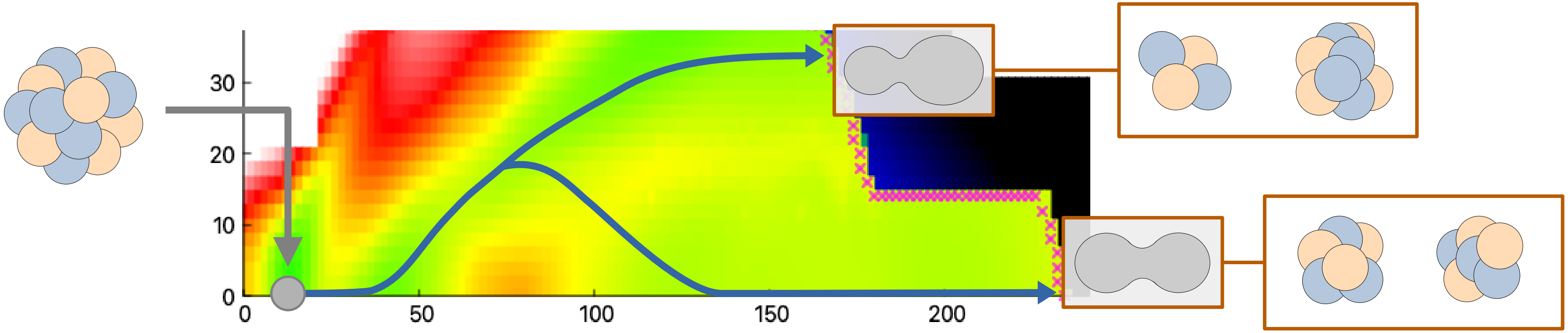
Improved modelling of nuclear fission with the “exact” TDGCM and projection techniques

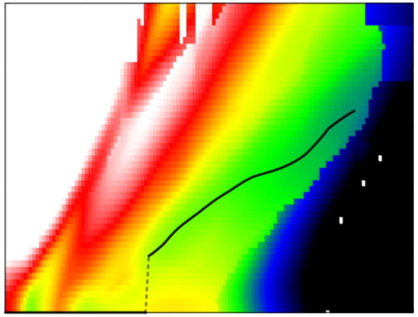
Ngee Wein Lau

Laboratoire des 2 Infinis Toulouse (L2IT)
IN2P3 – CNRS / Université de Toulouse



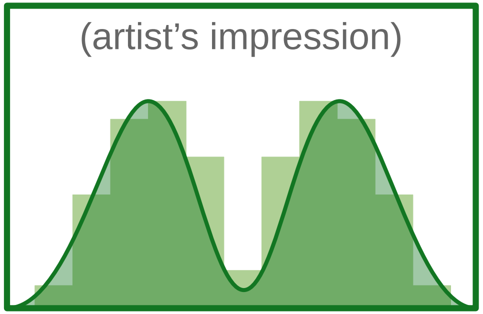
Research aims

potential energy surfaces (PESs)



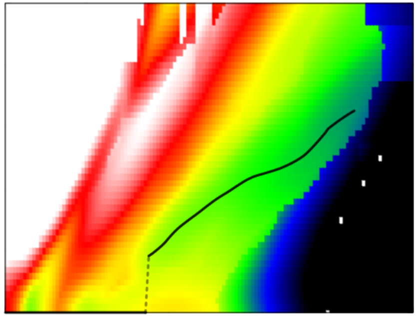
→ the time-dependent generator coordinate method (TDGCM) → GOA →

fission observables



Research aims

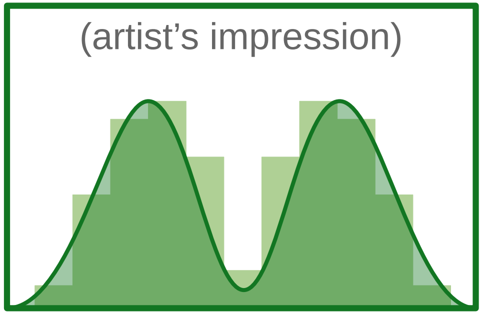
potential energy
surfaces (PESs)



the time-dependent
generator coordinate
method (TDGCM)

GOA

fission
observables

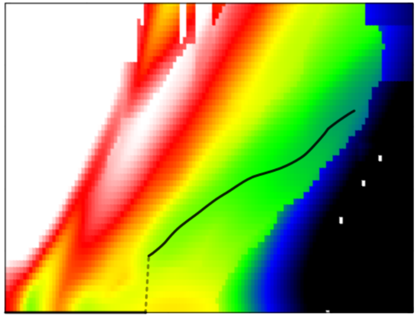


"exact" TDGCM:
without the GOA

improved accuracy,
compatibility with
future extensions

Research aims

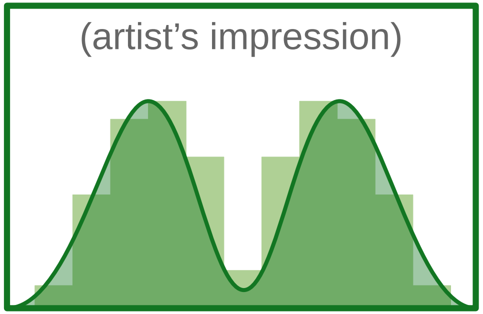
potential energy surfaces (PESs)



the time-dependent generator coordinate method (TDGCM)

GOA

fission observables



"exact" TDGCM: without the GOA

improved accuracy, compatibility with future extensions

- New implementation
- Exact solution of 1D model possible
- Generalisation to 2D in progress

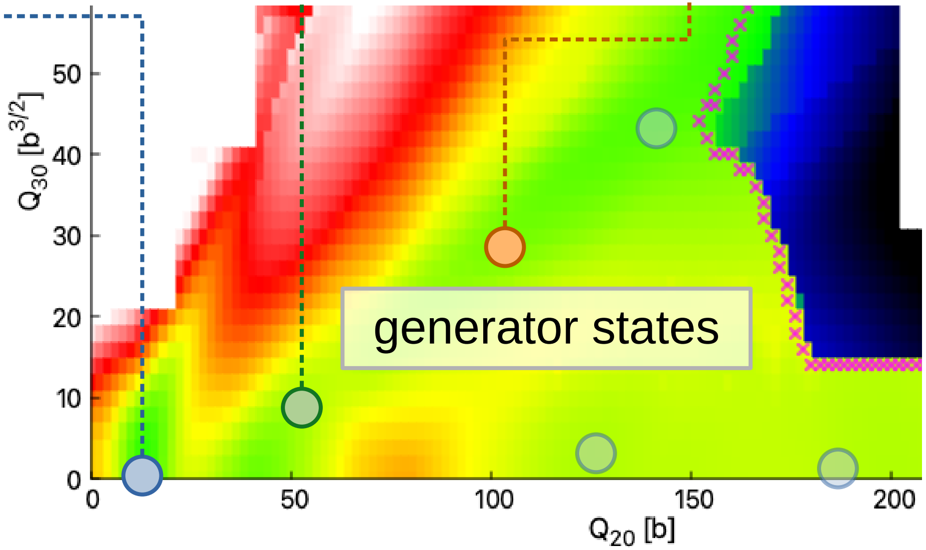
What is the TDGCM?

(time-dependent generator coordinate method)

$$|\Psi_{\mathrm{GCM}}(t)\rangle = f(\mathbf{q}_1,t)\,|\Phi(\mathbf{q}_1)\rangle + f(\mathbf{q}_2,t)\,|\Phi(\mathbf{q}_2)\rangle + f(\mathbf{q}_3,t)\,|\Phi(\mathbf{q}_3)\rangle + \ldots$$

$$|\Psi_{\mathrm{GCM}}(t)\rangle = \int d\mathbf{q}\; f(\mathbf{q},t)\,|\Phi(\mathbf{q})\rangle$$

weight function



P. Ring, P. Schuck, *The Nuclear Many-Body Problem (Ch. 10),* Springer, Berlin (2004)

P.-G. Reinhard, R. Cusson, K. Goeke, *Nucl. Phys. A* **398**, 141 (1983)

What is the TDGCM?

(time-dependent generator coordinate method)

Hill-Wheeler equation

$$\int d\mathbf{q}' \left(H(\mathbf{q},\mathbf{q}') - i\hbar N(\mathbf{q},\mathbf{q}') \frac{d}{dt} \right) f(\mathbf{q}',t) = 0$$

weight function

Hamiltonian kernel

$$H(\mathbf{q},\mathbf{q}') = \langle \Phi(\mathbf{q}) | \hat{H} | \Phi(\mathbf{q}') \rangle$$

overlap kernel

$$N(\mathbf{q},\mathbf{q}') = \langle \Phi(\mathbf{q}) | \Phi(\mathbf{q}') \rangle$$

P. Ring, P. Schuck, *The Nuclear Many-Body Problem (Ch. 10),* Springer, Berlin (2004)

P.-G. Reinhard, R. Cusson, K. Goeke, *Nucl. Phys. A* **398**, 141 (1983)

Exact solution of the TDGCM

$$\int d\mathbf{q}' \left(H(\mathbf{q}, \mathbf{q}') - i\hbar N(\mathbf{q}, \mathbf{q}') \frac{d}{dt} \right) f(\mathbf{q}', t) = 0$$

natural basis transformation

$$H_C(\mathbf{r}, \mathbf{r}') = \int d\mathbf{q}\, d\mathbf{q}'\, N^{-1/2}(\mathbf{r}, \mathbf{q}) H(\mathbf{q}, \mathbf{q}') N^{-1/2}(\mathbf{q}', \mathbf{r}')$$

$$g(\mathbf{r}, t) = \int d\mathbf{q}\, N^{1/2}(\mathbf{r}, \mathbf{q}) f(\mathbf{q}, t)$$

Exact solution of the TDGCM

$$\int d\mathbf{q}' \left(H(\mathbf{q},\mathbf{q}') - i\hbar N(\mathbf{q},\mathbf{q}') \frac{d}{dt} \right) f(\mathbf{q}',t) = 0$$

natural basis transformation

$$H_C(\mathbf{r},\mathbf{r}') = \int d\mathbf{q}\, d\mathbf{q}'\, N^{-1/2}(\mathbf{r},\mathbf{q}) H(\mathbf{q},\mathbf{q}') N^{-1/2}(\mathbf{q}',\mathbf{r}')$$

$$g(\mathbf{r},t) = \int d\mathbf{q}\, N^{1/2}(\mathbf{r},\mathbf{q}) f(\mathbf{q},t)$$

collective Schrödinger equation

$$\int d\mathbf{r}'\, H_C(\mathbf{r},\mathbf{r}') g(\mathbf{r}',t) = i\hbar \frac{d}{dt} g(\mathbf{r},t)$$

What problems are left to solve?

requires a smooth PES — solved in 1D with the link/drop method*

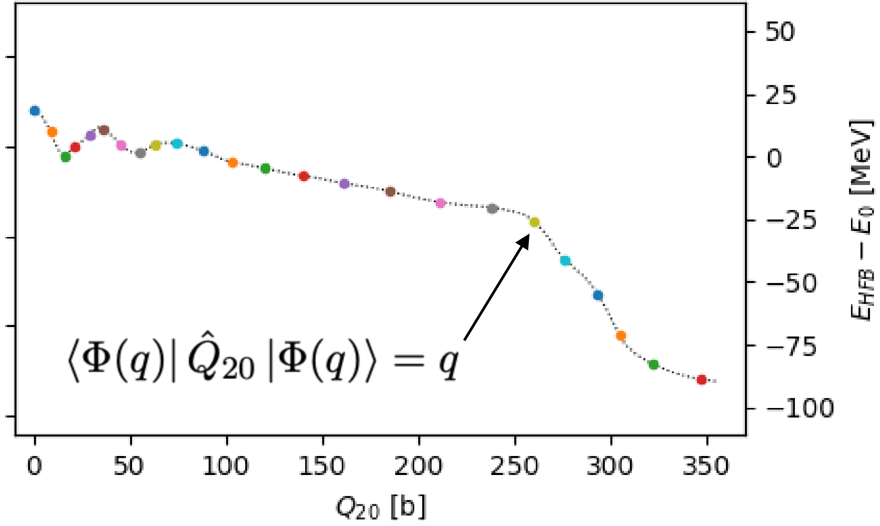
see also presentations by N. Pillet and P. N. Gallego

*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Phys. Rev. Lett.* **113**, 152501 (2024)

What problems are left to solve?

requires a smooth PES

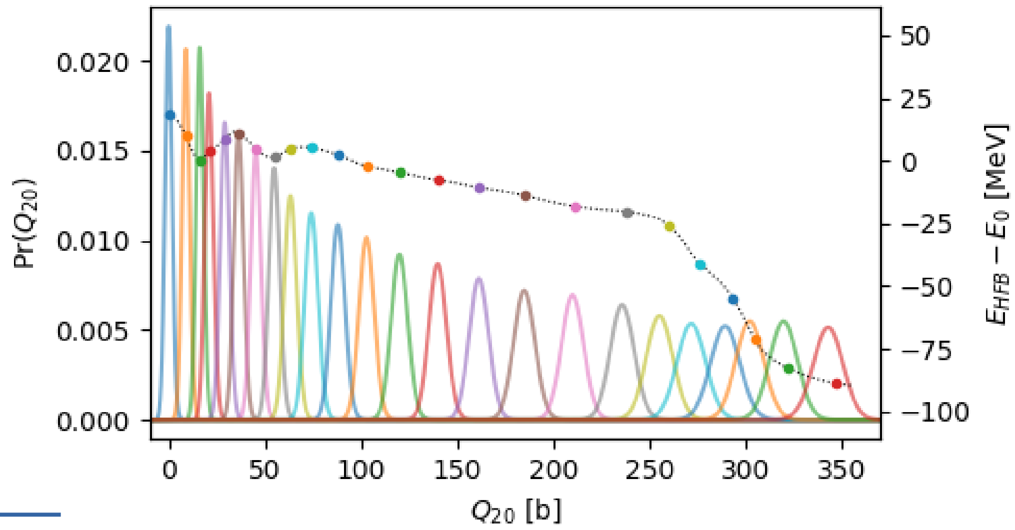
generator states are not well-defined in terms of generator coordinates



What problems are left to solve?

requires a smooth PES

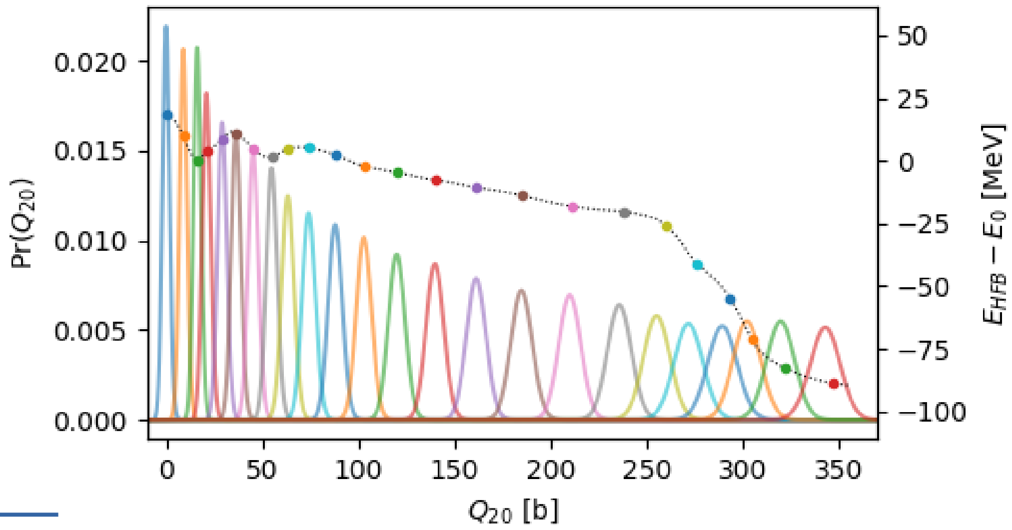
generator states are not well-defined in terms of generator coordinates



What problems are left to solve?

requires a smooth PES

generator states are not well-defined in terms of generator coordinates



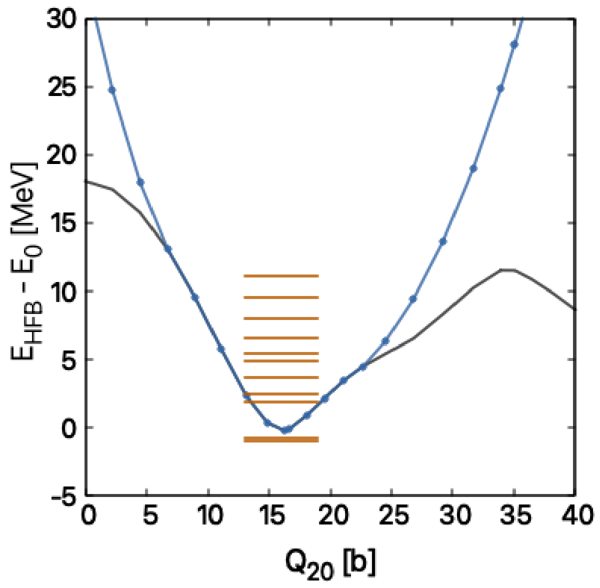
obtained by projection onto the generator coordinates

What problems are left to solve?

requires a smooth PES

generator states are not well-defined in terms of generator coordinates

modification of the Hamiltonian kernel is poorly defined without the GOA



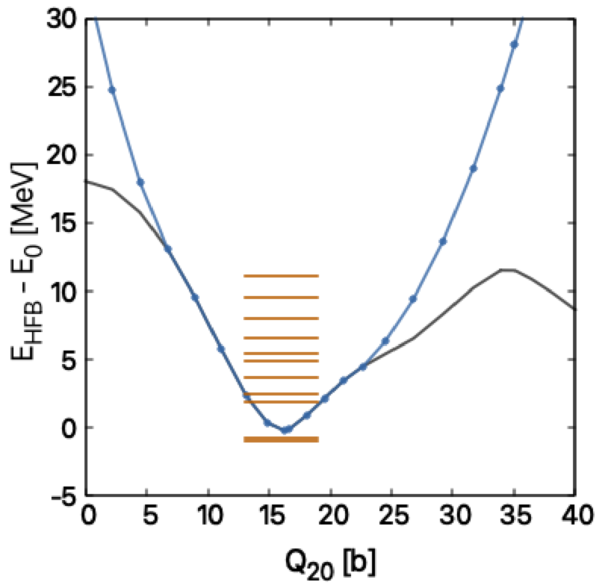
important for initial state construction and removing scissioned components

What problems are left to solve?

requires a smooth PES

generator states are not well-defined in terms of generator coordinates

modification of the Hamiltonian kernel is poorly defined without the GOA



projection techniques provide a rigorous definition

Projection and TDGCM

$$\hat{P}_{\hat{Q}_{20}}(q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\varphi \; e^{i\varphi(\hat{Q}_{20}-q)}$$

projection operator (continuous)

Projection and TDGCM

$$\hat{P}_{\hat{Q}_{20}}(q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\varphi\; e^{i\varphi(\hat{Q}_{20}-q)}$$

projection operator (continuous)

$$n(q) = \langle \psi(q)|\Psi\rangle$$

$$|\Psi\rangle = \int dq\; n(q)\,|\psi(q)\rangle$$

arbitrary state expressed
in operator eigenbasis

$$\Pr(q) = \langle\Psi|\,\hat{P}_{\hat{Q}_{20}}(q)\,|\Psi\rangle = |n(q)|^2$$

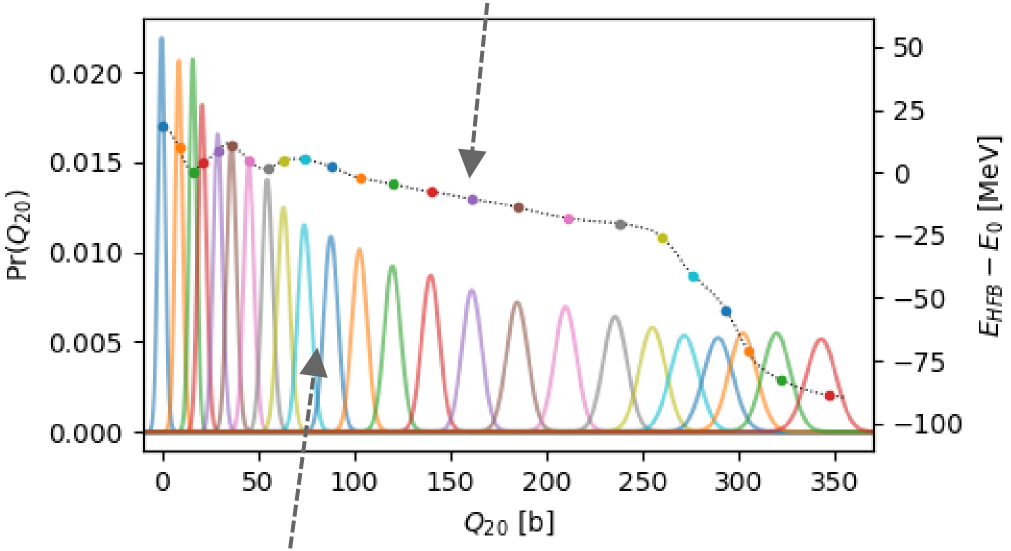
probability of measuring the
state with result q

Projection and TDGCM

$$\hat{P}_{\hat{Q}_{20}}(q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\varphi \; e^{i\varphi(\hat{Q}_{20}-q)}$$

projection operator (continuous)

original PES



Q_{20} distributions obtained from projection

Improved visualisation of fission dynamics

without projection

$$\Pr(q,t) \approx \left| f(q,t) \right|^2$$

not normalised and/or
not localised!

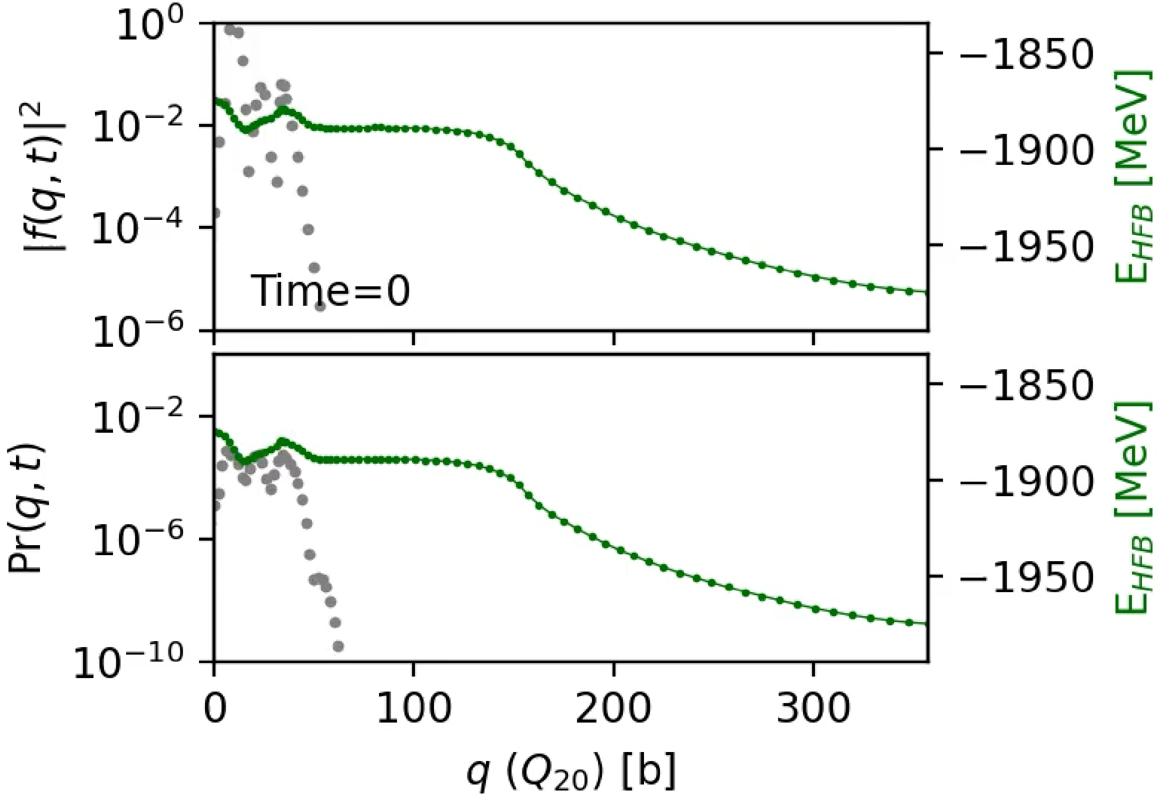
with projection

$$\Pr(q,t) = \left| n(q,t) \right|^2 = \left| \langle \Psi(t) | \psi(q) \rangle \right|^2$$

Improved visualisation of fission dynamics

without projection

with projection



Modification of Hamiltonian kernel

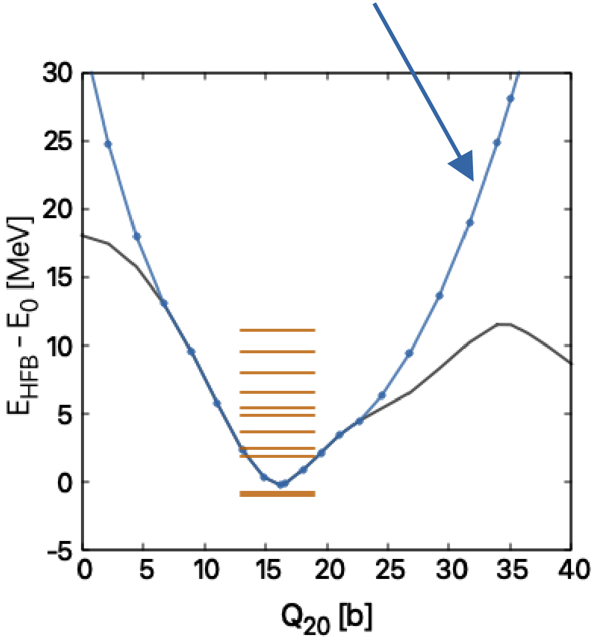
local Schrödinger equation

$$\hat{H}' = \hat{H} + \hat{V}'$$

$$H'(\mathbf{q}, \mathbf{q}') = H(\mathbf{q}, \mathbf{q}') + V'(\mathbf{q}, \mathbf{q}')$$

GCM formalism

modified potential to
determine bound states



Modification of Hamiltonian kernel

local Schrödinger equation

$$\hat{H}' = \hat{H} + \hat{V}'$$

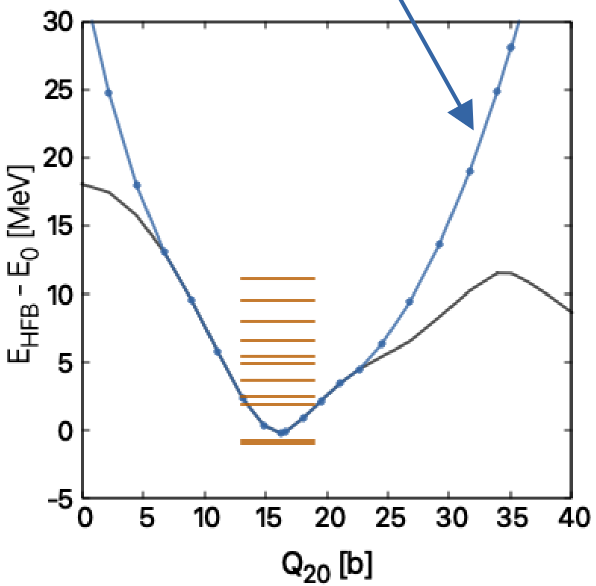
$$H'(\mathbf{q},\mathbf{q}') = H(\mathbf{q},\mathbf{q}') + V'(\mathbf{q},\mathbf{q}')$$

GCM formalism

how can we construct a kernel (matrix) from a function?

$$V'(\mathbf{q})$$

modified potential to determine bound states



Modification of Hamiltonian kernel

local Schrödinger equation

$$\hat{H}' = \hat{H} + \hat{V}'$$

$$H'(\mathbf{q}, \mathbf{q}') = H(\mathbf{q}, \mathbf{q}') + V'(\mathbf{q}, \mathbf{q}')$$

GCM formalism

$$V'(\mathbf{q}, \mathbf{q}') \sim \langle \Phi(\mathbf{q}) | \hat{V}' | \Phi(\mathbf{q}') \rangle$$

$$= \int d\mathbf{q}_2 \, \langle \Phi(\mathbf{q}) | \, \hat{P}_{\hat{Q}}(\mathbf{q}_2) V'(\mathbf{q}_2) \, | \Phi(\mathbf{q}') \rangle$$

kernel defined with projection operator

Exact solution of TDGCM dynamics

collective Schrödinger equation

$$\int d\mathbf{r}' \; H_C(\mathbf{r},\mathbf{r}')g(\mathbf{r}',t) = i\hbar\frac{d}{dt}g(\mathbf{r},t)$$

$$-\frac{i}{\hbar}H_C \cdot \mathbf{g}(t) = \frac{d\mathbf{g}}{dt}$$

Exact solution of TDGCM dynamics

collective Schrödinger equation

$$\int d\mathbf{r}'\ H_C(\mathbf{r},\mathbf{r}')g(\mathbf{r}',t) = i\hbar\frac{d}{dt}g(\mathbf{r},t)$$

$$-\frac{i}{\hbar}H_C \cdot \mathbf{g}(t) = \frac{d\mathbf{g}}{dt} \longrightarrow \mathbf{g}(t) = e^{-iH_C t/\hbar}\cdot \mathbf{g}(0)$$

exact solution

- Requires collective Hamiltonian to be diagonalisable
- Does not require iterative numerical solutions

Quasistatic approach to spontaneous fission

add imaginary “absorption” potential
after fission barrier(s)

$$H'(\mathbf{q},\mathbf{q}') = H(\mathbf{q},\mathbf{q}') + V'(\mathbf{q},\mathbf{q}')$$

only applied to 1D and 2D “toy model” potentials

G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

Quasistatic approach to spontaneous fission

add imaginary "absorption" potential
after fission barrier(s)

$$H'(\mathbf{q},\mathbf{q}') = H(\mathbf{q},\mathbf{q}') + \underbrace{V'(\mathbf{q},\mathbf{q}')}$$

$$H'_C(\mathbf{r},\mathbf{r}')$$

solve the exact *static* GCM by diagonalising the collective Hamiltonian...

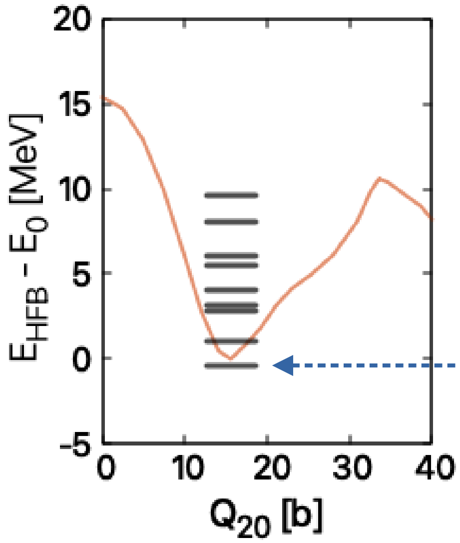
$$\downarrow$$

$$\boxed{\lambda_i,\ \mathbf{v}_i(\mathbf{r})}$$

...to produce energy eigenstates with complex eigenvalues

G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

Quasistatic approach to spontaneous fission



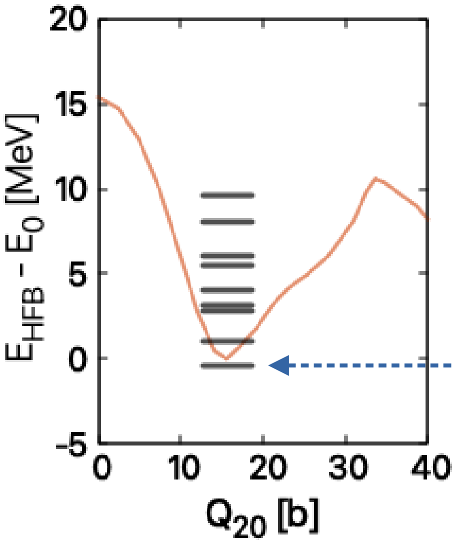
the quasistatic state
$\mathbf{v}_i(\mathbf{r})$ is in resonance...

$$\lambda_i = \underbrace{E_i} - \frac{i}{2}\Gamma_i$$

with the bound eigenstate that
has the same real energy

G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

Quasistatic approach to spontaneous fission



the quasistatic state $\mathbf{v}_i(\mathbf{r})$ is in resonance...

$$\lambda_i = E_i - \frac{i}{2}\Gamma_i$$

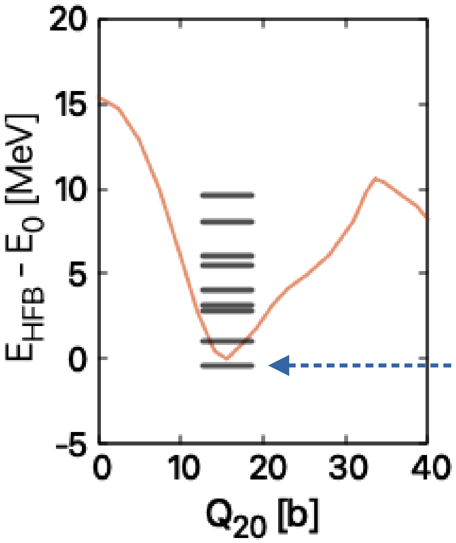
with the bound eigenstate that has the same real energy

with a lifetime determined by the resonance width

$$\tau_i = \frac{\hbar}{\Gamma_i}$$

G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

Quasistatic approach to spontaneous fission



the quasistatic state
$\mathbf{v}_i(\mathbf{r})$ is in resonance...

$$\lambda_i = E_i - \frac{i}{2}\Gamma_i$$

with a lifetime determined by the resonance width

with the bound eigenstate that has the same real energy

$$\tau_i = \frac{\hbar}{\Gamma_i}$$

spontaneous fission lifetime

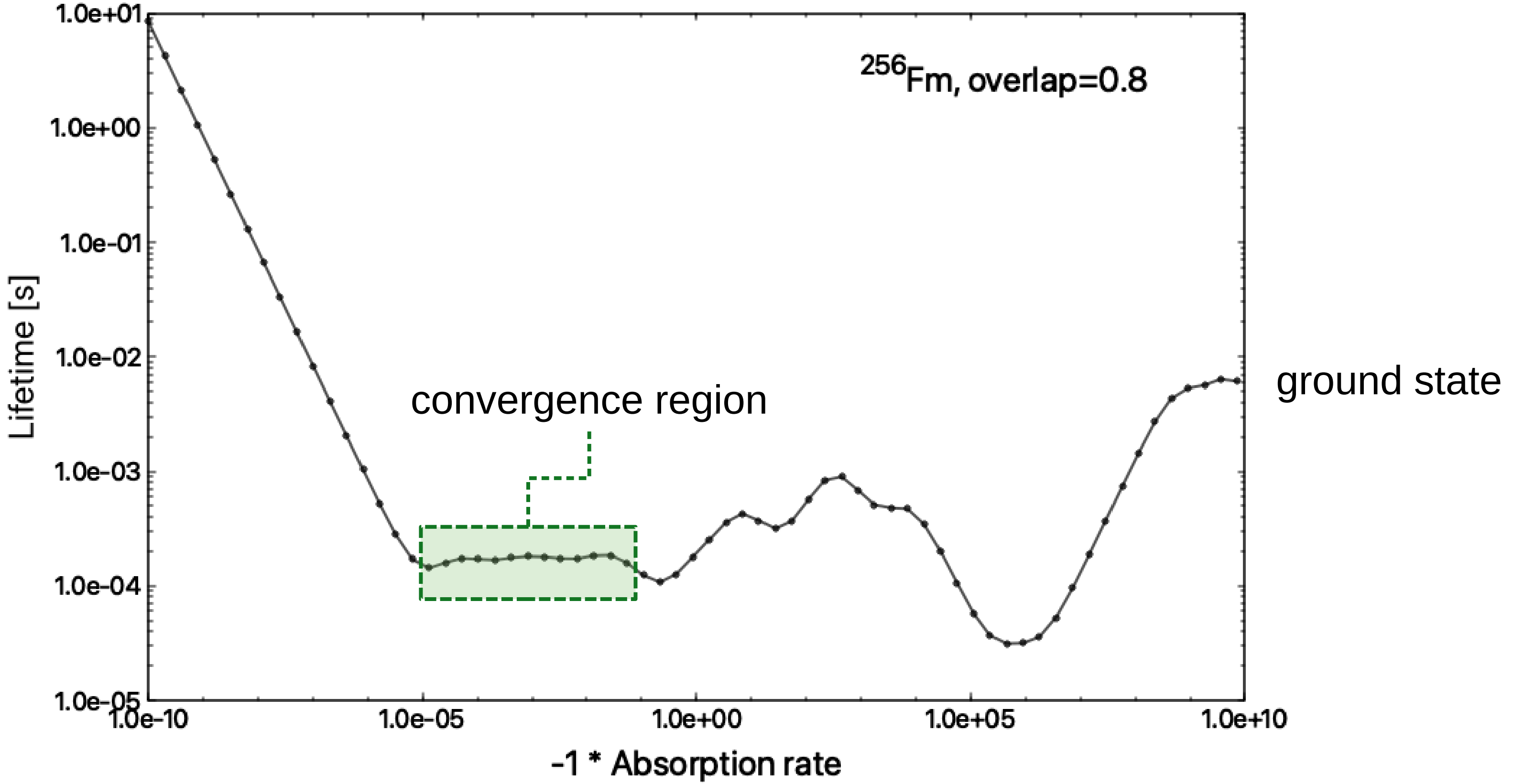
G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

Variation of lifetime with absorption rate

However:

is the spontaneous fission lifetime simply dependent on the strength of the absorption potential?

Variation of lifetime with absorption rate



Evaluation of preliminary results

nuclide	spontaneous fission half-life [s]		ratio (theory/expt.)
	this method	experimental*	
^{256}Cf	1.047×10^{-11}	7.38×10^{2}	**1.41×10^{-14}**
^{256}Fm	7.035×10^{-6}	9.426×10^{3}	**7.464×10^{-10}**

*Values taken from https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html, accessed 03/03/2026

Evaluation of preliminary results

nuclide	spontaneous fission half-life [s]		ratio (theory/expt.)
	this method	experimental*	
^{256}Cf	1.047×10^{-11}	7.38×10^{2}	**1.41×10^{-14}**
^{256}Fm	7.035×10^{-6}	9.426×10^{3}	**7.464×10^{-10}**

- Underestimation suggests presence of systematic errors
- Existing methods of calculating SF lifetimes are extremely sensitive to the variation of inputs!
- “Collective inertias” used for conventional lifetime calculations are underestimated by the GCM

*Values taken from https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html, accessed 03/03/2026

Summary

application of exact TDGCM to fission in 1 dimension

- Removal of the GOA
- Smooth 1D PESs obtained with link/drop method*

*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Phys. Rev. Lett.* **113**, 152501 (2024)

Summary

application of exact TDGCM to fission in 1 dimension

- Removal of the GOA
- Smooth 1D PESs obtained with link/drop method*

new uses for projection onto generator coordinates

- Explicit coordinate representation of basis and time-evolved states
- Rigorous method to modify Hamiltonian kernels

*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Phys. Rev. Lett.* **113**, 152501 (2024)

Summary

application of exact TDGCM to fission in 1 dimension

- Removal of the GOA
- Smooth 1D PESs obtained with link/drop method*

new uses for projection onto generator coordinates

- Explicit coordinate representation of basis and time-evolved states
- Rigorous method to modify Hamiltonian kernels

new approach to study spontaneous fission

- Application of quasistatic method† to a 1D PES with the exact GCM
- Analysis and improvements still in progress

*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Phys. Rev. Lett.* **113**, 152501 (2024)

†G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

Thank you!

Acknowledgements

Ph.D. supervisors (2021–2024 @ ANU)
- Prof. Cédric Simenel (ANU)
- Dr. Rémi Bernard (CEA Cadarache)
- Dr. Taiki Tanaka (JAEA)

Postdoctoral supervisor (2024–2026 @ L2IT)
- Dr. Guillaume Scamps (L2IT)

Collaborators
- Prof. Luis Robledo (UAM)
- Mr. Paul Tan (CEA Cadarache)

You, for listening!