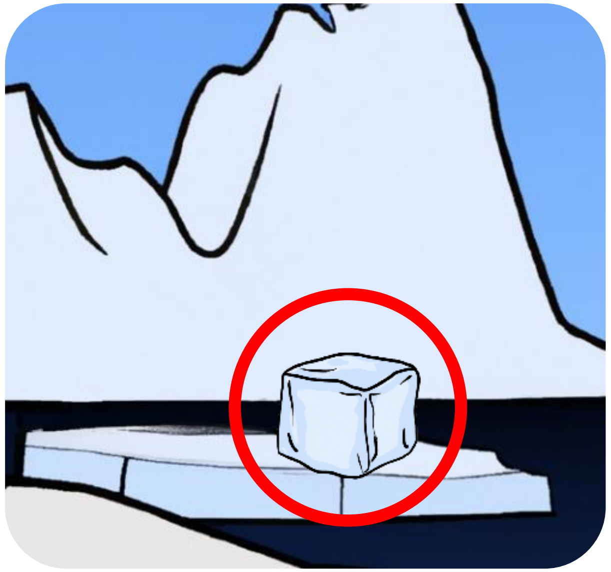
[2]Quantum Universe Center, KIAS

[3]School of Physics, KIAS

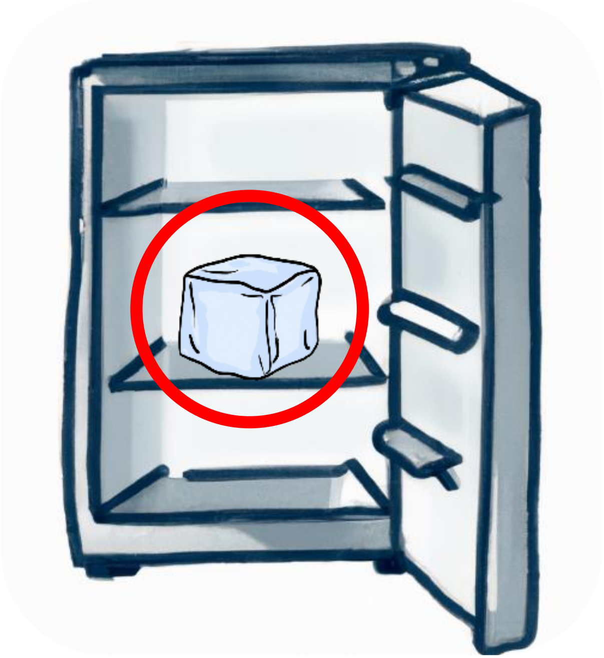
asia pacific center for theoretical physics

KOREA INSTITUTE FOR ADVANCED STUDY

Macroscopic system

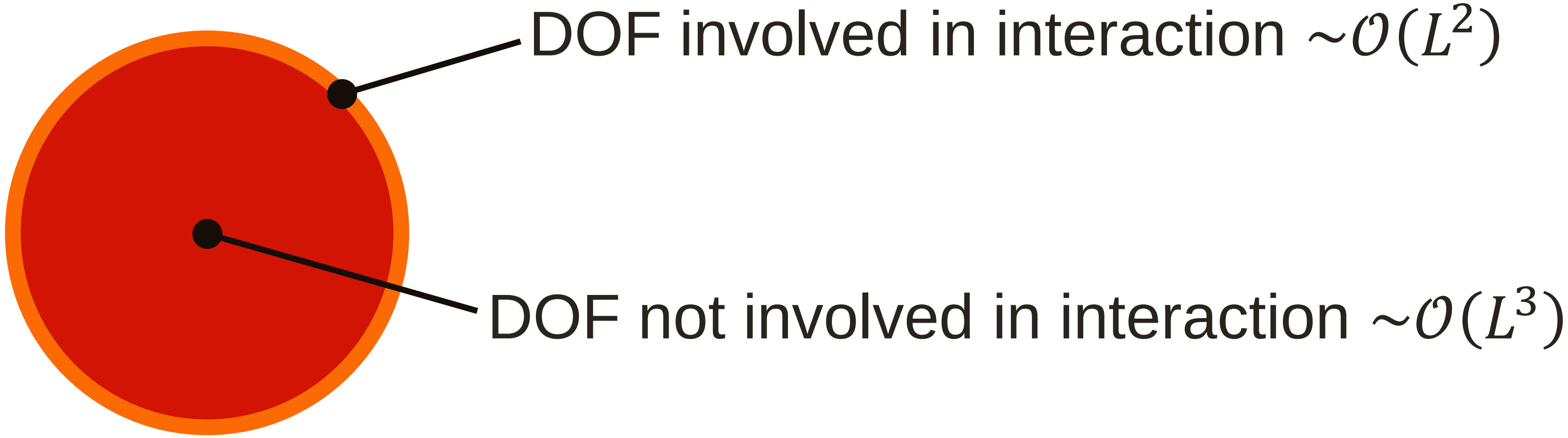


VS.



Weakly coupled systems

Equilibrium state is independent of the specifics of interaction



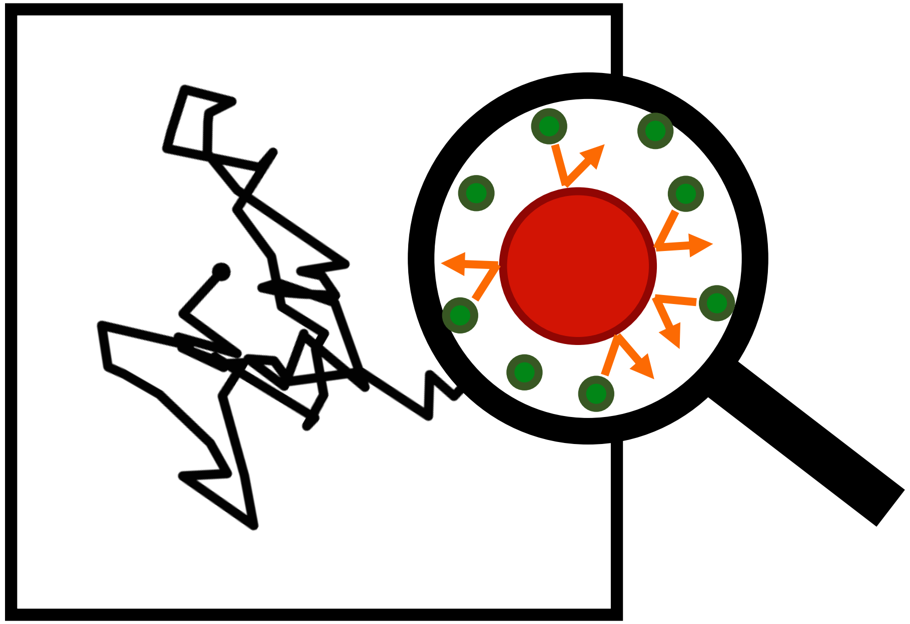
No sign of strong-coupling effects

Microscopic systems

Interaction is comparable

Microscopic systems are expected to be a strongly-coupled systems

free Brownian motion

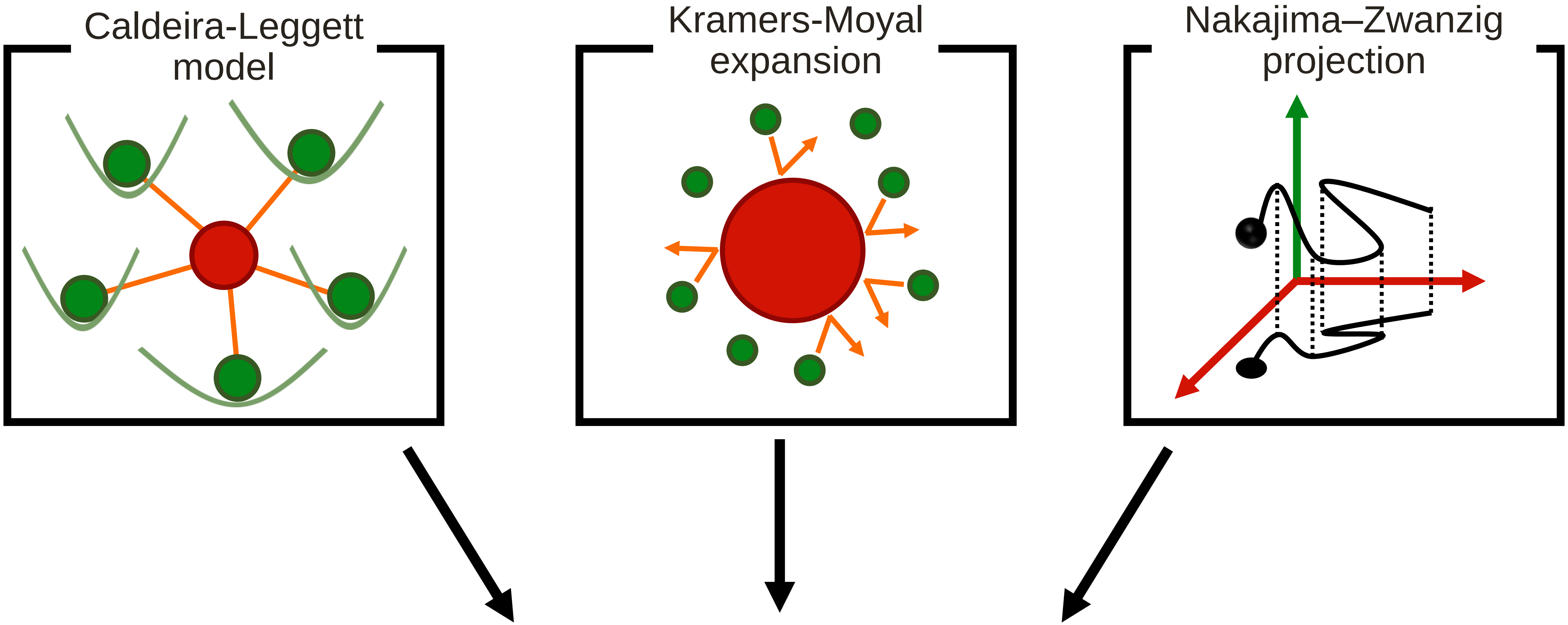


Langevin equation

$$m\dot{v}(t) = -\gamma v(t) + \sqrt{2\gamma T}\xi(t) \qquad (k_B = 1)$$

no strong-coupling effects!

Derivations of Langevin equation



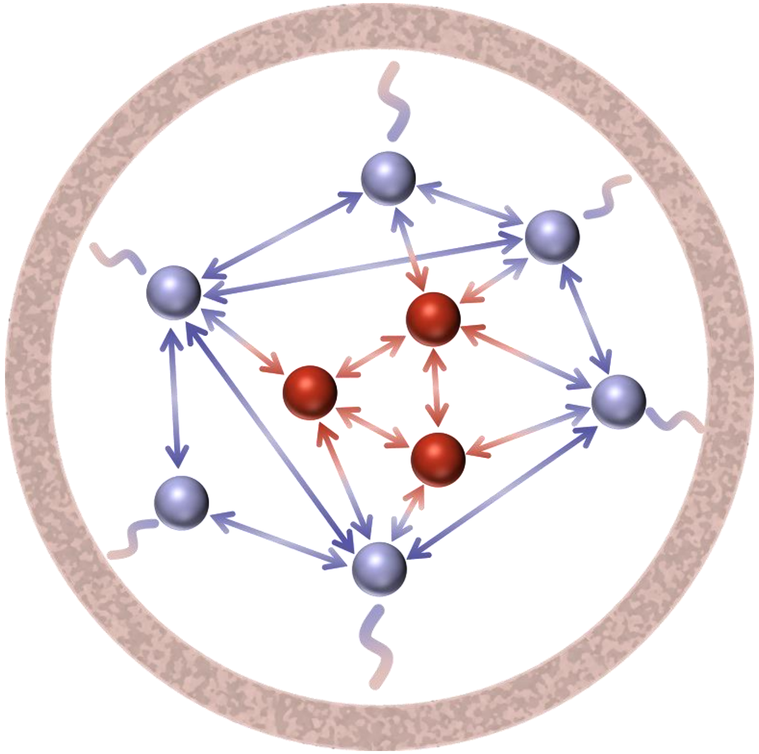
$$m\dot{v}(t) = -\gamma v(t) + \sqrt{2\gamma T}\,\xi(t)$$

Setup

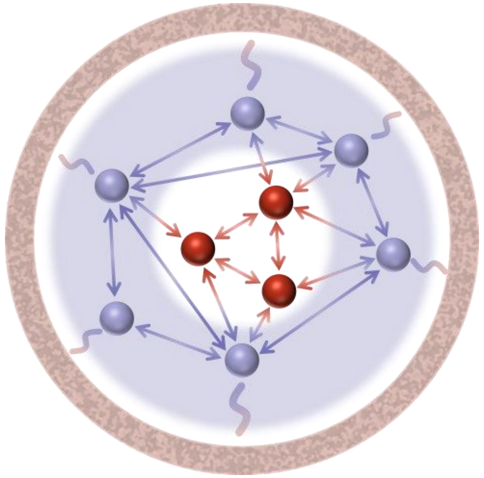
Microscopic description

$$m\dot{v}_n = f_n(\boldsymbol{x}, \boldsymbol{v}, t) - \partial_{x_n} V_I(\boldsymbol{x}, \tilde{\boldsymbol{x}})$$

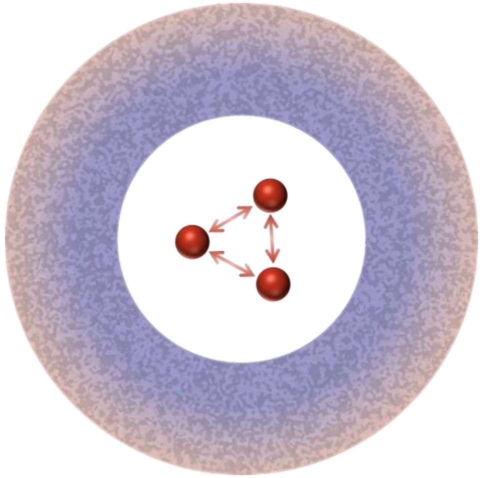
$$\tilde{m}\dot{\tilde{v}}_{\tilde{n}} = -\partial_{\tilde{x}_{\tilde{n}}}\left(V_I(\boldsymbol{x}, \tilde{\boldsymbol{x}}) + \tilde{V}(\tilde{\boldsymbol{x}})\right) - \tilde{\gamma}\tilde{v}_{\tilde{n}} + \sqrt{2\tilde{\gamma}\tilde{T}}\tilde{\xi}_{\tilde{n}}$$



fast relaxation limit of bath



$$\tau_{\mathrm{rel}}^{\mathrm{bath}} \ll \tau_{\mathrm{rel}}^{\mathrm{sys}}$$

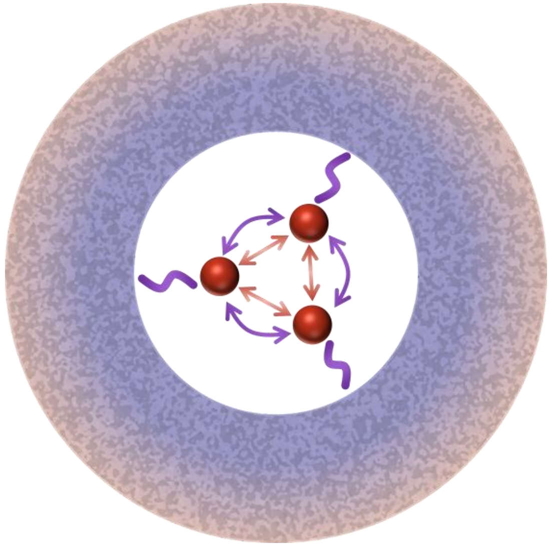


$$m\dot{v}_n = \textbf{?}$$

Main result

Langevin equation for strongly-coupled system

$$m_S \dot{\boldsymbol{v}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{v}, t) - \nabla\Delta(\boldsymbol{x}) - \mathbf{G}(\boldsymbol{x})\boldsymbol{v} + \sqrt{2\mathbf{G}(\boldsymbol{x})T}\boldsymbol{\xi}$$



mean force potential

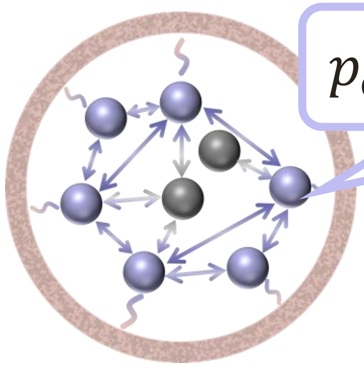
$$\Delta(\boldsymbol{x}) \equiv -\beta^{-1} \ln \int d\tilde{\boldsymbol{x}} \frac{1}{\mathcal{Z}_B} e^{-\beta\left(V_I(\boldsymbol{x},\tilde{\boldsymbol{x}}) + \tilde{V}(\tilde{\boldsymbol{x}})\right)}$$

effective damping coefficients

$$G_{nm}(\boldsymbol{x}) \equiv \frac{1}{T}\int_0^\infty dt\, C_{\partial_{x_n}V_I, \partial_{x_m}V_I}(t|\boldsymbol{x})$$

correlation function in equilibrium bath dynamics

$$C_{f,g}(t|\boldsymbol{x}) = \left\langle \delta f\left(\boldsymbol{x}, \tilde{\boldsymbol{x}}(t)\right) \delta g\left(\boldsymbol{x}, \tilde{\boldsymbol{x}}(0)\right) \right\rangle_{\text{eq}}$$



$$p_{\text{eq}}(\tilde{\boldsymbol{x}}|\boldsymbol{x}) \propto e^{-\beta\left(V_I(\boldsymbol{x},\tilde{\boldsymbol{x}}) + \tilde{V}(\tilde{\boldsymbol{x}})\right)}$$

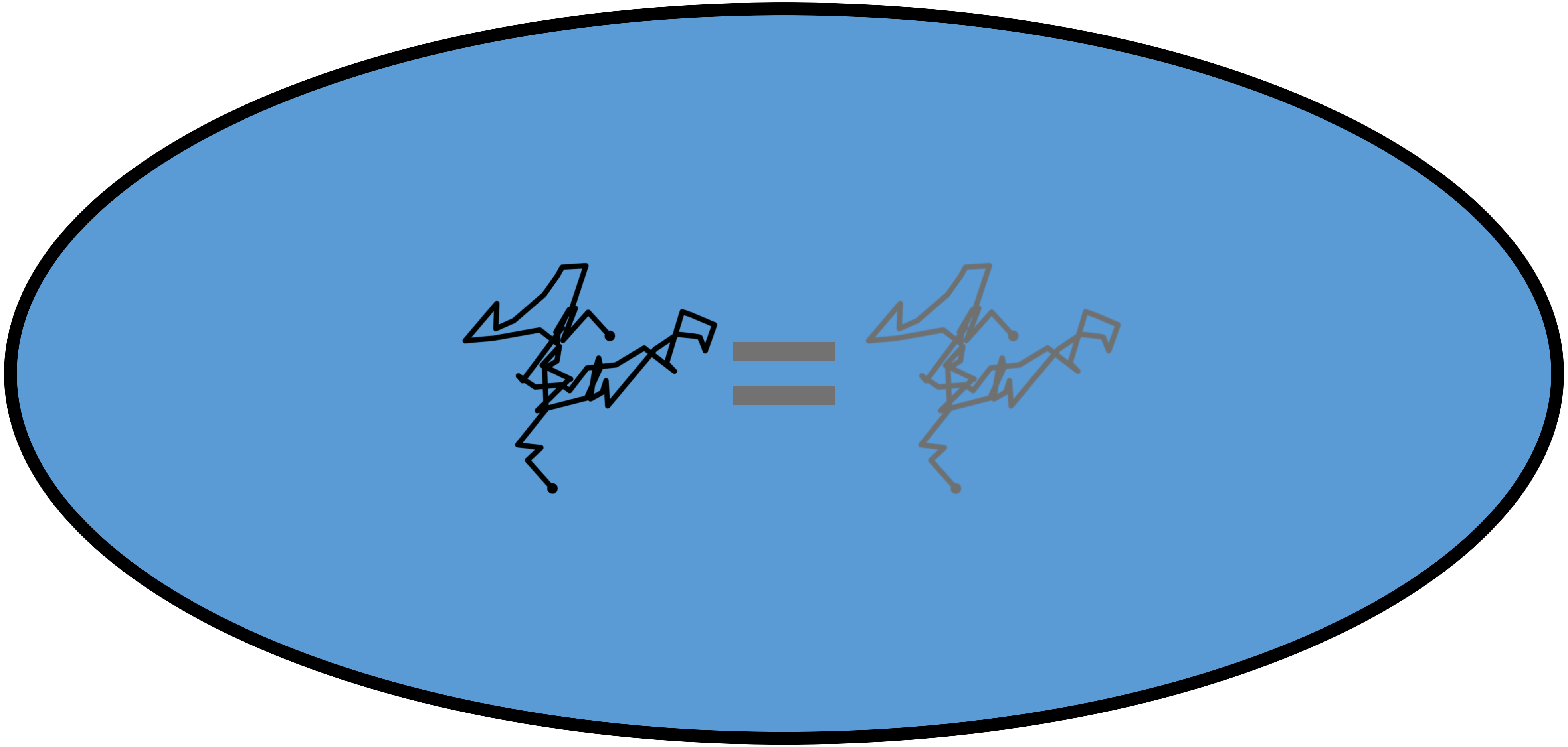
Conditions for vanishing strong-coupling effects

first condition **second condition**

Conditions for vanishing strong-coupling effects

first condition **second condition**

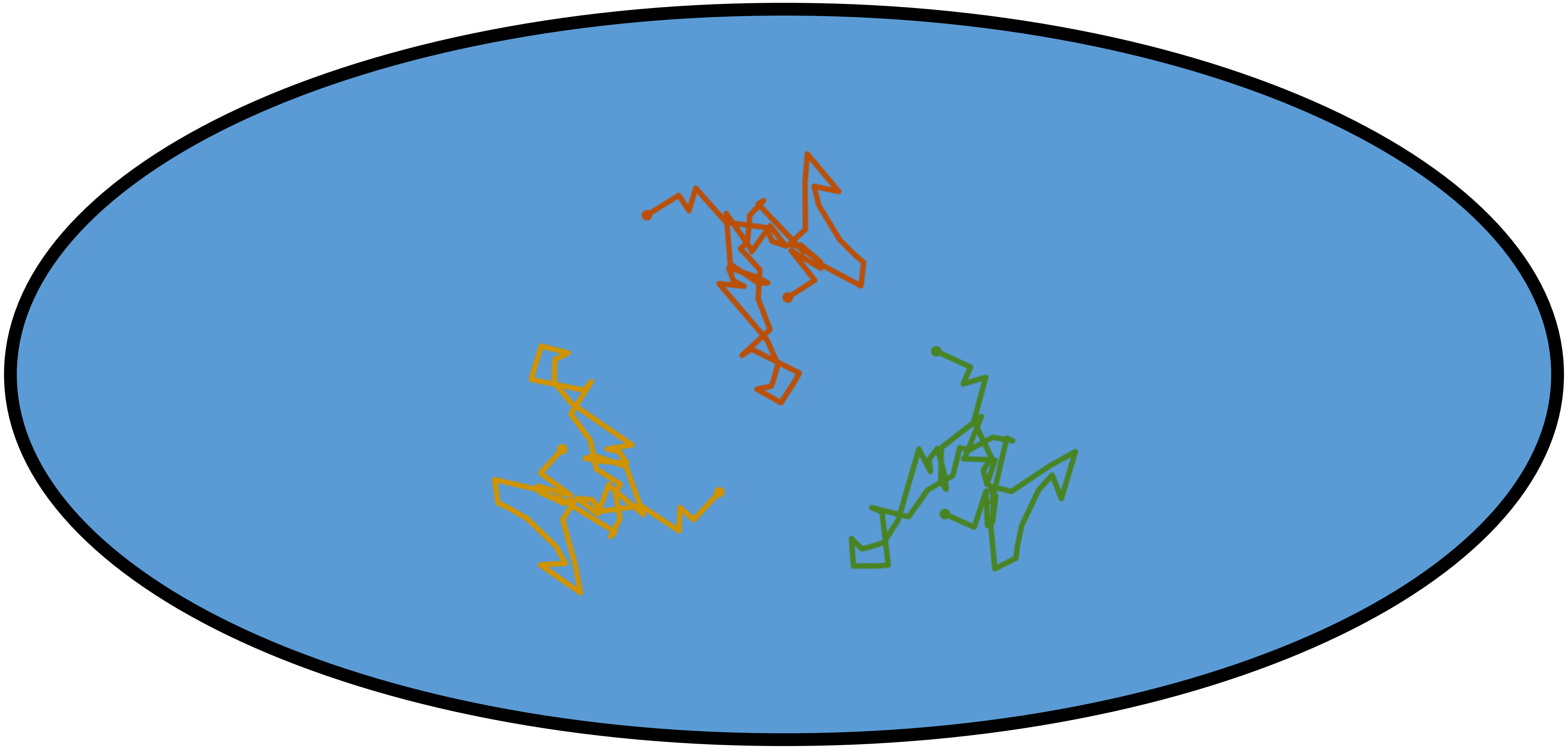
Translational invariance



Conditions for vanishing strong-coupling effects

first condition **second condition**

Mutual independence

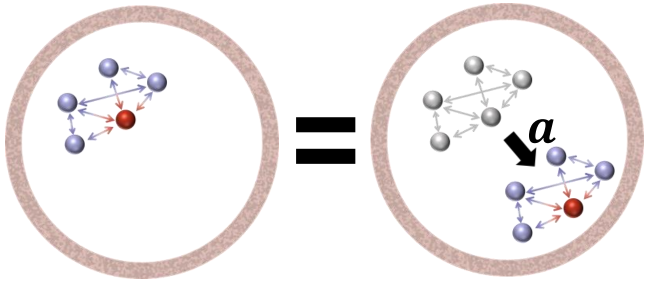


Conditions for vanishing strong-coupling effects

first condition
translational invariance

$$\Delta(\boldsymbol{x}+\boldsymbol{a}) = \Delta(\boldsymbol{x})$$

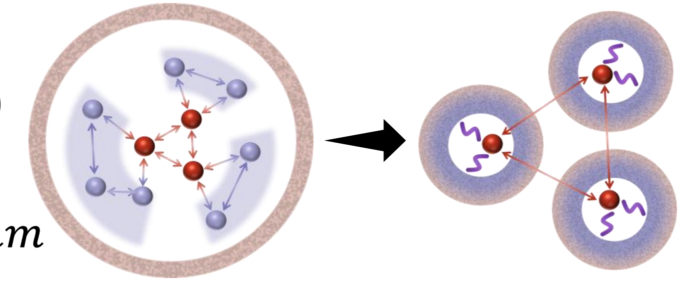
$$G_{nm}(\boldsymbol{x}+\boldsymbol{a}) = G_{nm}(\boldsymbol{x})$$



second condition
mutual independence

$$\Delta(\boldsymbol{x}) = \sum_n \Delta_n(x_n)$$

$$G_{nm}(\boldsymbol{x}) = \gamma_n(x_n)\delta_{nm}$$



condition I & II ⇒ $\Delta(\boldsymbol{x}) = \Delta, \qquad G_{nm}(\boldsymbol{x}) = \gamma_n \delta_{nm}$

restoration of the traditional Langevin equation

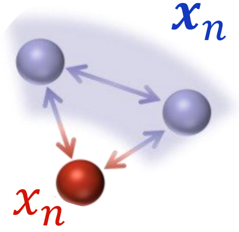
$\gamma_n\delta_{nm}$ $\gamma_n\delta_{nm}$

equation of motion $\quad m_S\dot{\boldsymbol{v}} = f(\boldsymbol{x},\boldsymbol{v},t) - \nabla\Delta(\boldsymbol{x}) - \mathbf{G}(\boldsymbol{x})\boldsymbol{v} + \sqrt{2\mathbf{G}(\boldsymbol{x})T}\boldsymbol{\xi}(t)$

condition I & II ⇒ $m\dot{v}_n = f_n(\boldsymbol{x},\boldsymbol{v},t) - \gamma_n v_n + \sqrt{2\gamma_n T}\xi_n$

Explicit form of the reduced damping constant

$$\gamma_n \equiv \frac{1}{T}\sum_{\tilde{n},\tilde{m}} \int_0^\infty dt \left\langle \delta\left(\partial_{x_n} V_I\left(x_n, \tilde{x}_{\tilde{n}}(t)\right)\right)\delta\left(\partial_{x_m} V_I\left(x_n, \tilde{x}_{\tilde{m}}(0)\right)\right)\right\rangle_{\mathrm{eq}}$$



$$= \frac{1}{T}\sum_{\tilde{n},\tilde{m}} \int_0^\infty dt \left\langle \delta f_{\tilde{n}}\left(x_n, \tilde{x}_{\tilde{n}}(t)\right)\delta f_{\tilde{m}}\left(x_n, \tilde{x}_{\tilde{m}}(0)\right)\right\rangle_{\mathrm{eq}}$$

Newton's third law

$$= \frac{1}{T}\sum_{\tilde{n},\tilde{m}} \tilde{\gamma} T \delta_{\tilde{n},\tilde{m}}$$

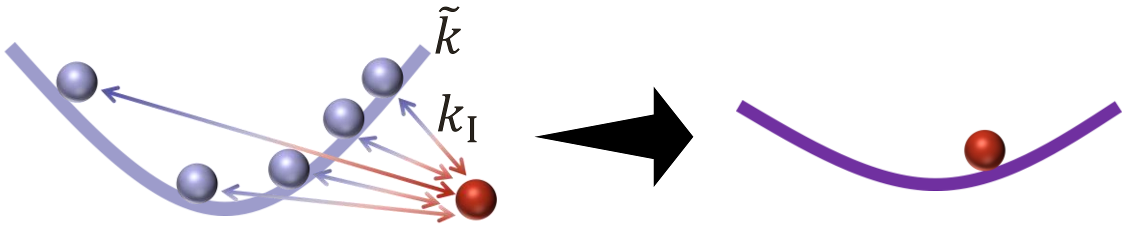
Green-Kubo relation

condition I & II ⇨ $m\dot{v}_n = f_n(\boldsymbol{x}, \boldsymbol{v}, t) - \gamma_n v_n + \sqrt{2\gamma_n T}\xi_n, \qquad \gamma_n = \tilde{N}_n \tilde{\gamma}$

$\tilde{N}_n$: number of bath particles interacting with n-th system particle

Example I: broken translational invariance

: single system particle + $\tilde{N}$-identical bath particles



mean force potential

$$\Delta(x) = \frac{1}{2}kx + c_1, \qquad k = \frac{\tilde{N}k_I\tilde{k}}{k_I + \tilde{k}}$$

effective damping coefficients

$$\gamma(x) = \tilde{N}\tilde{\gamma}\left(\frac{k_I}{k_I + \tilde{k}}\right)^2$$

symmetry restoration limit $\tilde{k} \to 0$

$$-\partial_x\Delta(x) = 0, \qquad \gamma(x) = \tilde{N}\tilde{\gamma}$$

weak-coupling limit $k_I \to 0$

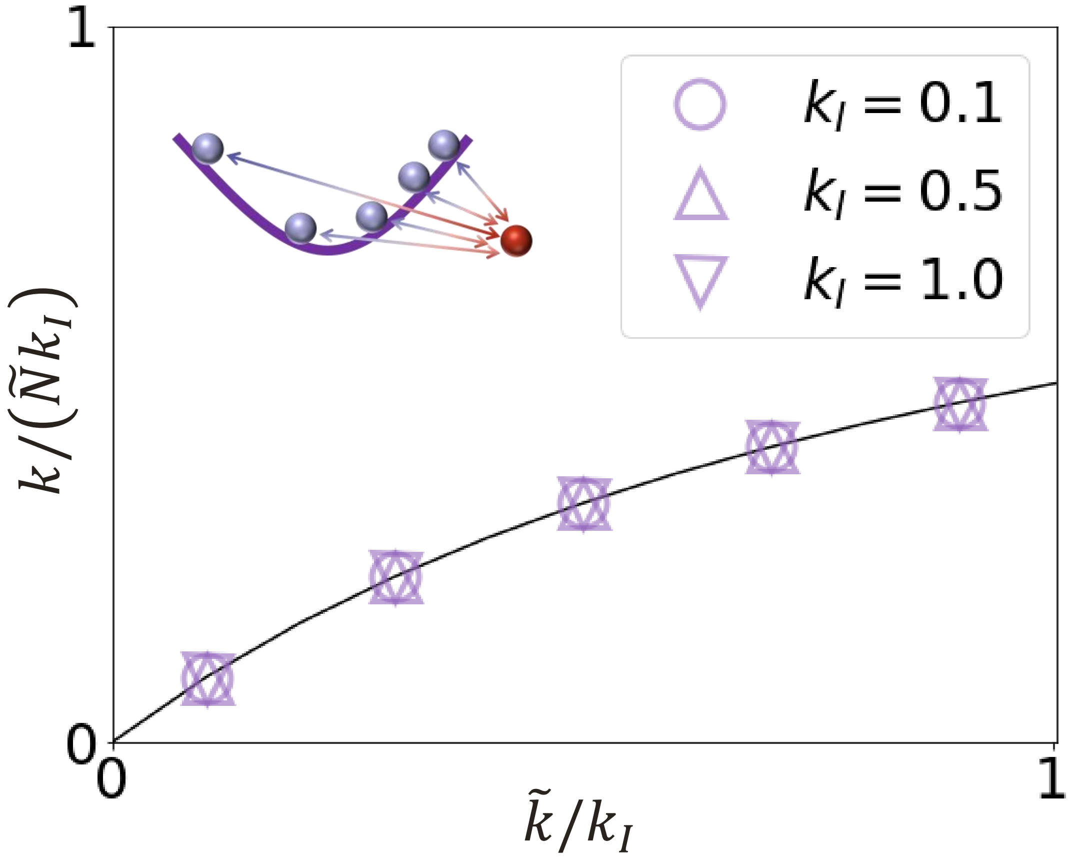
$$-\partial_x\Delta(x) = \mathcal{O}(k_I), \qquad \gamma(x) = \mathcal{O}(k_I^2)$$

Example I: broken translational invariance

: single system particle + $\widetilde{N}$-identical bath particles

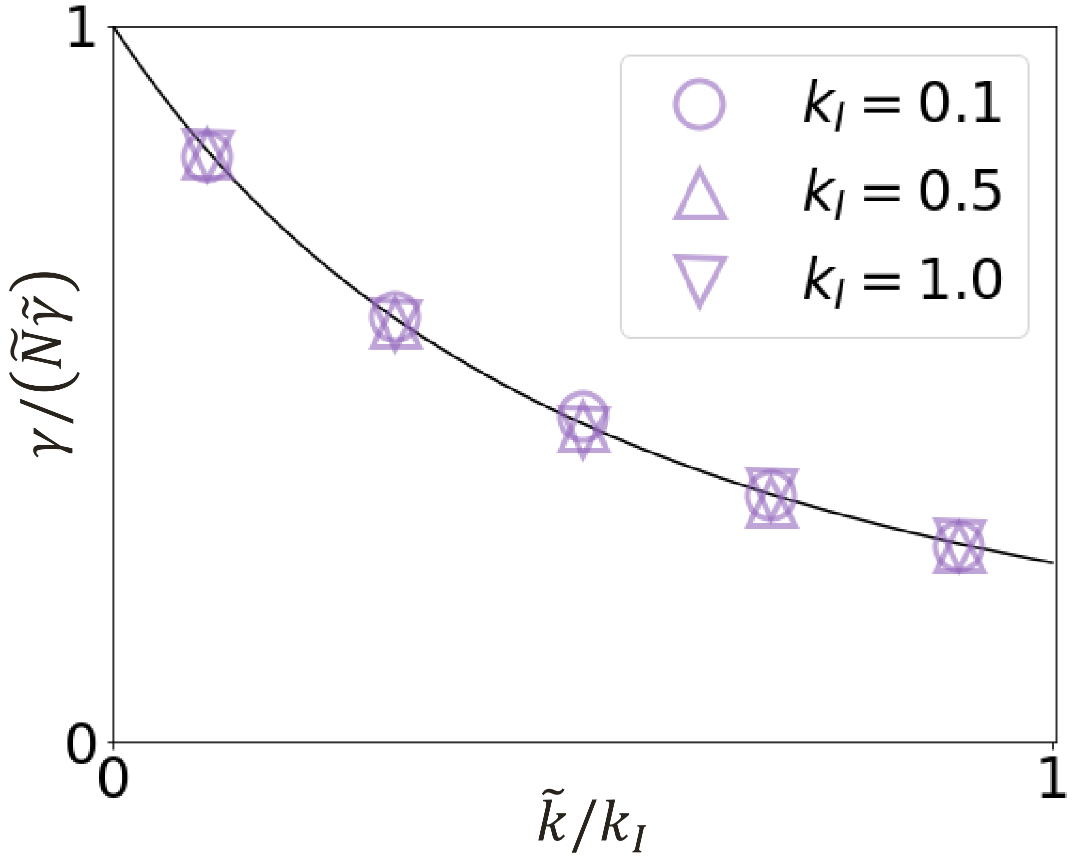
mean force potential

$$\Delta(x) = \frac{1}{2} k x^2 + c_1, \qquad k = \frac{\widetilde{N} k_I \tilde{k}}{k_I + \tilde{k}}$$



effective damping coefficients

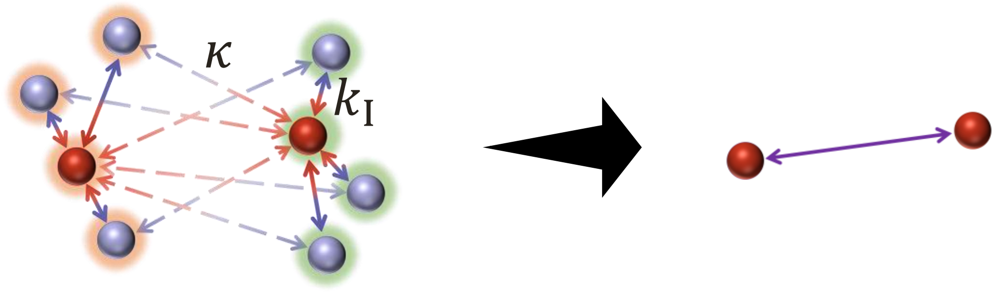
$$\gamma(x) = \widetilde{N}\tilde{\gamma}\left(\frac{k_I}{k_I + \tilde{k}}\right)^2$$



$f^{\text{ext}} = 0$
$\widetilde{N} = 10^4$
$\widetilde{m} = 10^{-4}$
$\tilde{\gamma} = 10^{-2}$
$m = 1$
$T = 1$

Example II: broken mutual independence

: two system particles + $\widetilde{N}$-bath particles of two species



mean force potential

$$\Delta(\boldsymbol{x}) = \frac{1}{2}k(x_1 - x_2)^2 + c_2, \qquad k = \frac{\widetilde{N}k_I\kappa}{k_I + \kappa}$$

effective damping coefficients

$$\mathbf{G}(x) = \frac{\widetilde{N}\tilde{\gamma}}{2(k_I+\kappa)^2}\begin{pmatrix} k_I^2+\kappa^2 & 2k_I\kappa \\ 2k_I\kappa & k_I^2+\kappa^2 \end{pmatrix}$$

independence restoration limit $\kappa \to 0$

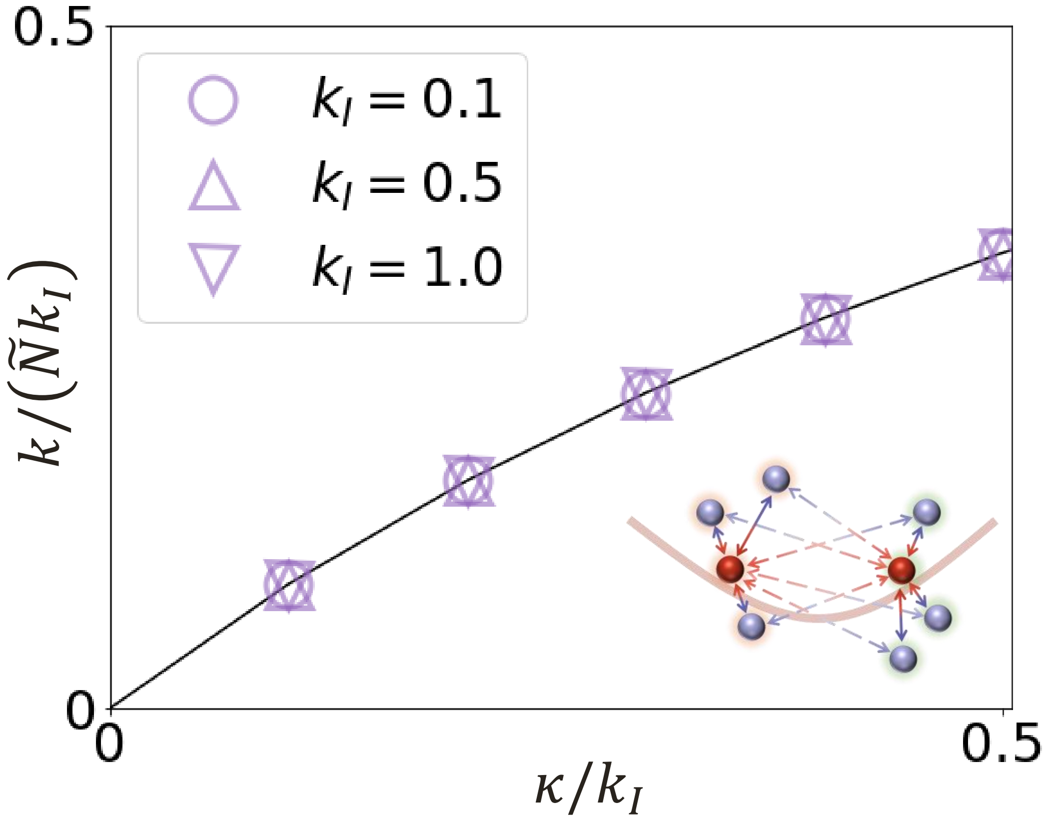
$$-\boldsymbol{\nabla}\Delta(x) = \mathbf{0}, \qquad G(x) = \frac{\widetilde{N}\tilde{\gamma}}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Example II: broken mutual independence

: two system particles + $\widetilde{N}$-bath particles of two species

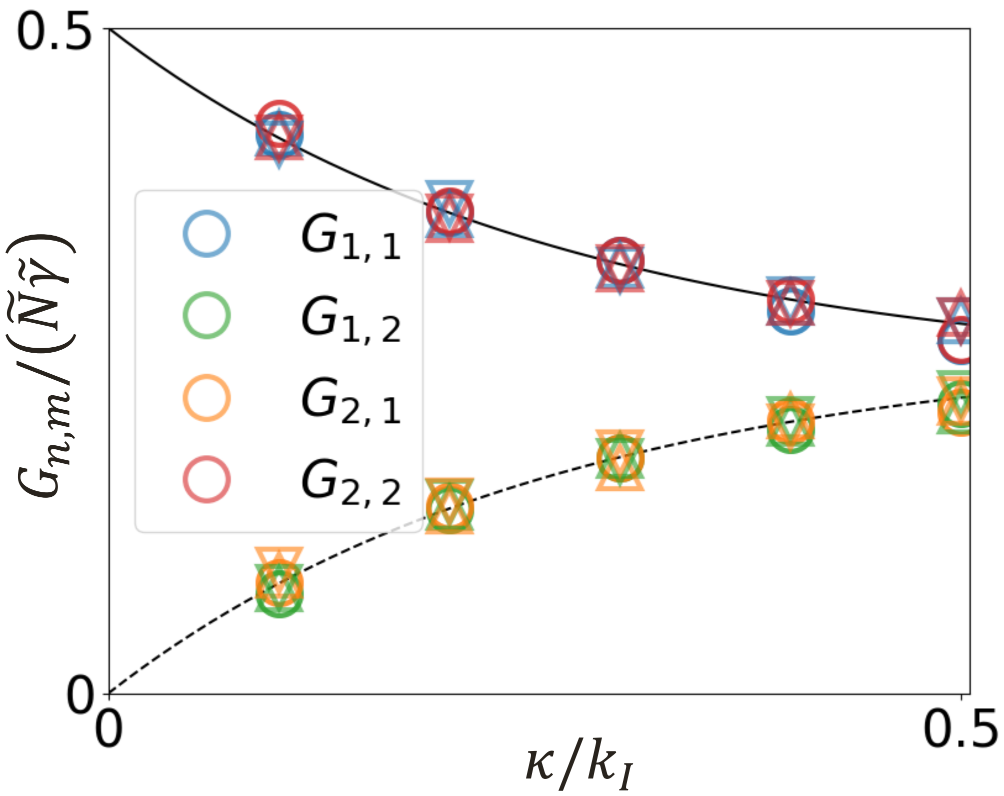
mean force potential

$$\Delta(x) = \frac{1}{2}k(x_1 - x_2)^2 + c_2, \qquad k = \frac{\widetilde{N}k_I\kappa}{k_I + \kappa}$$



effective damping coefficients

$$\mathbf{G}(x) = \frac{\widetilde{N}\tilde{\gamma}}{2(k_I + \kappa)^2}\begin{pmatrix} k_I^2 + \kappa^2 & 2k_I\kappa \\ 2k_I\kappa & k_I^2 + \kappa^2 \end{pmatrix}$$

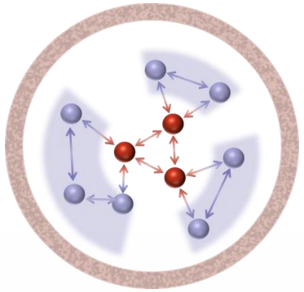


$\boldsymbol{f}^{\text{ext}} = -\boldsymbol{x}$
$\widetilde{N} = 10^4$
$\widetilde{m} = 10^{-4}$
$\tilde{\gamma} = 10^{-2}$
$m = 1$
$T = 1$

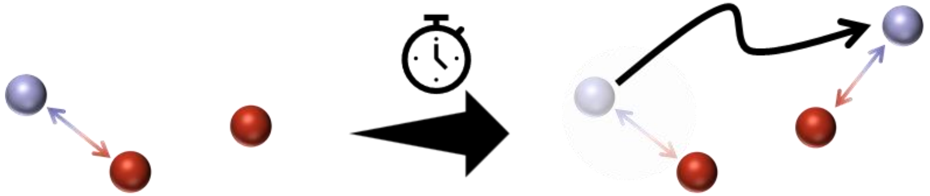
Example III: short-range interaction

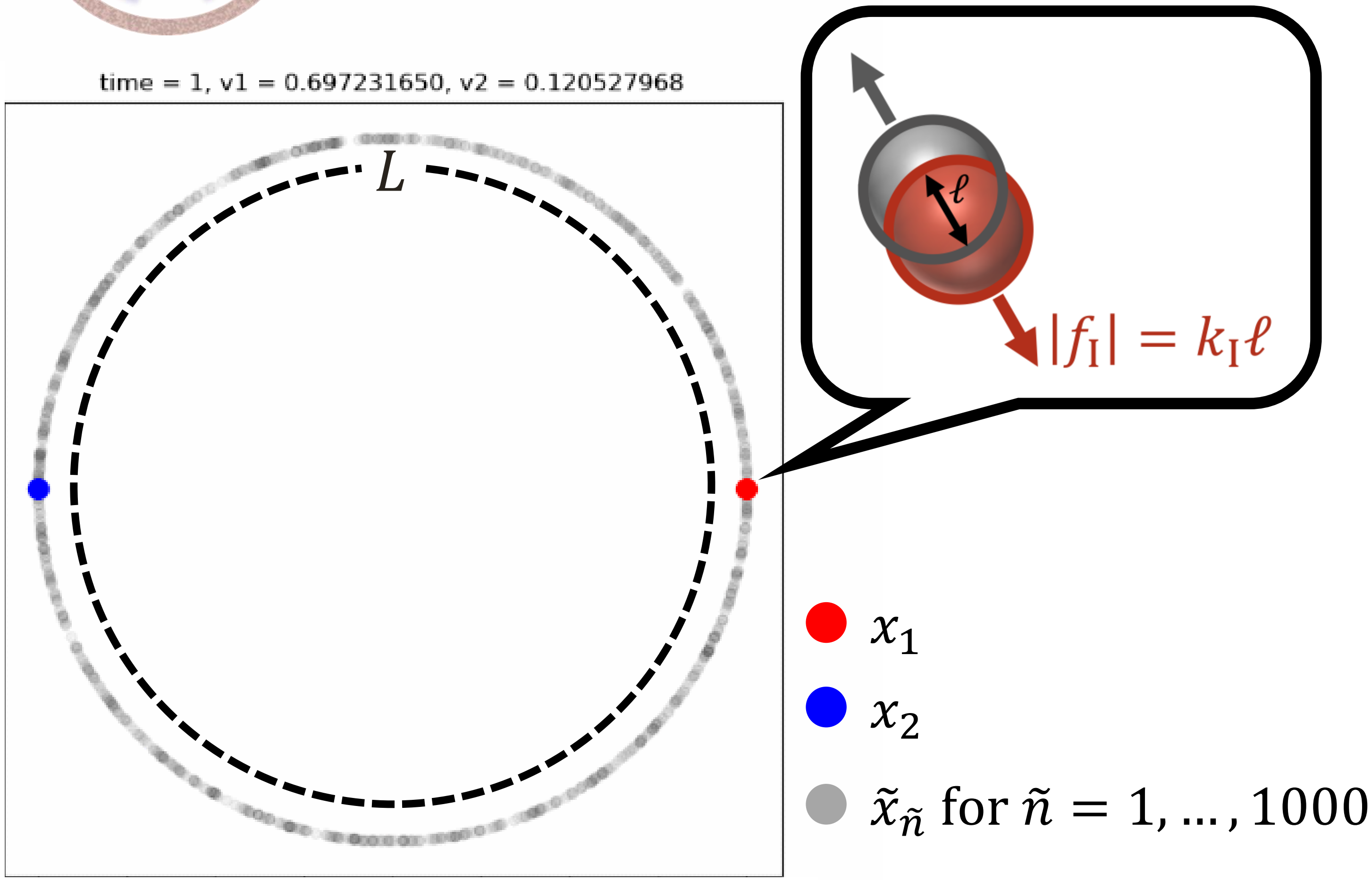
: short-range harmonic repulsion

Ideal condition



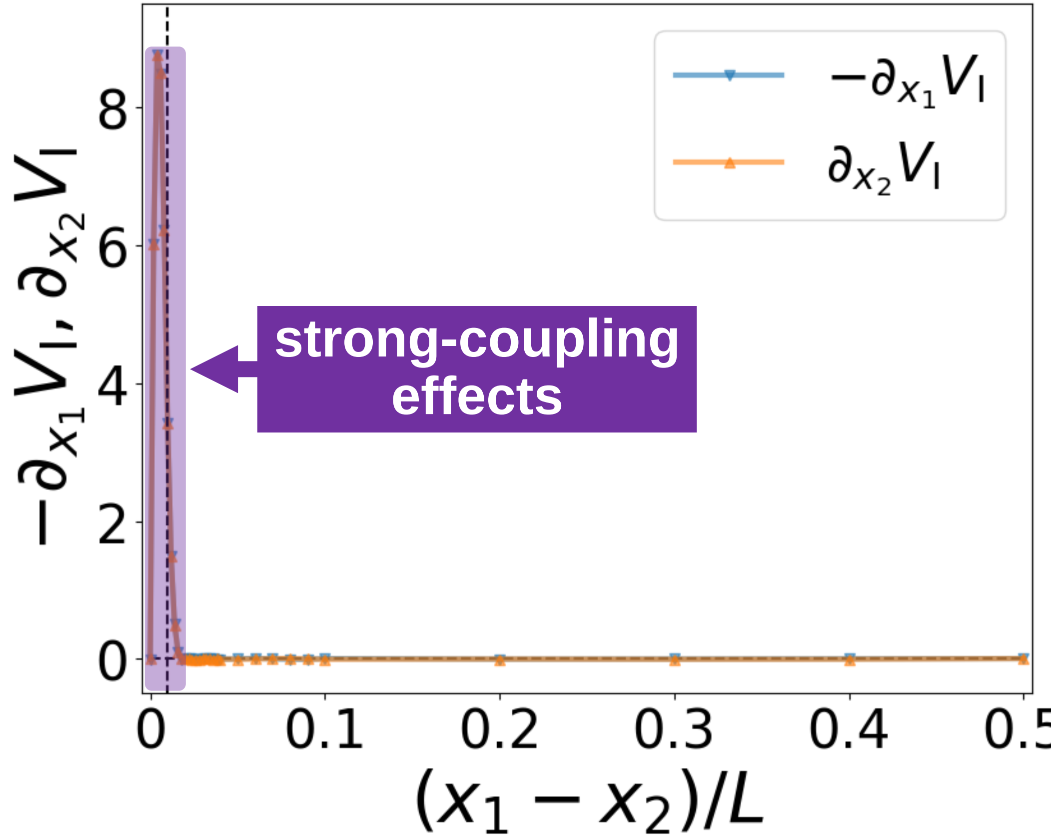
Realistic case

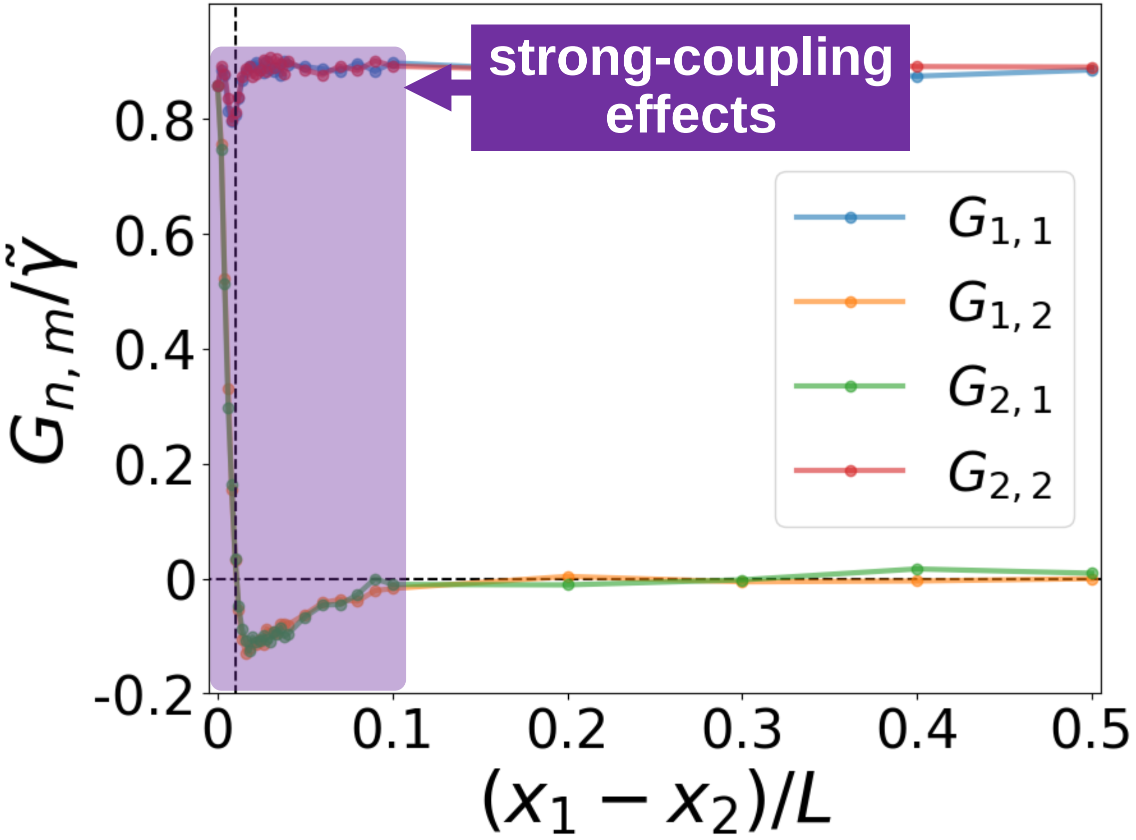




Example III: short-range interaction

: short-range harmonic repulsion





$\tilde{N} = 10^3$
$\tilde{\gamma} = 10^{-2}$
$m = 10^{-2}$
$T = 10$
$L = 100$
$r_I = 1$
$k_I = 10$

Summary

"We formulate a Langevin equation capturing strong coupling effects"

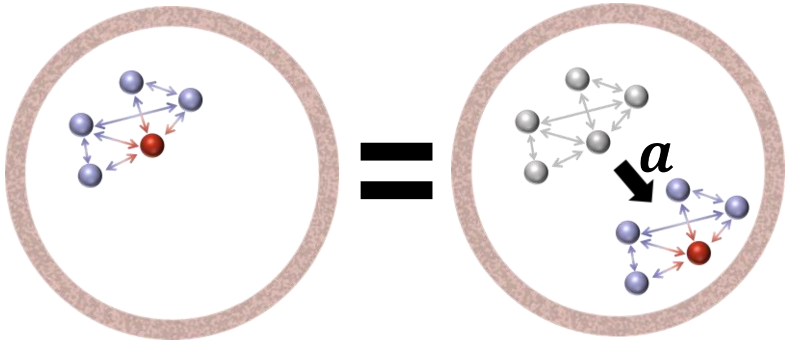
$$m_S\dot{\boldsymbol{v}} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{v},t) - \boldsymbol{\nabla}\Delta(\boldsymbol{x}) - \mathbf{G}(\boldsymbol{x})\boldsymbol{v} + \sqrt{2\mathbf{G}(\boldsymbol{x})T}\,\boldsymbol{\xi}(t)$$

mean force potential $\Delta(\boldsymbol{x})$

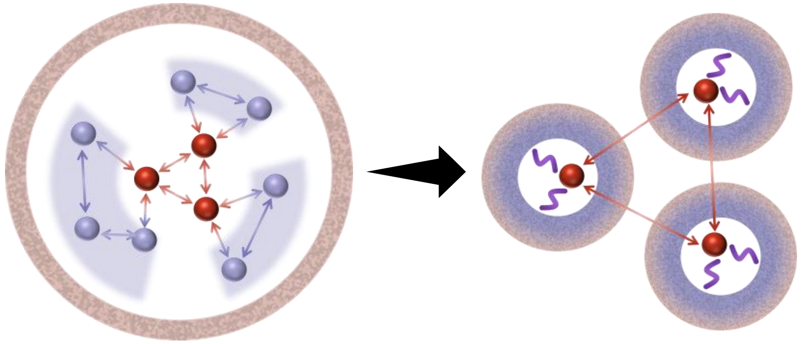
effective damping coefficients $\mathbf{G}(\boldsymbol{x})$

"Strong-coupling effects can disappear even with a finite coupling strength"

translational invariance



mutual independence



Thank you for your attention!!

jongmin.park@apctp.org

One postdoc position is available

For details
https://sites.google.com/view/jmpark/job-opening

Collaborators:

Hyunggyu Park
(KIAS)

Jae Sung Lee
(KIAS)

arXiv:2309.15359
(It will be appeared in PRE soon)