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

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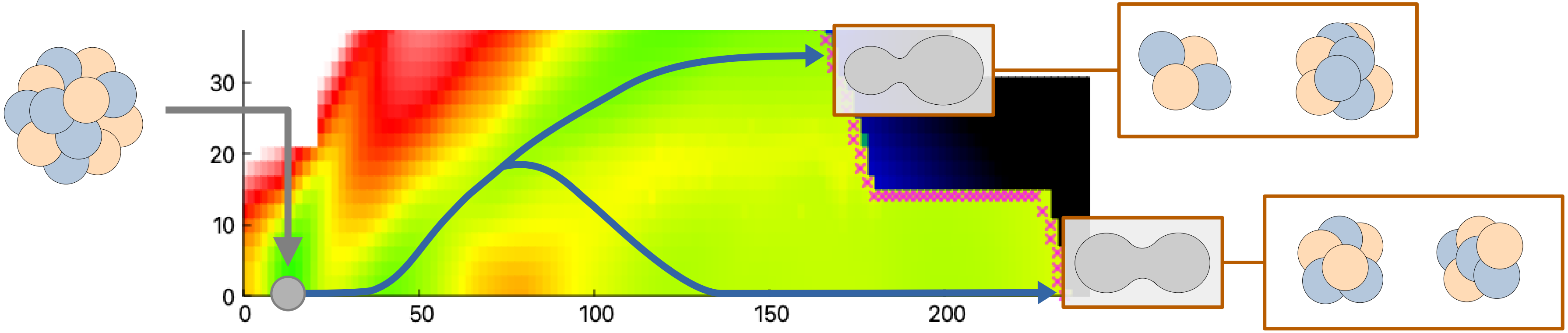
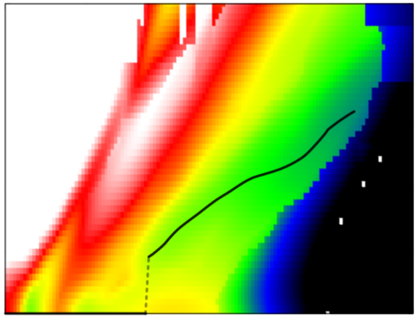


Research aims

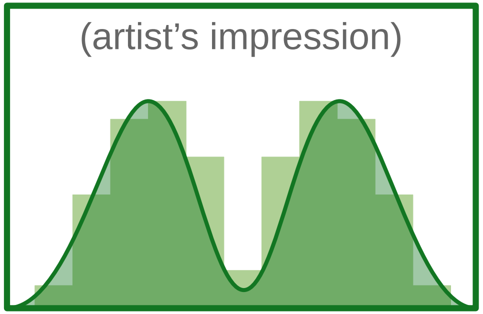
potential energy surfaces (PESs)



the time-dependent generator coordinate method (TDGCM)

GOA

fission observables



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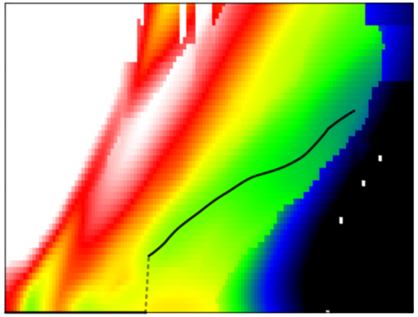

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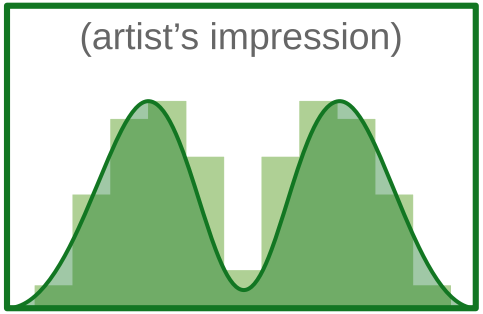

"exact" TDGCM: without the GOA

improved accuracy, compatibility with future extensions

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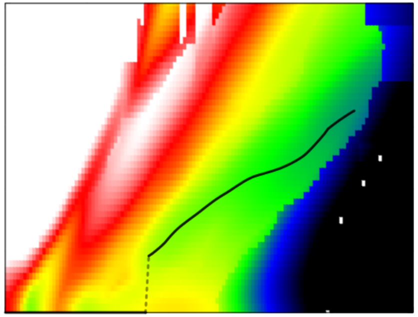

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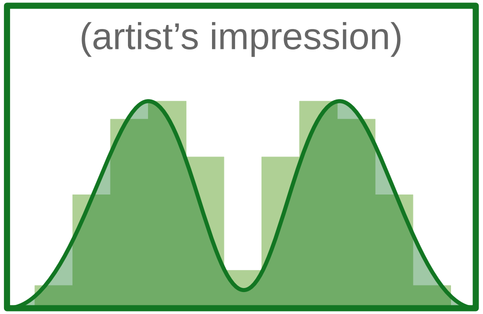


"exact" TDGCM: without the GOA

improved accuracy, compatibility with future extensions

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

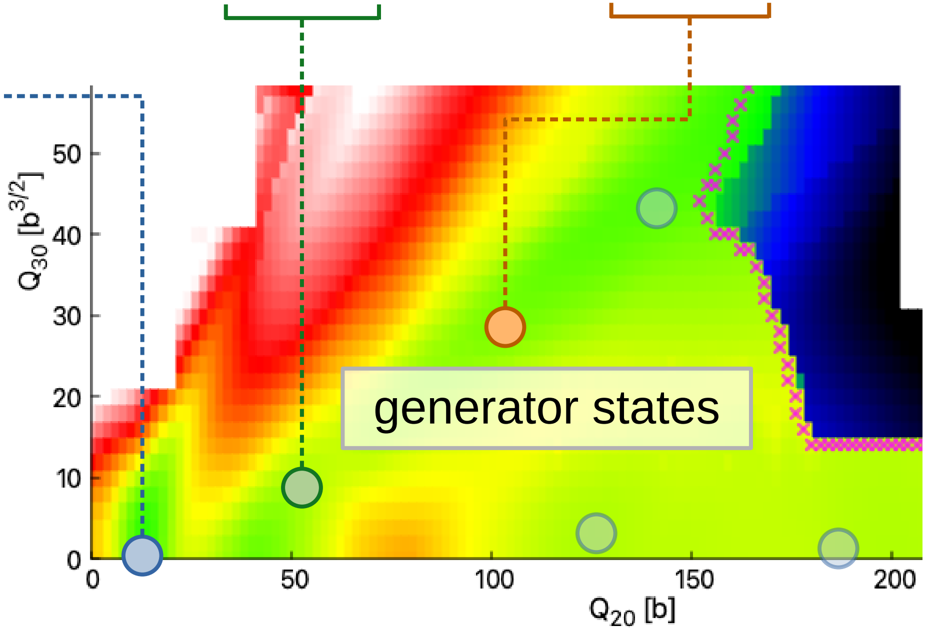
What is the TDGCM?

(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

$$\int d\mathbf{q}' \left(\underbrace{H(\mathbf{q},\mathbf{q}')}_{\text{Hamiltonian kernel}} - i\hbar \underbrace{N(\mathbf{q},\mathbf{q}')}_{\text{overlap kernel}} \frac{d}{dt} \right) \underbrace{f(\mathbf{q}',t)}_{\text{weight function}} = 0$$

weight function

Hamiltonian kernel

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

overlap kernel

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

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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

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

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?

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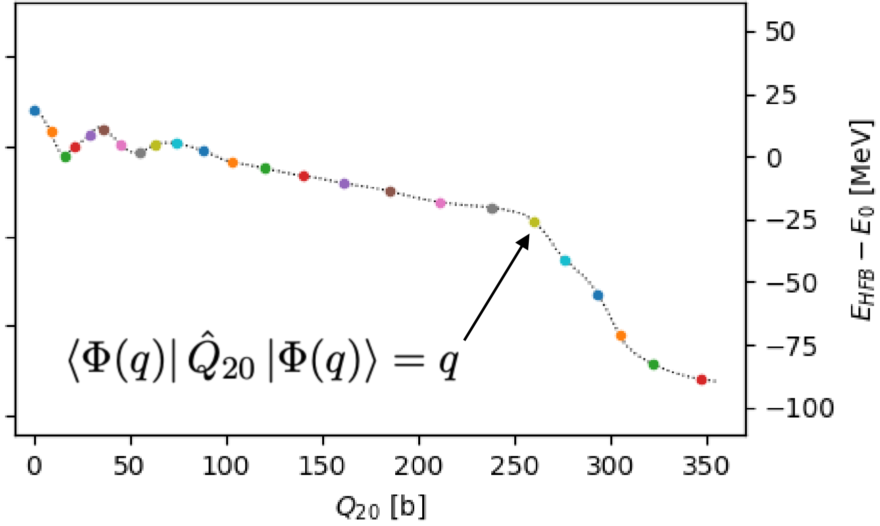
generator states are not well-defined in terms of generator coordinates



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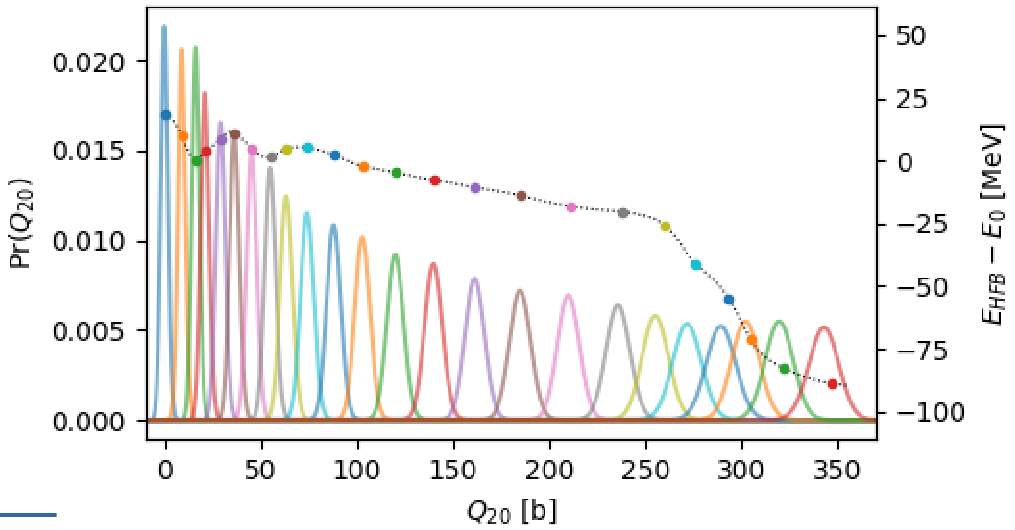

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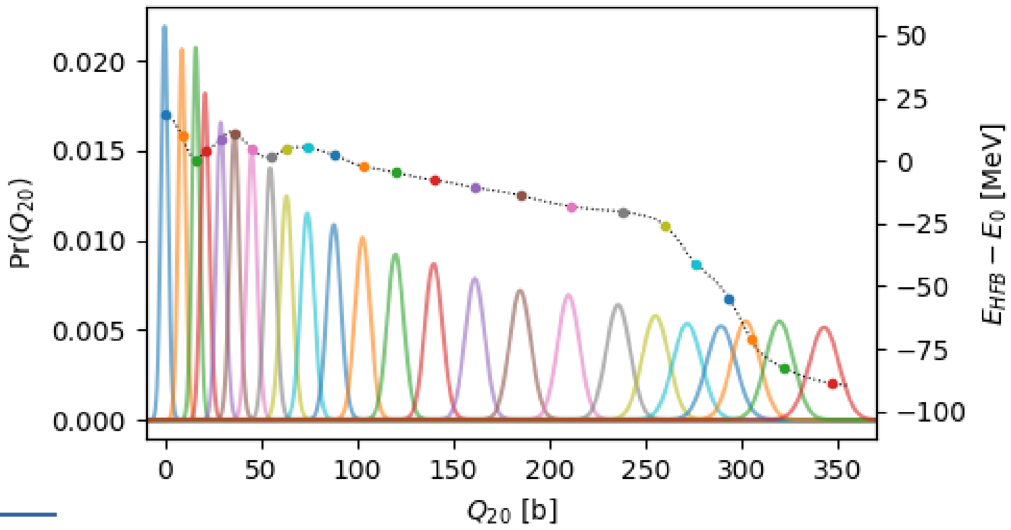

obtained by projection onto the generator coordinates

What problems are left to solve?

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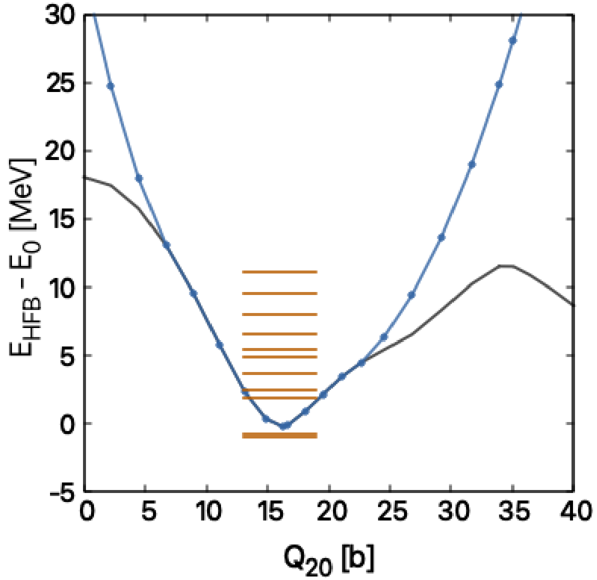
generator states are not well-defined in terms of generator coordinates

modification of the Hamiltonian kernel is poorly defined without the GOA



important for initial state construction and removing scissioned components

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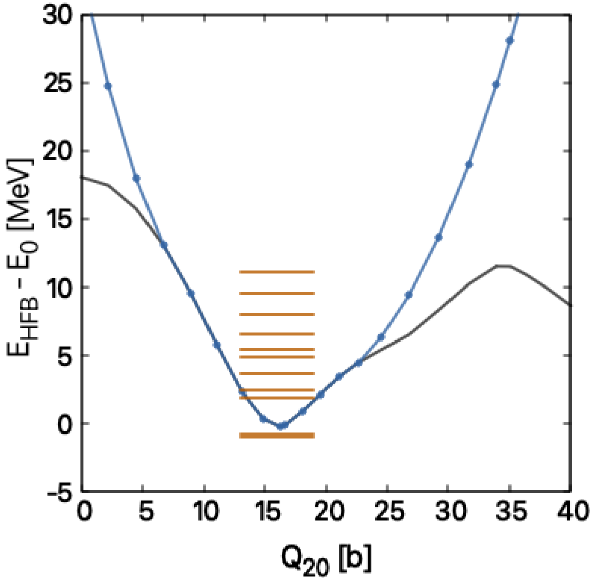


projection techniques provide a rigorous definition

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

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

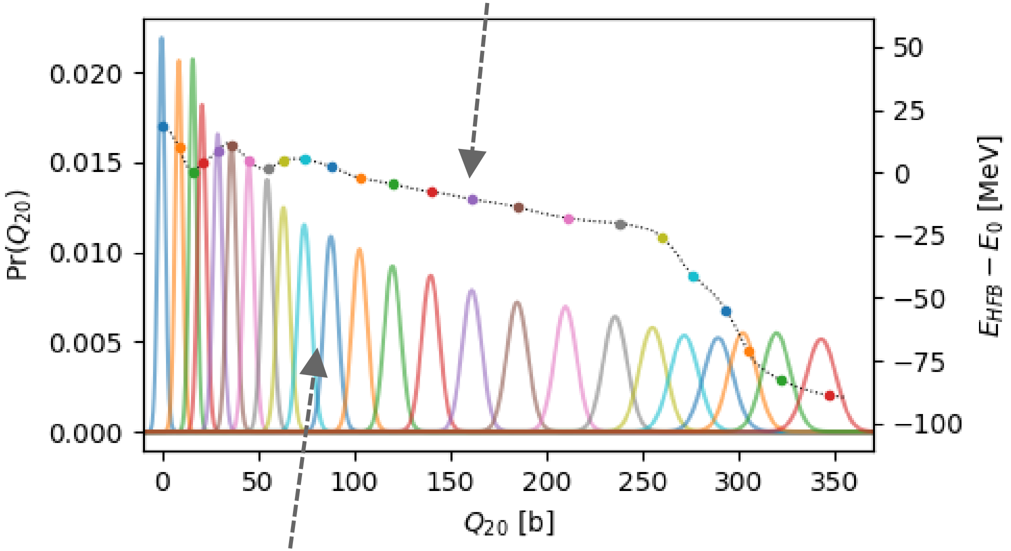
probability of measuring the state with result q

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!

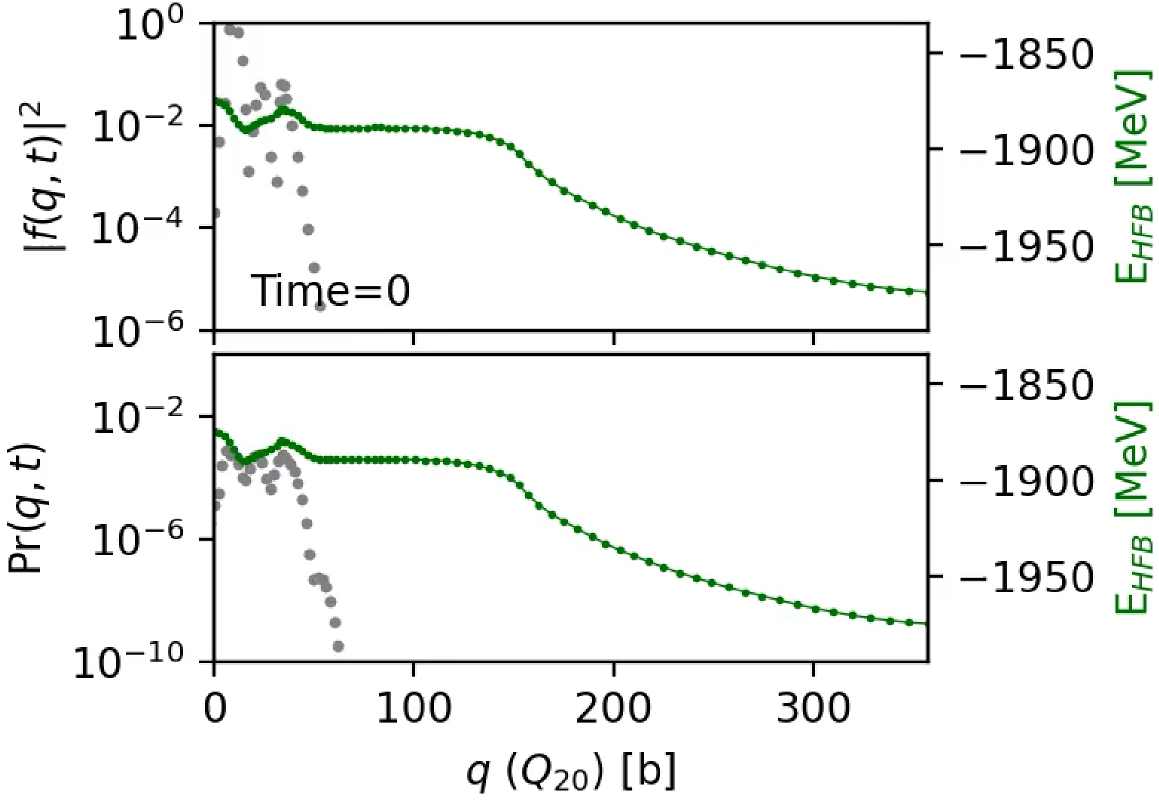
with projection

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

Improved visualisation of fission dynamics

without projection

with projection



Modification of Hamiltonian kernel

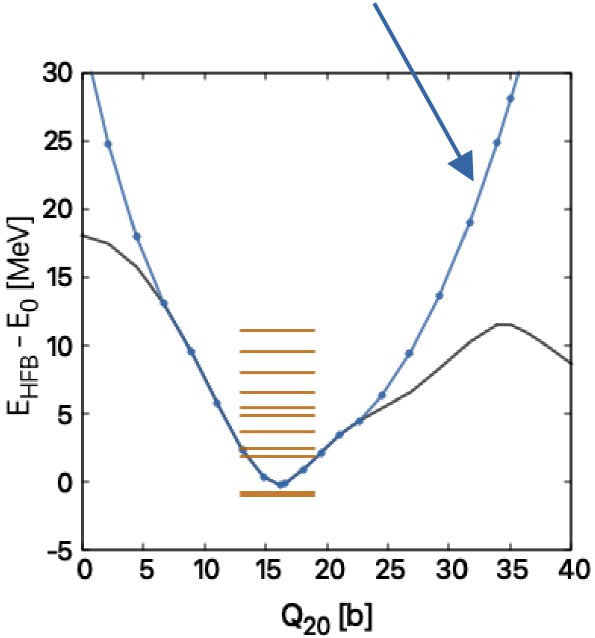
local Schrödinger equation

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

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

GCM formalism

modified potential to determine bound states



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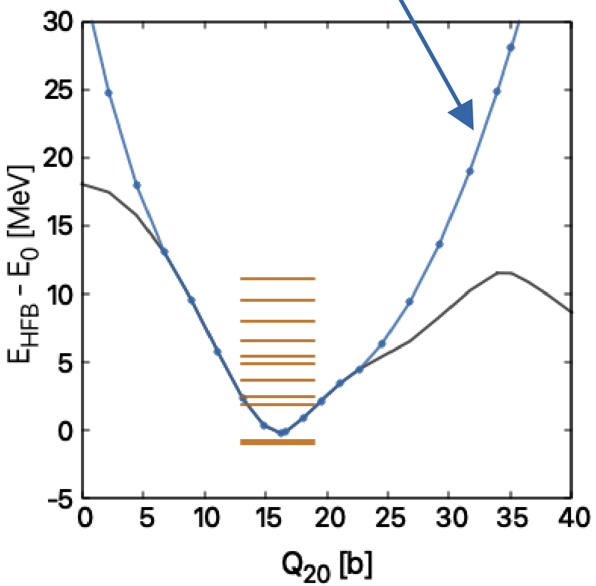
GCM formalism

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

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

modified potential to determine bound states



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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

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

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

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

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)

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

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

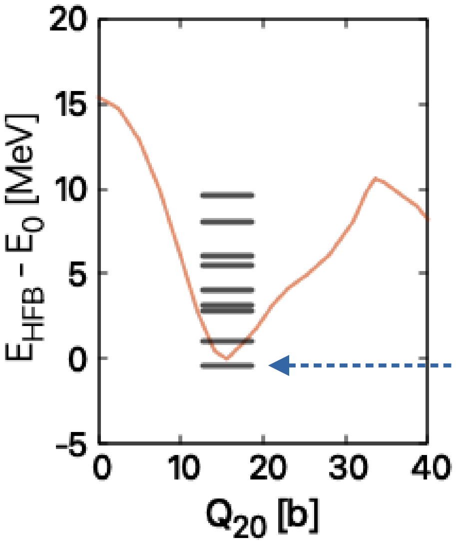
solve the exact *static* GCM by diagonalising
the collective Hamiltonian...

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

...to produce energy eigenstates
with complex eigenvalues

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

Quasistatic approach to spontaneous fission



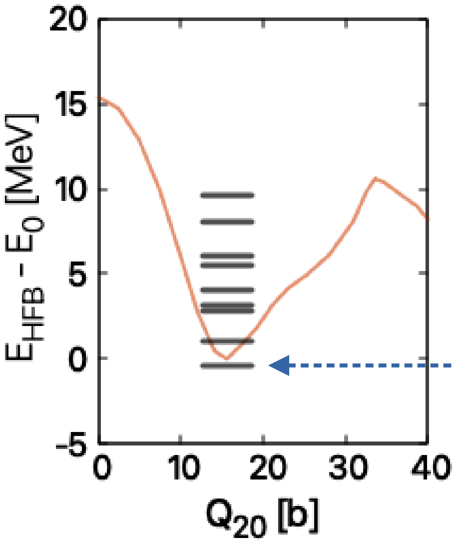
the quasistatic state $\mathbf{v}_i(\mathbf{r})$ is in resonance...

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

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 a lifetime determined by the resonance width

with the bound eigenstate that has the same real energy

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

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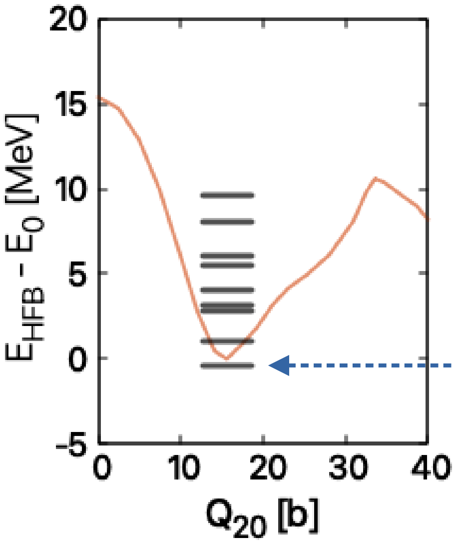
Quasistatic approach to spontaneous fission



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spontaneous fission lifetime

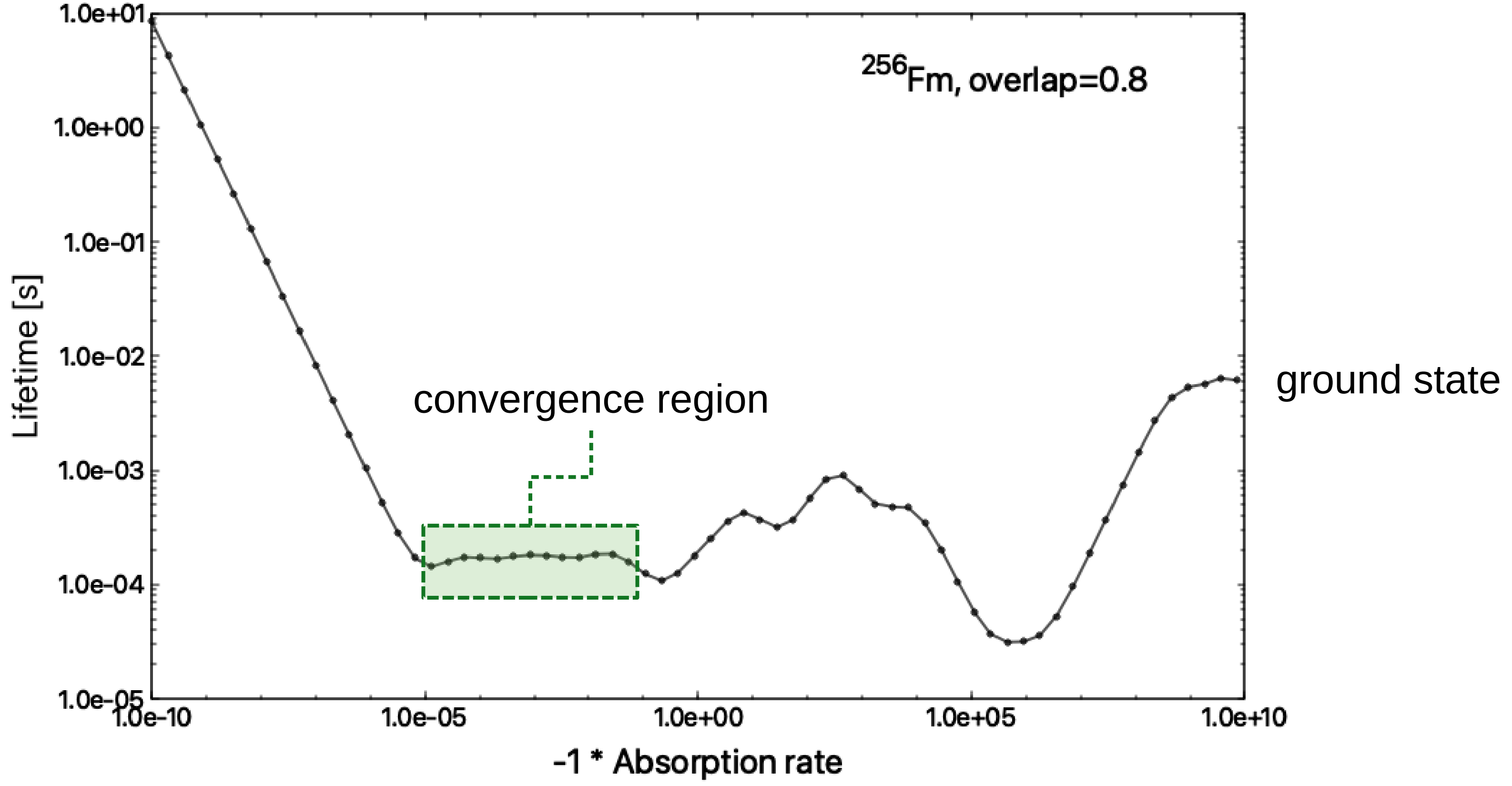
G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

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

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- 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)

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new uses for projection onto generator coordinates

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

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extended 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)

The workshop organisers

You, for listening!