“Numerically Exact” Methods for Open Quantum Dynamics: Applications to Low-Energy Nuclear Reactions

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Special thanks to
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Kazuki Okada
Shoki Koyanagi
Angela Riva

Overview

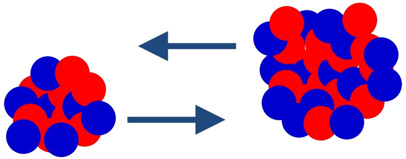
Conventional master equations: Born-Markov approximation

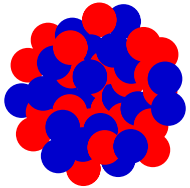
"Numerically exact" = Non-perturbative, non-Markovian

Bath oscillator model (Caldeira-Leggett model)

Low-energy nuclear reactions (fusion & fission)

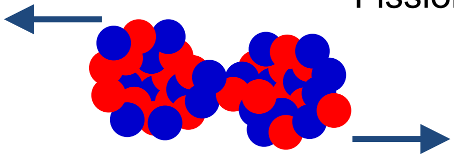
<u>Dissipative quantum tunneling</u>





Fusion!

Fission!



I will focus on methodologies ..

Perhaps inapplicable to your problems …

- Good to know what we can do in a simple setting
- You can play with it!

Outline

- **Why OQS for low-energy nuclear reactions?** (7 slides)

— Why quantum? — Why open? — Classical Langevin approach

- **Bath oscillator model** (4 slides)

— Thermalization — Quantum Brownian motion

- **Method 1: HEOM, pseudomode** (9 slides)

— Introduction — Application to fission

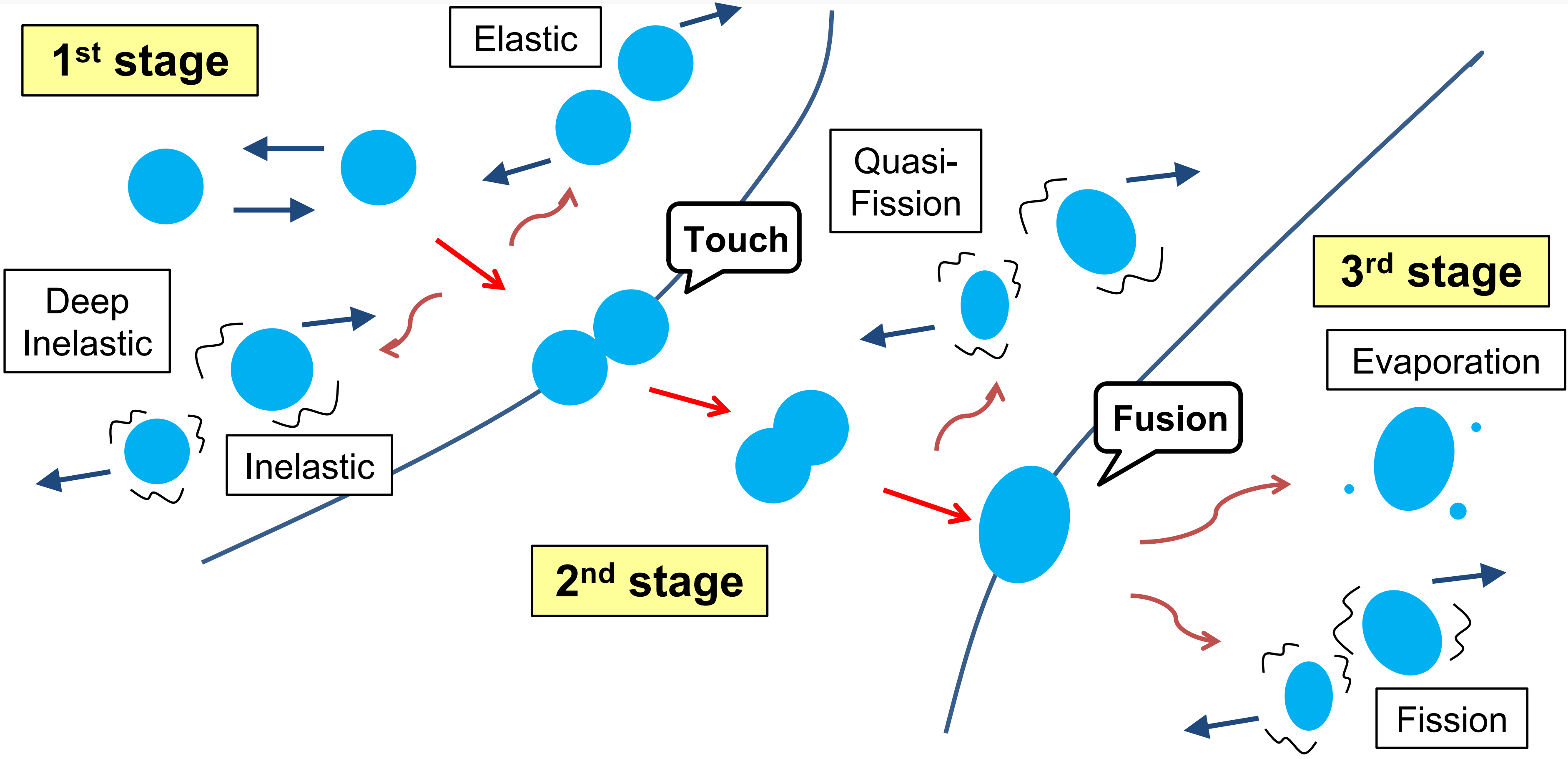
- **Method 2: TEDOPA** (5 slides)

— Introduction — Application to fusion

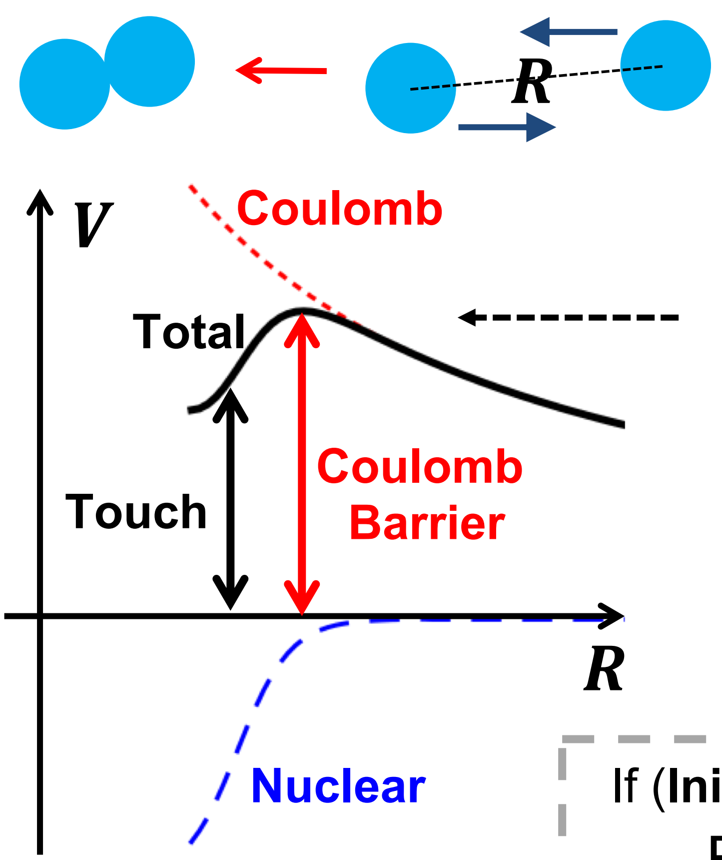
- **Summary**

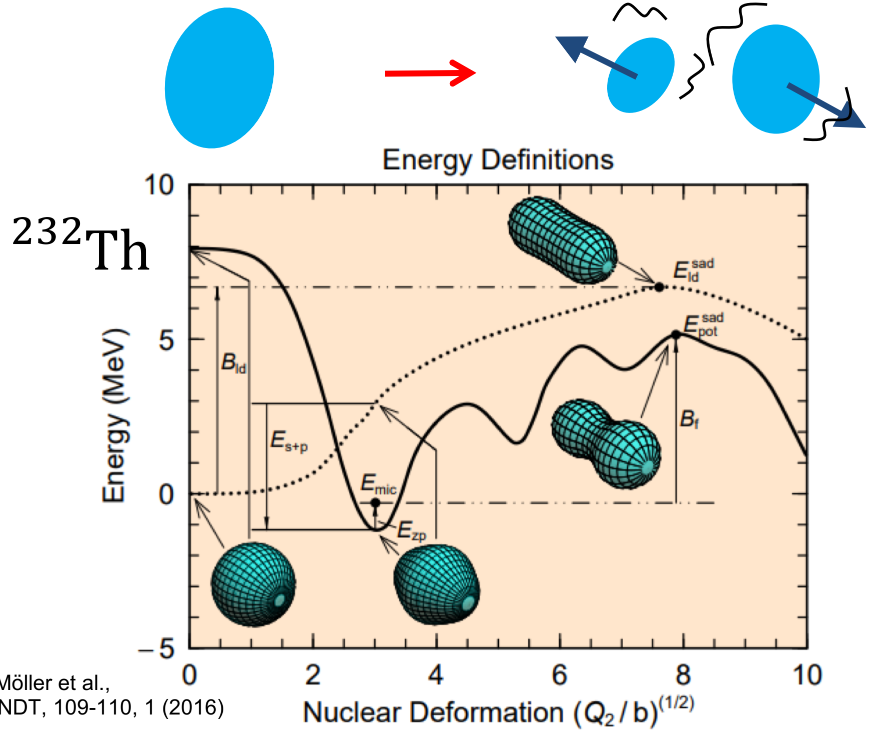
Outline

3 stages


1st stage
Elastic
Deep Inelastic
Inelastic
Touch
Quasi-Fission
2nd stage
Fusion
3rd stage
Evaporation
Fission

Why quantum ? (quantum tunneling at low-energy)



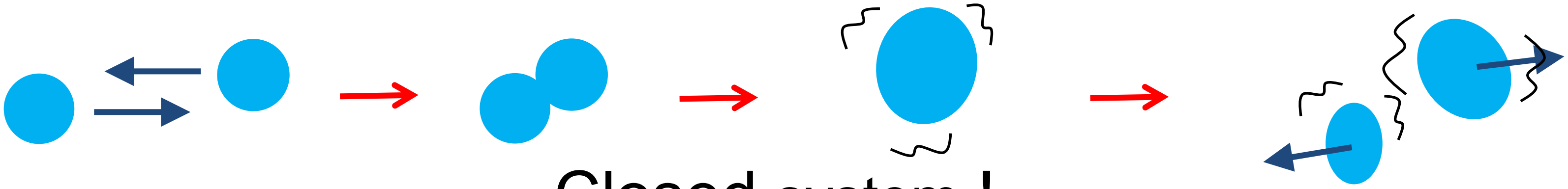


P. Möller et al.,
ADNDT, 109-110, 1 (2016)

If (**Initial energy**) < (**Barrier**) …

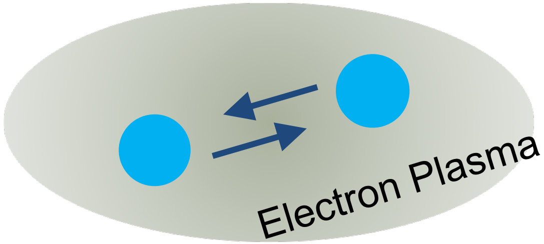
Reaction through **Quantum Tunneling**

Why open ? (phenomenological treatment of excitations)



Closed system !

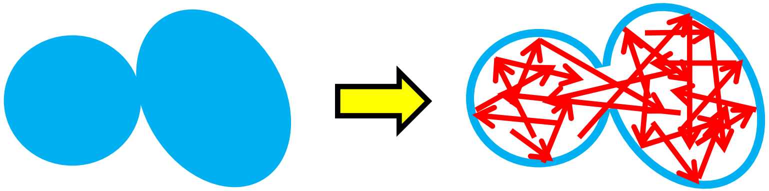
❖ **Nuclear reactions in a dense electron plasma**



Effects of surrounding electrons on the reaction rate ?

Iain Lee and Alexis Diaz-Torres, Phys. Lett. B**827** (2022) 136970
D. A. Baiko, MNRAS **508** (2021) 2134

➢ **Macroscopic approach**



Phenomenological description of complex internal excitations

D. A. Bromley, Treatise on Heavy-Ion Science Volume 2, (Plenum Press New York, 1984)
P. Frobrich and R. Lipperheide, Theory of Nuclear Reactions, (Oxford University Press, 1996)

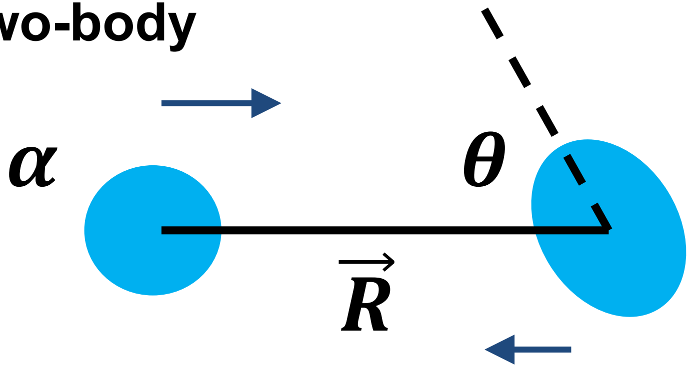
Collective coordinates

Macroscopic approach:

Select coordinates relevant to the dynamics ⟺ Microscopic approach:
Based on nucleonic degrees of freedom

(Collective coordinates)

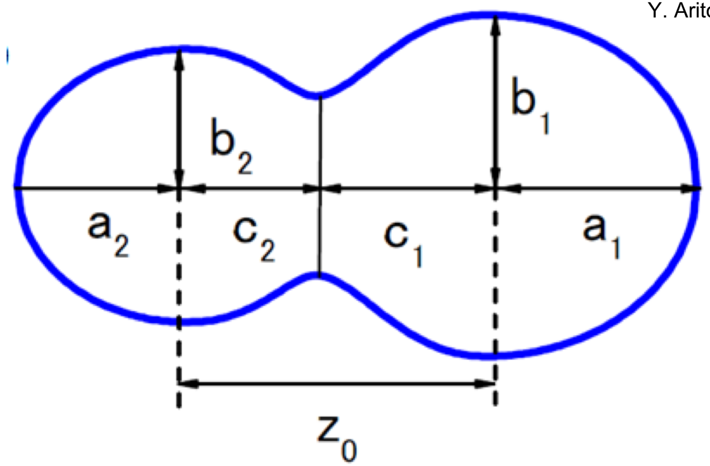
Two-body



$\vec{R}$: Relative motion
α: Surface vibration
θ: Rotation angle

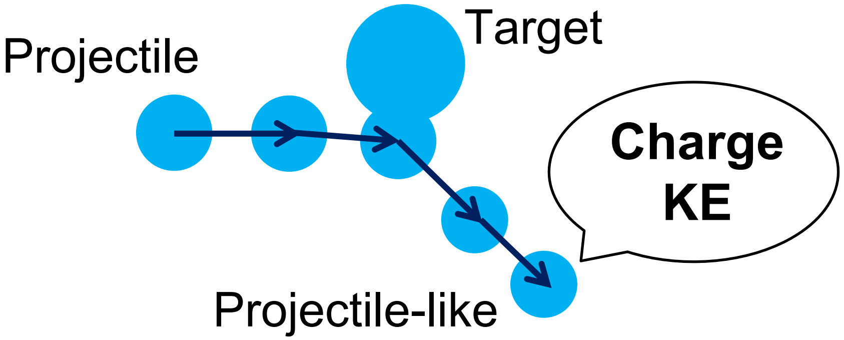
Mononucleus

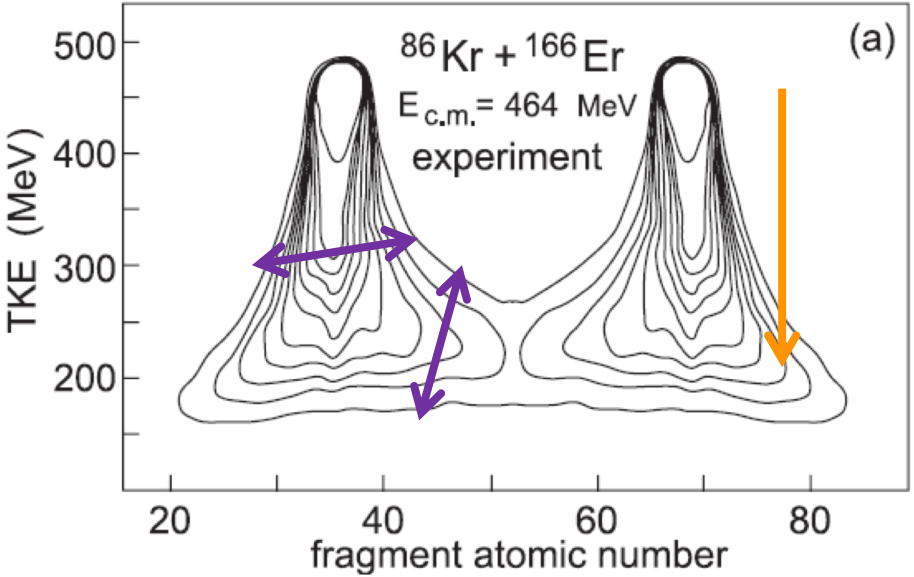
Y. Aritomo's slide



Shape coordinates

Dissipation and fluctuation





V. Zagrebaev & W. Greiner, J. Phys. G: Nucl. Part. Phys. **31,** 825 (2005)

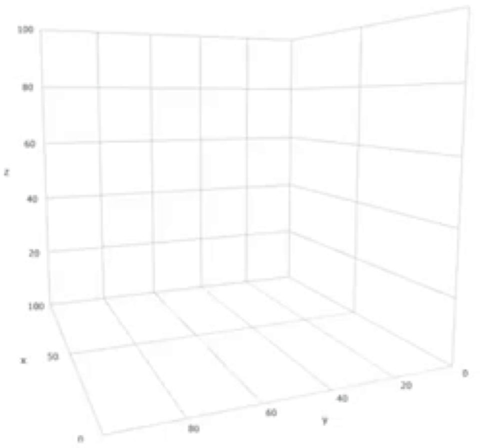
✓Energy dissipation

✓Fluctuation

Phenomenologically

Classical Langevin equation

https://www.youtube.com/watch?v=7A83IXbs6Ik



Collective coordinate(s): Q

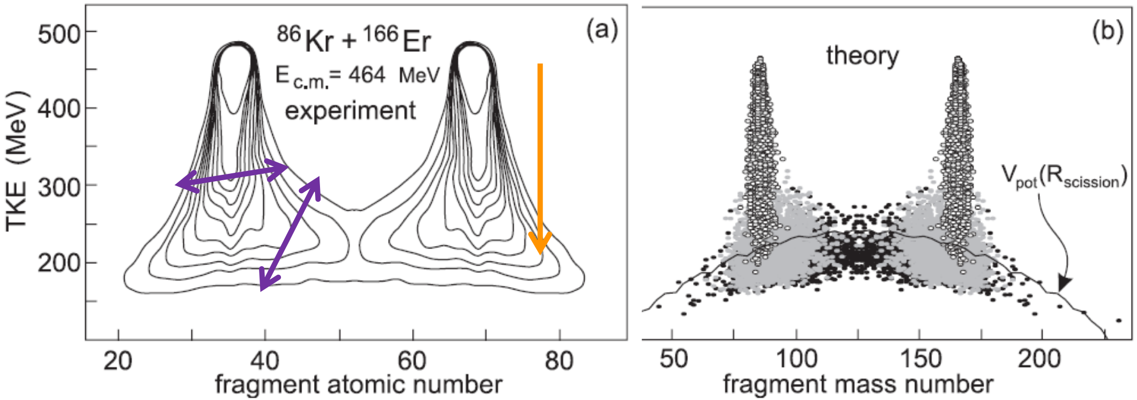
$$\begin{cases} \dot{Q} = P/M \\ \dot{P} = -V'(Q) - \underline{\gamma P} + \underline{\zeta(t)} \end{cases}$$

Energy dissipation

Fluctuation

$$\begin{cases} \langle \zeta(t) \rangle = 0 \\ \langle \zeta(t)\zeta(s) \rangle = (2M\gamma/\beta)\delta(t-s) \end{cases}$$

V. Zagrebaev & W. Greiner, J. Phys. G: Nucl. Part. Phys. **31,** 825 (2005)



Applicability:
- Deep inelastic
- Fusion
- Fission
- Quasi fission

at high energies

Goal Unified description of low-energy nuclear reactions

(from low to high energies)

✓ Low energy: Quantum mechanics

✓ High energy: Dissipation and fluctuation

Quantum mechanical description of dissipation and fluctuation

(OQS approach to low-energy nuclear reactions)

System: Collective motion

Bath: Internal motion

Outline

Bath oscillator model

Harmonic oscillator bath

R. P. Feynman & F. L. Vernon, Jr., Ann. Phys. 24, 118 (1963); P. Ullersma, Physica 32, 27 (1966); A. O. Caldeira & A. J. Leggett, Ann. Phys. 149, 374 (1983); G. W. Ford, J. T. Lewis, & R. F. O'Connell, Phys. Rev. A 37, 4419 (1988); U. Weiss, Quantum Dissipative Systems (World Scientific, Singapore, 2008)

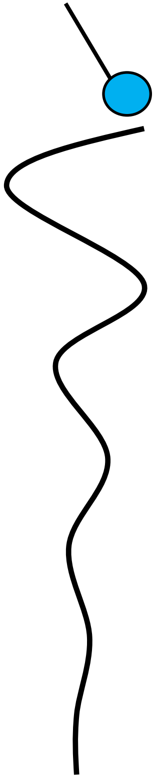
$$H = \frac{P^2}{2M} + V(Q) + \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2}{2} \left(q_i - \frac{c_i}{m_i \omega_i^2} h(Q) \right)^2 \right]$$

$$= H_S + H_B + H_I \quad \begin{cases} H_S = \underbrace{\frac{P^2}{2M} + V(Q)}_{H_{S,\mathrm{eff}}} + h^2(Q) \sum_i \frac{c_i^2}{2m_i \omega_i^2} \\ H_B = \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2 q_i^2}{2} \right], \quad H_I = -h(Q) \cdot \sum_i c_i q_i \end{cases}$$

Spectral density: $J(\omega) = \frac{\pi}{2} \sum_i \frac{c_i^2}{m_i \omega_i} [\delta(\omega - \omega_i) - \delta(\omega + \omega_i)]$

Assumed to be a smooth function of ω (continuous distribution)

Thermalization



Relaxation: steady state?

H. Grabert, P. Schramm, & G-L Ingold, Physics Reports 168, 115 (1988)
Y. Tanimura, J. Chem. Phys. 141, 044114 (2014)
A. S. Trushechkin, M. Merkli, J. D. Cresser, & J. Anders, AVS Quantum Sci. 4, 012301 (2022)

Empirically known …

Let $\rho(0) = \rho_S(0) \otimes \overbrace{\exp(-\beta H_B)/\blacksquare}^{\rho_{B,\mathrm{G}}}$. If

- $\lim\limits_{t\to\infty} \frac{d}{dt}\rho_S(t) = 0$ (Existence of steady state)
- $\lim\limits_{t\to\infty} \rho_S(t)$ is independent of $\rho_S(0)$ (Uniqueness),

Smooth $J(\omega)$ (?)

No system symmetry (?)

then

Mean-**F**orce **G**ibbs state

$$\lim_{t\to\infty} \rho_S(t) = \mathrm{tr}_B[\exp(-\beta H)]/\blacksquare = \rho_{S,\mathrm{MFG}}$$

⟹ Thermalization!

※ Noneq quantum thermodynamics:

S. Koyanagi & Y. Tanimura, J. Chem. Phys. 161, 114113 (2024)
M. T., arXiv:2511.15084 [quant-ph]

Remarks

- ➢ Classically, $\rho_{S,\mathrm{MFG}} = \exp\left(-\beta H_{S,\mathrm{eff}}\right)/\blacksquare$. No longer the case in the quantum treatment.
- ➢ It doesn't imply $\lim\limits_{t\to\infty} \rho(t) = \exp(-\beta H)\,/\blacksquare$ (later).

Langevin equation: General form

Classical e.o.m

$$\dot{P}(t) = -\frac{\partial H}{\partial Q}, \quad \dot{p}_i(t) = -\frac{\partial H}{\partial q_i}$$

① Solve it formally

② Inserting the solution

③ Then …

$$\dot{P}(t) = \underbrace{-V'(Q(t))}_{\text{Potential}} \underbrace{- \int_0^t ds\, \eta(t,s) P(s)}_{\text{Frictional force}} + h'\big(Q(t)\big)\Big[\underbrace{\zeta(t)}_{\text{Random force}} - \Delta(t) h\big(Q(0)\big)\Big]$$

$$\eta(t,s) = \frac{\Delta(t-s)}{M} h'\big(Q(t)\big) h'\big(Q(s)\big), \qquad \Delta(t) = \frac{2}{\pi}\int_0^\infty d\omega\, \frac{J(\omega)}{\omega}\cos(\omega t)$$

$$\zeta(t) = \sum_i c_i \left[q_i(0)\cos(\omega_i t) + \frac{p_i(0)}{m_i \omega_i}\sin(\omega_i t)\right]$$

Langevin equation: Brownian motion

$$\eta(t,s) = \frac{\Delta(t-s)}{M} h'(Q(t))h'(Q(s)),\ \ \Delta(t) = \frac{2}{\pi}\int_0^\infty d\omega\ \frac{J(\omega)}{\omega}\cos(\omega t)$$

$$\dot{P}(t) = \underbrace{-V'(Q(t))}_{\text{Potential}} - \underbrace{\int_0^t ds\, \eta(t,s)P(s) + h'(Q(t))}_{\text{Frictional force}}[\underbrace{\zeta(t)}_{\text{Random force}} - \Delta(t)h(Q(0))]$$

Initial product state: $\rho(0) = \rho_S(0) \otimes \rho_{B,\mathrm{G}}$

$$\begin{cases} \mathrm{tr}[\zeta(t)\rho_{B,\mathrm{G}}] = 0 \\ \mathrm{tr}[\zeta(t)\zeta(s)\rho_{B,\mathrm{G}}] = \Delta(t-s)/\beta \\ \zeta(t)\text{: Gaussian} \end{cases}$$

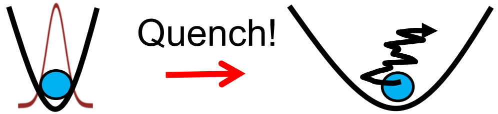
Let $J(\omega) = M\gamma\omega$ (Ohmic) and $h(Q) = Q$.
Then $\Delta(t) = 2M\gamma\delta(t)$ and, for $t > 0$,

$$\begin{cases} \dot{P}(t) = -V'(Q(t)) - \gamma P(t) + \zeta(t) \\ \mathrm{tr}[\zeta(t)\zeta(s)\rho_{B,\mathrm{G}}] = (2M\gamma/\beta)\delta(t-s) \end{cases} \Rightarrow$$

Brownian motion!

※ $\rho(0) = \exp(-\beta(H_S' + H_B + H_I))/\blacksquare$

e.g.



$$H_S' = \frac{P^2}{2M} + \frac{M\Omega'^2 Q^2}{2} \qquad H_S = \frac{P^2}{2M} + \frac{M\Omega^2 Q^2}{2}$$

$$\xi(t) = \zeta(t) - \Delta(t)h(Q(0))$$

$$\mathrm{tr}[\xi(t)\rho(0)] = 0$$

$$\mathrm{tr}[\xi(t)\xi(s)\rho(0)] = \Delta(t-s)/\beta$$

U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 2008)

Quantum mechanical treatment …

Quantum Brownian motion!

Outline

Influence functional

Initial product state: $\rho(0) = \rho_S(0) \otimes \rho_{B,\mathrm{G}}$

$$\rho_S(Q_a, Q_b; t) = \int dQ_c dQ_d\, \mathcal{J}_S(Q_aQ_b, Q_cQ_d; t)\rho_S(Q_c, Q_d; t = 0)$$

Path integral representation:

Isolated system

$$\mathcal{J}_S(Q_aQ_b, Q_cQ_d; t) = \int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[\bar{Q}]\}/\hbar}$$

➡

Open system R. P. Feynman & F. L. Vernon, Jr., Ann. Phys. 24, 118 (1963)

$$\mathcal{J}_S(Q_aQ_b, Q_cQ_d; t) = \int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[\bar{Q}]\}/\hbar} e^{-\Phi[Q,\bar{Q}]/\hbar}$$

Influence of the bath

Bath oscillator model ($H = H_S + H_B - h \cdot X_B$ with $H_B = \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2 q_i^2}{2}\right]$ & $X_B = \sum_i c_i q_i$)

$$\Phi[Q, \bar{Q}] = \int_0^t d\tau \int_0^\tau ds\, \{h(Q(\tau)) - h(\bar{Q}(\tau))\}\{L(\tau - s)h(Q(s)) - L^*(\tau - s)h(\bar{Q}(s))\}$$

where

Bath correlation function

$$L(t) = \frac{1}{\hbar}\mathrm{tr}_B\left[X_B^I(t)X_B\rho_{B,\mathrm{G}}\right]$$
$$= \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\{\coth(\beta\hbar\omega/2)\cos(\omega t) - i\sin(\omega t)\}$$

Heisenberg e.o.m ($h(Q) = Q$ for simplicity): $\Delta(t) = \frac{2}{\pi}\int_0^\infty d\omega\,\frac{J(\omega)}{\omega}\cos(\omega t)$

$$\dot{P}^H(t) = -V'\left(Q^H(t)\right) - \frac{1}{M}\int_0^t ds\,\Delta(t-s)P^H(s) + [\zeta(t) - \Delta(t)h(Q)]$$

Frictional force: $\dot{\Delta}(t) = 2\mathrm{Im}[L(t)]$

Random force: $\mathrm{tr}_B\left[\frac{[\zeta(t),\zeta(s)]_+}{2}\rho_{B,\mathrm{G}}\right] = \hbar\mathrm{Re}[L(t)]$

Fourier transform

$\Rightarrow$ $\mathcal{F}\left[\hbar\mathrm{Re}[L]\right](\omega) = \frac{\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)\mathcal{F}[\Delta](\omega)$

(Quantum) Fluctuation-dissipation relation

- High temperature limit ($\beta\hbar \to 0$) yields $\hbar\omega/2\coth(\beta\hbar\omega/2) \sim 1/\beta$, and we recover
$$\mathrm{tr}_B\left[\frac{[\zeta(t),\zeta(s)]_+}{2}\rho_{B,\mathrm{G}}\right] = \frac{\Delta(t-s)}{\beta}$$
- Physically impossible for both $\Delta(t)$ and $\mathrm{Re}[L(t)]$ to be delta functional simultaneously.

Quantum processes are fundamentally non-Markovian!

High temperature limit

$\mathcal{J}_S(Q_aQ_b, Q_cQ_d; t) =$
$\int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[Q]\}/\hbar} e^{-\Phi[Q,Q]/\hbar}$
$\Phi[Q,\bar{Q}] = \int_0^t d\tau \int_0^\tau ds \{h(Q(\tau)) - h(\bar{Q}(\tau))\}$
$\times\{L(\tau-s)h(Q(s)) - L^*(\tau-s)h(\bar{Q}(s))\}$

Markovian case

A. O. Caldeira & A. J. Leggett, Physica 121, 587 (1983)

$$\Delta(t) = 2M\gamma\delta(t)\ (J(\omega) = M\gamma\omega) \Longrightarrow L(t) \simeq M\gamma(2\delta(t)/\beta\hbar + i\dot{\delta}(t))$$

$$\Phi[Q,\bar{Q}] = \int_0^t d\tau\, f(Q(\tau), \bar{Q}(\tau))$$

$$\frac{d}{dt}\mathcal{J}_S(Q_aQ_b, Q_cQ_d; t) = \int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[\bar{Q}]\}/\hbar} e^{-\Phi[Q,\bar{Q}]/\hbar} \underline{\left[\frac{i}{\hbar}\{L_S(Q(t)) - L_S(\bar{Q}(t))\} - \frac{1}{\hbar} f(Q(t), \bar{Q}(t))\right]}$$

This part can be taken outside

Closed equation for $\rho_S(t)$ (Caldeira-Leggett master equation)

Non-Markovian case

Y. Tanimura, J. Phys. Soc. Jpn. 75, 082001 (2006)

$$\Delta(t) = 2\lambda e^{-\gamma|t|}\ (J(\omega) = 2\lambda\gamma\omega/(\gamma^2+\omega^2)\ ) \Longrightarrow L(t \geq 0) \simeq c e^{-\gamma t}\ (c = \lambda\gamma(2/\beta\hbar\gamma - i))$$

$$\Phi[Q,\bar{Q}] = \int_0^t d\tau \{h(Q(\tau)) - h(\bar{Q}(\tau))\} y[Q,\bar{Q},\tau], \quad y[Q,\bar{Q},\tau] = \int_0^\tau ds\, e^{-\gamma(\tau-s)}\{c\, h(Q(s)) - c^* h(\bar{Q}(s))\}$$

$$\frac{d}{dt}\mathcal{J}_S(Q_aQ_b, Q_cQ_d; t) = \int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[\bar{Q}]\}/\hbar} e^{-\Phi[Q,\bar{Q}]/\hbar}$$
$$\times\left[\frac{i}{\hbar}\{L_S(Q(t)) - L_S(\bar{Q}(t))\} - \frac{1}{\hbar}\{h(Q(t)) - h(\bar{Q}(t))\}\underbrace{y[Q,\bar{Q},t]}\right]$$

Not Closed!

This part cannot be taken outside

$$y[Q,\bar{Q},t] = \int_0^t ds\, e^{-\gamma(t-s)} \times\{c\, h(Q(s)) - c^* h(\bar{Q}(s))\}$$

Introducing auxiliary quantities to close the equation!

- $\rho_{n\in\mathbb{Z}_{\geq 0}}(Q_a, Q_b; t) = \int dQ_c dQ_d\, \mathcal{J}_n(Q_a Q_b, Q_c Q_d; t)\rho_S(Q_c, Q_d; t=0)$
- $\mathcal{J}_{n\in\mathbb{Z}_{\geq 0}}(Q_a Q_b, Q_c Q_d; t) = \int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[\bar{Q}]\}/\hbar} e^{-\Phi[Q,\bar{Q}]/\hbar} \frac{[y[Q,\bar{Q},t]]^n}{\sqrt{n!}}$

$$\Rightarrow \quad \rho_0(t) = \rho_S(t) \qquad \rho_n(0) = \begin{cases} \rho_S(0) & (n=0) \\ 0 & (n>0) \end{cases}$$

$$\frac{d}{dt} y = -\gamma y + [c\, h(Q(t)) - c^* h(\bar{Q}(t))]$$

$$\frac{d}{dt}\mathcal{J}_n(Q_a Q_b, Q_c Q_d; t) = \int D[Q] \int D[\bar{Q}]\, e^{i\{S_S[Q]-S_S[\bar{Q}]\}/\hbar} e^{-\Phi[Q,\bar{Q}]/\hbar}$$

$$\times\left[\left(\frac{i}{\hbar}\{L_S(Q(t)) - L_S(\bar{Q}(t))\} - n\gamma\right)\underbrace{\frac{[y[Q,\bar{Q},t]]^n}{\sqrt{n!}}}_{\mathcal{J}_n} - \frac{\sqrt{n+1}}{\hbar}\{h(Q(t)) - h(\bar{Q}(t))\}\underbrace{\frac{[y[Q,\bar{Q},t]]^{n+1}}{\sqrt{(n+1)!}}}_{\mathcal{J}_{n+1}} + \sqrt{n}[c\, h(Q(t)) - c^* h(\bar{Q}(t))]\underbrace{\frac{[y[Q,\bar{Q},t]]^{n-1}}{\sqrt{(n-1)!}}}_{\mathcal{J}_{n-1}}\right]$$

$$\frac{d}{dt}\rho_n(t) = -\frac{i}{\hbar}[H_S, \rho_n(t)] - n\gamma\rho_n(t) - \frac{\sqrt{n+1}}{\hbar}[h, \rho_{n+1}(t)] + \sqrt{n}[c\, h\rho_{n-1}(t) - c^*\rho_{n-1}(t)h]$$

Hierarchical Equations Of Motion (HEOM)

Y. Tanimura & R. Kubo, J. Phys. Soc. Jpn. 58, 101 (1989)
Y. Tanimura, J. Phys. Soc. Jpn. 75, 082001 (2006)

Markovian embedding

Classical e.o.m ($h(Q) = Q$ for simplicity)

$$\dot{P}(t) = -V'\big(Q(t)\big) - \int_0^t ds\, \Delta(t-s)\frac{P(s)}{M} + [\zeta(t) - \Delta(t)Q(0)]$$

$$\mathrm{tr}\big[\zeta(t)\zeta(s)\rho_{B,\mathrm{G}}\big] = \Delta(t-s)/\beta$$

$\frac{P(s)}{M} = \frac{d}{ds}Q(s)$ and $\int_0^t ds\, \Delta(t-s)\frac{P(s)}{M} = \Delta(0)Q(t) - \Delta(t)Q(0) + \int_0^t ds\, \dot{\Delta}(t-s)Q(s)$

$$\dot{P}(t) = -U'\big(Q(t)\big) + X(t) \quad \begin{cases} U(Q) = V(Q) - \Delta(0)Q^2/2 \\ X(t) = \zeta(t) - \int_0^t ds\, \dot{\Delta}(t-s)Q(s) \end{cases}$$

When $\Delta(t) = 2\lambda e^{-\gamma|t|}$ …

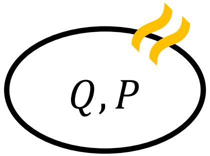
$$\dot{X}(t) = -\gamma X(t) + 2\lambda\gamma Q(t) + \zeta_D(t)$$

where $\zeta_D(t) = \dot{\zeta}(t) + \gamma\zeta(t)$ satisfies

$$\mathrm{tr}\big[\zeta_D(t)\zeta_D(s)\rho_{B,\mathrm{G}}\big] = (\lambda\gamma/\beta)\delta(t-s)$$

Markovian!

Non-Markovian bath

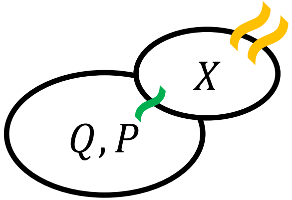


$\dot{Q}(t) = \cdots$

$\dot{P}(t) = \cdots + \zeta(t)$

$\mathrm{tr}\big[\zeta(t)\zeta(s)\rho_{B,\mathrm{G}}\big] \propto e^{-\gamma|t-s|}$

Markovian bath



$\dot{Q}(t) = \cdots,\quad \dot{P}(t) = \cdots + \boldsymbol{X(t)}$

$\dot{X}(t) = \cdots + \boldsymbol{\zeta_D(t)}$

$\mathrm{tr}\big[\zeta_D(t)\zeta_D(s)\rho_{B,\mathrm{G}}\big] \propto \delta(t-s)$

Pseudomode

Alternatively, we can design the extended space …

$$\mathcal{D}[L]\blacksquare = L\blacksquare L^\dagger - \left(L^\dagger L\blacksquare + \blacksquare L^\dagger L\right)/2$$

$$\frac{d}{dt}\varrho(t) = -\frac{i}{\hbar}\left[H_S - h\cdot X_{ps}, \varrho(t)\right] + \mathcal{L}_{ps}\varrho(t) \quad \begin{cases} \mathcal{L}_{ps}\varrho = \sum_{k=1}^{K}\left\{-i\left[\omega_k b_k^\dagger b_k, \varrho\right] + 2\kappa_k \mathcal{D}[b_k]\varrho\right\} \\ X_{ps} = \sum_{k=1}^{K} g_k\left(b_k^\dagger + b_k\right) \end{cases}$$

Initial state: $\varrho(t) = \rho_S(0)\otimes|\mathbf{0}\rangle\langle\mathbf{0}|$

$$\Phi[Q,\bar{Q}] = \int_0^t d\tau \int_0^\tau ds\,\{h(Q(\tau)) - h(\bar{Q}(\tau))\} \times\{L(\tau-s)h(Q(s)) - L^*(\tau-s)h(\bar{Q}(s))\}$$

We can similarly derive the Influence functional, which takes the same Gaussian form but with

$$L(t)\to C(t\geq 0) = \frac{1}{\hbar}\mathrm{tr}_{ps}\left[X_{ps}e^{\mathcal{L}_{ps}t}\left(X_{ps}|\mathbf{0}\rangle\langle\mathbf{0}|\right)\right] = \frac{1}{\hbar}\sum_{k=1}^{K} g_k^2 e^{-(\kappa_k + i\omega_k)t}$$

If $C(t) = L(t)$, then $\rho_S(t) = \mathrm{tr}_{ps}[\varrho(t)]$!

D. Tamascelli, A. Smirne, S. F. Huelga, M. B. Plenio, Phys. Rev. Lett. 120, 030402 (2018)

Testing $L(t)$

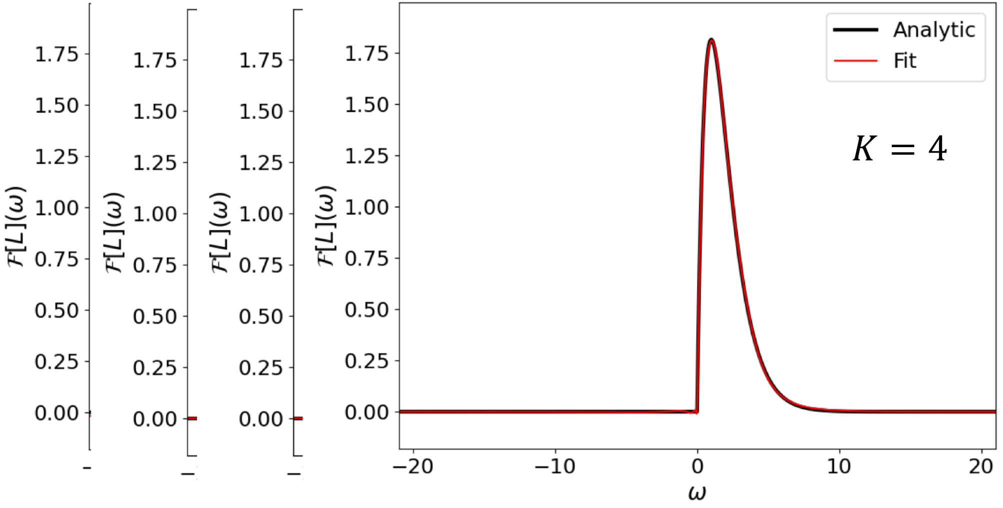
$$L(t) = \sum_{k=1}^{K} d_k e^{-z_k t} \quad (d_k, z_k \in \mathbb{C}) \quad \text{or} \quad \frac{2J(\omega)}{1-e^{-\beta\hbar\omega}} = \mathcal{F}[L](\omega) = \sum_{k=1}^{K} 2\mathrm{Re}\left[\frac{d_k}{z_k - i\omega}\right]$$

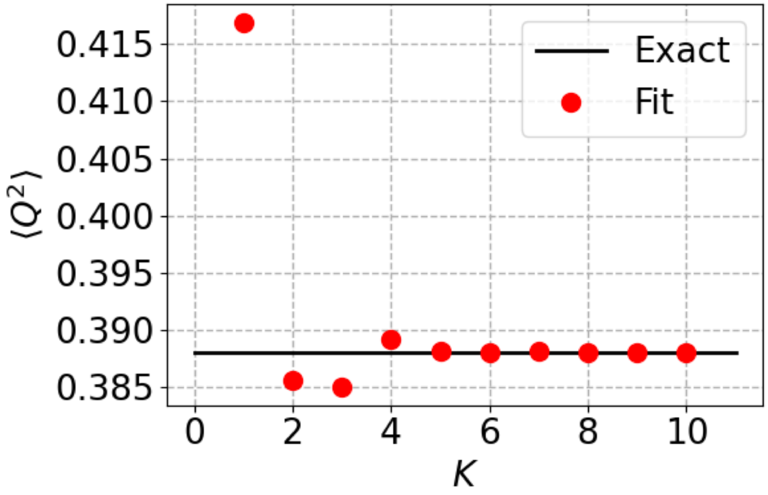
Various fitting methods …

M. Xu, Y. Yan, Q. Shi, J. Ankerhold, & J. T. Stockburger, Phys. Rev. Lett. 129, 230601 (2022)
H. Takahashi, S. Rudge, C. Kaspar, M. Thoss, & R. Borrelli, J. Chem. Phys. 160, 204105 (2024)
B. L. Dé, A. Jaouadi, E. Mangaud, A. W. Chin, M. D-Lecomte, J. Chem. Phys. 160, 244102 (2024)

Example: $J(\omega \geq 0) = \omega e^{-\omega}$, $\beta = \infty$

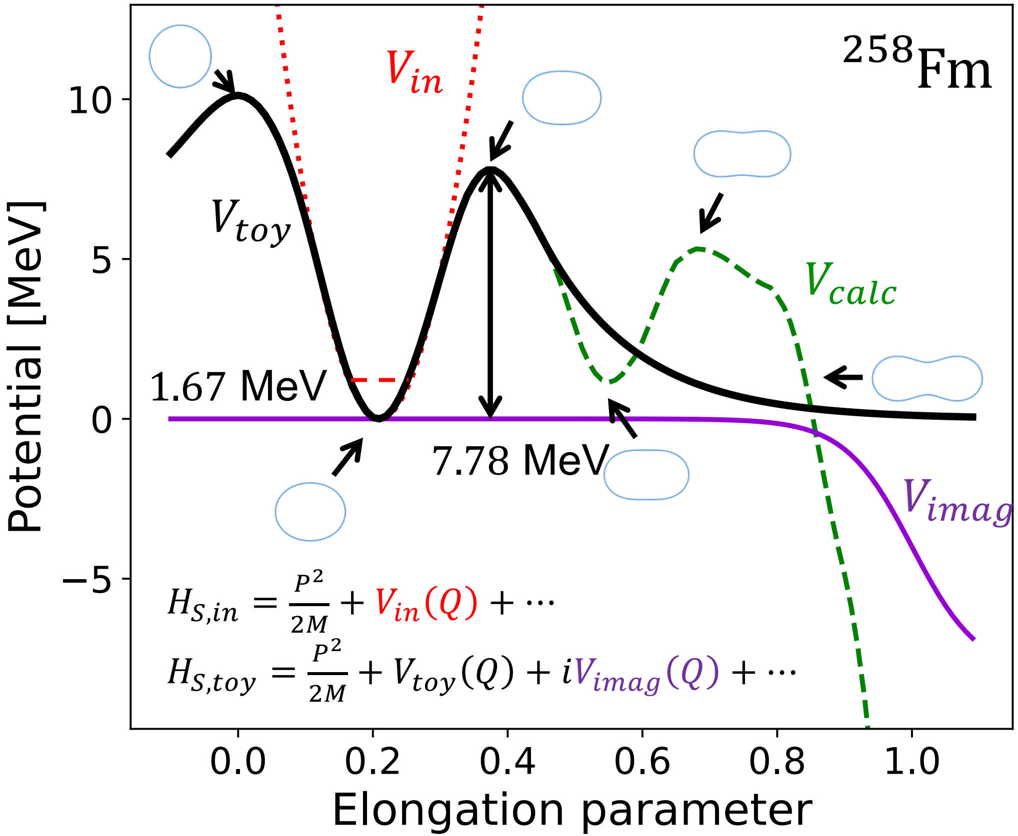
$H_{S,\mathrm{eff}} = \frac{P^2+Q^2}{2}$, $h(Q) = Q$

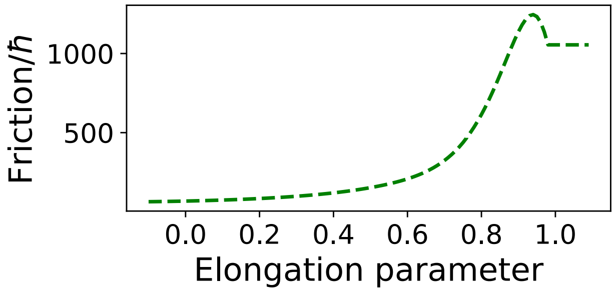




github.com/masaaki93/TestingBCF

Fission (toy model)





h_{calc}

$$h_{toy} = \frac{h_{calc}}{10}$$

Product initial state

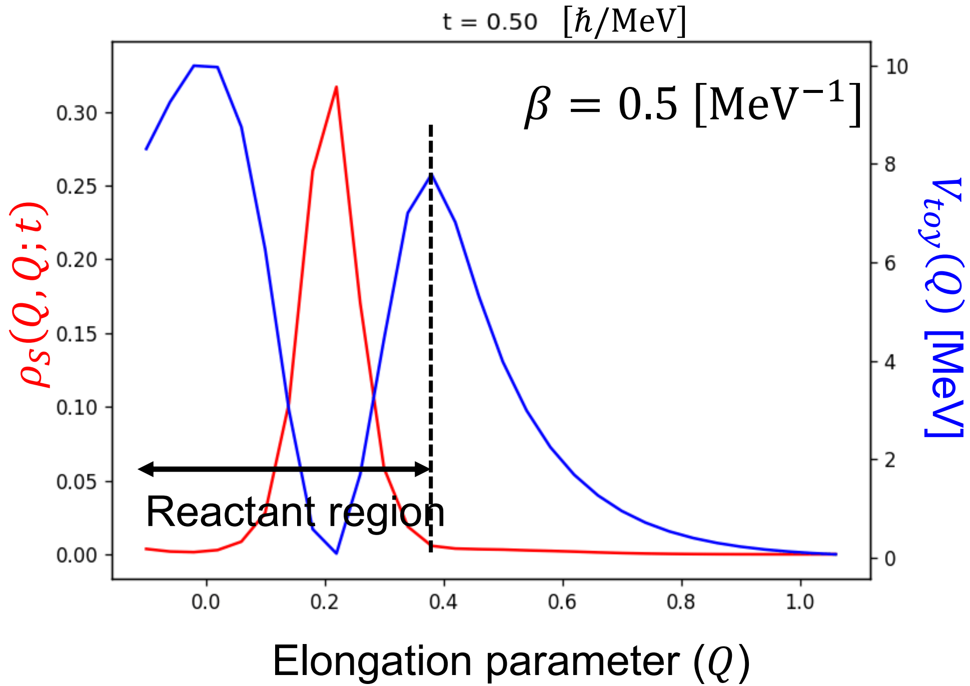
$$\rho(0) \propto \exp\left(-\beta\left(H_{S,in} + H_B\right)\right) / \blacksquare$$

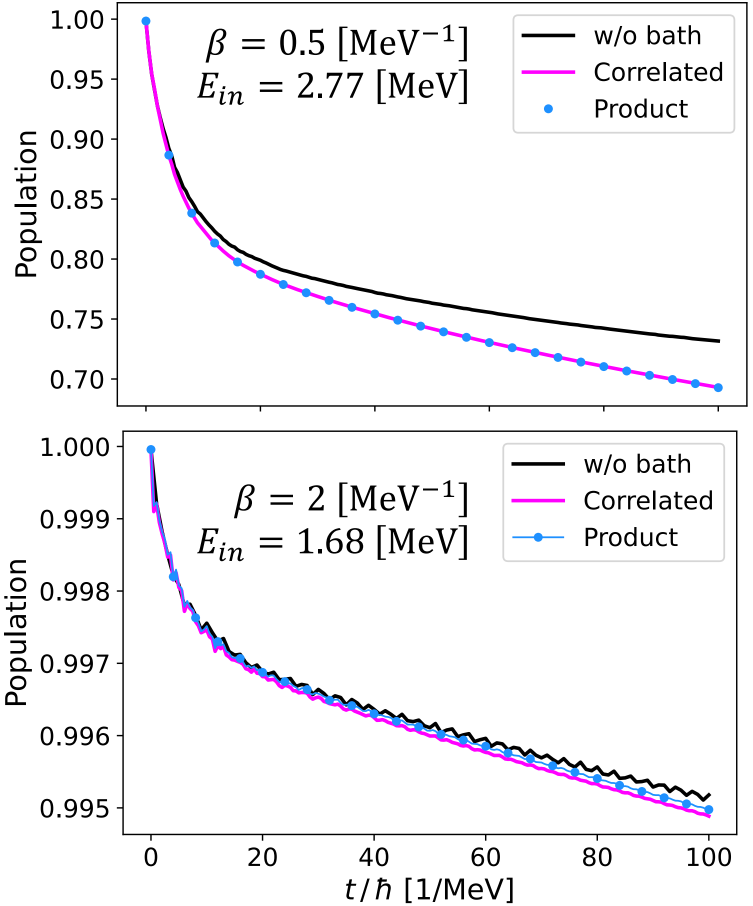
Solve HEOM with $H_{S,in}$ (Thermalize)

Solve HEOM with $H_{S,toy}$ (Transmission)

Provided by Kazuki Okada

Results





- (Correlated) $\simeq$ (Product) at $\beta = 0.5$, while the deviation is seen at $\beta = 2$.
- Transmission is enhanced by the bath?

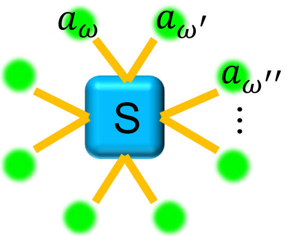
Outline

Wave-function approach: TEDOPA

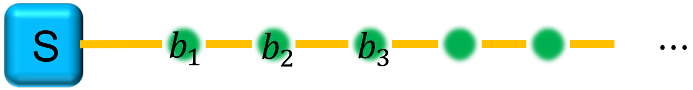
$$H = H_S + H_B + H_I \quad \begin{cases} H_B = \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2 q_i^2}{2}\right] \sim \int_0^\Omega d\omega\, \hbar\omega a_\omega^\dagger a_\omega \\ H_I = -h \cdot \sum_i c_i q_i \sim -h \cdot \int_0^\Omega d\omega \sqrt{K(\omega)}\,(a_\omega + a_\omega^\dagger) \end{cases}$$

$\boxed{K(\omega)} \propto J(\omega)$ (spectral density)

Star



Mapping!



N-N coupling 1D chain

$$\boxed{H_B = \sum_{n=1}^{\infty}\left[\hbar\epsilon_n b_n^\dagger b_n + \hbar t_n\left(b_{n+1}^\dagger b_n + b_n^\dagger b_{n+1}\right)\right]}$$

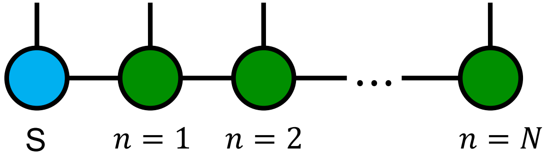
$$\boxed{H_I = -h \cdot g\left(b_1 + b_1^\dagger\right)}$$

Possible with orthogonal polynomials for $\langle f_1, f_2\rangle_K \equiv \int_0^\Omega d\omega \boxed{K(\omega)} f_1(\omega) f_2(\omega)$!

Alex W. Chin, Ángel Rivas, Susana F. Huelga, and Martin B. Plenio, J. Math. Phys. 51, 092109 (2010)
Javier Prior, Alex W. Chin, Susana F. Huelga, and Martin B. Plenio, Phys. Rev. Lett. 105, 050404 (2010)

Time **E**volving **D**ensity matrix with **O**rthogonal **P**olynomials **A**lgorithm (**TEDOPA**)

More about TEDOPA

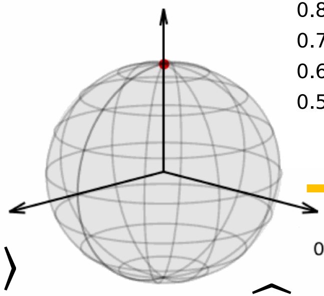
$|\Psi(t)\rangle =$ 

$J(\omega)$: finite support, no gap …

$\epsilon_n, \ t_n \xrightarrow{n\to\infty}$ finite

e.g. Two-level system ($\beta = \infty$)

$$|\Psi(0)\rangle = |\uparrow\rangle \otimes |0_\omega 0_{\omega'} \cdots\rangle$$
$$= |\uparrow\rangle \otimes |0_{n=1} 0_{n=2} \cdots\rangle$$



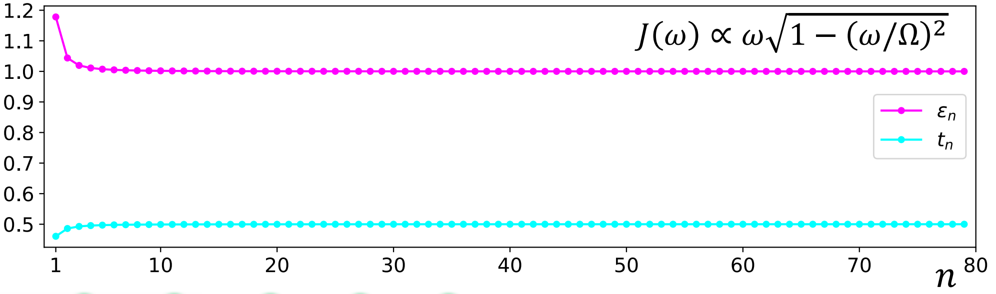
Infinitely long recurrence time

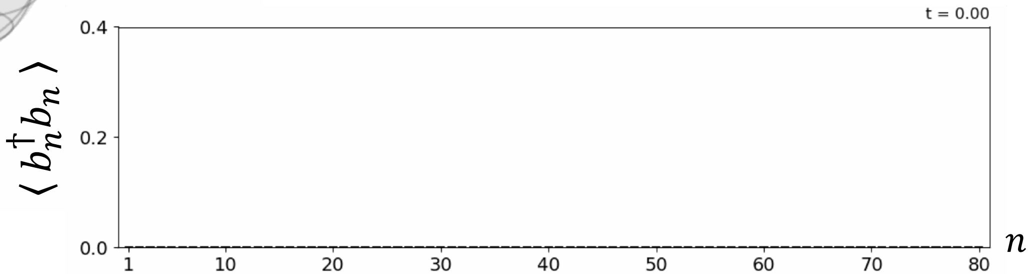
$\Rightarrow$ Irreversible loss!

Open source packages are now available!

MPSDynamics.jl

Thibaut Lacroix, Brieuc Le Dé, Angela Riva, Angus J. Dunnett, & Alex W. Chin, J. Chem. Phys. 161, 084116 (2024)





Thermalization in TEDOPA

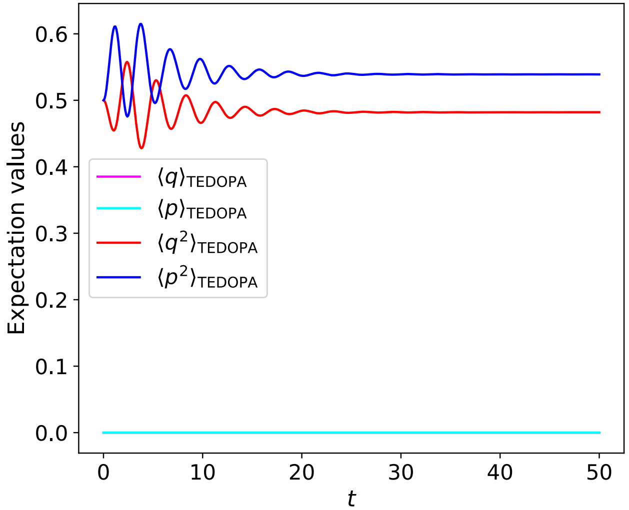
A part of the bath degrees of freedom keeps evolving. How is it reconciled with thermalization?

$$\lim_{t\to\infty} \rho_S(t) = \mathrm{tr}_B[\exp(-\beta H)]/\blacksquare$$

Harmonic oscillator: $H_{S,\mathrm{eff}} = \frac{p^2+q^2}{2}$, $h(q) = q$

Exact solutions available! H. Grabert, P. Schramm, G-L Ingold, Physics Reports 168, 115 (1988)

- $\langle \mathcal{O} \rangle_{\mathrm{Gibbs}} = \mathrm{tr}[\mathcal{O}\exp(-\beta H)]/\blacksquare$

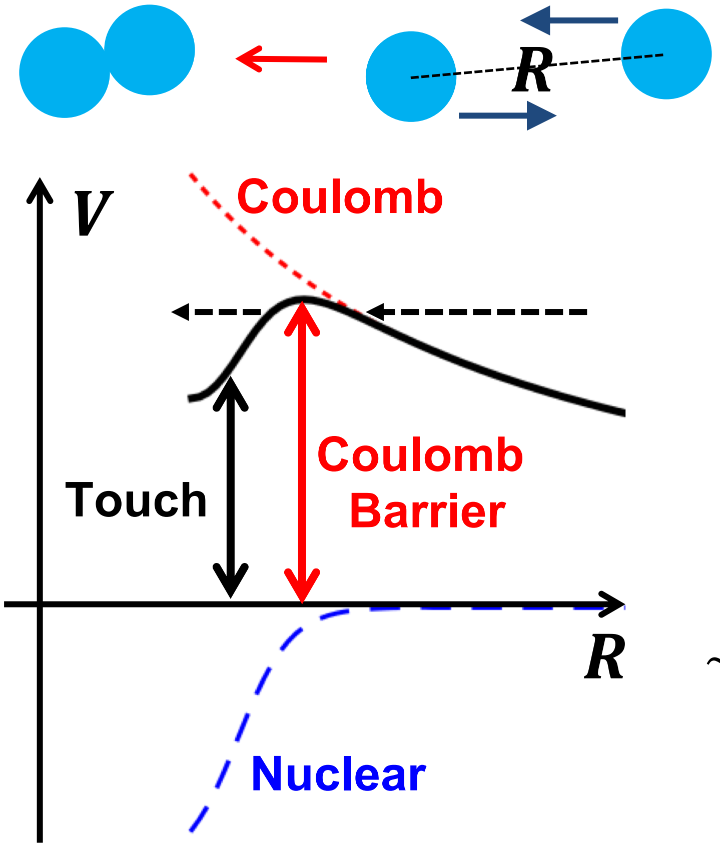


$\mathcal{O}$	$\langle \mathcal{O} \rangle_{\mathrm{Gibbs}}$	$\langle \mathcal{O} \rangle_{\mathrm{TEDOPA}}$
$\boldsymbol{q}$	0	$\sim 10^{-6}$
$\boldsymbol{p}$	0	$\sim 10^{-6}$
$\boldsymbol{q^2}$	0.48199	0.48198
$\boldsymbol{p^2}$	0.53903	0.53905

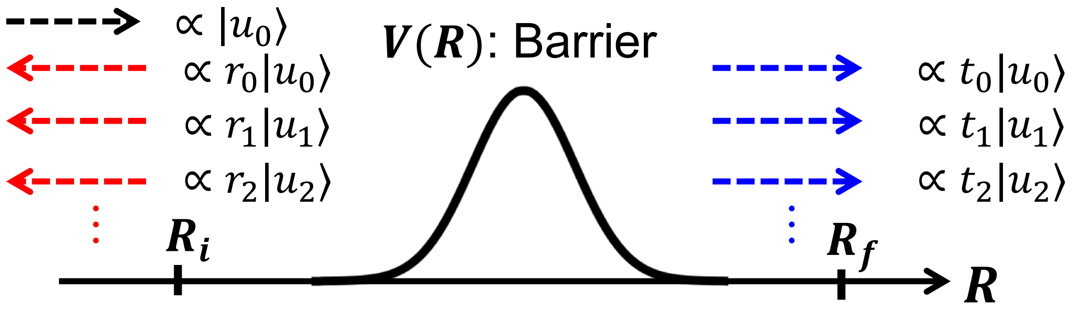
$\lim_{t\gg 1} \rho_S(t) = \mathrm{tr}_B[\exp(-\beta H)]/\blacksquare$ but $\rho(t) \neq \exp(-\beta H)\,/\blacksquare$

Continuously distributed modes and $t \to \infty$?

Fusion (toy model)



1D barrier transmission problem



Difficulty (energy projection)

G.S. ($\beta = \infty$)

$|\Psi(0)\rangle = |\psi_S\rangle|u_0\rangle$

Localized around R_i

$$t_f(E) \sim \int_0^\infty d\tau\, e^{iE\tau/\hbar}\langle R_f u_f|e^{-iH\tau/\hbar}|\Psi(0)\rangle$$

$$\longrightarrow \quad T(E) = \sum_f |t_f(E)|^2$$

$$\sim \int_0^\infty d\tau_1 \int_0^\infty d\tau_2\, e^{iE(\tau_1-\tau_2)/\hbar}\underline{\rho_S(R_f\tau_1, R_f\tau_2)}$$

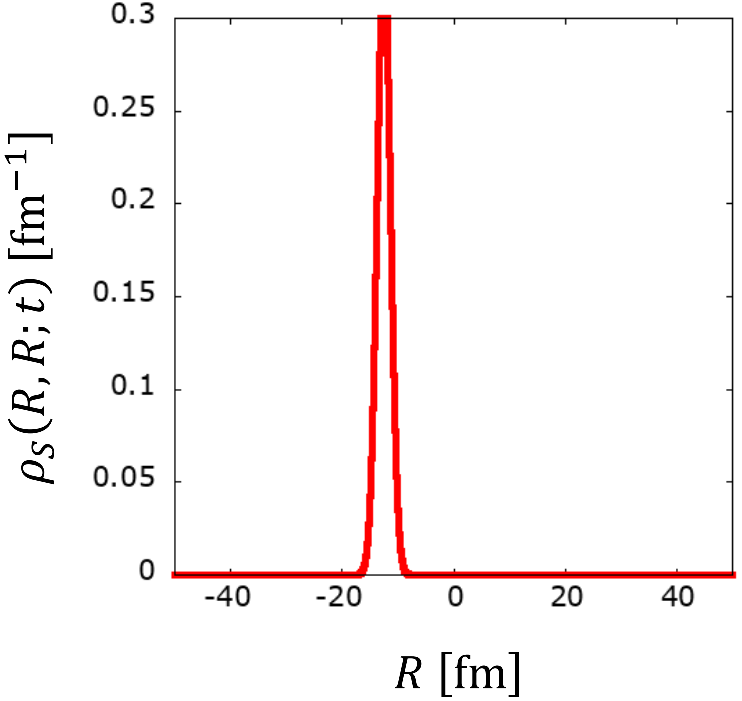
$$\rho_S(\tau_1,\tau_2) = \mathrm{tr}_B[e^{-iH\tau_1/\hbar}|\Psi(0)\rangle\langle\Psi(0)|e^{iH\tau_2/\hbar}]$$

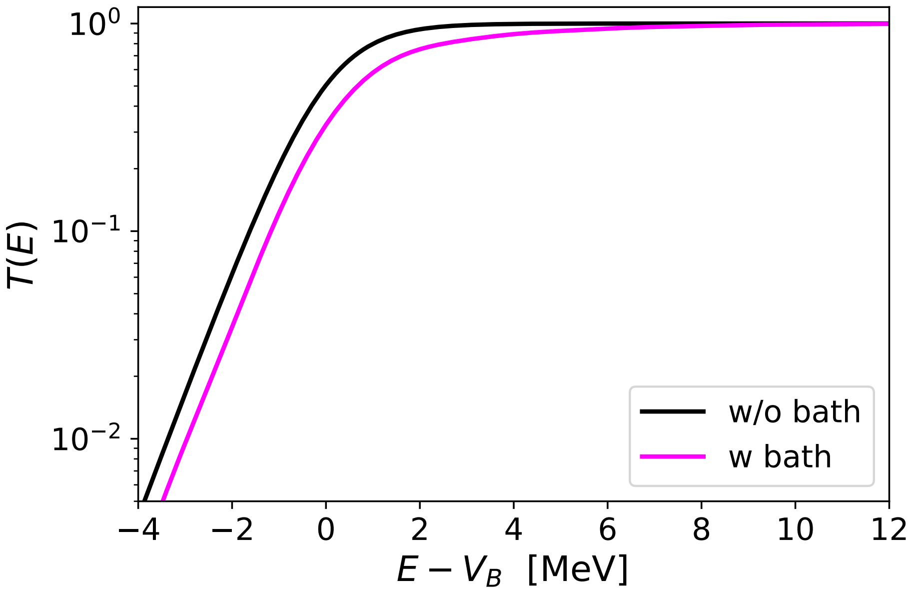
Two-time reduced density matrix

A. B. Balantekin & N. Takigawa, Ann. Phys. (N.Y.) 160, 441 (1985)

M.T. & K. Hagino, Ann. Phys. 412, 168005 (2020)

Results





- Transmission is suppressed by the bath

Summary

HEOM, pseudomode

Markovian embedding

Density matrix $\propto d_S^2$

From short to long times

$L(t) \simeq c_1 e^{-\mu_1 t} + c_2 e^{-\mu_2 t} + \cdots$

TEDOPA

Star to chain transformation

Wave function $\propto d_S$

Hard at long times

$J(\omega)$: finite support

Ambitious direction: Going beyond the Gaussian bath model

One possible approach: A pseudomode description for your problem?