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Thermodynamics of Mpemba effect : Revisit to Lu & Raz theory

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In Frontiers in Non-equilibrium Physics 2024, **Talk on June 24th**

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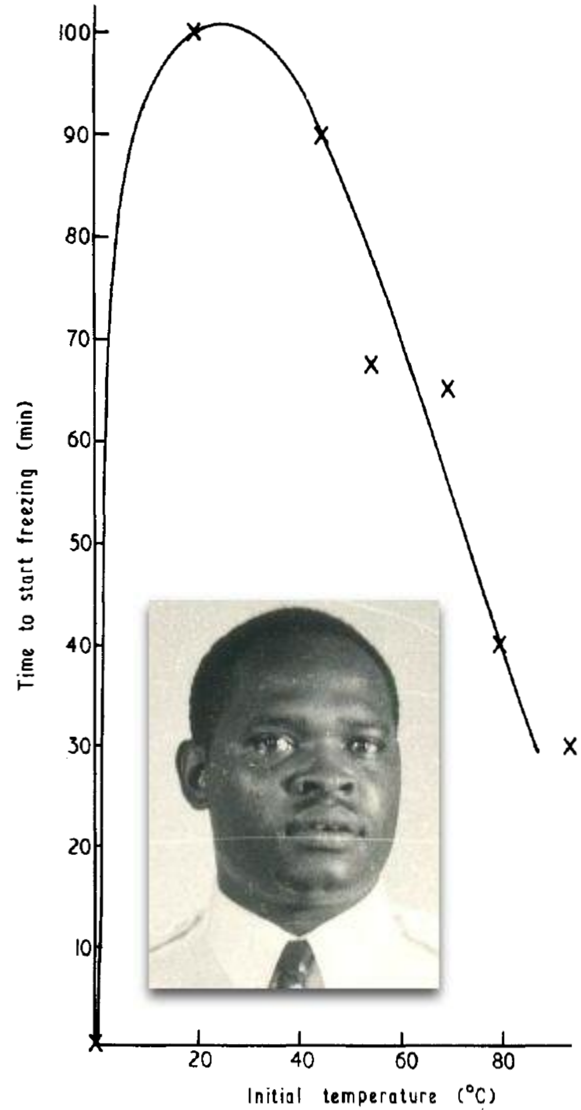
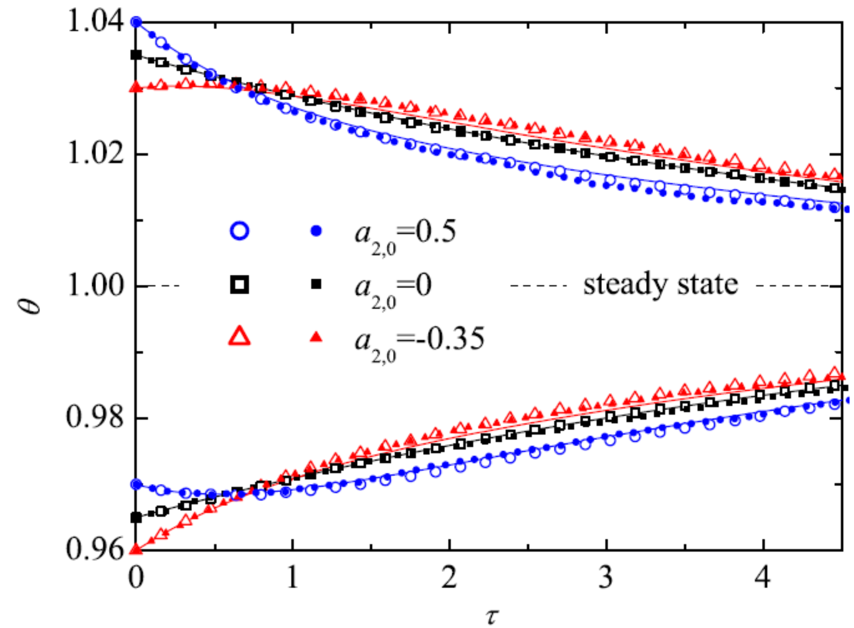
What is the Mpemba effect?

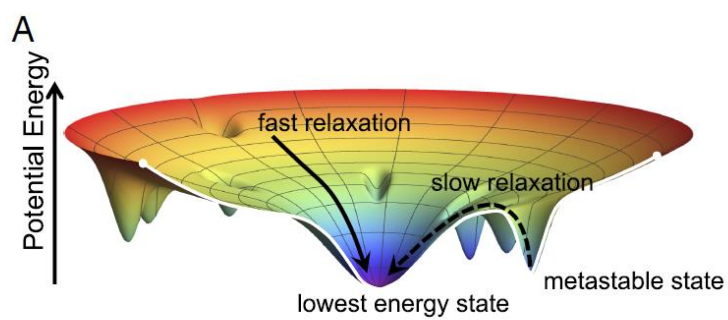
- What is Mpemba effect?
  - Erasto B. Mpemba found that some hot suspensions (*ice cream mix*) can freeze faster than cold (1963).
  - With the help of D. G. Osborne he has published a scientific paper (1969).



Some theoretical studies

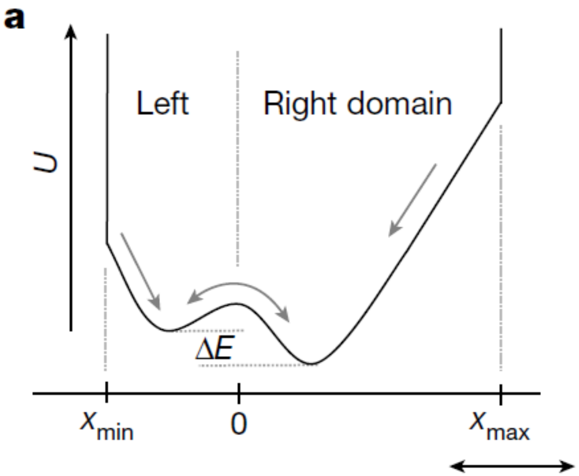
- Lasanta et al. PRL **119**, 148001 (2017) found that a granular gas can have both ME and the inverse ME by controlling *kurtosis*.
- Lu & Raz, PNAS **114**, 5083 (2017) indicated that the slow relaxation can take place by trapping at local minima.

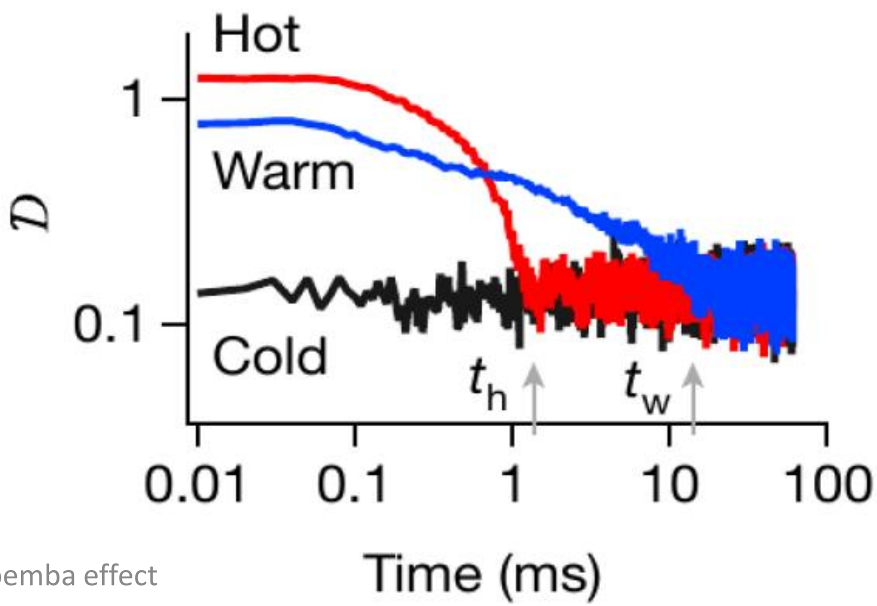




Experimental confirmation

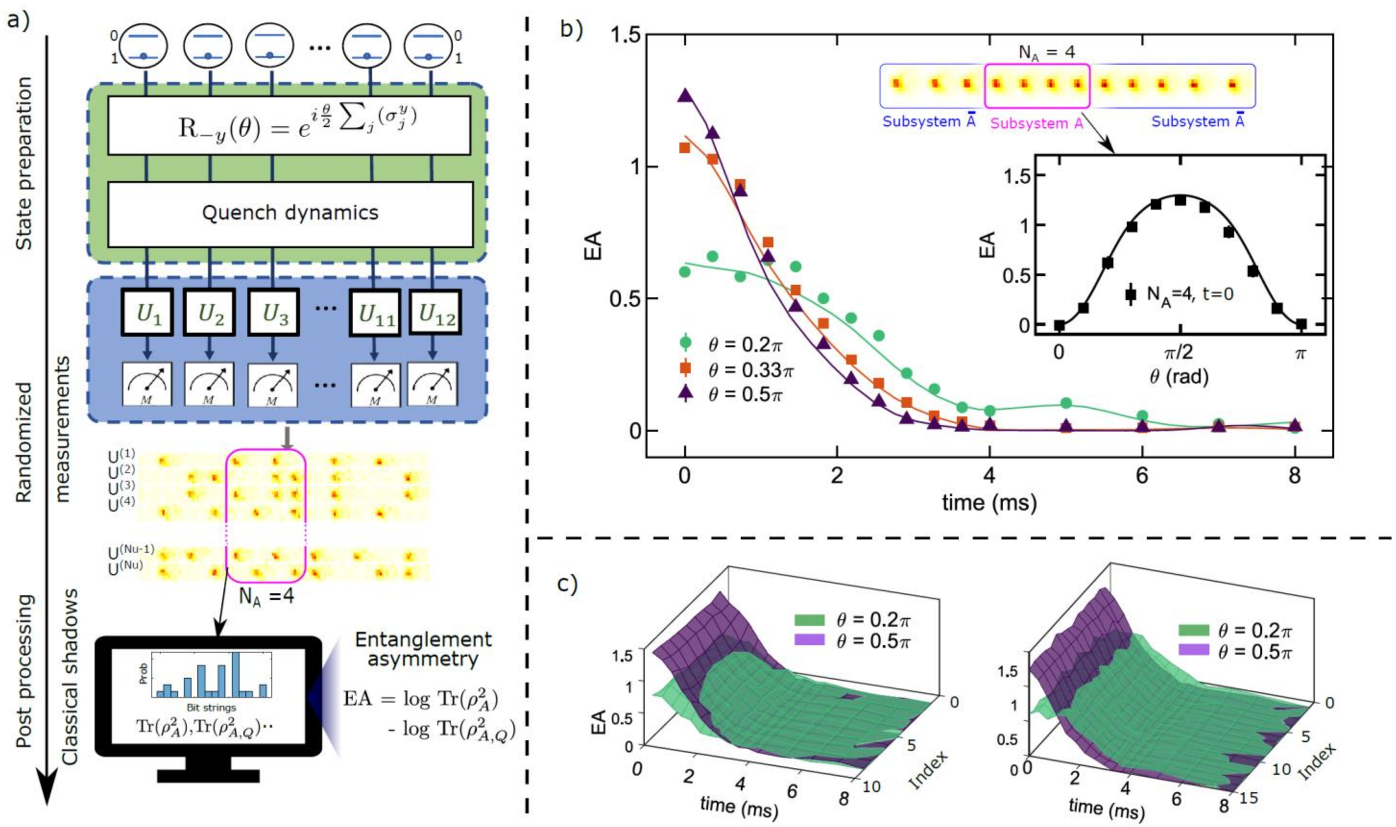
- Kumar & Bechhoefer, Nature **584**, 64 (2020).
- They have analyzed trapped colloids in a double well potential.
- They observed the distance between the distribution and equilibrium one.



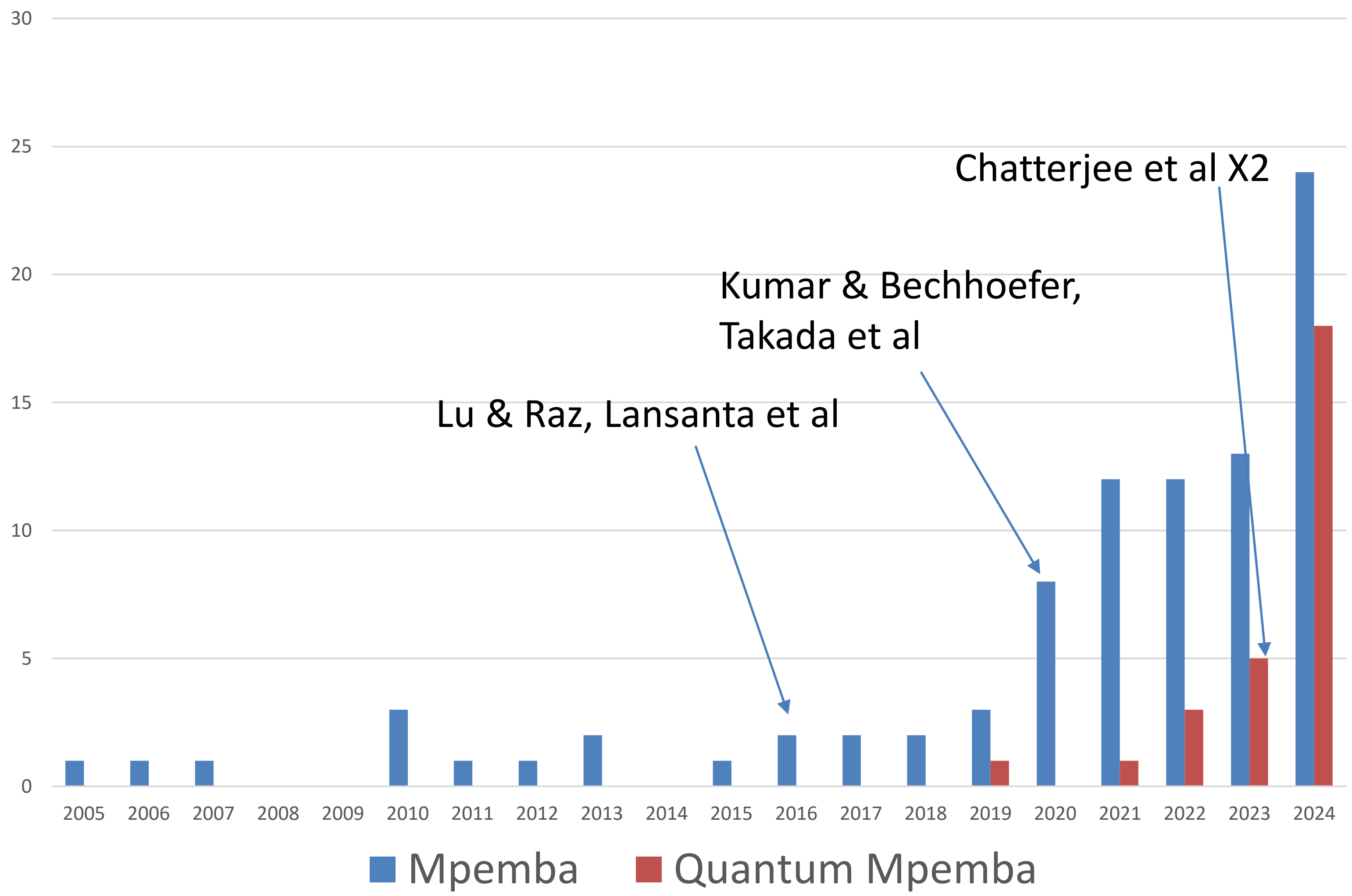


Experimental QMPE

- The first experimental reports on QMPE exists this year (PRL **133**, 010403 (2024), ibid 010402 (2024)).
- This is observed in a trapped atomic gas for quantum simulator.



Papers on Mpemba effect in arXiv (one month ago)



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- Introduction
- Scenarios for the Mpemba effect
- Our model analysis
  – Analysis for a square-well potential
  – Analysis for a triple-harmonic potential
- Summary

Two scenarios

- Scenario 1: to use the different initial conditions
  - Santos, Ares, Chatterjee, Goold, Yamashika, Turkeshi
  - The symmetry in the initial condition is different.
  - The slow mode is not always important (=> next talk)
  - This is easier scenario to obtain the Mpemba.
- Scenario 2: to use potential landscape starting from equilibrium conditions.
  - Lu, Bechhoefer, Vuceljia
  - I adopt this scenario in this talk.

Illustration of Mpemba effect in the first scenario

- We can write the energy equation (for an uniform system):

$\dot{\gamma}$: shear rate

$$c_V \dot{T} = -\frac{\dot{\gamma}}{n} P_{xy} + 2 c_V \zeta (T_{\rm env} - T),$$

$\gtrsim 0$

- If the system is at equilibrium, the viscous heating is absent (P_{xy}=0).
- If the system is in non-equilibrium, the heating term must exist.
- Then, the system at equilibrium must have faster cooling than that at non-equilibrium.

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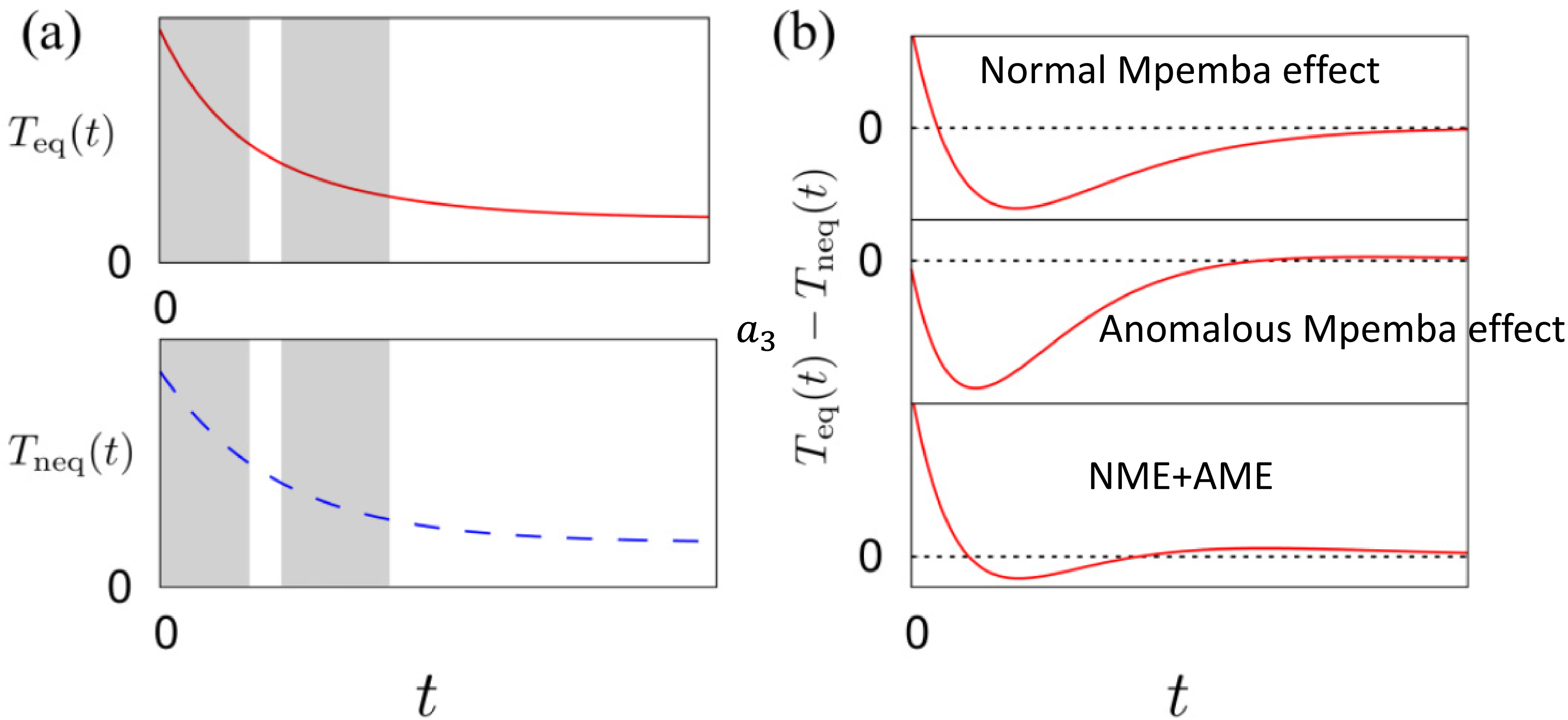
Essence of Mpemba effect



Quantitative argument following this scenario can be found in Takada, Hayakawa & Santos, PRE**103**, 032901 (2021)

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Model for the second scenario

- We use the Fokker-Planck equation:

$$\partial_t p = \mathbb{W}(\beta) p, \qquad \mathbb{W}(\beta) := \partial_x (V'(x) + T\partial_x)$$

- Because FP eq. does not have any degeneracy, we can write

$$p(x, \beta; t) = \sum_n \mathrm{e}^{-\lambda_n t} r_n(x, \beta) a_n$$

$$a_n := \int \mathrm{d}x' \ell_n(x', \beta) p_i(x', \beta_i)$$

l_n and r_n are the left and right eigenvectors.

$$p(x, t) \approx p_{\mathrm{eq}}(x, \beta) + \mathrm{e}^{-\lambda_2 t} r_2(x) a_2(\beta_i, \beta), \qquad a_2(\beta_i, \beta) := \int \mathrm{d}x' \ell_2(x', \beta) p_i(x')$$

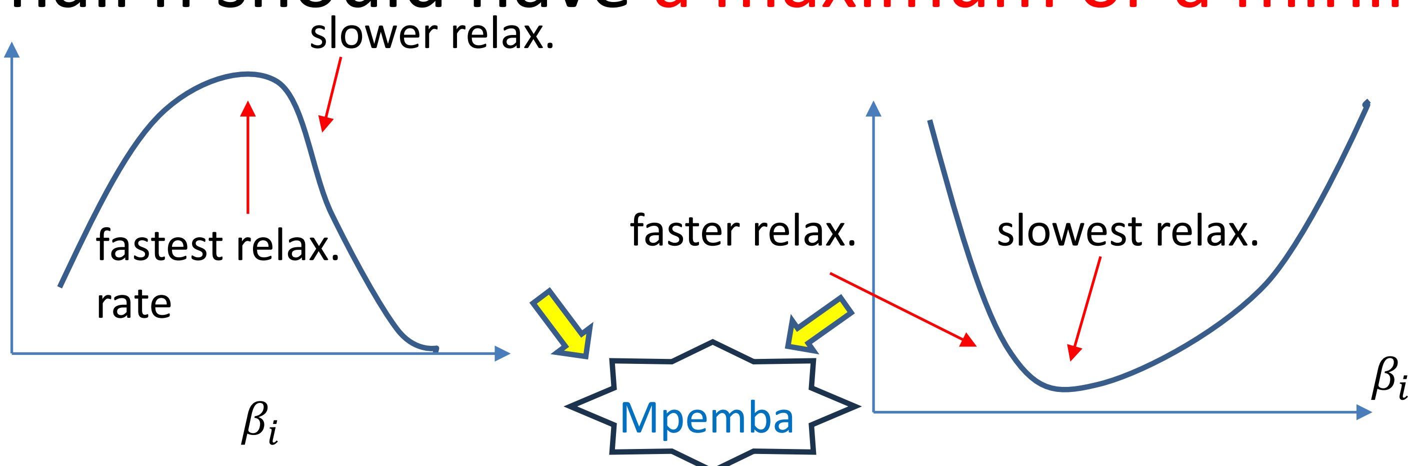
$$p_i := e^{-\beta_i V} / Z(\beta_i)$$

Observable dynamics & condition of Mpemba effect

- An observable A obeys:

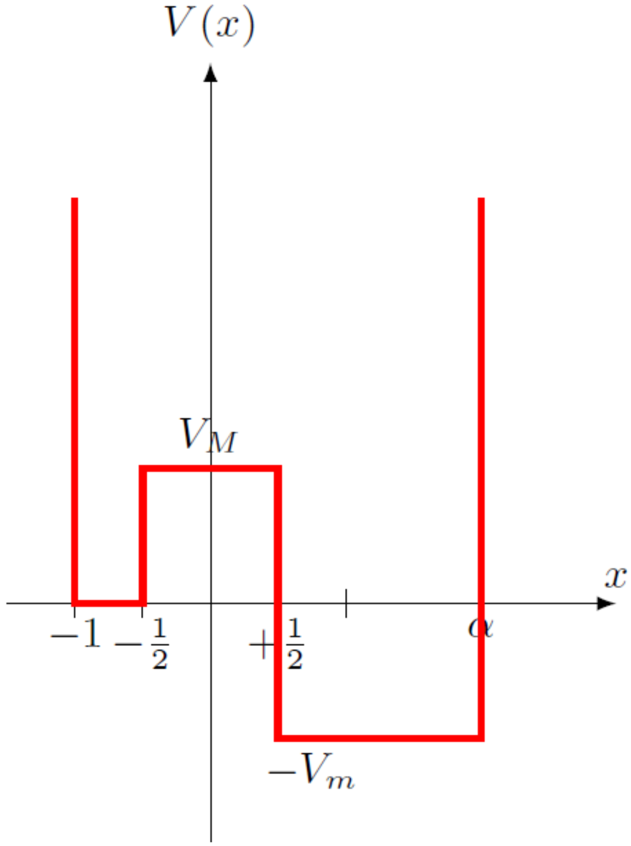
$$\langle A\rangle(t) = \langle A\rangle_{\mathrm{eq}} + \sum_n \mathrm{e}^{-\lambda_n t} a_n(\beta_i, \beta) \int \mathrm{d}x r_n(x) A(x)$$

- To observe the Mpemba condition a_n with small n should have a maximum or a minimum.



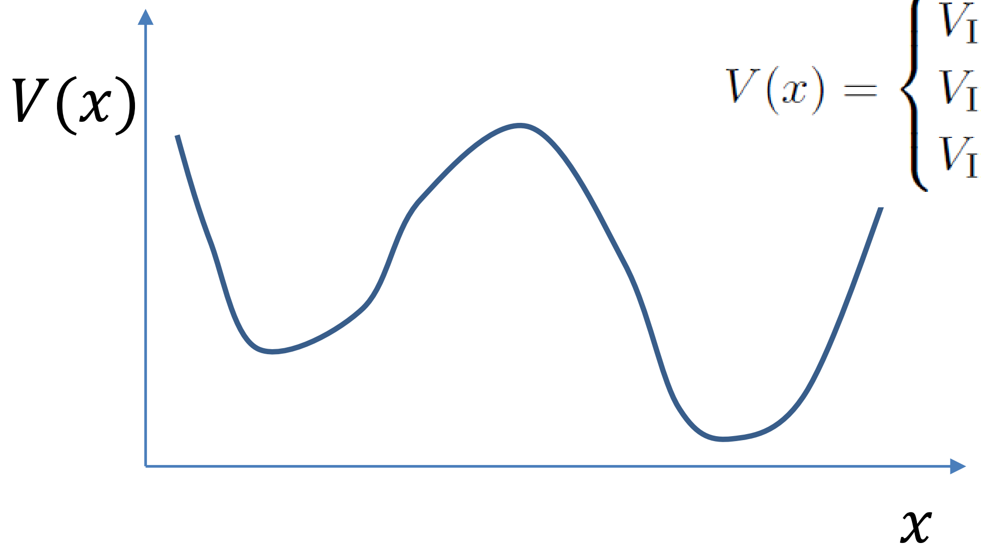
Our model analysis (1)

- We analyze two models.
- First one: asymmetric square potential
  - See Walker & Vucelja, J. Stat. Mech. (2021) 11315.
  - See also Biswas et al. JCP **159**, 044210 (2023) for a piece-wise linear potential.



Our model analysis (2)

- We also analyze a continuous bistable potential.
- For explicit calculation we adopt a triple harmonic potential



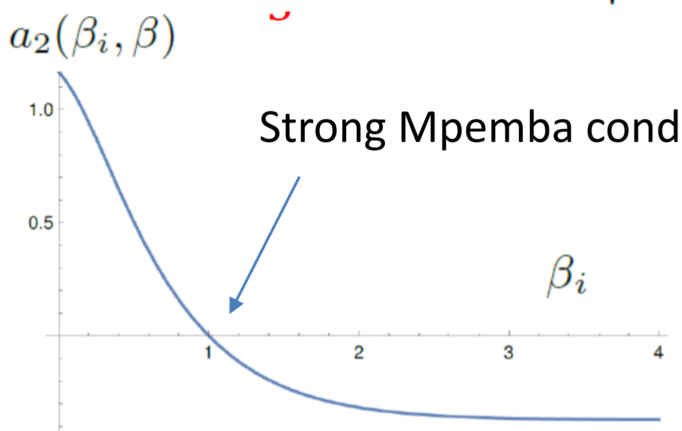
$$V(x) = \begin{cases} V_{\mathrm{I}}(x) := \frac{k_{\mathrm{I}}}{2}(x+1)^2, \\ V_{\mathrm{II}}(x) := V_M - \frac{k_{\mathrm{II}}}{2}x^2, \\ V_{\mathrm{III}}(x) := -V_m + \frac{k_{\mathrm{III}}}{2}(x-\alpha)^2, \end{cases}$$

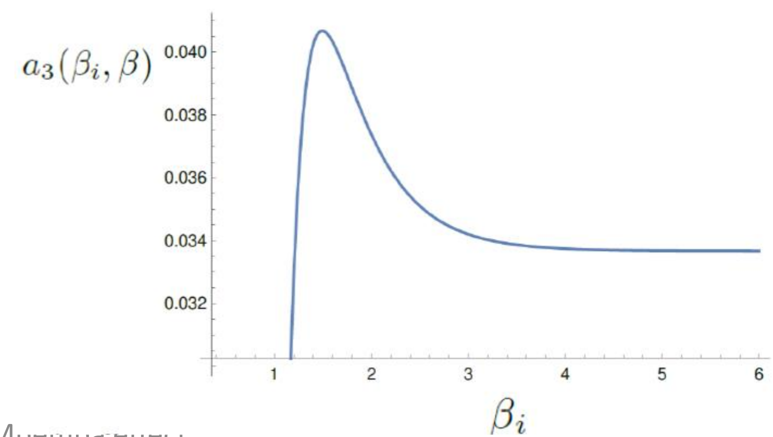
Square well potential (symmetric case)

- We can solve the problem exactly.
  - Three regions can be connected by 6 conditions.

$$a_2(\beta_i,\beta)=\frac{[1+e^{\beta V_m}+2e^{-\beta V_M}]^{1/2}(e^{\beta V_M}-e^{\beta(V_m+V_M)}-e^{\beta_i V_M}+e^{\beta_i(V_m+V_M)}+e^{(\beta+\beta_i)V_M})(-e^{\beta V_m}+e^{\beta_i V_m})}{\frac{\pi\nu}{2}(2+e^{\beta_i V_M}+e^{\beta_i(V_m+V_M)})\left[(1+e^{\beta V_M})(1+e^{\beta(V_m+V_M)})(1+e^{\beta V_m}+2e^{\beta(V_m+V_M)})\right]^{1/2}}$$

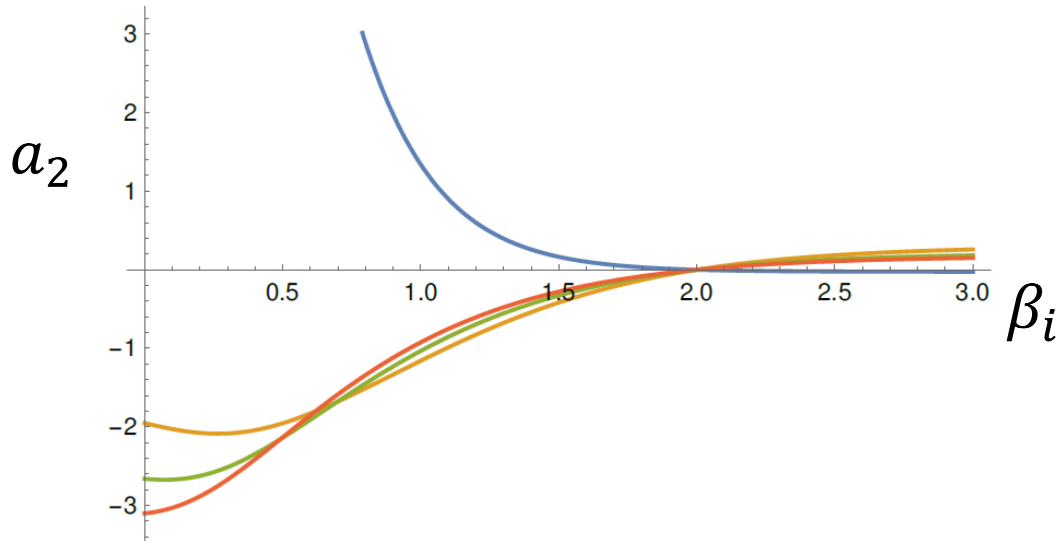
$$a_3(\beta_i,\beta)=\frac{2\sqrt{2}}{\pi}e^{-\frac{1}{2}(\beta-2\beta_i)(V_m+V_M)}\sqrt{\frac{2+e^{\beta V_M}+e^{\beta(V_m+V_M)}}{1+e^{\beta_i V_M}+e^{\beta_i(V_m+V_M)}}}\frac{1+e^{(\beta-\beta_i)V_m}-2e^{(\beta-\beta_i)(V_m+V_M)}}{2+e^{\beta_i V_M}+e^{\beta_i(V_m+V_M)}}$$





Square well potential ($\alpha \neq 1$)

- We can obtain the exact results even for asymmetric case ($\alpha \neq 1$).
- In this case $a_2(\beta_i)$ can have a minimum.



(blue: $\alpha = 0.5$; yellow: $\alpha = 0.6$; green: $\alpha = 0.7$; red: $\alpha = 0.8$)

Continuous potential

- We can use the mapping onto Schrödinger equation with

$$g(x,t) := e^{-\beta V(x)/2} p(x,t)$$

$$T\partial_t g(x,t) = [T^2\partial_x^2 - U(x)]g(x,t) = T\mathbb{L}g(x,t)$$

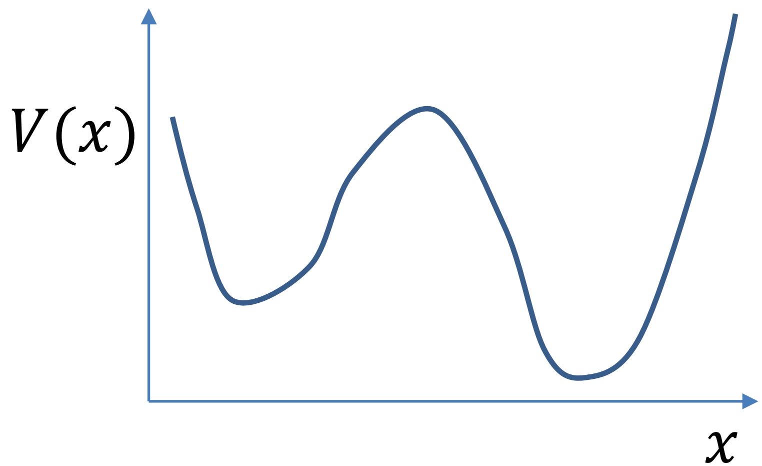
Effective potential $U(x) := \frac{1}{4}V'(x)^2 - \frac{1}{2}TV''(x)$

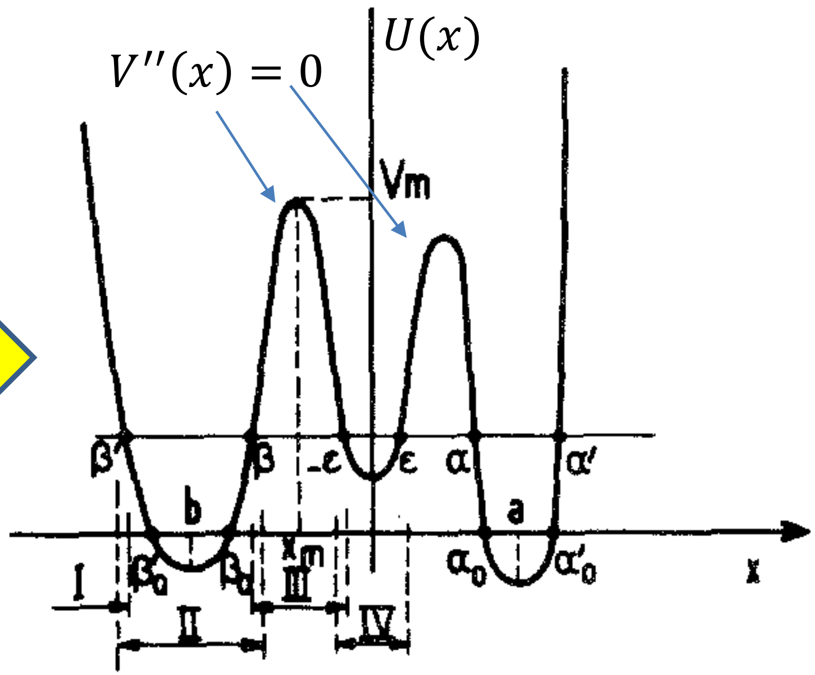
$$P(x,t|x_0) = \exp\left[\frac{V(x_0)-V(x)}{2T}\right]\sum_{n\geq 0}\varphi_n(x_0)\varphi_n(x)e^{-\lambda_n t},$$

$$\mathbb{L}\varphi_n(x) = -\lambda_n\varphi(x)$$

Potential landcape

- Effective potential has more complicated structure than V(x) as





- Then we may use WKB analysis.
  – This is not pleasant.

Triple harmonic potential

- If we adopt a triple-harmonic potential, the effective potential is still harmonic.

$$V(x) = \begin{cases} V_{\mathrm{I}}(x) := \frac{k_{\mathrm{I}}}{2}(x+1)^2, & \text{if } x < x_- \\ V_{\mathrm{II}}(x) := V_M - \frac{k_{\mathrm{II}}}{2}x^2, & \text{if } x_- \leq x \leq x_+, \\ V_{\mathrm{III}}(x) := -V_m + \frac{k_{\mathrm{III}}}{2}(x-\alpha)^2, & \text{if } x > x_+, \end{cases}$$

$$\Downarrow$$

$$U(x) = \begin{cases} U_{\mathrm{I}}(x) := \frac{k_{\mathrm{I}}^2}{4}(x+1)^2 - T\frac{k_{\mathrm{I}}}{2}, & \text{if } x < x_- \\ U_{\mathrm{II}}(x) := \frac{k_{\mathrm{II}}^2}{4}x^2 + \frac{T}{2}k_{\mathrm{II}}, & \text{if } x_- \leq x \leq x_+, \\ U_{\mathrm{III}}(x) := \frac{k_{\mathrm{III}}^2}{4}(x-\alpha)^2 - \frac{T}{2}k_{\mathrm{III}}, & \text{if } x > x_+, \end{cases}$$

Solution of the triple harmonic model

- Eigenvalues and approximate eigenfunctions

$$\lambda_n^{\mathrm{I}} = k_{\mathrm{I}}(n-1), \quad \varphi_n^{\mathrm{I}}(x) = \left(\frac{k_{\mathrm{I}}}{2\pi T}\right)^{1/4} \frac{1}{\sqrt{2^{n-1}(n-1)!}} H_{n-1}(\xi_{\mathrm{I}}) e^{-\xi_{\mathrm{I}}^2/2}$$

$$\lambda_n^{\mathrm{II}} = k_{\mathrm{II}} n, \quad \varphi_n^{\mathrm{II}}(x) = \left(\frac{k_{\mathrm{II}}}{2\pi T}\right)^{1/4} \frac{1}{\sqrt{2^{n-1}(n-1)!}} H_{n-1}(\xi_{\mathrm{II}}) e^{-\xi_{\mathrm{II}}^2/2},$$

$$\lambda_n^{\mathrm{III}} = k_{\mathrm{III}}(n-1), \quad \varphi_n^{\mathrm{III}}(x) = \left(\frac{k_{\mathrm{I}}}{2\pi T}\right)^{1/4} \frac{1}{\sqrt{2^{n-1}(n-1)!}} H_{n-1}(\xi_{\mathrm{III}}) e^{-\xi_{\mathrm{III}}^2/2}$$

n=1,2,…; n=2 is the slowest eigenmode.

$$\xi_{\mathrm{I}} := \sqrt{k_{\mathrm{I}}/T}(x+1),\ \xi_{\mathrm{II}} := \sqrt{k_{\mathrm{II}}/T}x, \text{ and } \xi_{\mathrm{III}} := \sqrt{k_{\mathrm{III}}/T}(x-\alpha)$$

$H_m(x)$ is the Hermite polynomial

The explicit a_2

- We can obtain the explicit a_2 and $\partial a_2/\partial\beta_i$

$$\overline{a_2}(\beta_i) = \frac{e^{-\frac{\beta_i k_\mathrm{I} k_\mathrm{II}^2}{2(k_\mathrm{I}+k_\mathrm{II})^2}}\left[k_\mathrm{I}(k_\mathrm{II}+k_\mathrm{III})\exp\left[\frac{1}{2}\beta_i k_\mathrm{II}\left(\frac{\alpha^2 k_\mathrm{III}^2}{(k_\mathrm{II}+k_\mathrm{III})^2}-\frac{k_\mathrm{I}^2}{(k_\mathrm{I}+k_\mathrm{II}^2)}\right)\right]-k_\mathrm{III}(k_\mathrm{I}+k_\mathrm{II})\right]}{\beta_i k_\mathrm{I} k_\mathrm{II} k_\mathrm{III}},$$

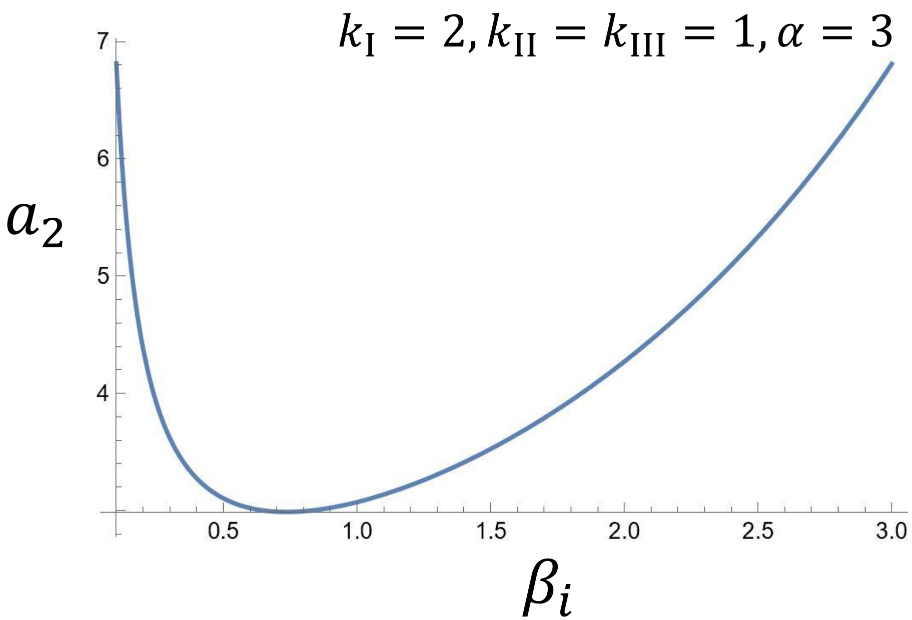
$$\text{where } \overline{a_2}(\beta_i) := a_2/A_\mathrm{I}\left(\frac{k_\mathrm{I}}{T}\right)^{3/4}$$

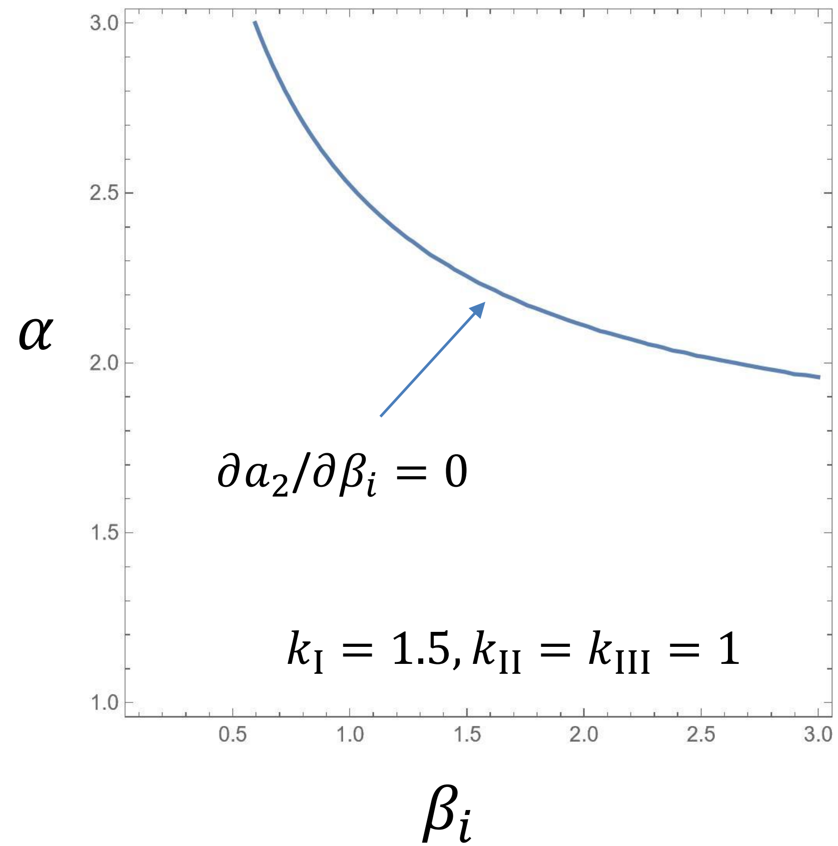
$$\frac{\partial\overline{a}_2(\beta_i)}{\partial\beta_i} = \frac{e^{-\frac{\beta_i k_\mathrm{I} k_\mathrm{II}^2}{2(k_\mathrm{I}+k_\mathrm{II})^2}}A_1 - \exp\left[\frac{1}{2}\beta_i k_\mathrm{II}\left(\frac{\alpha^2 k_\mathrm{III}^2}{(k_\mathrm{II}+k_\mathrm{III})^2}-\frac{k_\mathrm{I}^2}{(k_\mathrm{I}+k_\mathrm{II}^2)}\right)\right]A_2 + A_3}{2\beta_i^2 k_\mathrm{I} k_\mathrm{II} k_\mathrm{III}(k_\mathrm{I}+k_\mathrm{II})(k_\mathrm{II}+k_\mathrm{III})}$$

We can determine A_i with $i = 1,2,3$.

Results (1)

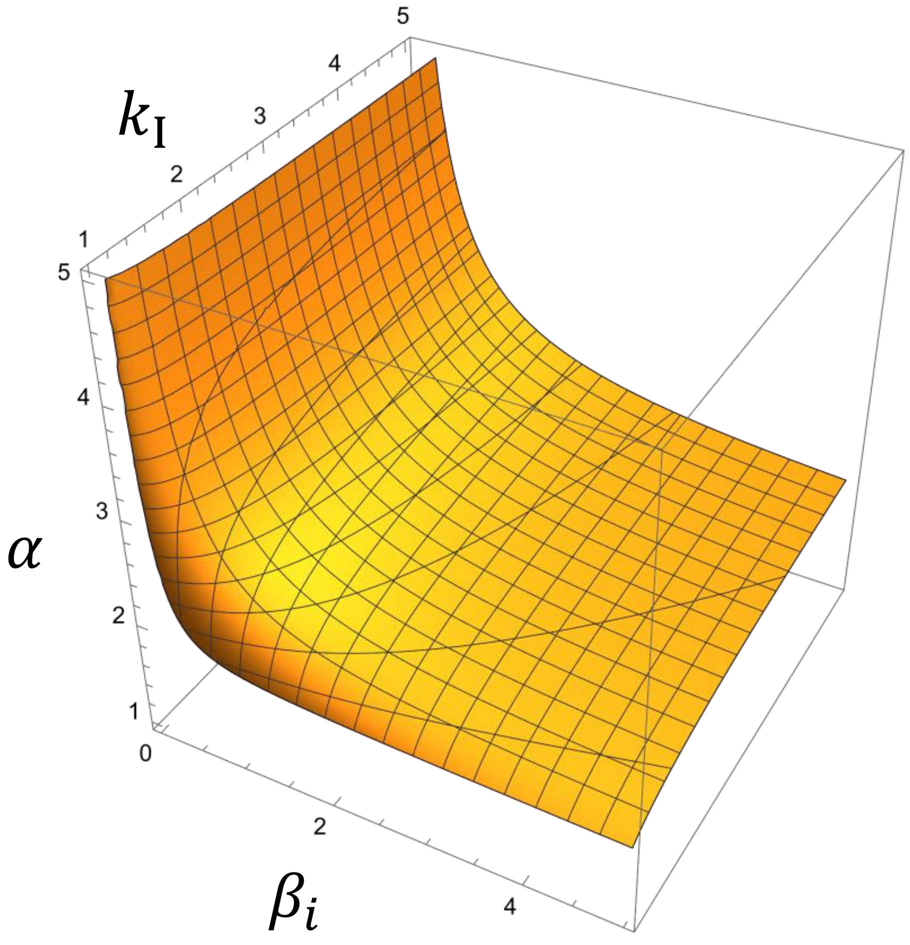
- We find there is the minimum for a_2 if $k_{\mathrm{I}} > 1$.





Result (2)

- Figure is the hyper-surface of $\partial a_2/\partial \beta_i = 0$ in the parameter space $(\beta_i, k_{\mathrm{I}}, \alpha)$.
- This surface indicates the existence of the Mpemba effect.



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Summary

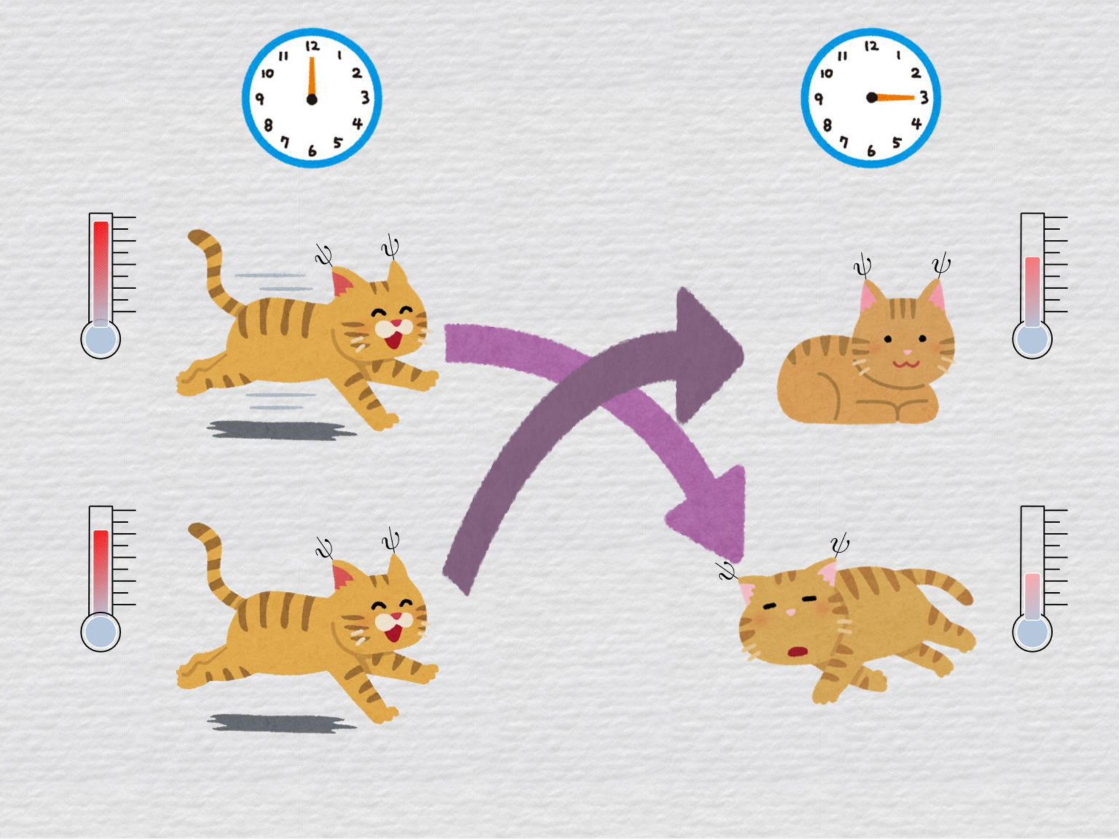
- We solved two bistable potential models using Fokker-Planck equation with relatively precise and simple analytic calculation.
- The asymmetricity of the potential is important.

Future directions

- We need to clarify the general condition for MPE starting from two equilibrium initial conditions.
  - Ohga et al. obtained some interesting results.
- How can we extend this analysis to quantum systems?
  - It is obvious that this is related to a problem of tunneling effect.
  - If we consider a non-Hermitian Hamiltonian, we can argue a relaxation process as the MPE.

Direct application to QMPE

- Listen to the next talk!



Thank you for your attention.

Quantum Mpemba effect

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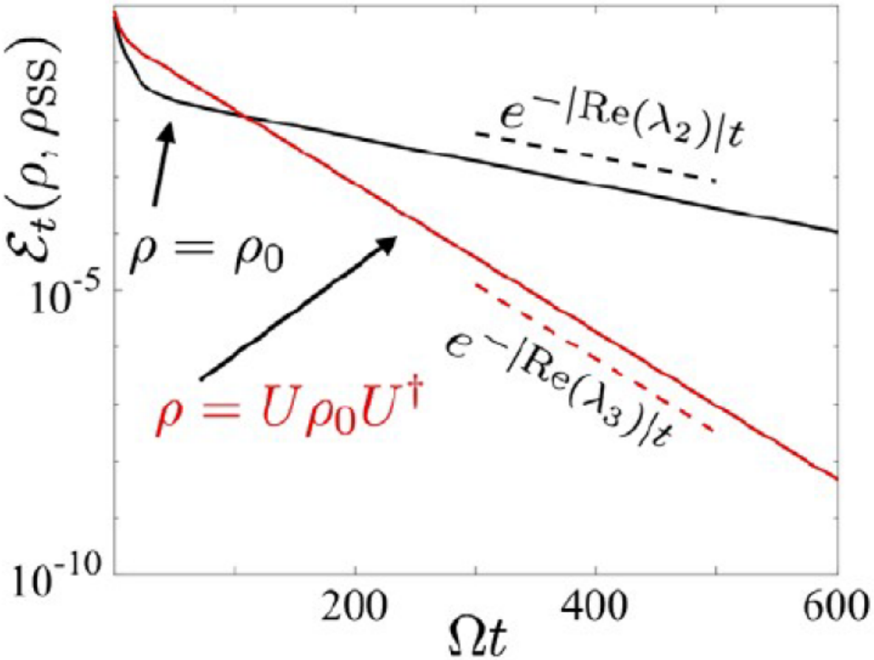
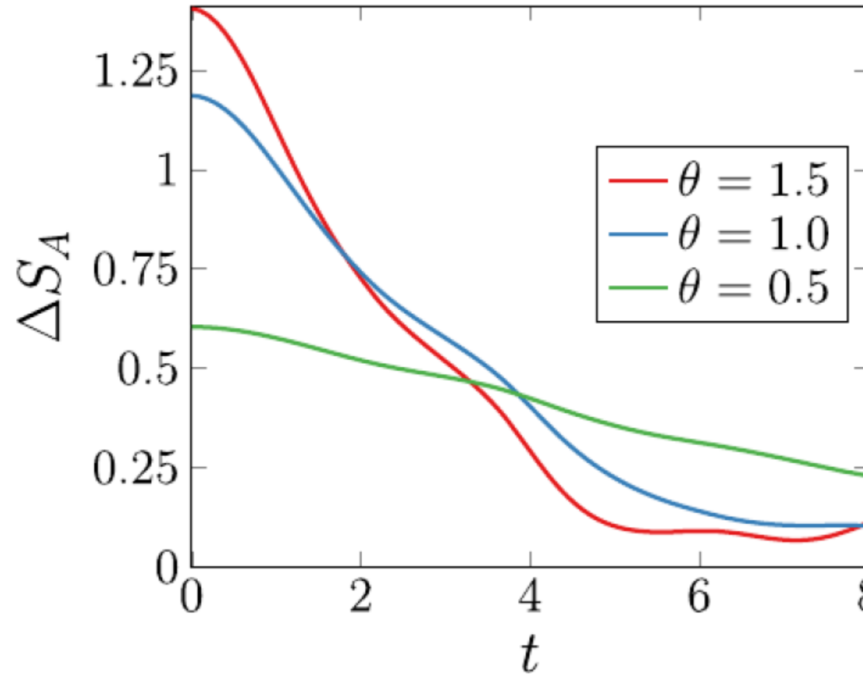


Distance from equilibrium in dissipative Dicke model



Entangle asymmetry in XXZ spin chain

[Carollo, Lasanta and Lesanovsky, PRL 127, 060401 (2021)]

[Ares, Murciano and Calabrese, Nature Communications 14, 2036 (2023)]