

# Role of quantum mechanics in a diffusion process for superheavy elements

Kouichi Hagino

Kyoto University, Kyoto, Japan

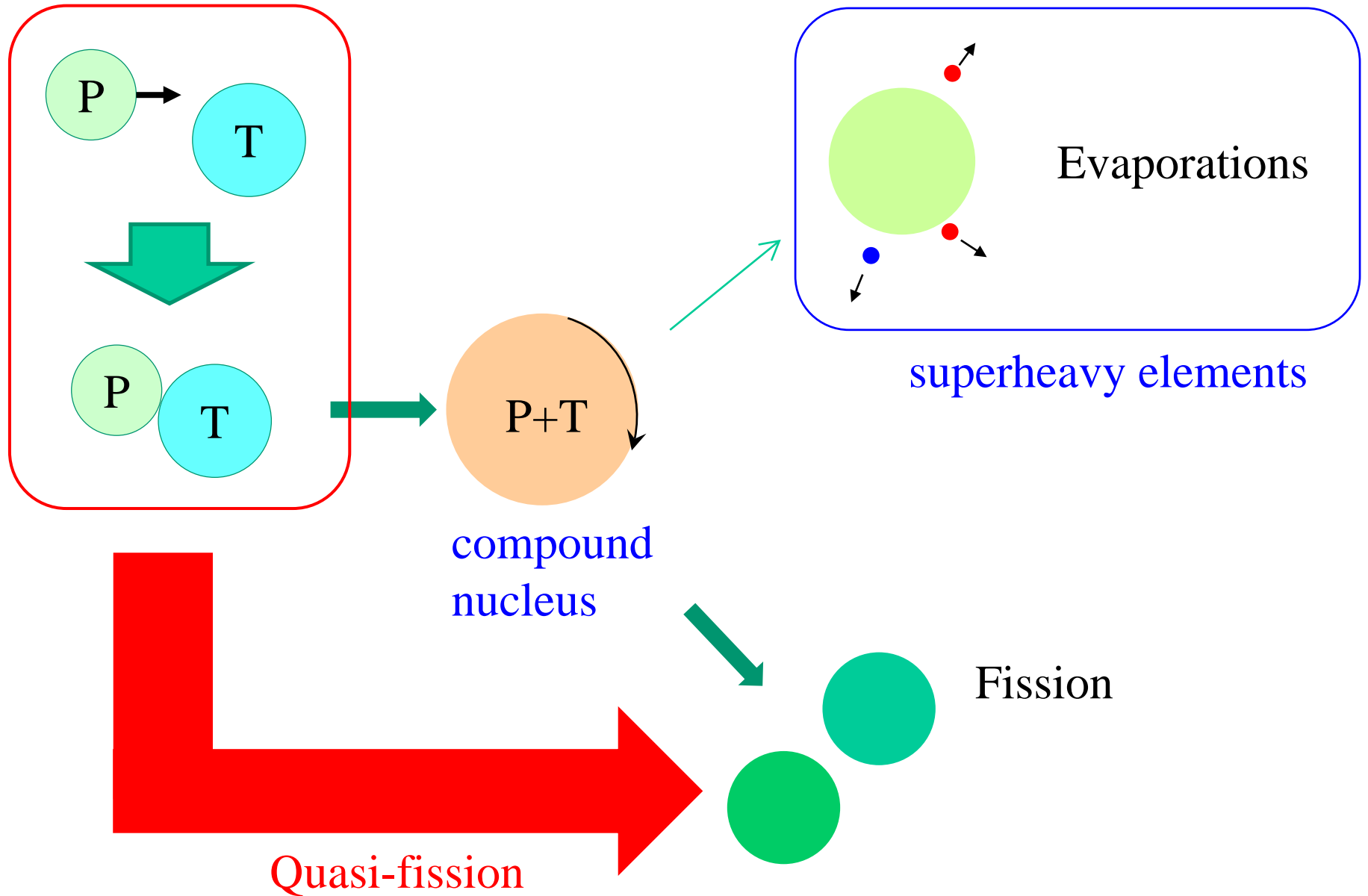


K. Washiyama (Kyushu)

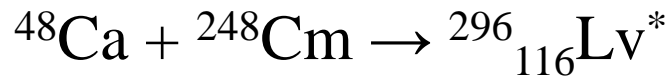
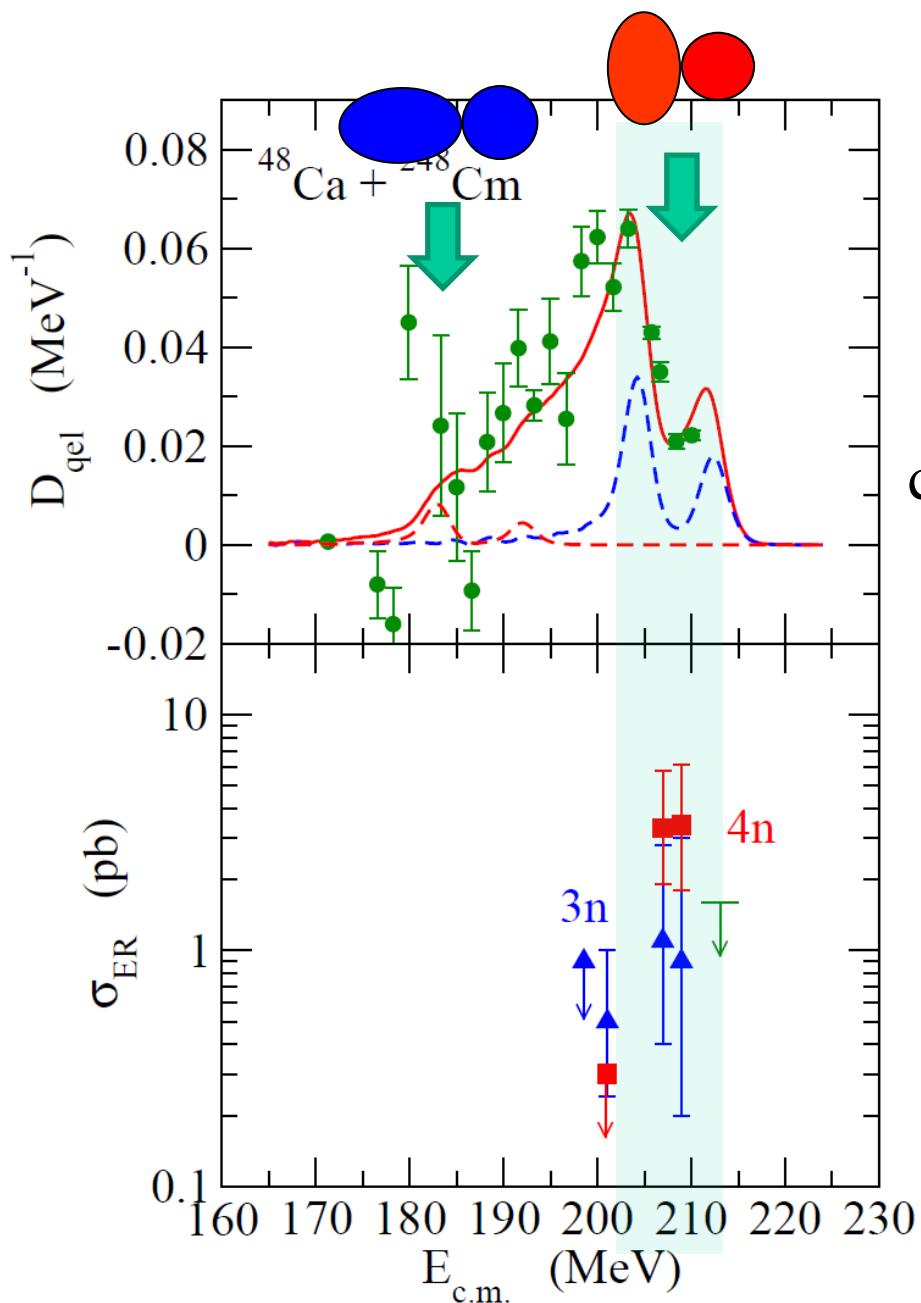
M. Tokieda (Tohoku)

1. Diffusion over the saddle: Langevin approach
2. Generalized Langevin approach and cold fusion
3. Towards quantum Langevin method
4. Summary

# Fusion for Superheavy elements



# Entrance channel dynamics: capture barrier distribution

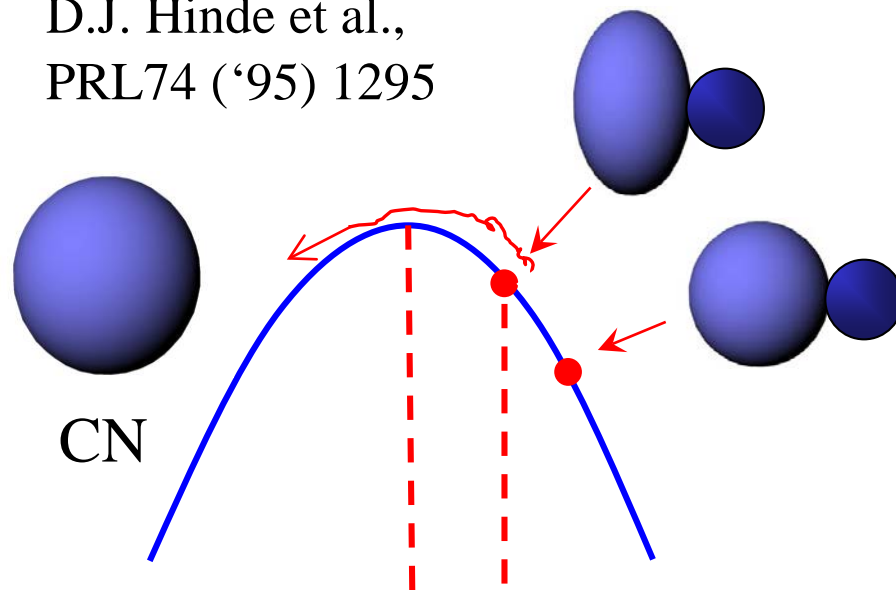


T. Tanaka, ..., K.H., et al.,  
 JPSJ 87 ('18) 014201  
 PRL124 ('20) 052502



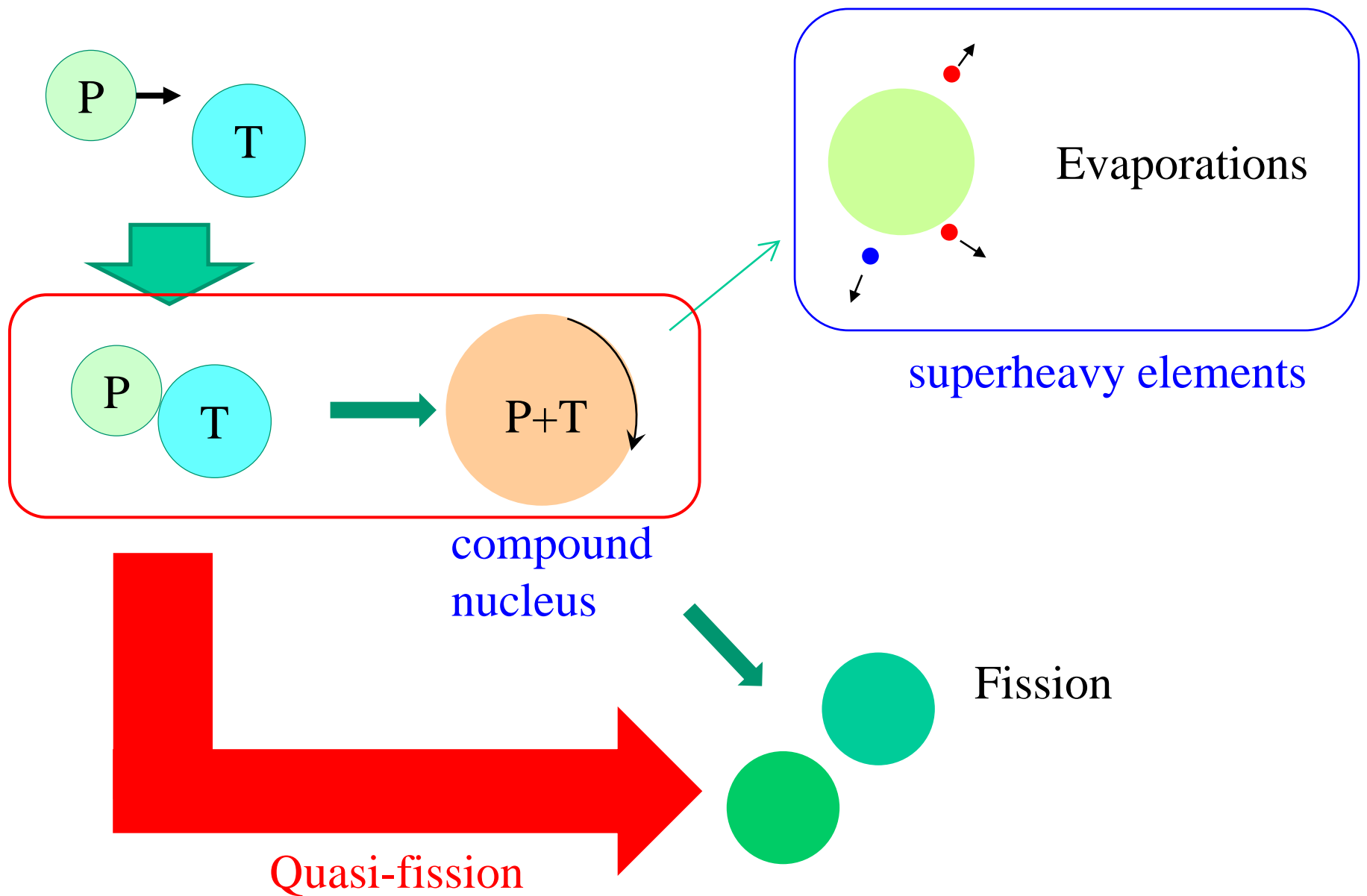
cf. notion of compactness:

D.J. Hinde et al.,  
 PRL74 ('95) 1295

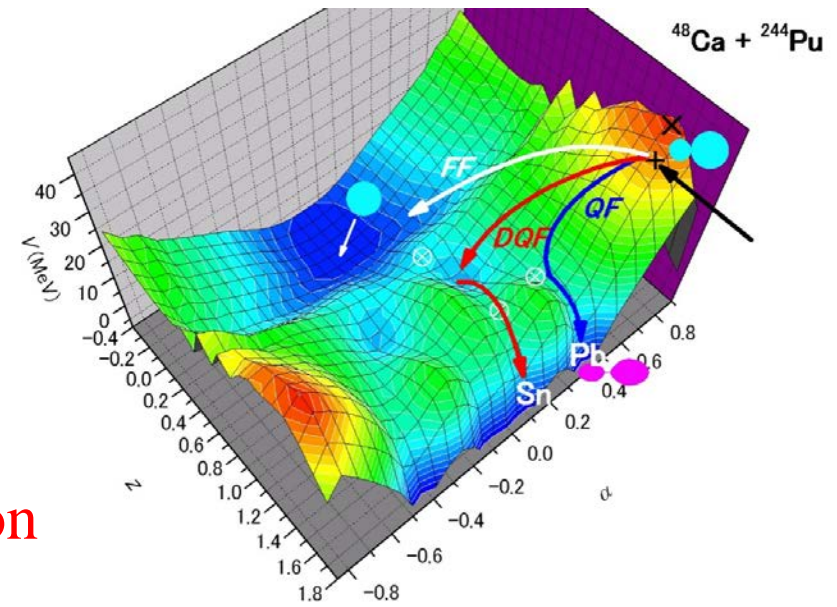
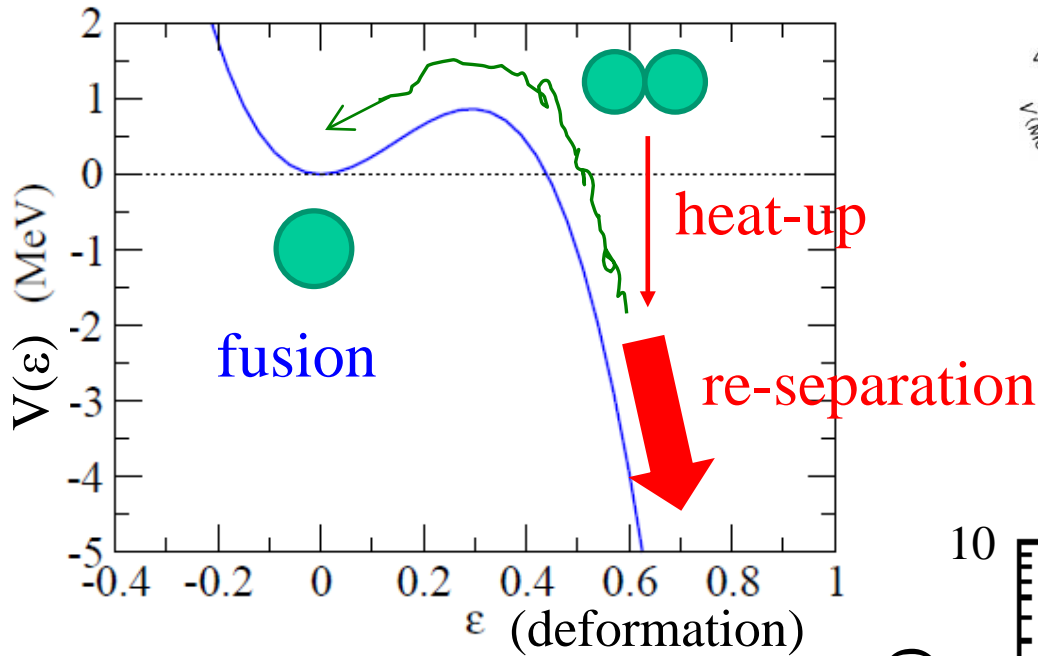


the next talk by Tanaka

# Fusion for Superheavy elements



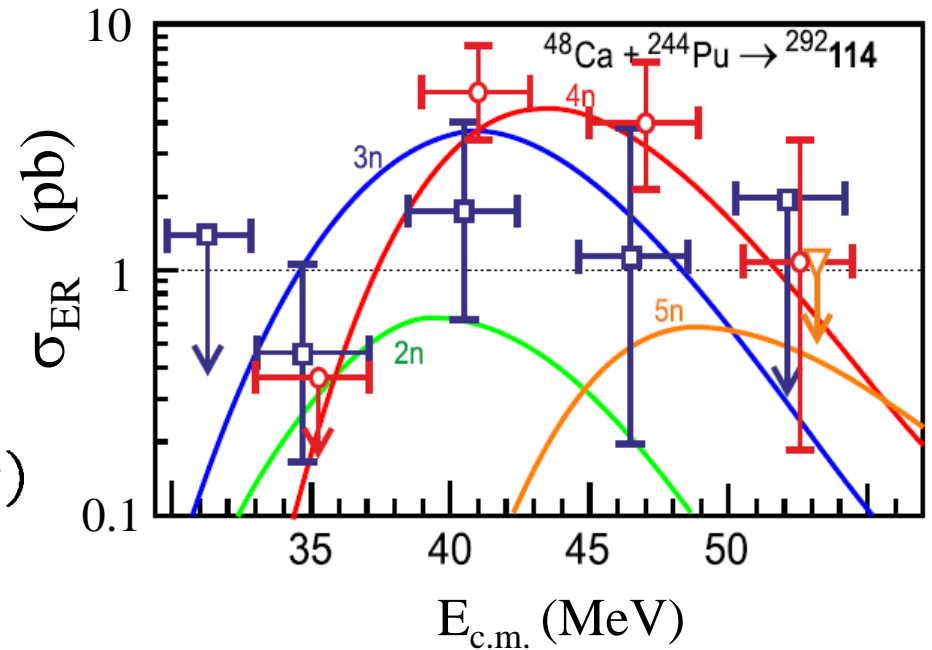
# Langevin approach



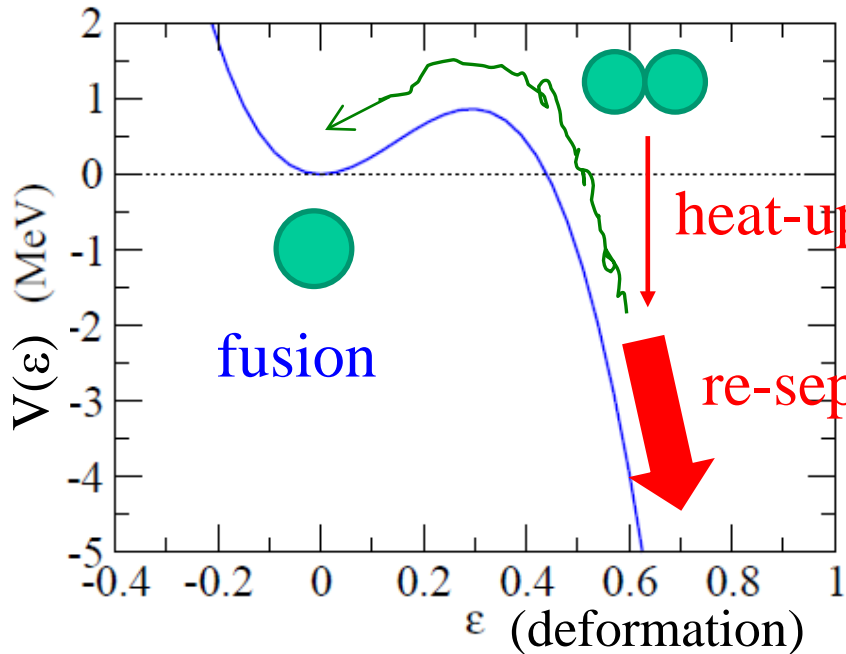
## thermal fluctuation

→ *classical Langevin method*

$$m \frac{d^2 q}{dt^2} = - \frac{dV(q)}{dq} - \gamma \frac{dq}{dt} + R(t)$$



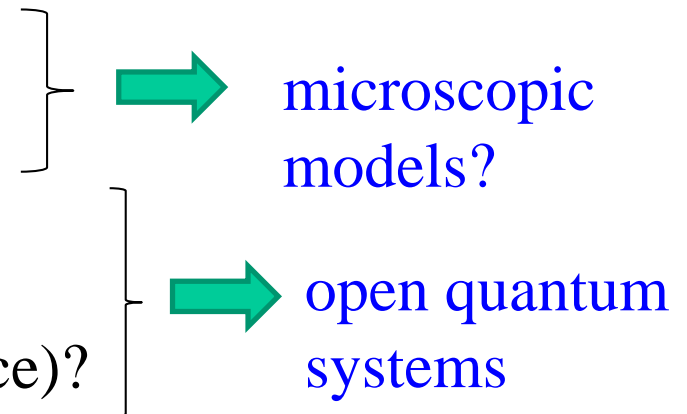
# Langevin approach



$$m \frac{d^2 q}{dt^2} = - \frac{dV(q)}{dq} - \gamma \frac{dq}{dt} + R(t)$$

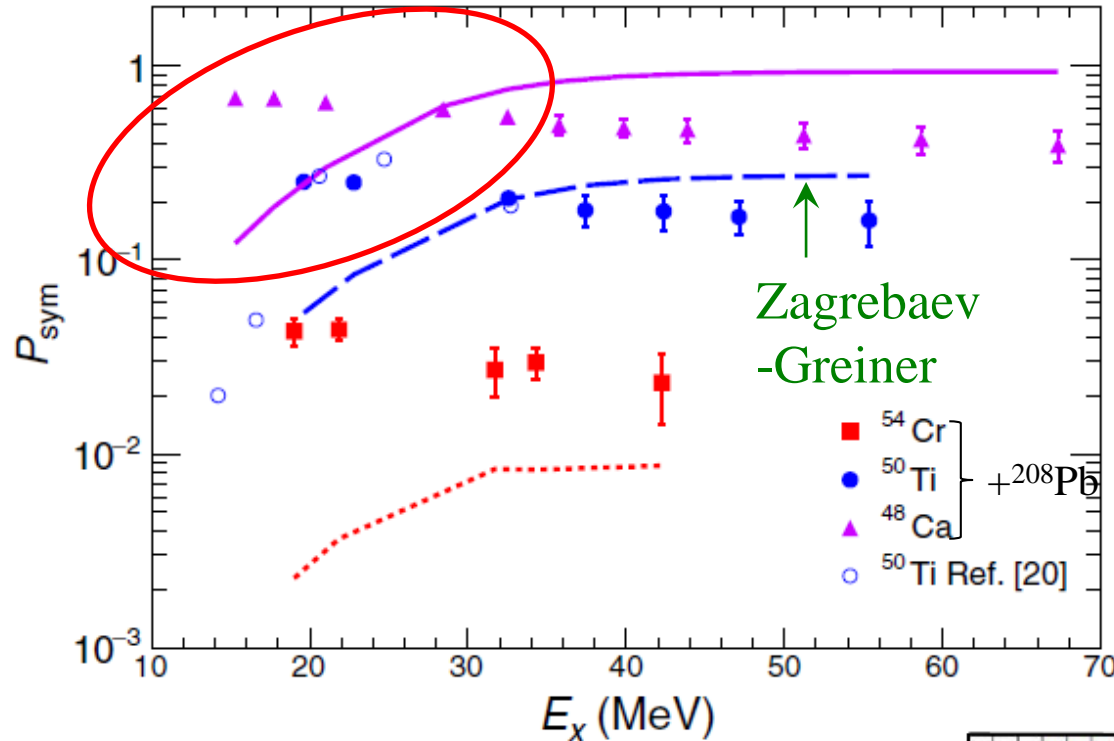
## Theoretical issues

- ✓ how to thermaize? mechanisms?
- ✓ is thermal equilibrium OK?
- ✓ Is Markovian approximation OK?
- ✓ **quantum effects?**
- ✓ quantal-to-classical transitions (decoherence)?

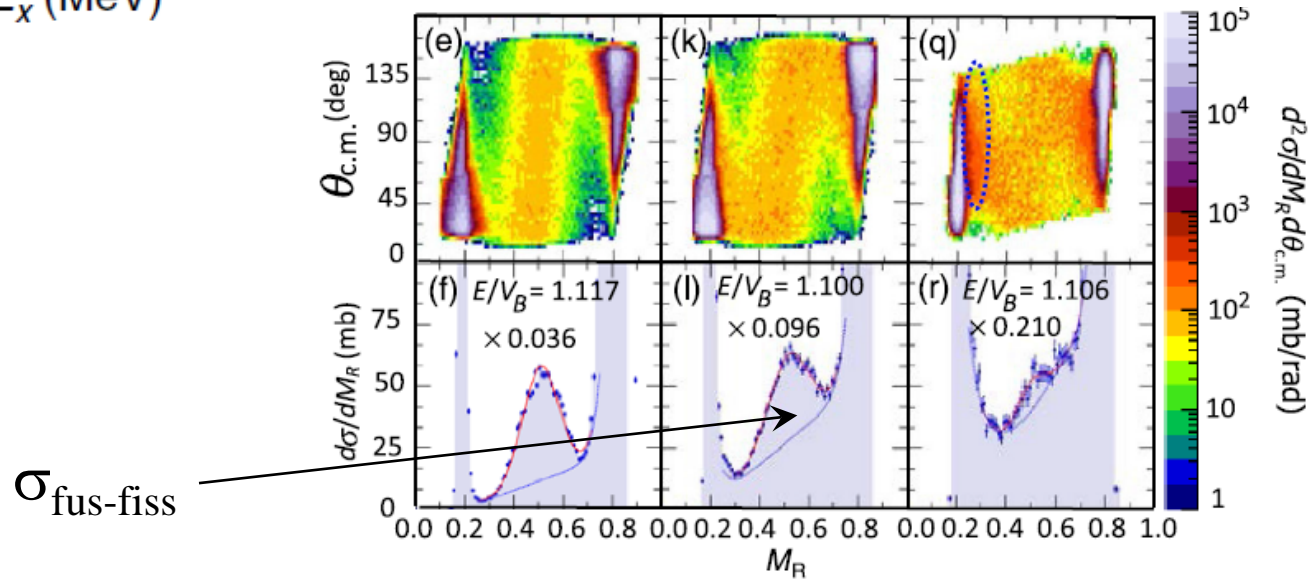


# Recent publication by Banerjee et al. (ANU)

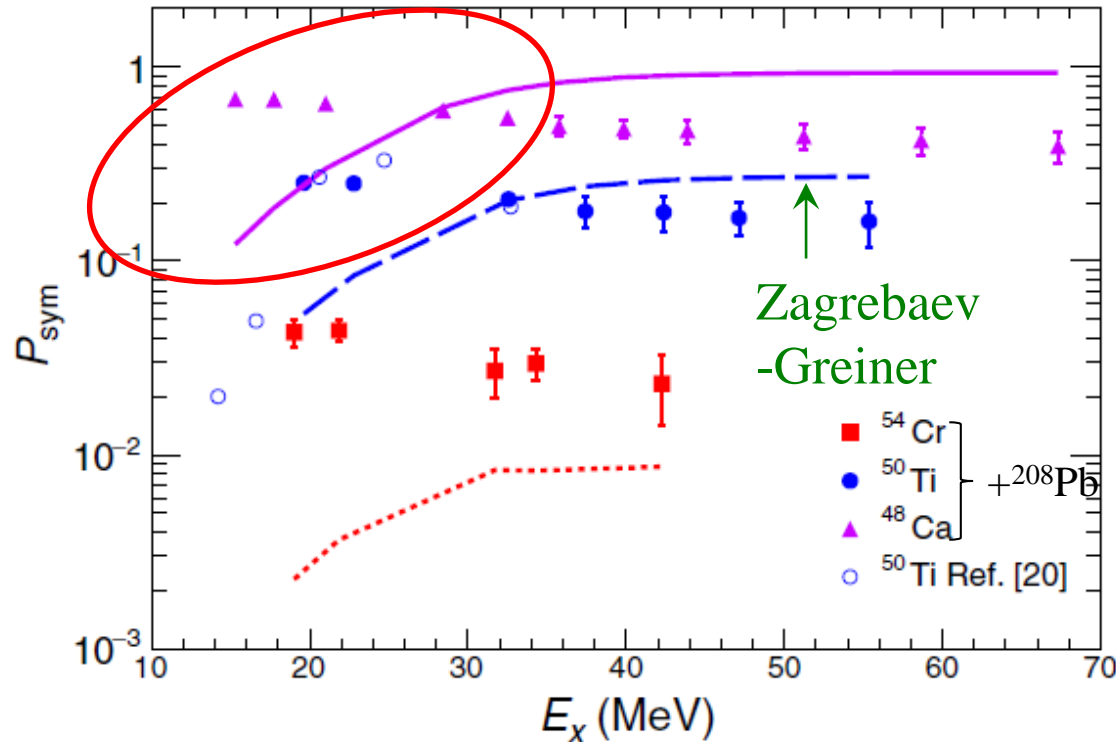
K. Banerjee, D.J. Hinde, et al.,  
PRL122, 232503 (2019)



“cold fusion reactions  
(involving  $^{208}\text{Pb}$ ) are not  
driven by a diffusion process”



## Recent publication by Banerjee et al. (ANU)



K. Banerjee, D.J. Hinde, et al.,  
PRL122, 232503 (2019)

“cold fusion reactions  
(involving  $^{208}\text{Pb}$ ) are not  
driven by a diffusion process”

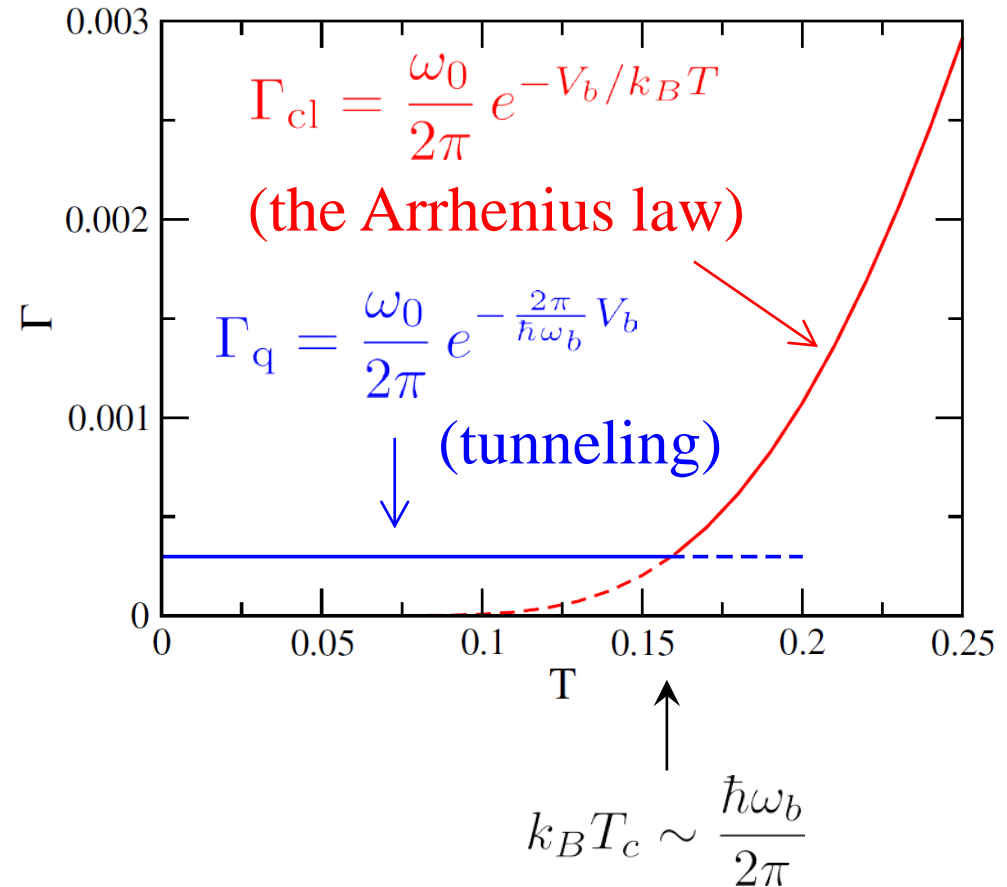
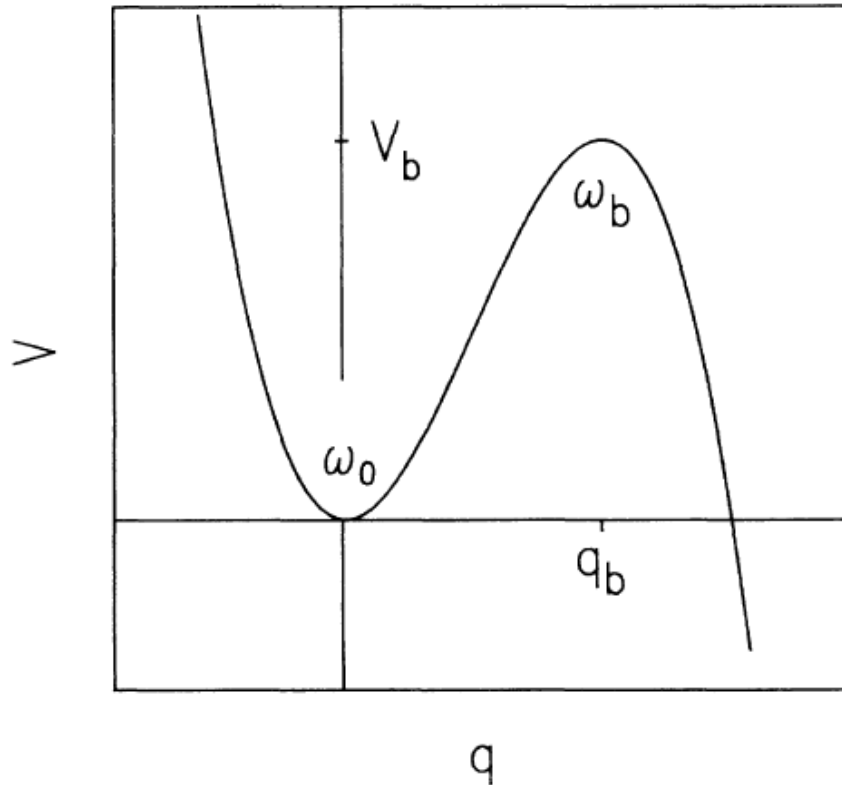
comparisons: to a classical Langevin calculation

→ quantum effect should be crucial at low  $E_x$



# Decay of a metastable state at finite temperatures

cf. induced fission



H. Grabert, P. Olschowski, and U. Weiss, PRB36, 1931 (1987)

 quantum Langevin for low temperatures?

## classical Langevin equation

$$m \frac{d^2 q}{dt^2} = - \frac{dV(q)}{dq} - \underbrace{\gamma \frac{dq}{dt}}_{\text{friction}} + \underbrace{R(t)}_{\text{random interaction}}$$

random interaction  $\rightarrow \langle R(t) \rangle = 0$

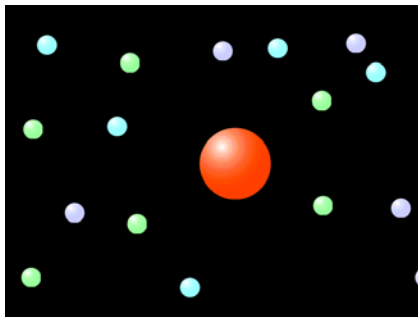
classical:

$$\langle R(t)R(t') \rangle = 2D \delta(t - t') \equiv 2D \chi(t - t')$$

$$D = \gamma T \quad (\text{Einstein relation})$$

(white noise; no memory)

Brownian motion



interaction of a Brownian  
particle with atoms

## classical Langevin equation

$$m \frac{d^2 q}{dt^2} = - \frac{dV(q)}{dq} - \underbrace{\gamma \frac{dq}{dt}}_{\text{friction}} + \underbrace{R(t)}_{\text{random interaction}}$$

friction random interaction  $\rightarrow \langle R(t) \rangle = 0$

classical:  $\langle R(t)R(t') \rangle = 2D \delta(t - t') \equiv 2D \chi(t - t')$

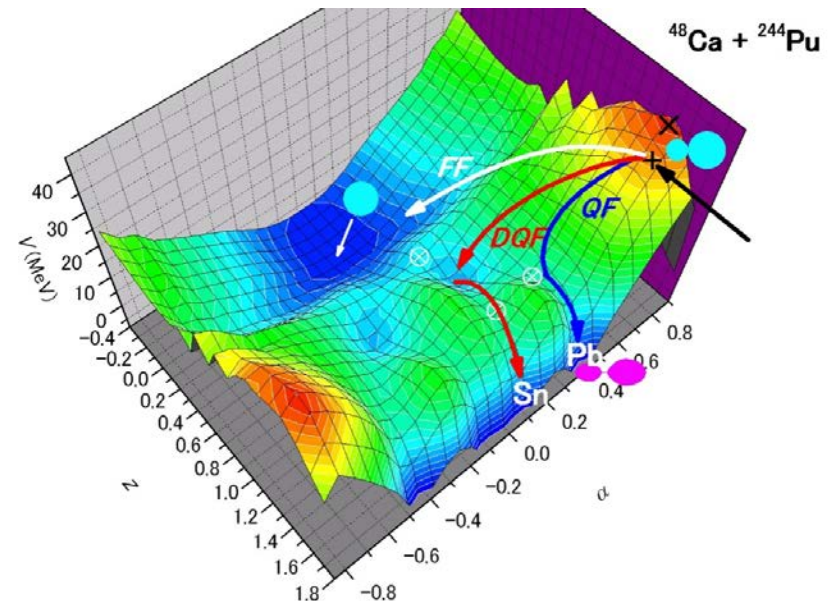
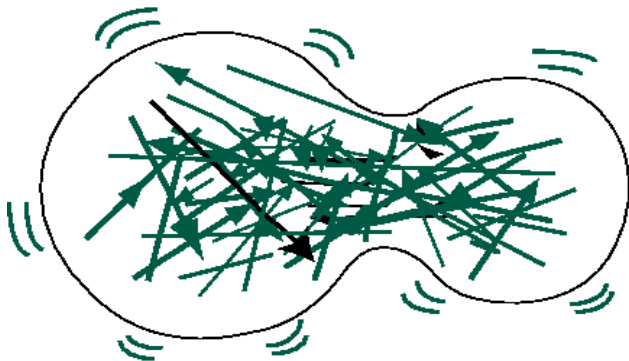
$$D = \gamma T \quad (\text{Einstein relation})$$

(white noise; no memory)

## nuclear reactions:

$q$  = the relative distance etc.

“atoms” = nucleonic d.o.f



$$m \frac{d^2 q}{dt^2} = -\frac{dV(q)}{dq} - \gamma \frac{dq}{dt} + R(t) \quad \langle R(t) \rangle = 0$$

**classical:**  $\langle R(t)R(t') \rangle = 2D \delta(t - t') \equiv 2D \chi(t - t')$

**quantal:**  $D = \gamma T$  (Einstein relation)

$\chi(t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T} \exp \left[ -\frac{(\hbar\omega)^2}{2\Delta^2} \right] e^{-i\omega(t-t')}$		
	Fermi statics	high energy cut-off

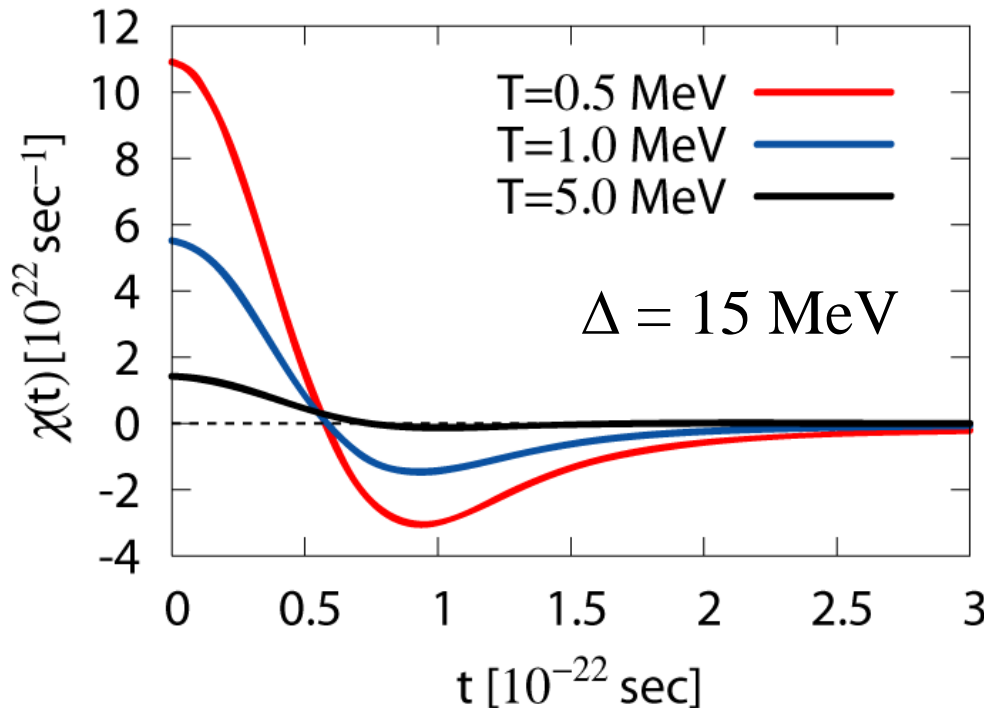
$\rightarrow \delta(t - t') \quad (T \rightarrow \infty)$

$$m \frac{d^2 q}{dt^2} = -\frac{dV(q)}{dq} - \gamma \frac{dq}{dt} + R(t) \quad \langle R(t) \rangle = 0$$

classical:  $\langle R(t)R(t') \rangle = 2D \delta(t - t') \equiv 2D \chi(t - t')$

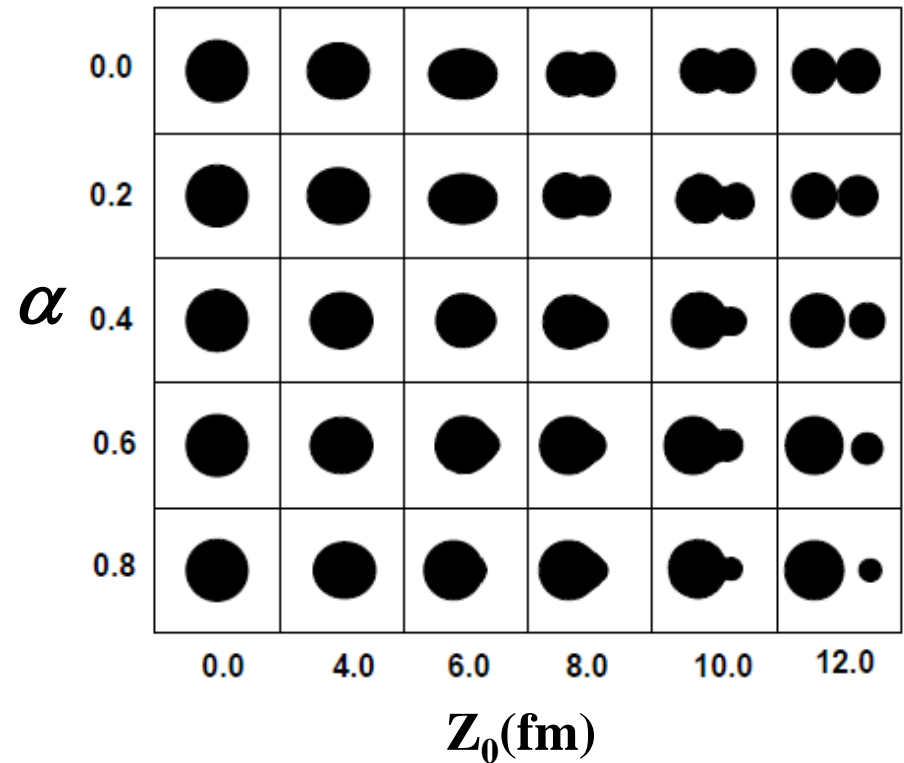
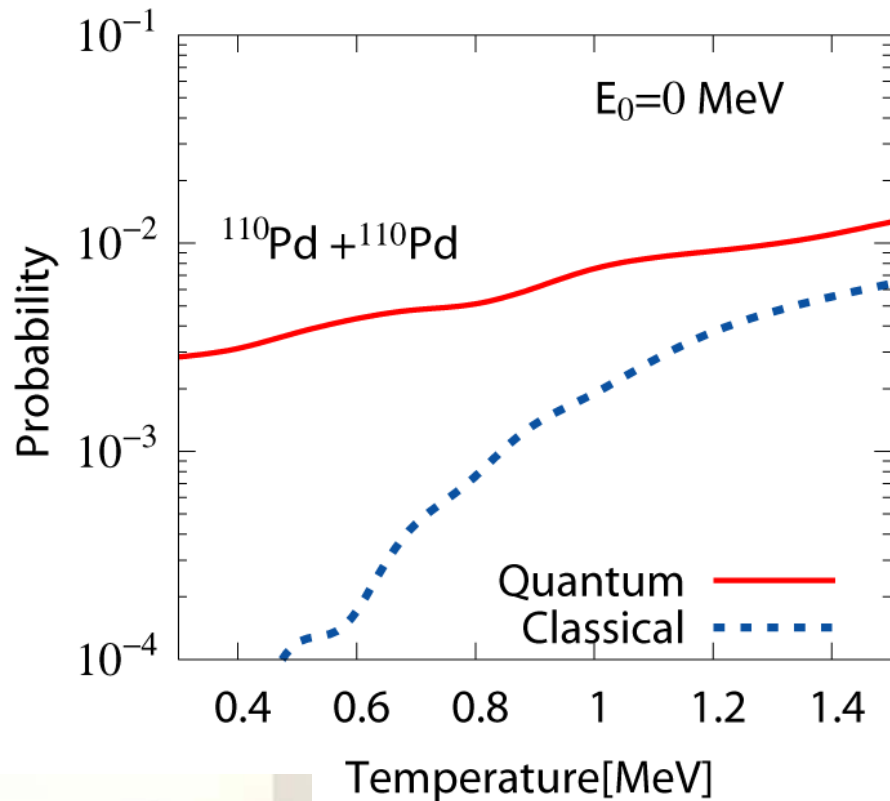
quantal:

$$\chi(t - t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T} \exp \left[ -\frac{(\hbar\omega)^2}{2\Delta^2} \right] e^{-i\omega(t-t')}$$

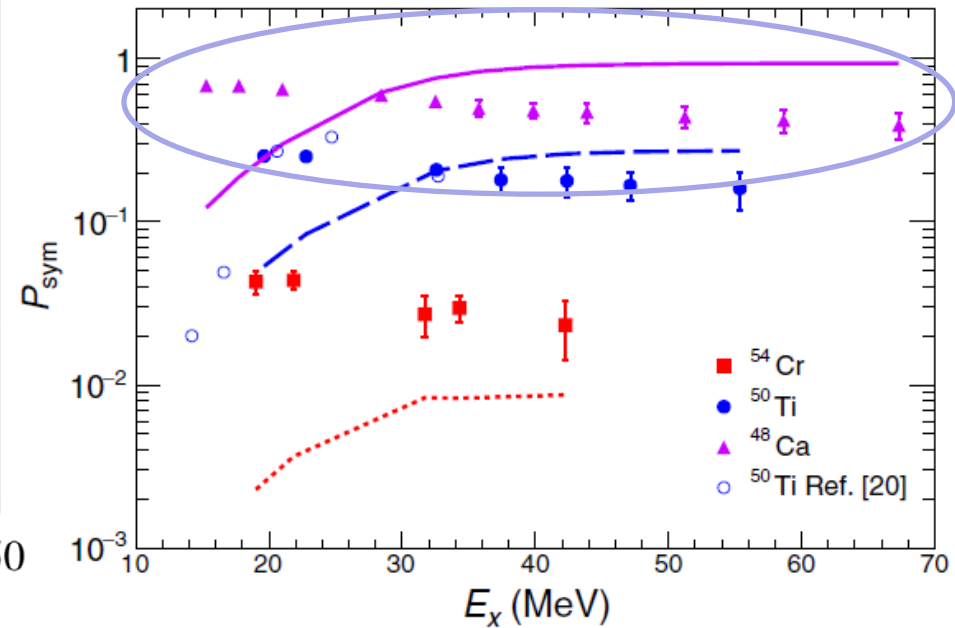
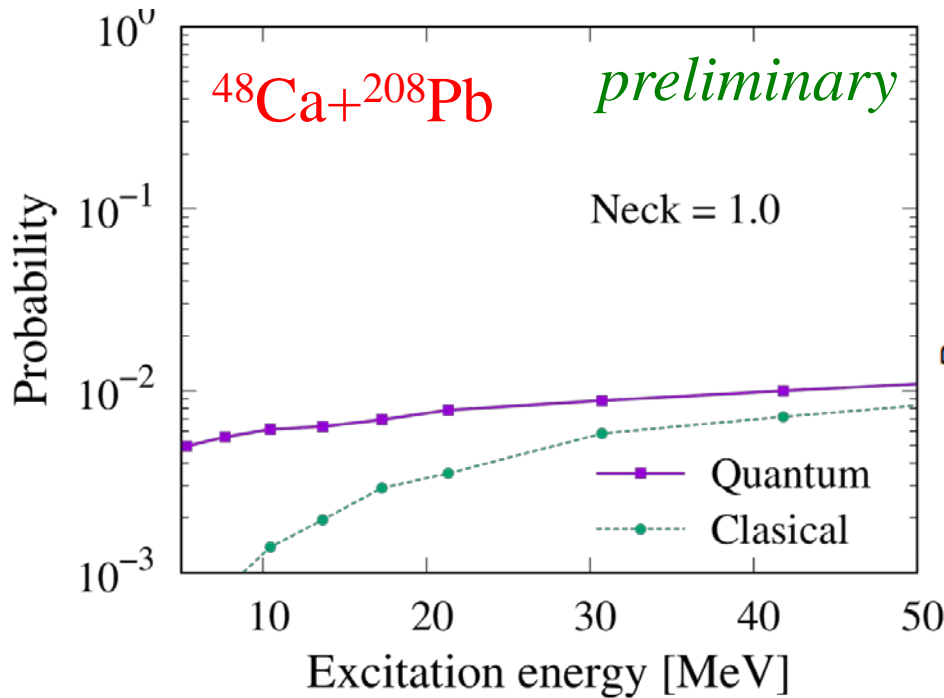


a long memory time  
at low  $T$

# 2D Langevin calculations with the rel. coordinate and the mass asym.



# 2D Langevin calculations with the rel. coordinate and the mass asym.



K. Banerjee, D.J. Hinde, et al.,  
PRL122, 232503 (2019)

qualitatively good,  
but quantitatively bad

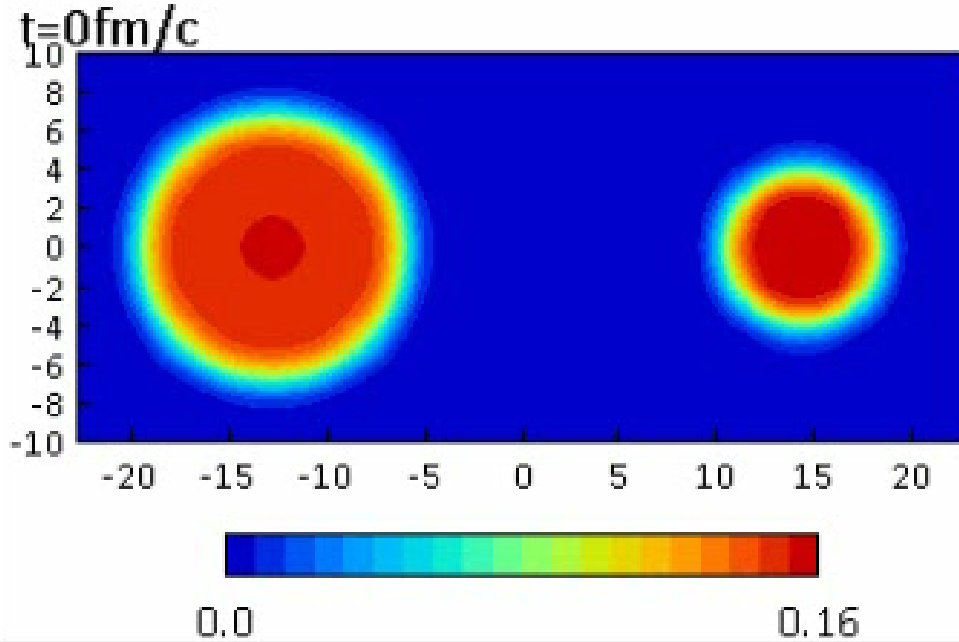
→ neck d.o.f?



K. Washiyama and K.H., in preparation

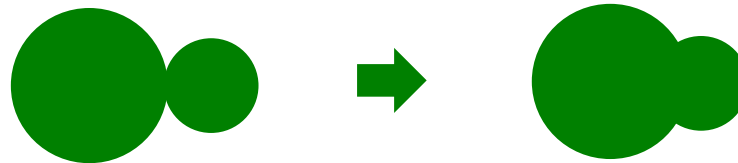
# TDHF calculation for $^{48}\text{Ca}+^{208}\text{Pb}$

$$E_{\text{cm}} = 178 \text{ MeV}$$



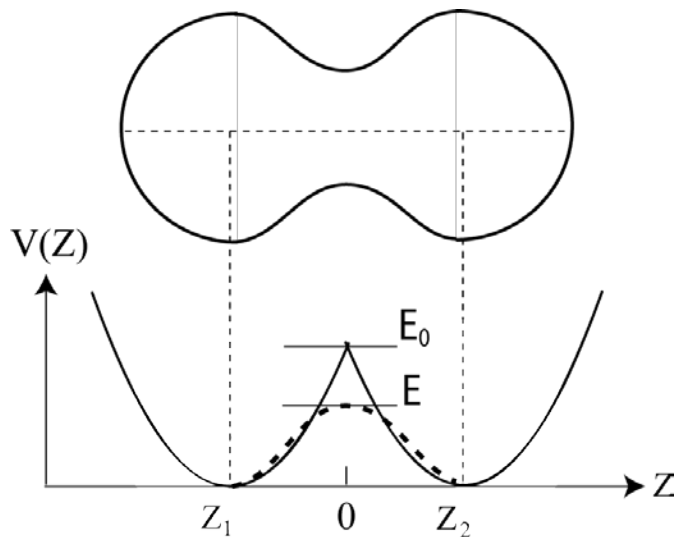
- ✓ Skyrme interaction (SLy4d)
- ✓ TDHF3D code

The neck d.o.f. is fast.



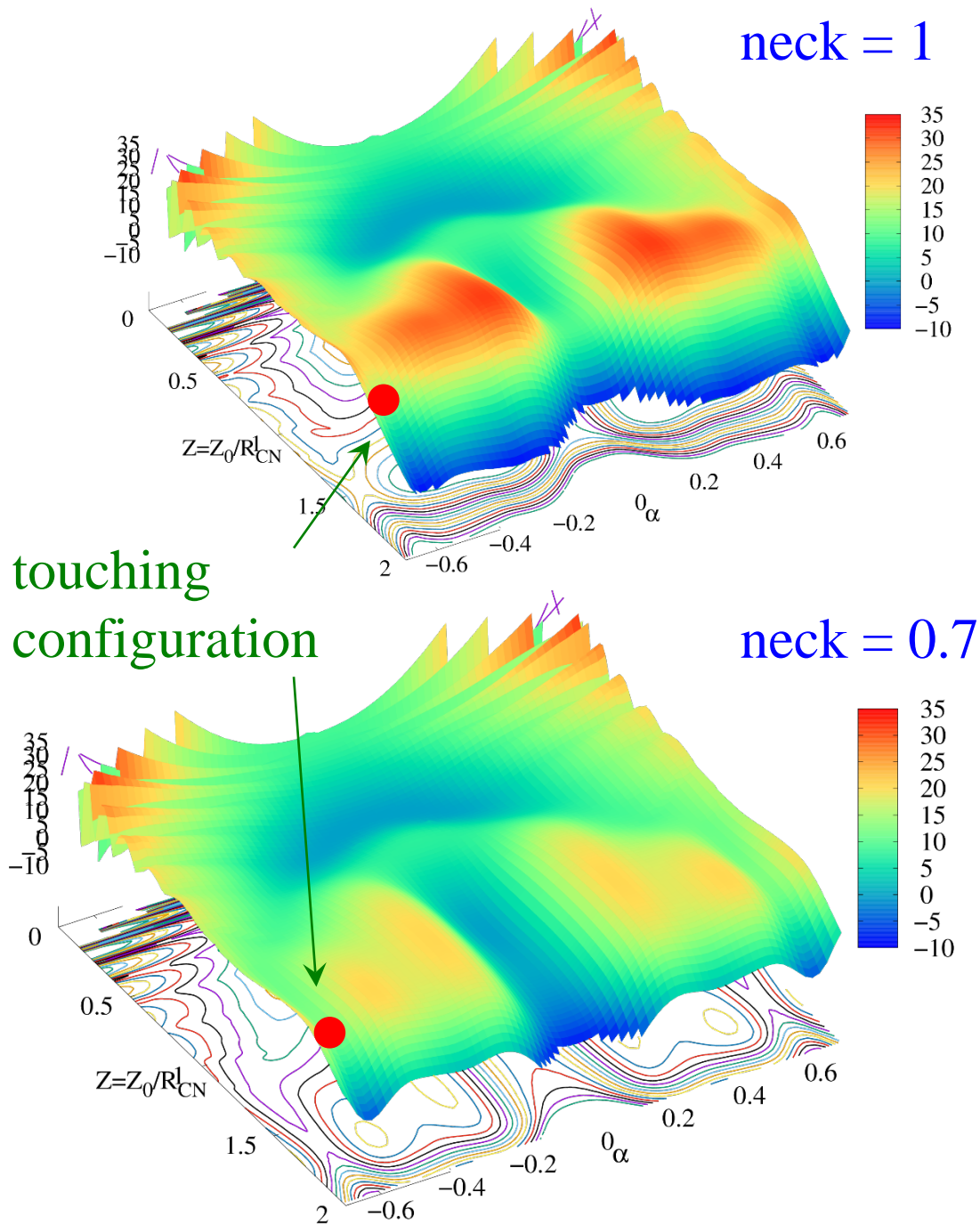
cf. D. Boilley et al., PRC84 ('11) 054608





$$\text{Neck} = E/E_0$$

*on going work*



## More quantal approach?

generalized Langevin approach:  $m \frac{d^2 q}{dt^2} = -\frac{dV(q)}{dq} - \gamma \frac{dq}{dt} + R(t)$

$$\langle R(t)R(t') \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T} \exp \left[ -\frac{(\hbar\omega)^2}{2\Delta^2} \right] e^{-i\omega(t-t')}$$

still classical motion (e.g., no tunneling)



more quantal approach: return to the original Hamiltonian

$$H = \frac{p^2}{2m} + V(q) + \underbrace{\sum_i \hbar\omega_i a_i^\dagger a_i}_{\text{H.O.}} + h(q) \underbrace{\sum_i d_i (a_i + a_i^\dagger)}_{\text{linear coupling}}$$

H.O.

linear coupling

A.O. Caldeira and A.J. Leggett, Ann. Phys. 149 ('83) 374



solve  $H$  quantum mechanically  $\longleftrightarrow$  “quantum Langevin”

## More quantal approach?

$$H = \frac{p^2}{2m} + V(q) + \sum_i \hbar\omega_i a_i^\dagger a_i + h(q) \sum_i d_i (a_i + a_i^\dagger)$$

➔ solve  $H$  quantum mechanically  $\longleftrightarrow$  “quantum Langevin”

time-dependent coupled-channels equations with an efficient basis

$$\Psi_{\text{tot}}(q, t) = \sum_{\{\tilde{n}_k\}} \tilde{\psi}_{\{\tilde{n}_k\}}(q, t) |\{\tilde{n}_k\}\rangle$$

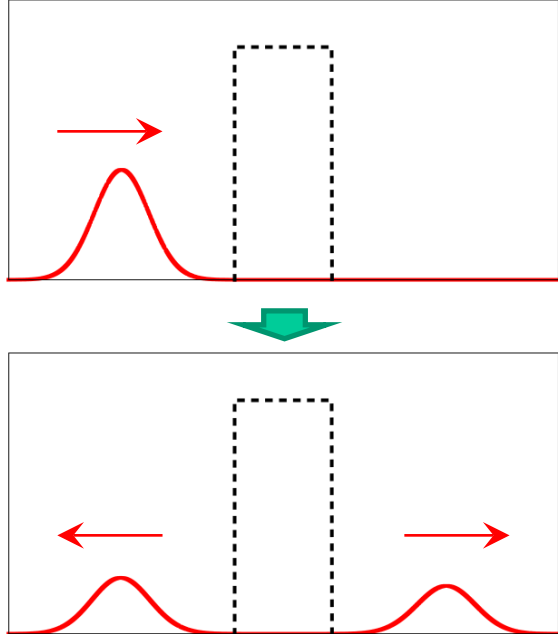
$$|\{\tilde{n}_k\}\rangle = \prod_{k=1}^K \frac{1}{\sqrt{\tilde{n}_k!}} (b_k^\dagger)^{\tilde{n}_k} |0\rangle$$

$$b_k^\dagger = \sum_i C_{ki} a_i^\dagger$$

M. Tokieda and K. Hagino, Ann. of Phys. 412 (2020) 168005  
Front. in Phys. 8 (2020) 8.

# Application to heavy-ion fusion reactions

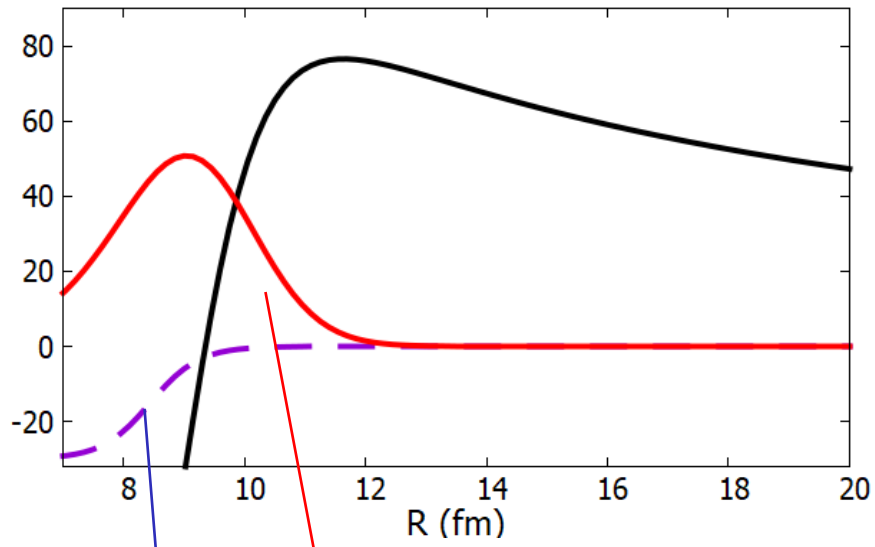
## time-dep. wave packet approach



$$R(E) \propto \langle \psi_R(t_f) | \delta(H - E) | \psi_R(t_f) \rangle$$

3D: radial coordinate for each partial wave  
(NB. no tangential friction)

$^{16}\text{O} + ^{208}\text{Pb}$



coupling to the bath

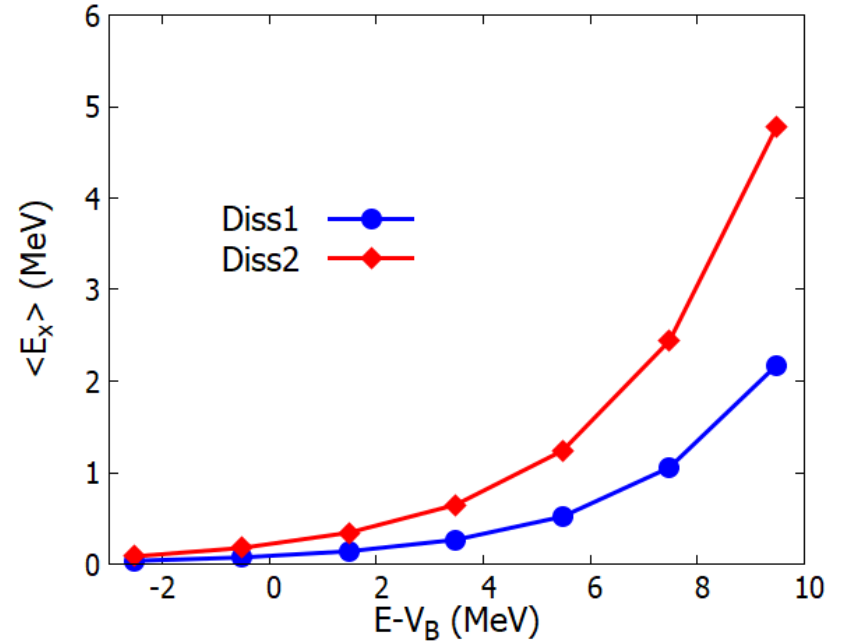
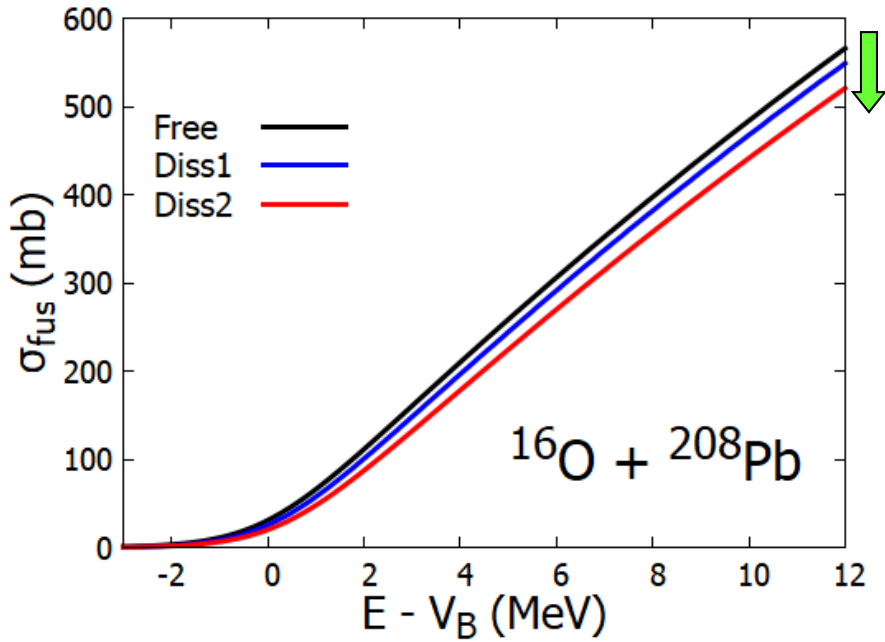
$$h(r) \propto V'_N(r)^2$$

cf. the surface friction model

absorption to simulate fusion

# fusion cross sections

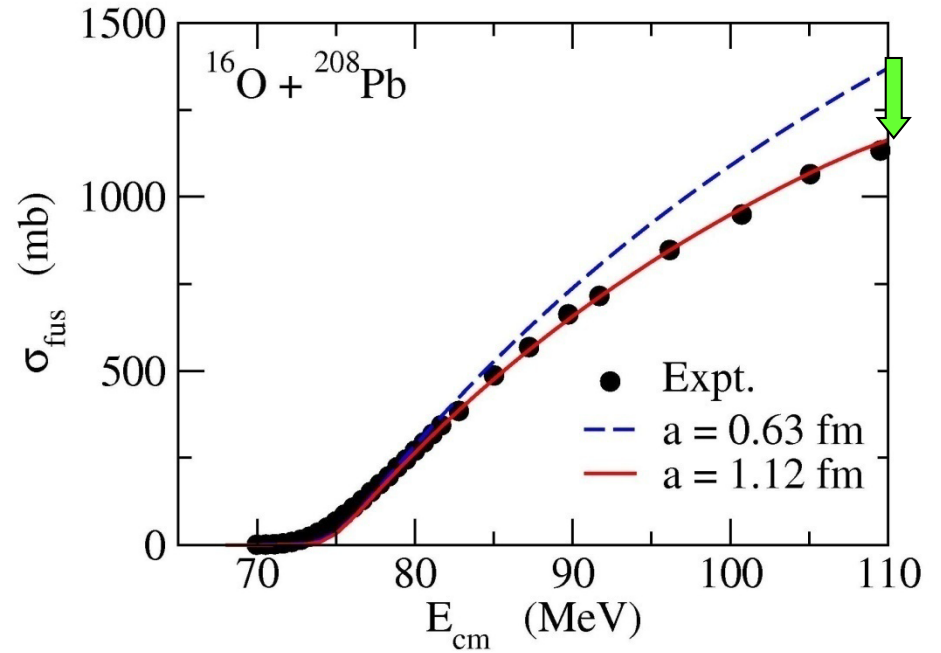
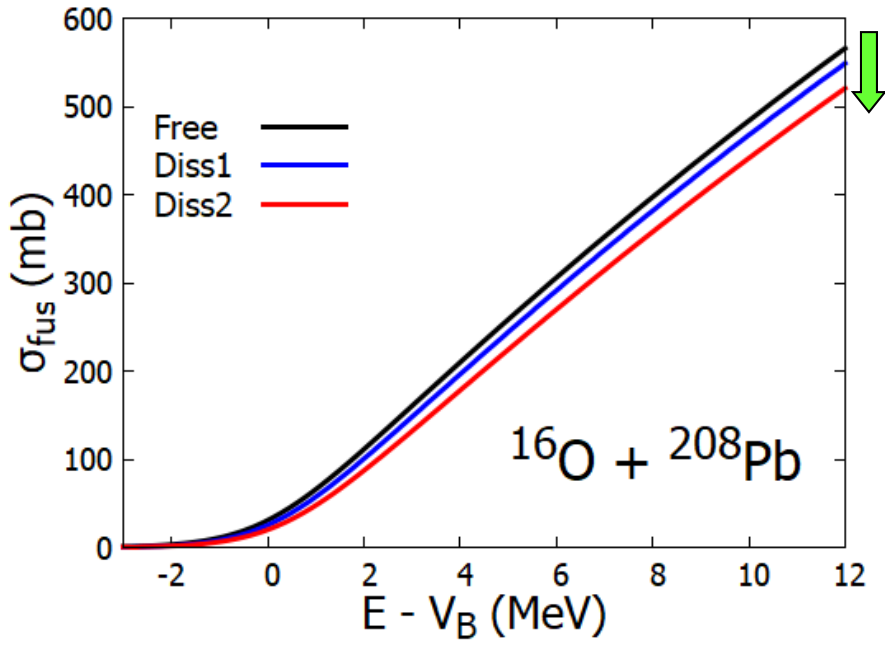
$$\sigma_{\text{fus}}(E) = \frac{\pi}{k^2} \sum_l (2l + 1)(1 - R_l(E))$$



M. Tokieda, Ph.D. thesis (2021), Tohoku University

# fusion cross sections

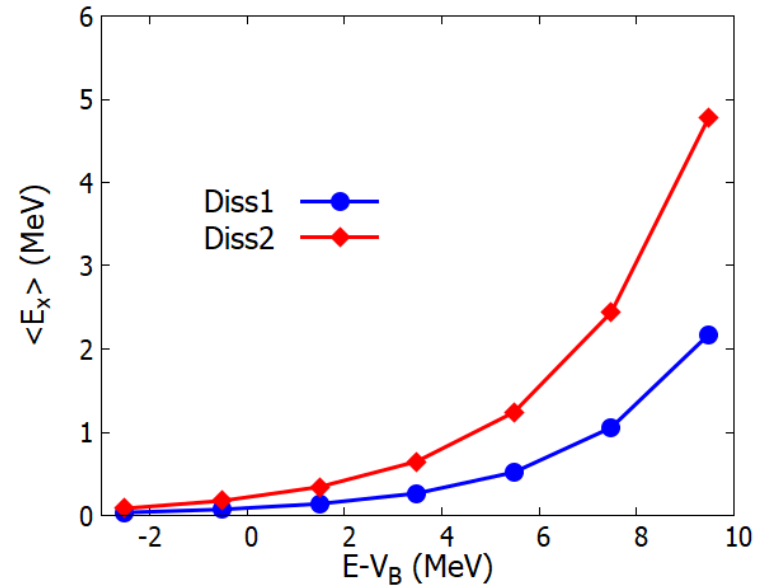
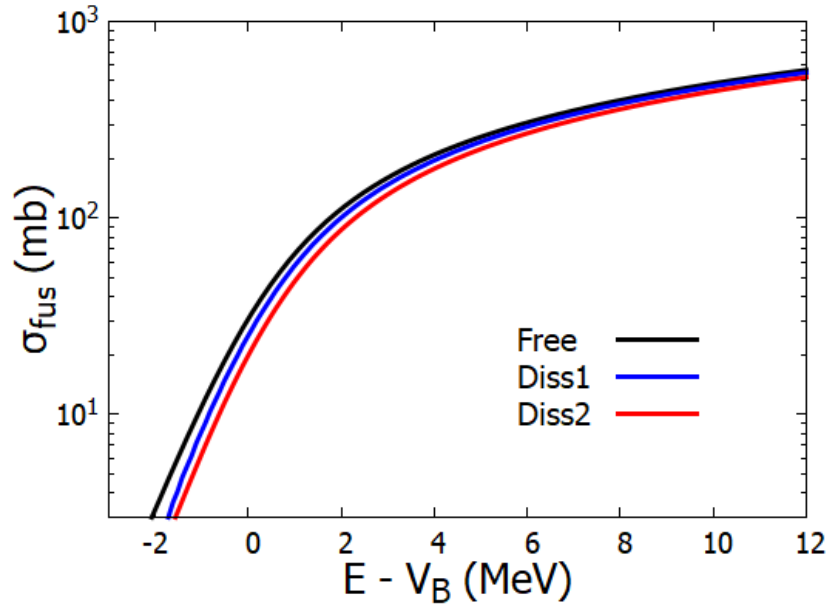
$$\sigma_{\text{fus}}(E) = \frac{\pi}{k^2} \sum_l (2l + 1)(1 - R_l(E))$$



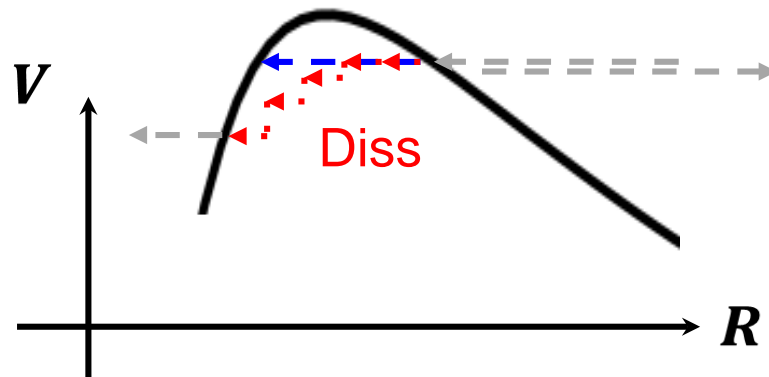
M. Tokieda, Ph.D. thesis (2021), Tohoku University

# fusion cross sections

$$\sigma_{\text{fus}}(E) = \frac{\pi}{k^2} \sum_l (2l + 1)(1 - R_l(E))$$



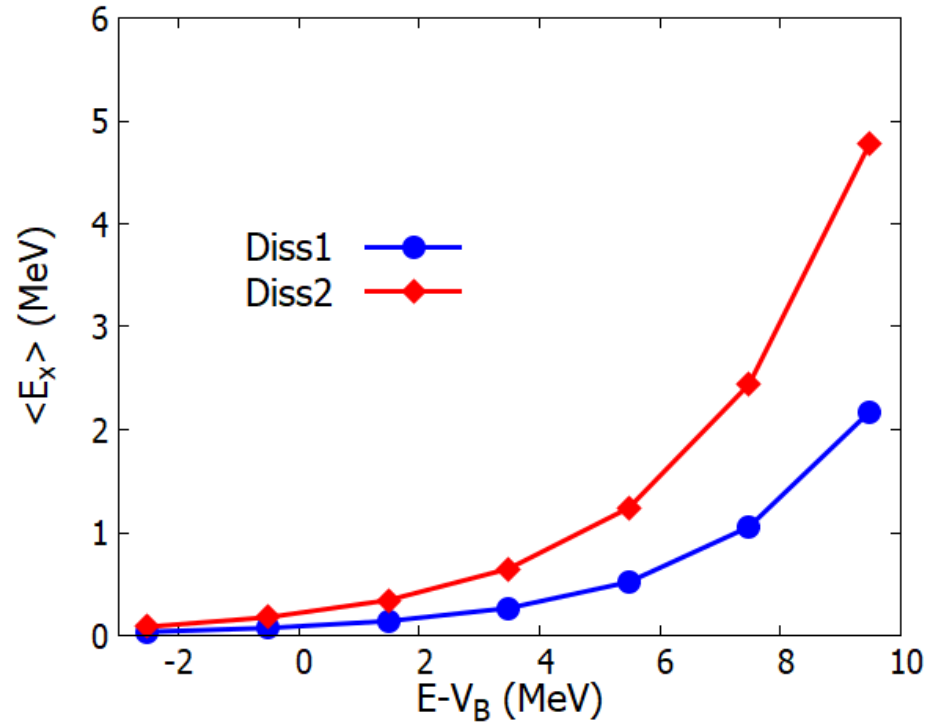
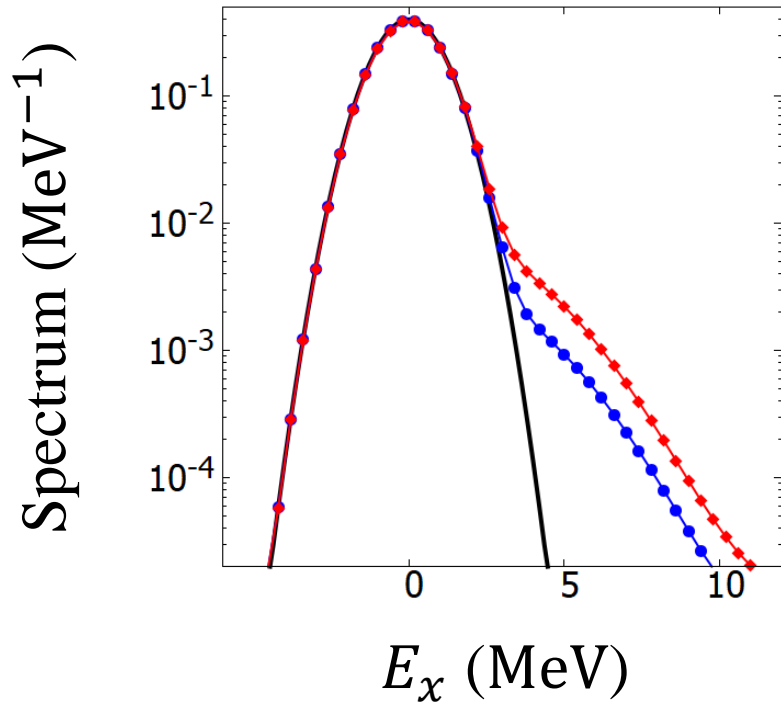
NB. Fusion cross sections: largely influenced even when  $\langle E_x \rangle$  is small



# Q-value distribution

$$\langle E_x \rangle = \frac{\langle \psi_R(t_f) | \delta(H_B - E) | \psi_R(t_f) \rangle}{\langle \psi_R(t_f) | \psi_R(t_f) \rangle}$$

$$E/V_B \simeq 0.96$$



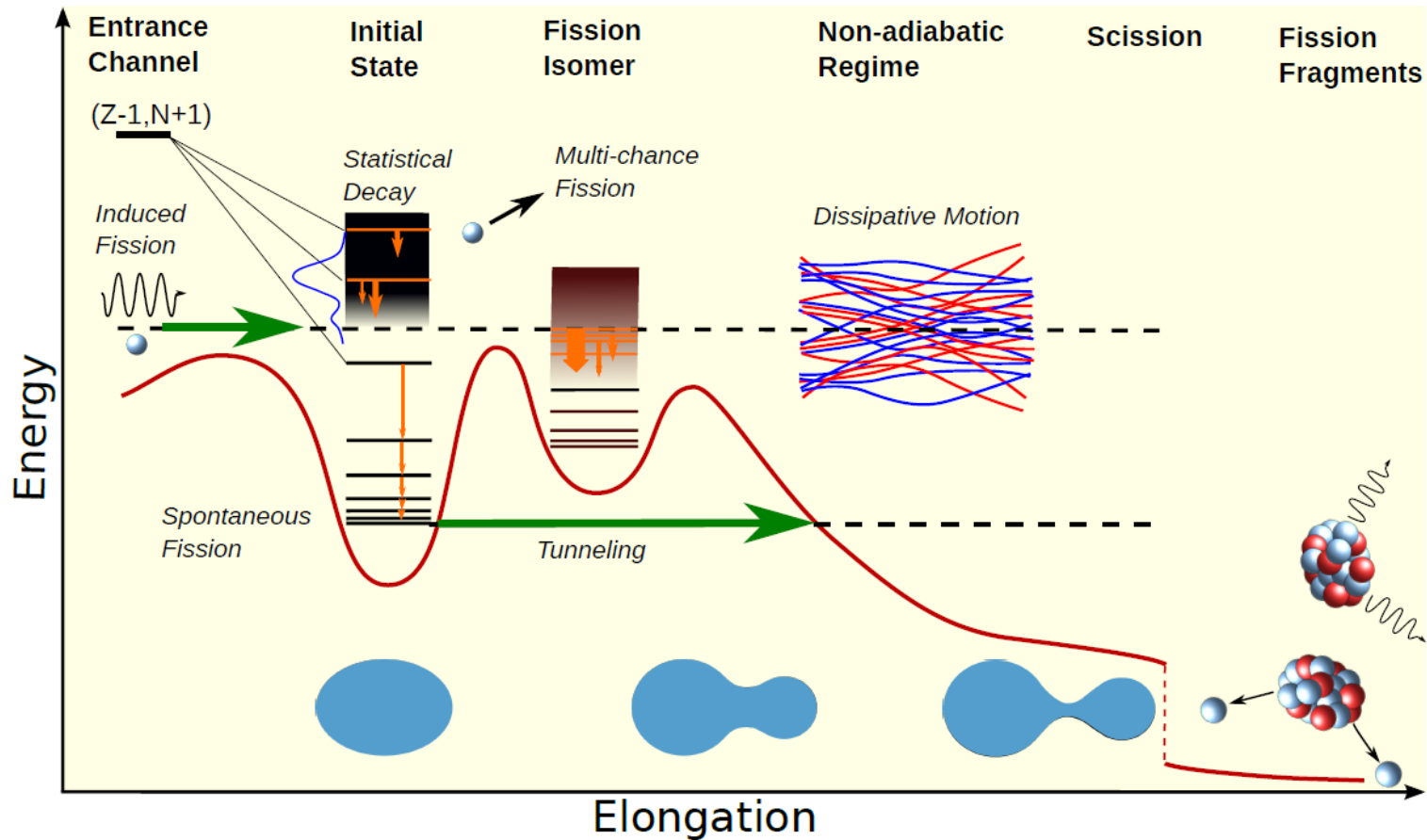
the next step: a comparison to the experimental data

M. Tokieda, Ph.D. thesis (2021), Tohoku University



# fission: a very complicated dynamics

a microscopic understanding → far from complete



M. Bender et al., J. of Phys. G47, 113002 (2020)

quantum Langevin: a unified description?

# Summary

fusion for SHE

→ a very complicated many-body dynamics

the *classical* Langevin: standard

➤ quantum extension?

→ maybe important for cold fusion reactions

- generalized Langevin calculations

enhanced  $P_{\text{CN}}$  for  $^{48}\text{Ca}+^{208}\text{Pb}$

- quantum Langevin approach

CC with Caldeira-Legett Hamiltonian

friction: hinders subbarrier fusion cross sections

→ a unified description from low- $E$  to high- $E$

