Quantum mechanical extension of the Langevin approach based on the Caldeira-Leggett model

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Langevin method

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

Quantum extension

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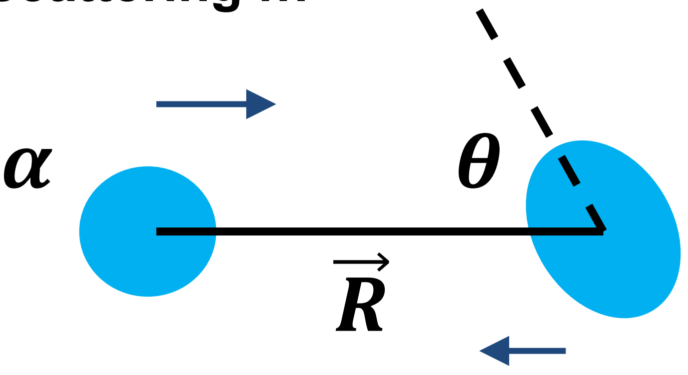
Macroscopic Approach: Collective Coordinates

Select d.o.f which are expected to be relevant to the reaction

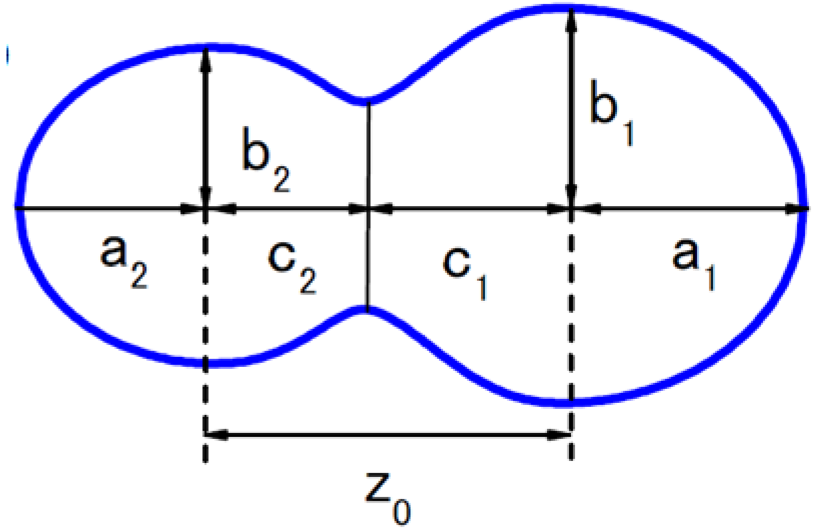
If scattering …



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

If fission …

Y. Aritomo's slide



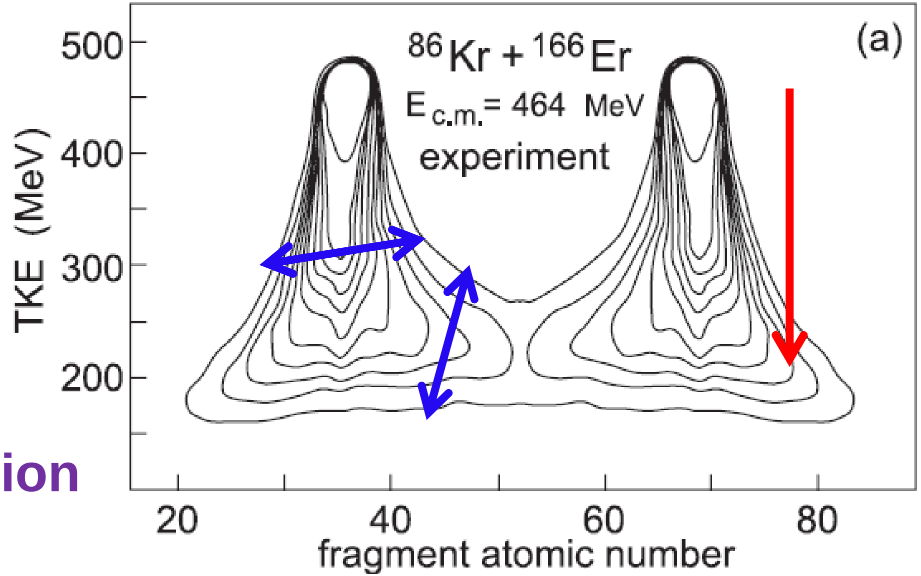
Shape coordinates

Fluctuation and Dissipation in Nuclear Reactions

Beyond collective coordinates

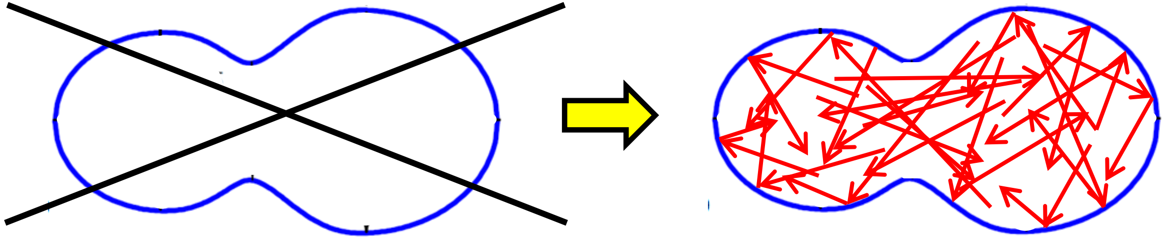
- ✓ **Energy dissipation**
- ✓ **Fluctuation**

which are originated from **internal motion**



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

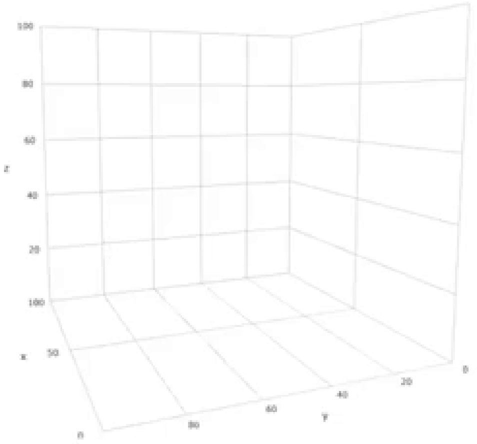
If fission …



Phenomenologically

Application of the Langevin Method

https://www.youtube.com/watch?v=7A83lXbs6Ik



Langevin method

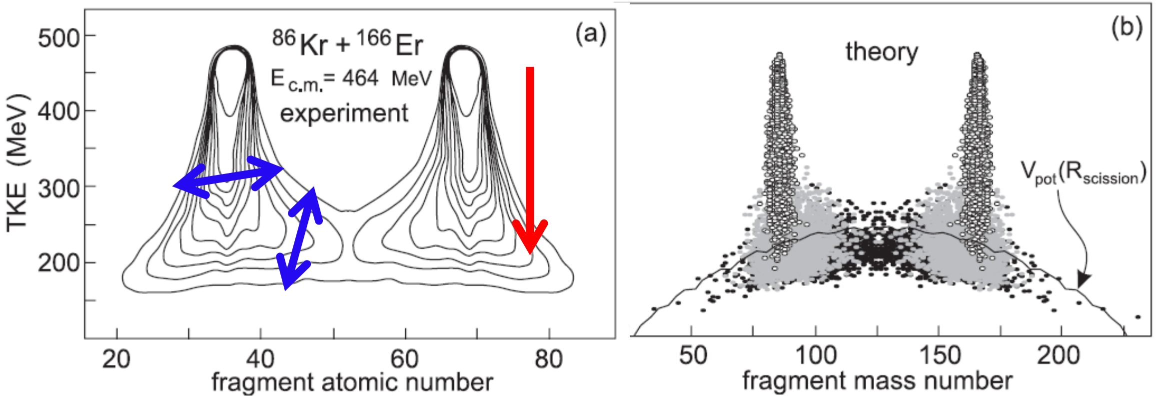
$$\begin{cases} \dot{x} = p/M \\ \dot{p} = -V'(x) - \underline{\gamma p} + \underline{\zeta(t)} \end{cases}$$

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



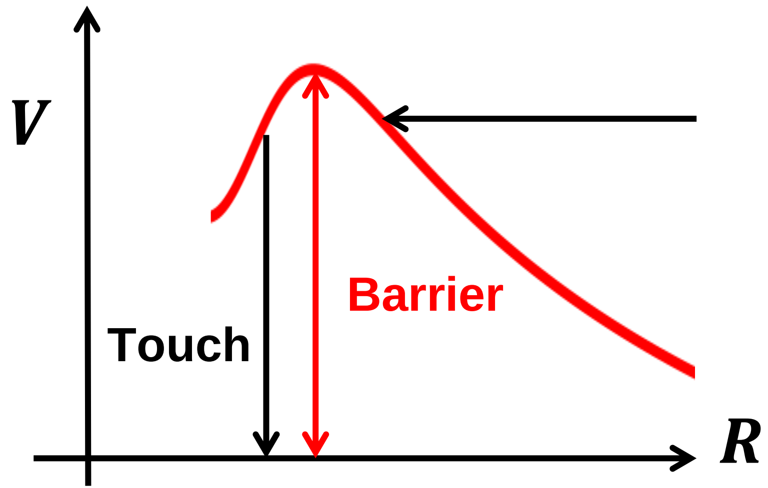
Applicability:

- Fission
- Fusion
- Quasi fission
- Deep inelastic sc

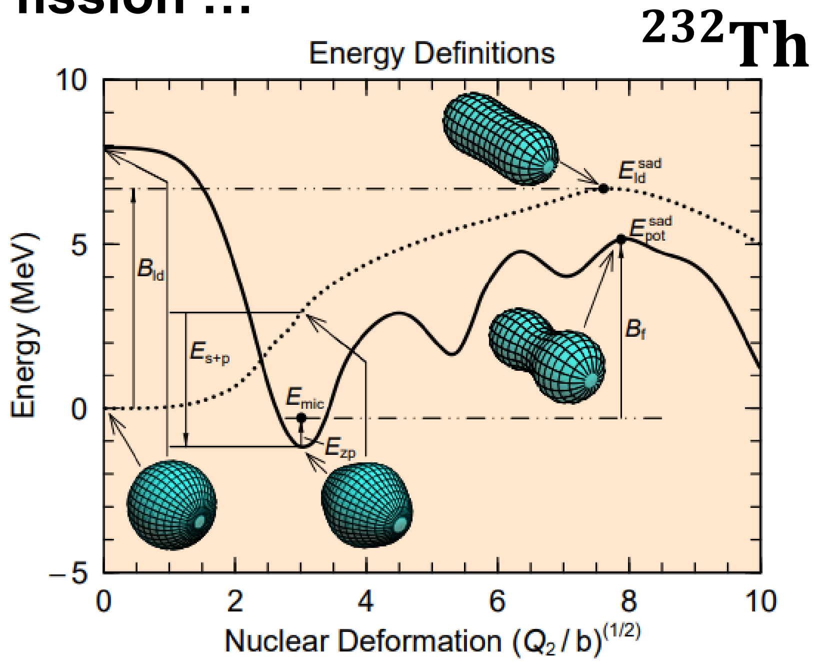
at above barrier

Necessity of Quantum Treatment (Low Energy)

If scattering …



If fission …



P.Moller,A.J.Sierk,T.Ichikawa,H.Sagawa,arXiv:nucl-th/1508.06294

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

Penetration through **Quantum Tunneling**

Our Goal

Our GOAL is

To describe low-energy nuclear reactions with single method (from **subbarrier** to **above barrier**)

What is problem ?

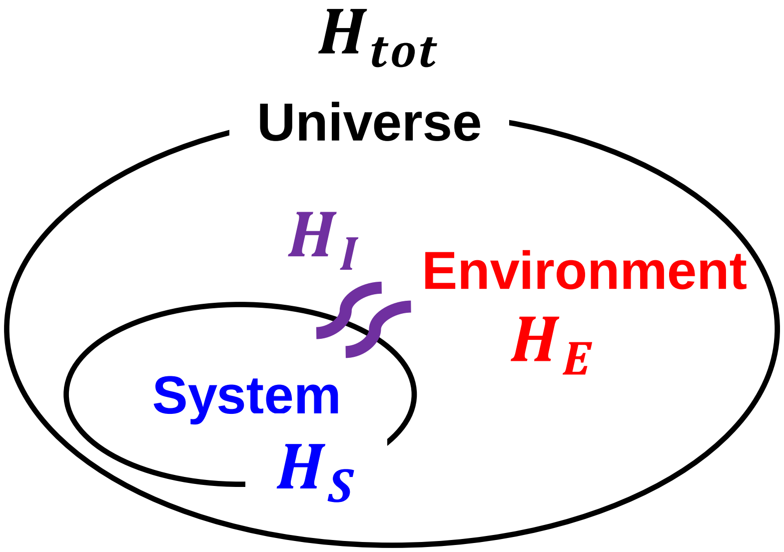
The present Langevin approach is based on classical mechanics, and is inapplicable to subbarrier reactions

How to achieve ?

Quantum mechanical extension of the Langevin approach

Open Quantum System

From more general point of view …



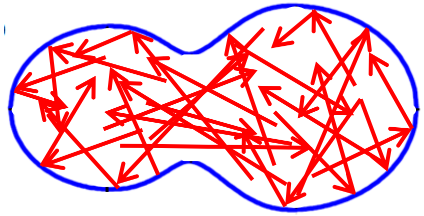
Open Quantum System

For nuclear reactions …

System: collective motion

Environment: internal motion

If fission …

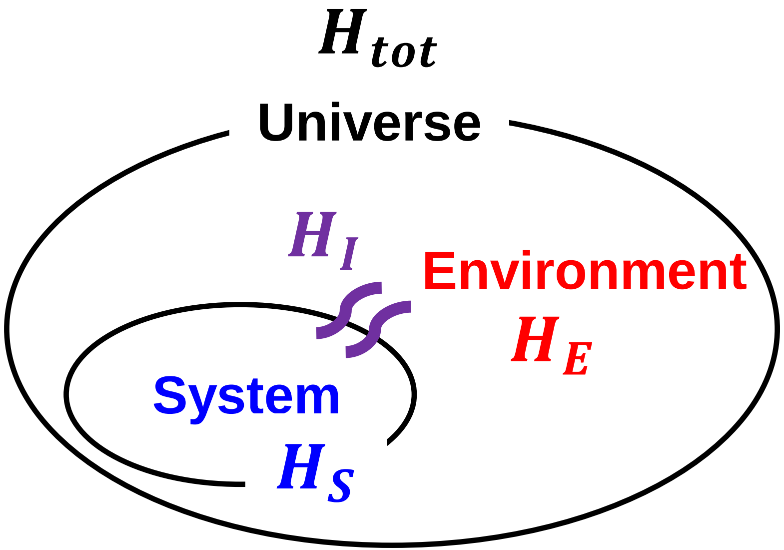


S plus E model

$$H_{tot} = H_S + H_E + H_I$$

Choose <u>simple</u> and <u>reasonable</u> $H_E,\ H_I$

The Caldeira-Leggett Model



$$H_{tot} = H_S + H_E + H_I$$

A.O.Caldeira and A.J.Leggett, Physica **121A**, 587 (1983)
A.O.Caldeira and A.J.Leggett, Ann. Phys. **149**, 374 (1983)

System of interest (arbitrary)

$$H_S = \frac{p^2}{2M} + U(x)$$

Environment (HO bath)

$$H_E = \sum_i \hbar\omega_i a_i^{\dagger} a_i$$

$$[a_i, a_j] = 0 \,, [a_i, a_j^{\dagger}] = \delta_{i,j}$$

Interaction (linear)

$$H_I = h(x) \sum_i d_i (a_i + a_i^{\dagger})$$

Derivation of the Langevin Equation 1

$$\boldsymbol{H_{\mathrm{CL}} = \frac{p^2}{2M} + U(x) + \sum_i \hbar\omega_i {a_i}^\dagger a_i + h(x) \sum_i d_i(a_i + {a_i}^\dagger)}$$

Heisenberg equation of motion …

$$\begin{cases} \textbf{Sys:} & \dot{p}_t = -U'(x_t) - h'(x_t)\sum_i d_i\left(a_{i,t} + a^\dagger{}_{i,t}\right) \quad \cdots \quad (\ast) \\ \textbf{Env:} & \dot{a}_{i,t} = -i\omega_i a_i - (id_i/\hbar)h(x_t) \end{cases}$$

Environment part can be solved analytically …

$$a_{i,t} = \underline{a_i} \exp(-i\omega_i t) - \underline{(id_i/\hbar)\int_0^t ds \exp\left(i\omega_i(s-t)\right)h(x_s)}$$

Initial condition of env — **Sys-Env Coupling**

Substituting this into Eq.(∗) and sorting out …

$$\dot{p}_t = (\textbf{Potential}) + (\textbf{Coupling}) + (\textbf{Initial env})$$

Derivation of the Langevin Equation 2

$$\boldsymbol{H_{\mathrm{CL}} = \frac{p^2}{2M} + U(x) + \sum_i \hbar\omega_i a_i^\dagger a_i + h(x)\sum_i d_i(a_i + a_i^\dagger)}$$

In the classical limit …

G.W.Ford, J.T.Lewis, and R. F.O'Connell, PRA **37**, 4419 (1988)

$$\boldsymbol{\dot{p}_t = -\underline{V'(x_t)} - \underline{\int_0^t ds\,\gamma(t,s)\,p_s} + \underline{h'(x_t)\zeta(t)}}$$

Potential

$$V(x) = U(x) - h^2(x)K(0)/2$$

Coupling

$$K(t) = 2\sum_i (d_i^2/\hbar\omega_i)\cos(\omega_i t)$$

$$\gamma(t,s) = K(t-s)h'(x_t)h'(x_s)/M$$

Initial env Suppose $h(x_{t=0}) = 0$

$$\zeta(t) = \sum_i d_i(a_i e^{-i\omega_i t} + a_i^\dagger e^{i\omega_i t})$$

$\rho_E \propto \exp(-\beta H_E)$ → Gaussian

$$\begin{cases} \langle\zeta(t)\rangle = 0 \\ \langle\zeta(t)\zeta(0)\rangle = K(t)/\beta \end{cases}$$

$\langle\mathcal{O}\rangle = \mathrm{Tr_E}[\mathcal{O}\rho_E]$

If HOs are distributed as $K(t) \propto \delta(t)$ ⇒ **Classical Langevin**

Coupled Channels Method

$$H_{\mathrm{CL}} = \frac{p^2}{2M} + V(x) + \sum_i \hbar\omega_i a_i{}^\dagger a_i + h(x)\sum_i d_i(a_i + a_i{}^\dagger)$$

✓ **Coupled channels method**

$$a_i{}^\dagger a_i|n_i\rangle = n_i|n_i\rangle$$

$$\langle x|\Psi(t)\rangle = \sum_{n_1,n_2,\ldots} \phi_{n_1,n_2,\ldots}(x,t)|n_1,n_2,\ldots\rangle$$

Total WF

Not for a large number of HOs

✓ **New basis** (M.T and K.Hagino, arXiv:quant-ph/1909.10418)

$$e^{-i\omega t} \simeq \sum_{k=1}^{K} \eta_k(\omega)u_k(t)$$

$$b^\dagger{}_k = \sum_i \eta_k(\omega_i)a_i^\dagger$$

$$[b_k, b_q{}^\dagger] = \delta_{k,q}$$

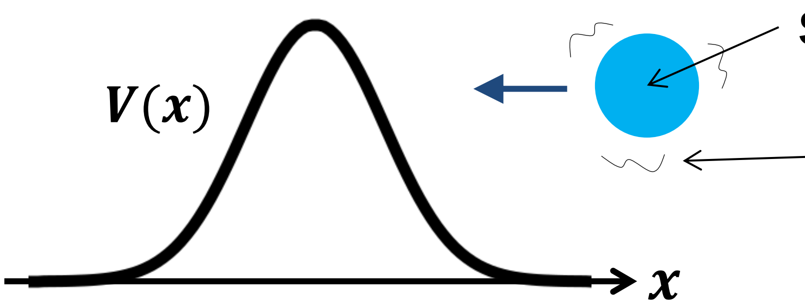
$$b_k{}^\dagger b_k|j_k\rangle = j_k|j_k\rangle$$

$$\langle x|\Psi(t)\rangle = \sum_{j_1,\ldots,j_K} \psi_{j_1,\ldots,j_K}(x,t)|j_1,\ldots,j_K\rangle$$

The number of basis vectors is …

- independent of **the number of HOs**
- dependent on $\max(\omega_i)$ ×(Running time) and d_i

Application to 1D Barrier Transmission Problem



Scattering (System)

Internal motion (Environment)

- ✓ **Solving Schrödinger equation**

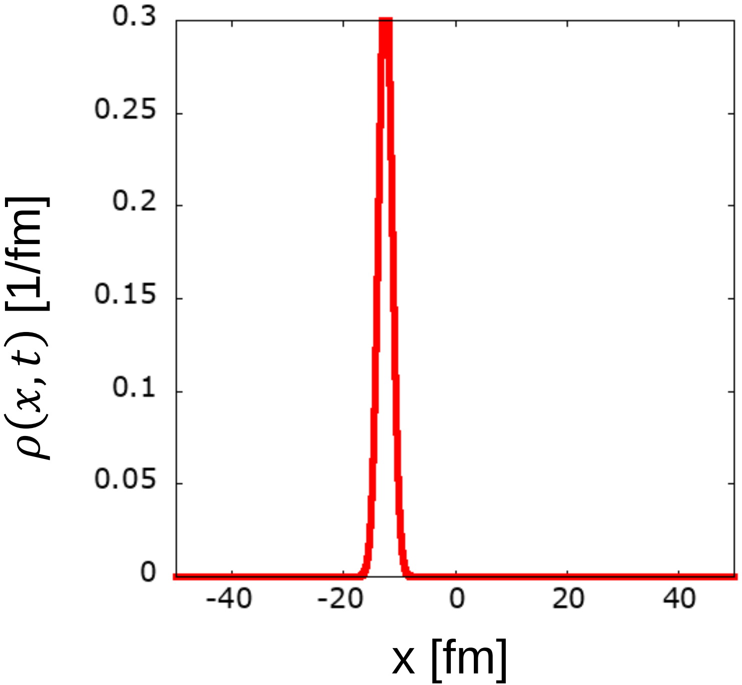
$$\langle x|\Psi(t)\rangle = \sum_{j_1,\ldots,j_K} \psi_{j_1,\ldots,j_K}(x,t)|j_1,\ldots,j_K\rangle$$

- ✓ **Energy projection** $H_0 = \frac{p^2}{2M} + \sum_i \hbar\omega_i a_i^\dagger a_i$

$$P(E) \propto \langle\Psi_T|\delta(H_0 - E)|\Psi_T\rangle$$

K. Yabana, Prog. Theor. Phys. **97**, 437 (1997)

Calculating penetrability $P(E)$ similar to this method

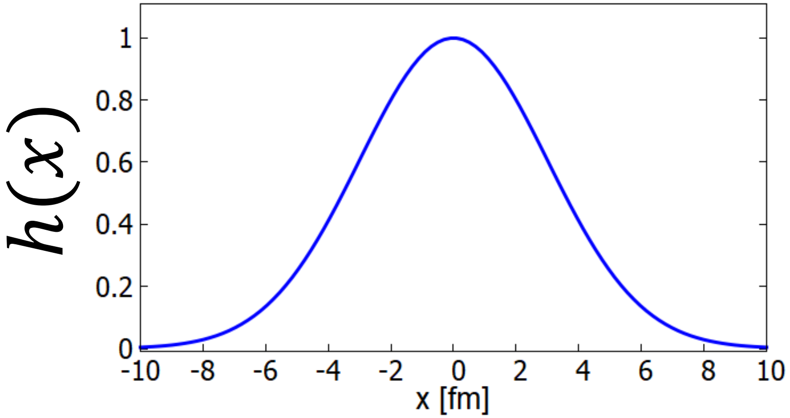


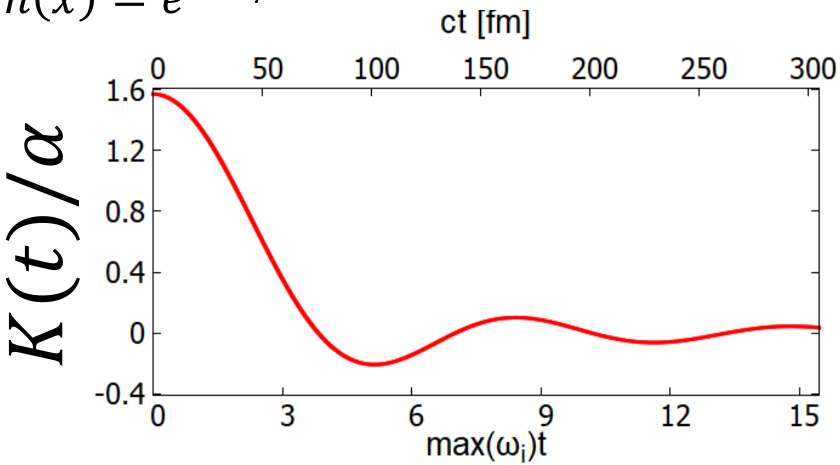
Setup

(Classical) $$\dot{p}_t = -V'(x_t) - \int_0^t ds\, \gamma(t,s)\, p_s + h'(x_t)\zeta(t)$$

$$\gamma(t,s) = K(t-s)h'(x_t)h'(x_s)/M \qquad \langle \zeta(t)\zeta(0)\rangle = K(t)/\beta$$

System: $^{58}\mathrm{Ni} + {}^{58}\mathrm{Ni}$
$$\begin{cases} V(x) = 100\, h(x)\ \text{MeV} \\ h(x) = e^{-x^2/2\times 3^2} \end{cases}$$

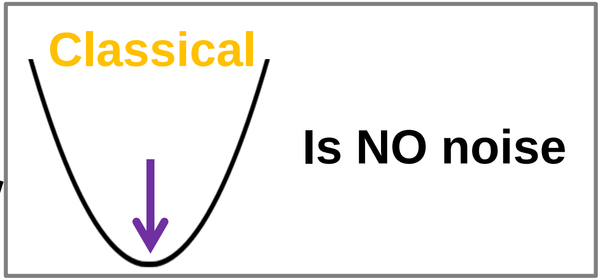




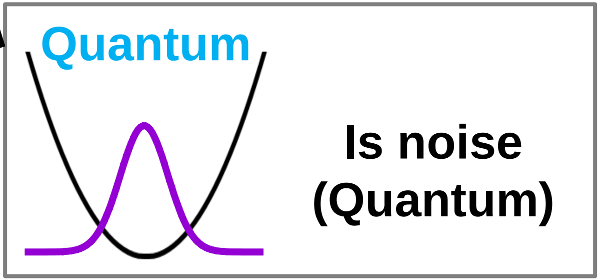
Classical (C), Semi-Classical (SC), Quantum (Q)

Total = Scattering (x, p) $\otimes$ Internal $(\{a_i\}_{i=1,2,\ldots})$

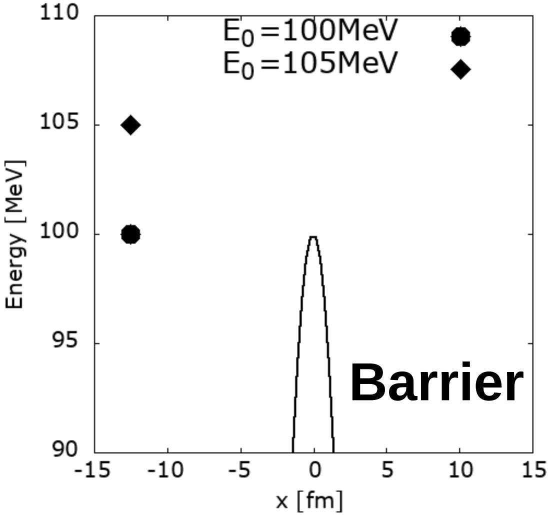
	Scattering	Internal
C	**Classical**	**Classical**
SC	**Classical**	**Quantum**
Q	**Quantum**	**Quantum**



Zero temperature
(Ground state initially)



What to solve ?



Classical

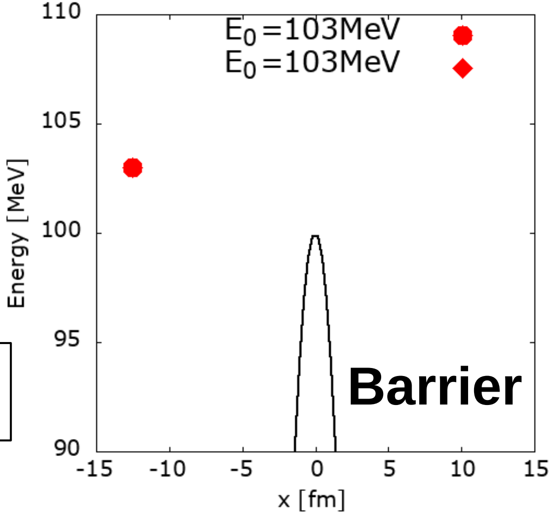
Classical e.o.m + Friction

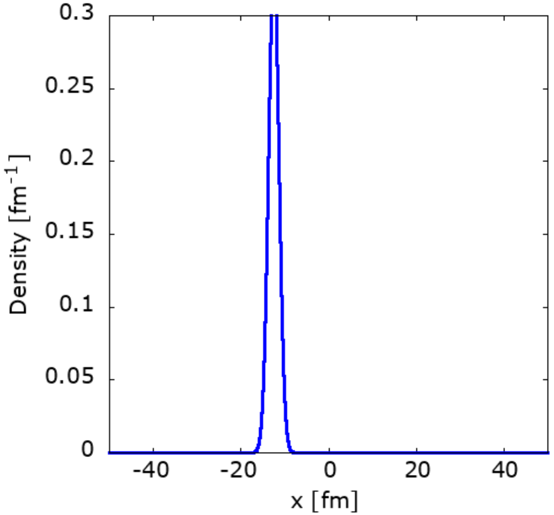
$$\dot{p}_t = -V'(x_t) - \int_0^t ds\, \gamma(t,s)\, p_s$$

Semi-Classical

Langevin (Q noise)

$$\dot{p}_t = -V'(x_t) - \int_0^t ds\, \gamma(t,s) p_s + h'(x_t)\zeta(t)$$



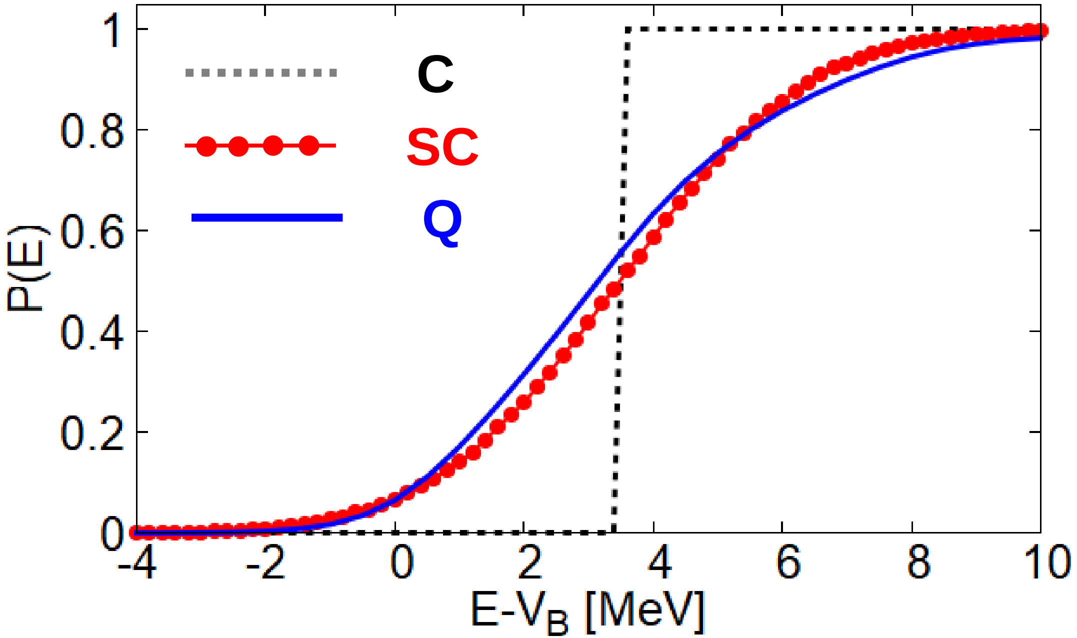


Quantum

Coupled channels

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = H_{\mathrm{CL}}|\Psi(t)\rangle$$

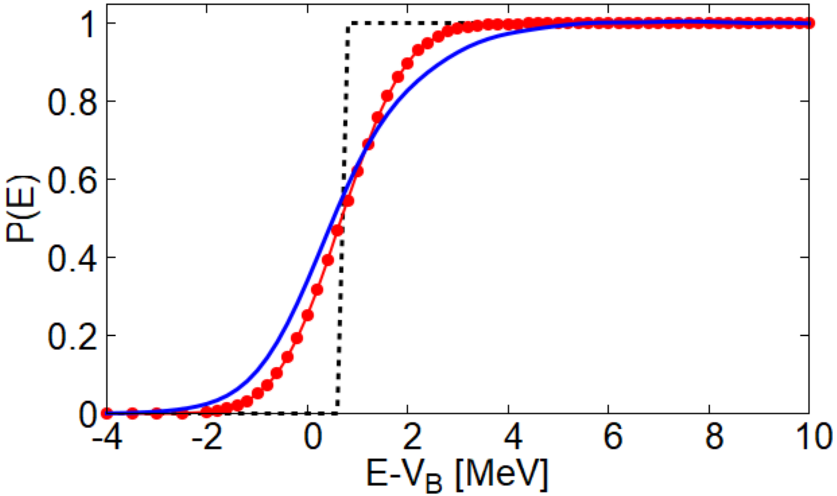
Energy Dependence of the penetrability 1

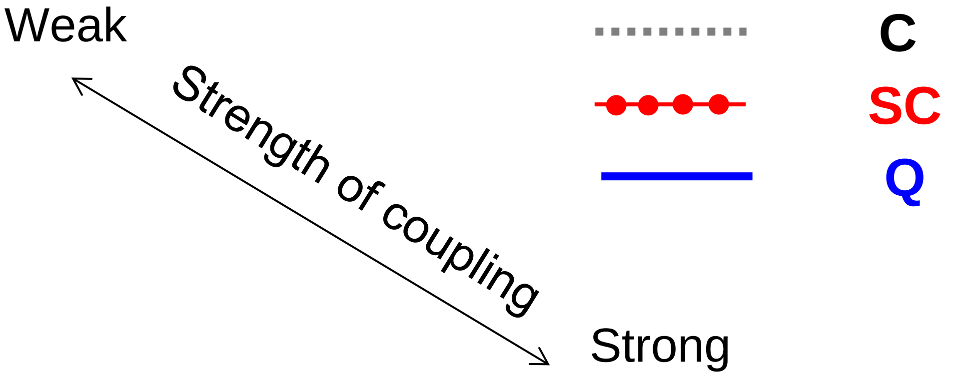


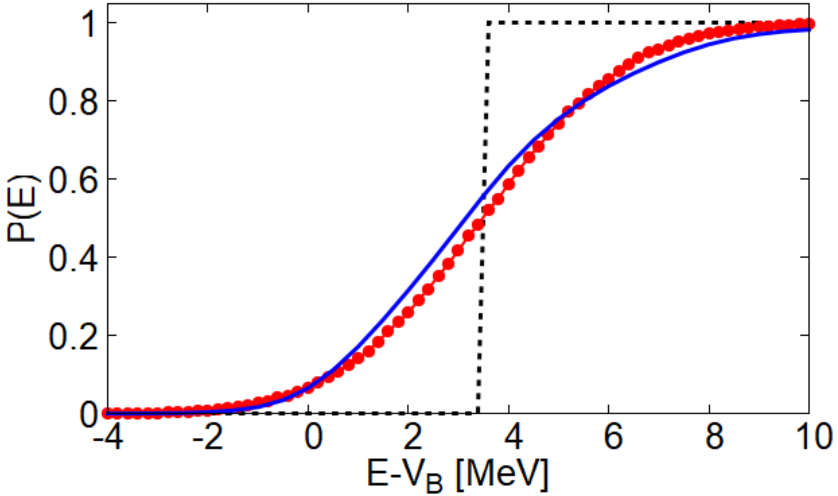
(SC) ≈ (Q)

The Langevin method with quantum noise looks very similar to the **quantum result**

Energy Dependence of the penetrability 2







Fluctuation: **SysQ**, **EnvQ**
SC: Only **EnvQ**
Q: **SysQ** and **EnvQ**
→ **SysQ** is masked by **EnvQ**

Summary

To achieve quantum extension of the Langevin method …

$$\boldsymbol{H}_{\mathbf{CL}} = \frac{\boldsymbol{p}^2}{2\boldsymbol{M}} + \boldsymbol{U}(\boldsymbol{x}) + \sum_i \hbar\boldsymbol{\omega}_i \boldsymbol{a}_i{}^\dagger \boldsymbol{a}_i + \boldsymbol{h}(\boldsymbol{x}) \sum_i \boldsymbol{d}_i(\boldsymbol{a}_i + \boldsymbol{a}_i{}^\dagger)$$

H_{CL} Classically, Langevin equation ⇒ H_{CL} Quantization ⇒ **Quantum Langevin**

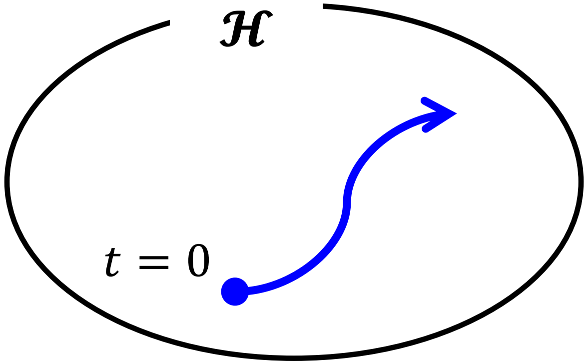
New basis: the number of basis vectors is independent of **the number of HOs**

- ✓ Application to a 1D barrier transmission problem

Around the barrier … **(SC) ≈ (Q)**

Left blank

How the new basis works ?



In general …

No idea how it evolves in the Hilbert space ($\mathcal{H}$)

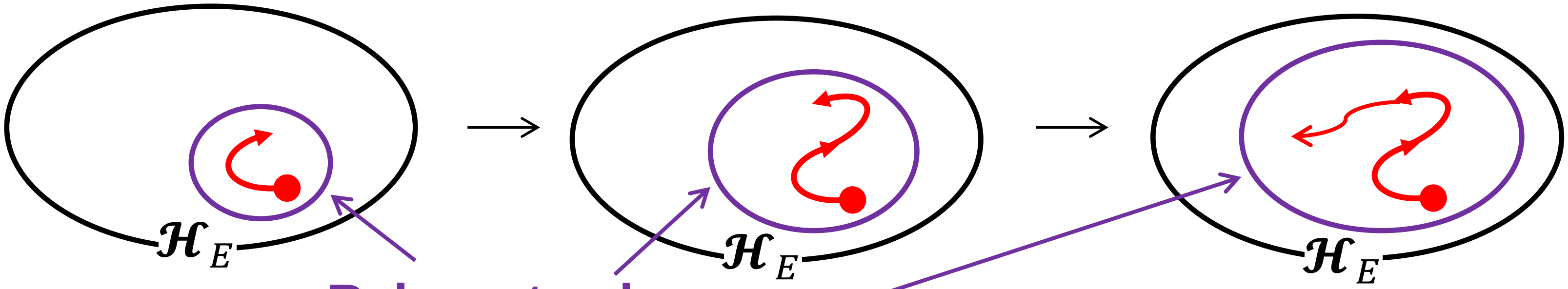
→ The model space as large as possible

$$\langle x|\Psi(t)\rangle = \sum_{n_1,n_2,\dots} \phi_{n_1,n_2,\dots}(x,t)|n_1,n_2,\dots\rangle$$

The Caldeira-Leggett model …

$$\sum_i \hbar\boldsymbol{\omega}_i \boldsymbol{a}_i{}^\dagger \boldsymbol{a}_i\,,\quad \sum_i \boldsymbol{d}_i(\boldsymbol{a}_i + \boldsymbol{a}_i{}^\dagger)$$

Simple !



Relevant subspace
expands with time

$$\langle x|\Psi(t)\rangle = \sum_{j_1,\dots,j_K} \psi_{j_1,\dots,j_K}(x,t)|j_1,\dots,j_K\rangle$$

Quantum Langevin Equation

$$H_{\mathrm{CL}} = \frac{p^2}{2M} + U(x) + \sum_i \hbar\omega_i a_i^\dagger a_i + h(x) \sum_i d_i(a_i + a_i^\dagger)$$

$$\dot{p}_t = -V'(x_t) - \int_0^t ds\, K(t-s)\{h'(x_t),\{h'(x_s),p_s\}\}/4M + \{h'(x_t),\zeta(t)\}/2$$

$$K(t) = 2\sum_i (d_i^2/\hbar\omega_i)\cos(\omega_i t)$$

Initial env Suppose $h(x_{t=0}) = 0$ $\zeta(t) = \sum_i d_i(a_i e^{-i\omega_i t} + a_i^\dagger e^{i\omega_i t})$

$\langle \mathcal{O} \rangle = \mathrm{Tr}_{\mathrm{E}}[\mathcal{O}\rho_E]$

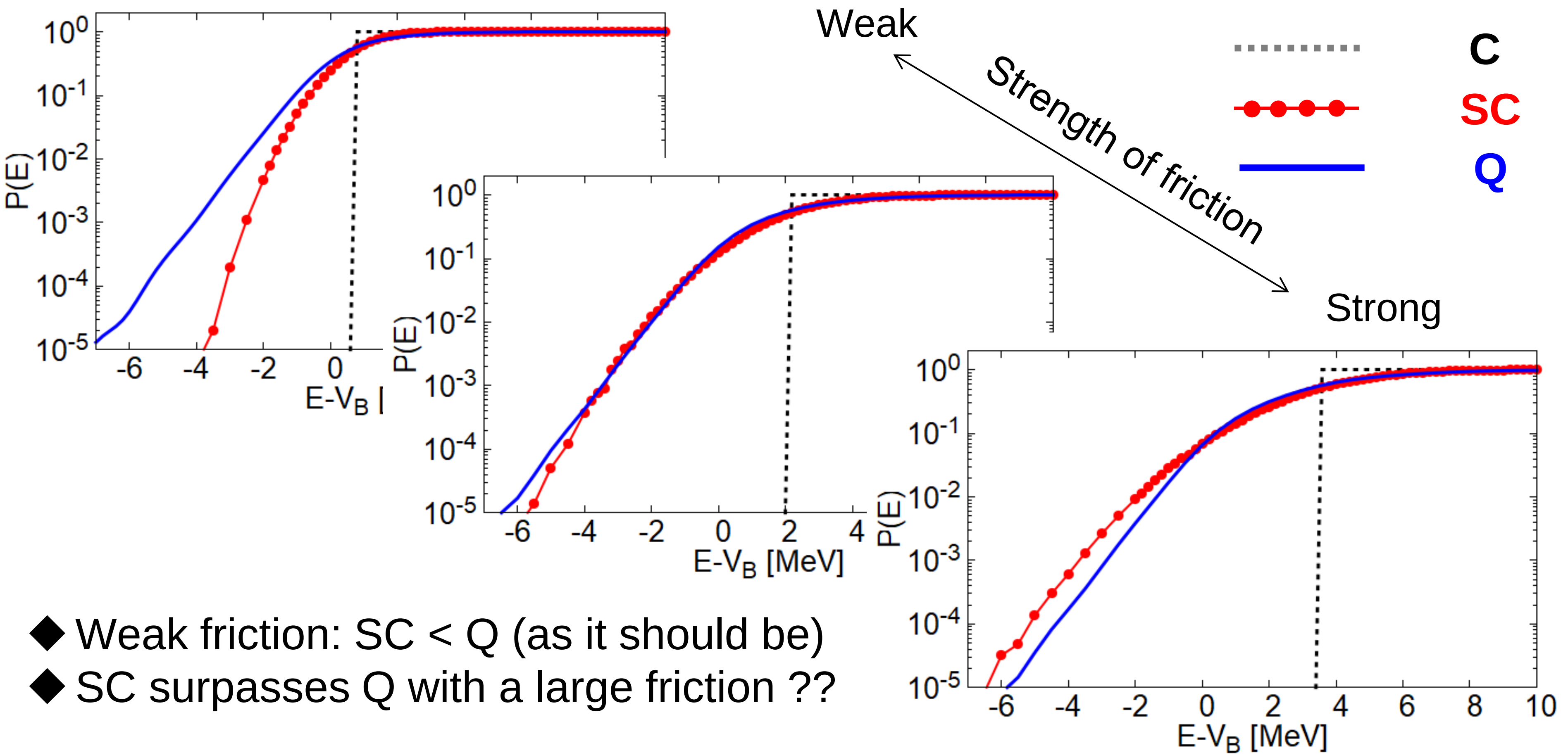
$\rho_E \propto \exp(-\beta H_E)$ → Gaussian

$$\begin{cases} \langle \zeta(t) \rangle = 0 \\ \langle \{\zeta(t),\zeta(0)\} \rangle = (4/\beta)\sum_i (d_i^2/\hbar\omega_i)\cos(\omega_i t)\,(\beta\hbar\omega_i/2)\coth(\beta\hbar\omega_i/2) \end{cases}$$

$$\langle \{\zeta(t),\zeta(0)\} \rangle/2 \begin{array}{ll} \to 2\sum_i d_i^2 \cos(\omega_i t) \neq 0 & (\beta \to \infty) \\ \to (2/\beta)\sum_i (d_i^2/\hbar\omega_i)\cos(\omega_i t) & (\beta \to 0) \end{array}$$

(classical)

Subbarrier energies



- Weak friction: SC < Q (as it should be)
- SC surpasses Q with a large friction ??

Numerical details

Classical, and semiclassical calculation

$c\Delta t = 0.75$ fm

One calculation takes less than 0.2 sec

Quantum calculation

(for energy projection)

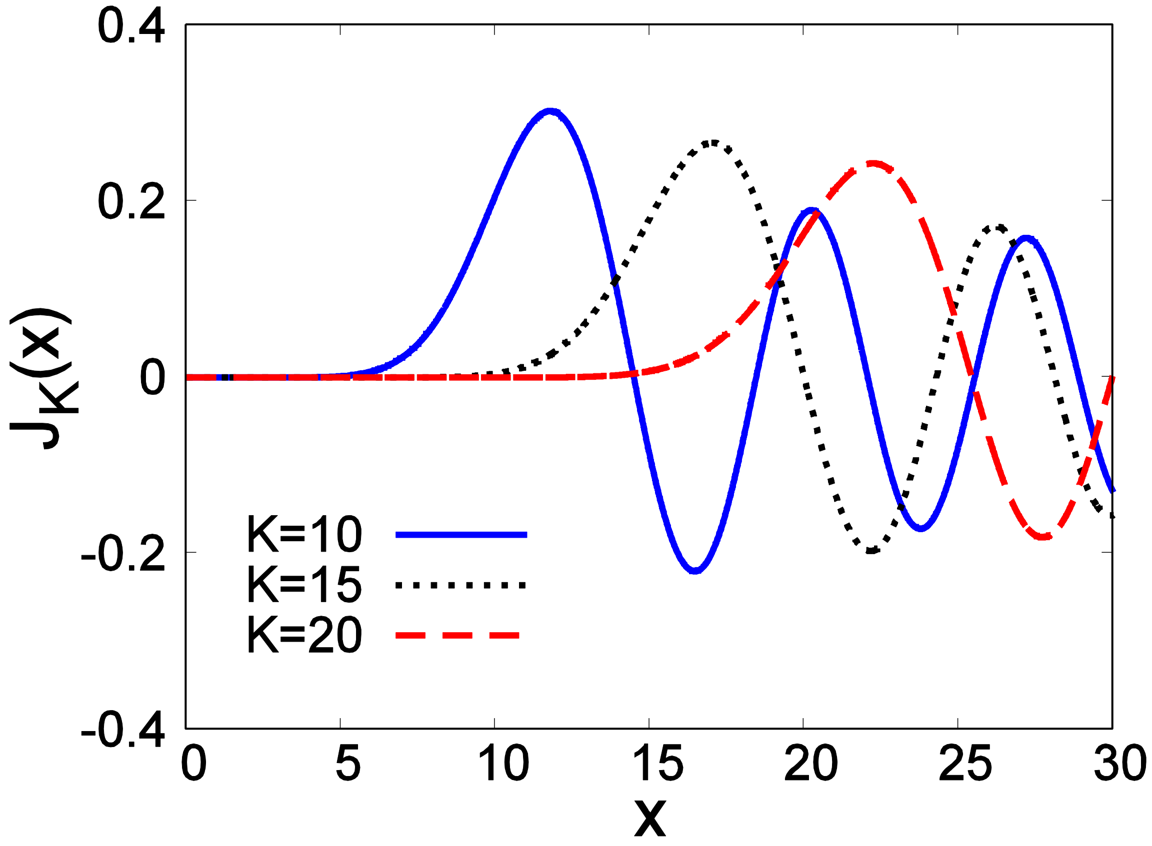
$\Delta r = 0.125$ fm, $c\Delta t = 0.1$ fm

$-25 < r\ (\mathrm{fm}) < 50$

Without energy projection, it takes about one night (~6 hours)

With energy projection, it takes about 1 - 2 days

Property of the Bessel functions

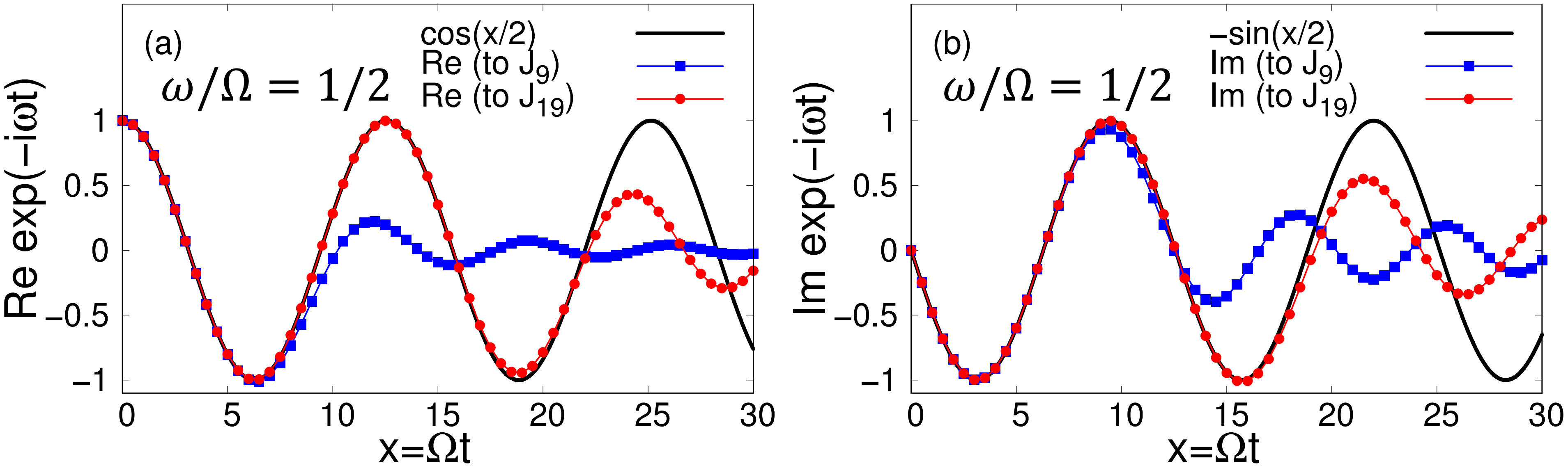


Expansion of $\exp(-i\omega_i t)$

Expand … $$\exp(-i\omega_i t) = \sum_{k=1}^{K} \eta_k(\omega_i) u_k(t) = \vec{\eta}(\omega_i) \cdot \vec{u}(t)$$

e.g. $$\exp(-i\omega_i t) = J_0(\Omega t) + 2\sum_{k=1}^{\infty}(-i)^k T_k(\omega_i/\Omega) J_k(\Omega t)$$

T_k: Chebyshev polynomials J_k: Bessel functions Ω : cutoff frequency



Memory Effects and Energy Dissipation

$$\dot{\mathrm{v}}_t = -\int_0^t ds\, K(t-s)\, \mathrm{v}_s$$

$$K(t) = 2\sum_i (d_i^2/\hbar\omega_i)\cos(\omega_i t)$$

✓ Single $K(t) \propto \cos(\Gamma t)$

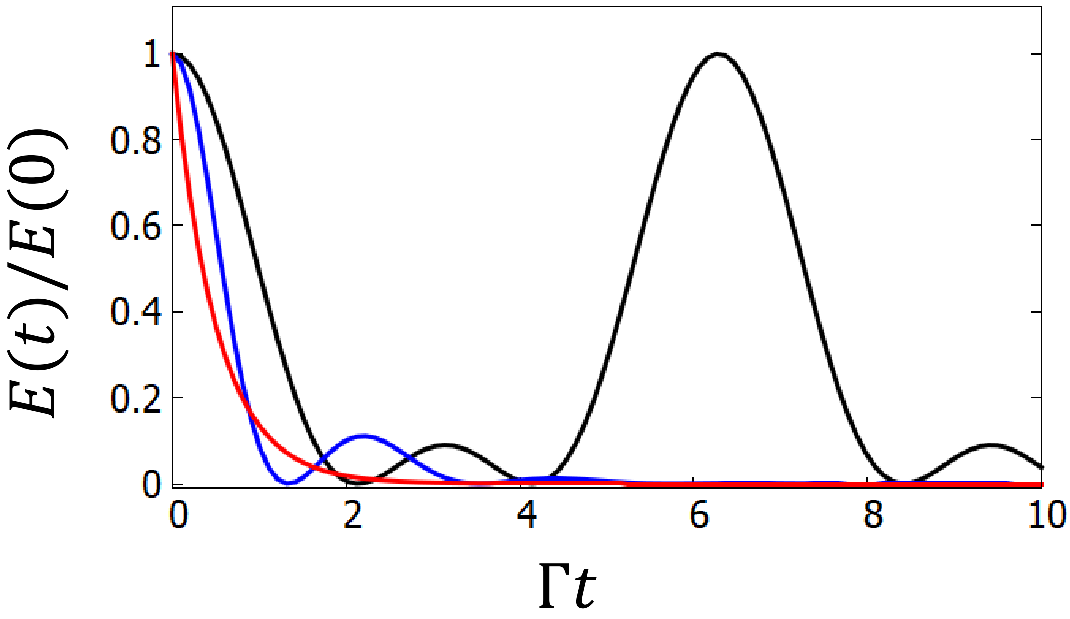
$$\mathrm{v_t/v_0} = \theta + (1-\theta)\cos(\Gamma t)$$

✓ Non-Markov $K(t) \propto e^{-\Gamma t}$

$$\mathrm{v_t/v_0} = \mathrm{e}^{-\Gamma t/2} \times [\cos(\Gamma t/2\theta) + \theta \sin(\Gamma t/2\theta)]$$

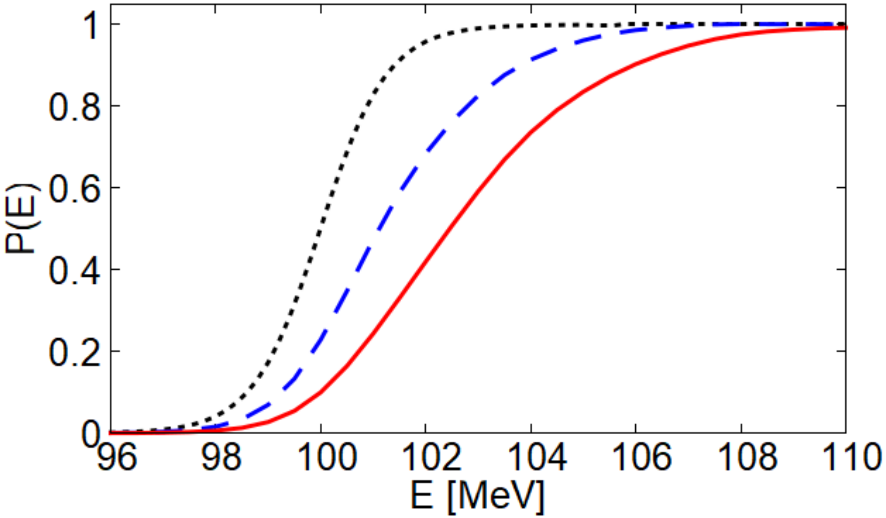
✓ Markov $K(t) \propto \Gamma\delta(t)$

$$\mathrm{v_t/v_0} = e^{-\Gamma t}$$

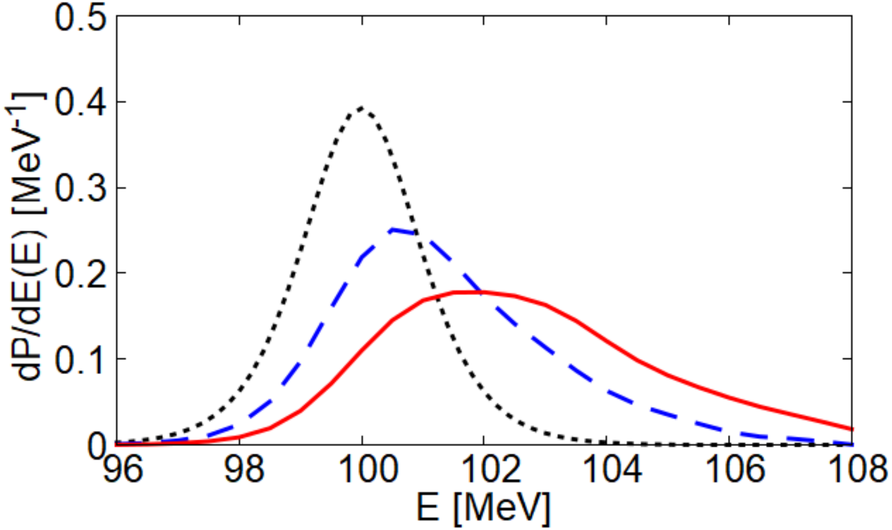


Effects of Fluctuation-Dissipation

Penetrability



Barrier distribution



- The stronger friction ➡ the higher effective barrier
- The stronger friction ➡ the broader effective barrier