A description of spontaneous fission with the “exact” TDGCM and projection techniques

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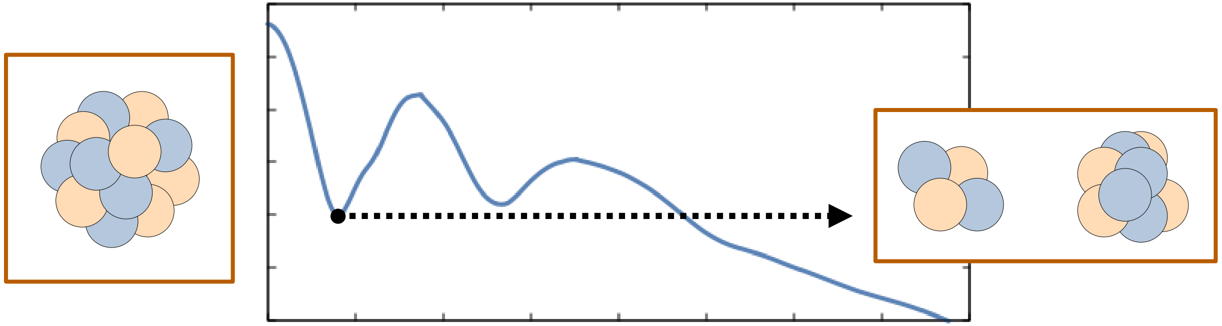
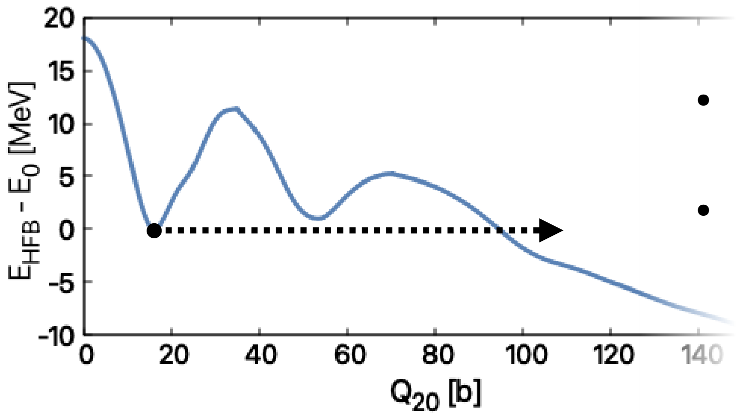


Motivation

microscopic description of *spontaneous* fission



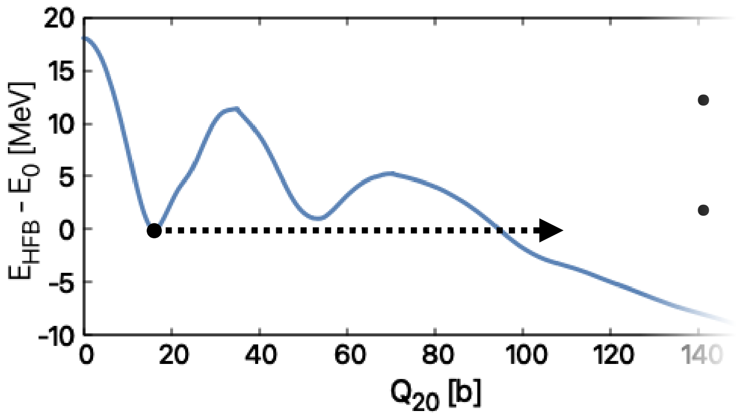
- Requires modelling of sub-barrier collective tunnelling
- Much longer evolution time than induced fission
- Prior work: “quasistatic approach”* applied to toy 1D and 2D potentials

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

Motivation

the time-dependent generator coordinate method (TDGCM) + [ ] → microscopic description of *spontaneous* fission

- New “exact” formalism excluding the GOA
- Necessary for future extensions to the theory
- Suitable for modelling tunnelling behaviours across the PES



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Motivation

the time-dependent generator coordinate method (TDGCM) + projection onto the collective coordinates → microscopic description of *spontaneous* fission

the time-dependent generator coordinate method (TDGCM)

- New “exact” formalism excluding the GOA
- Necessary for future extensions to the theory
- Suitable for modelling tunnelling behaviours across the PES

projection onto the collective coordinates

- Improves on some of the shortcomings of the exact TDGCM
- Needed to create modified potentials for the quasistatic approach

microscopic description of *spontaneous* fission

- Requires modelling of sub-barrier collective tunnelling
- Much longer evolution time than induced fission
- Prior work: “quasistatic approach”* applied to toy 1D and 2D potentials

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

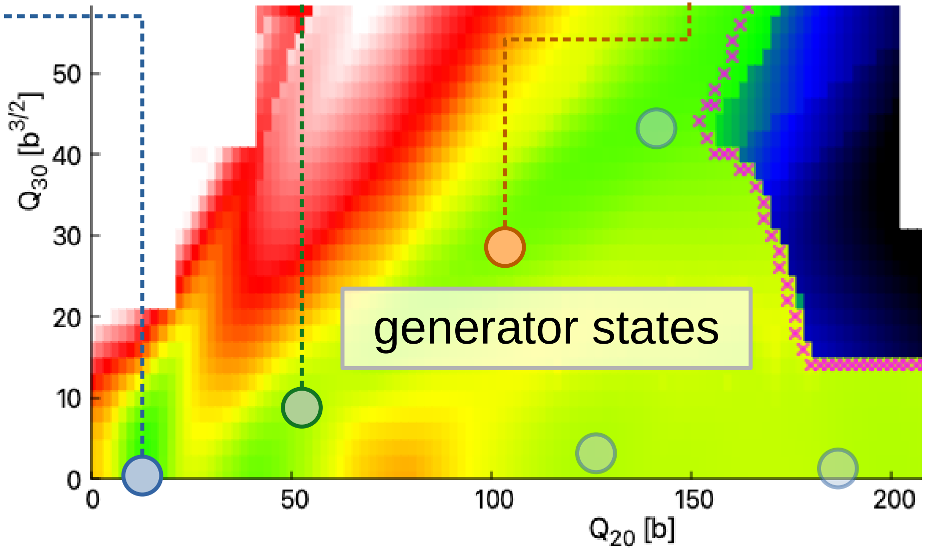
What is the TDGCM?

(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

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

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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

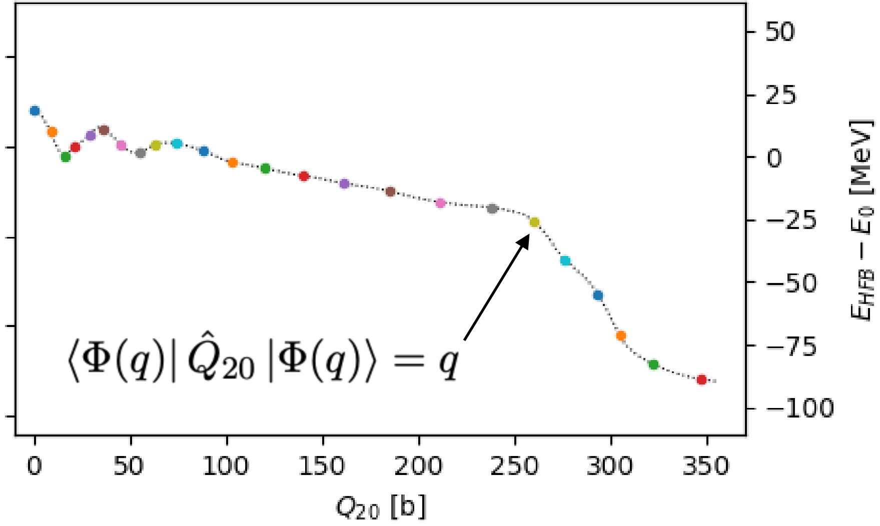
obtained in 1D with the link/drop method*
2D generalisation needed in future!

*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



$|\Phi(q)\rangle$ is not an eigenstate of $\hat{Q}_{20}$

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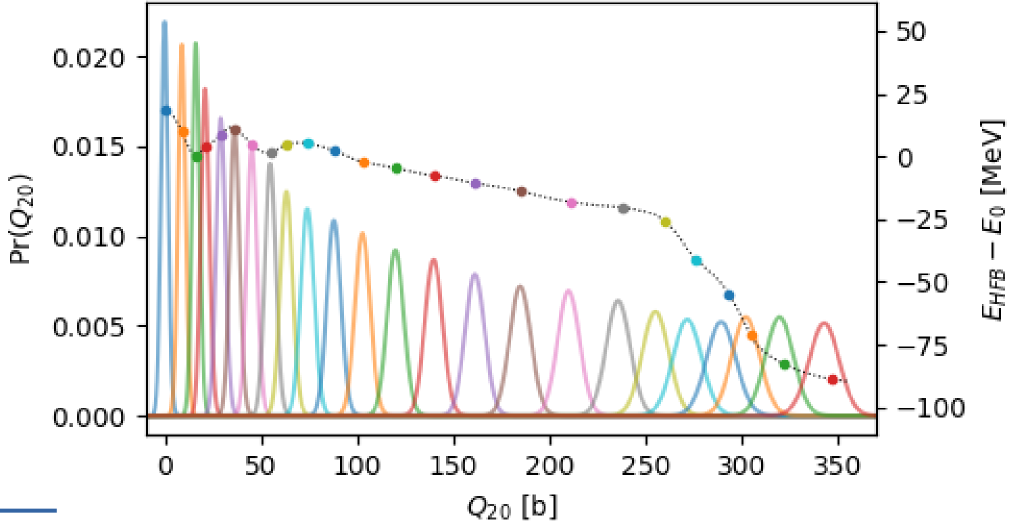

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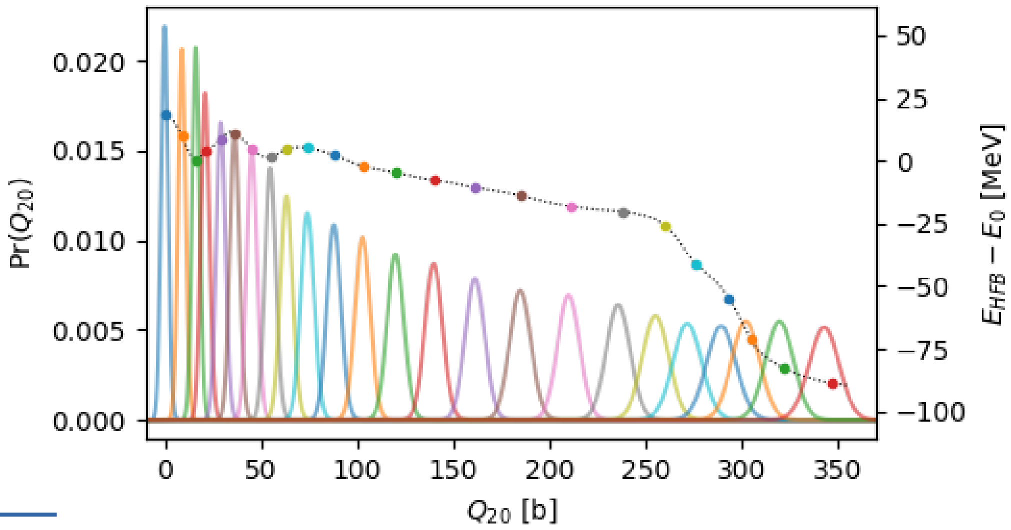

obtained by projection onto the generator coordinates

What problems are left to solve?

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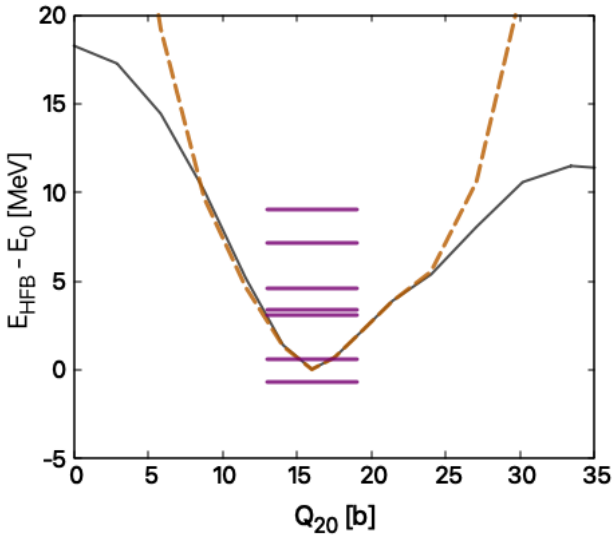
generator states are not well-defined in terms of generator coordinates

modification of the Hamiltonian kernel is poorly defined without the GOA



important for initial state construction and removing scissioned components

What problems are left to solve?

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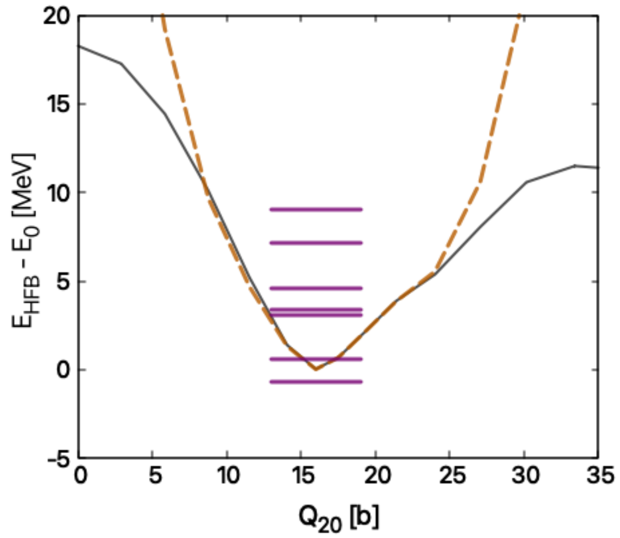

projection techniques provide a rigorous definition

The projection operator

1. standard projection operator

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

$$\delta(x - x_0) = \int_{-\infty}^{\infty} d\varphi \ e^{2i\pi\varphi(x-x_0)}$$

Dirac delta function as an inverse Fourier transform

The projection operator

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Dirac delta function as an inverse Fourier transform

eigenvalues Q of operator $\hat{Q}$ are real, continuous, and unbounded

different to other commonly projected observables (angular momentum, particle number, parity)!

The projection operator

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eigenvalues Q of operator $\hat{Q}$ are real, continuous, and unbounded

$$\hat{P}_{\hat{Q}}(Q) = \lim_{N\to\infty}\frac{1}{N}\sum_{j=1}^{N} e^{2i\pi j(\hat{Q}-Q)/N\Delta Q}$$

2. discrete projection operator

eigenvalues Q of operator $\hat{Q}$ occupy discrete points on an unbounded real mesh with interval ΔQ

The projection operator

2. discrete projection operator

$$\hat{P}_{\hat{Q}}(Q) = \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} e^{2i\pi j(\hat{Q}-Q)/N\Delta Q}$$

$$\hat{P}^{L}_{\hat{Q}}(Q) = \frac{1}{L} \sum_{j=1}^{L} e^{2i\pi j(\hat{Q}-Q)/L\Delta Q}$$

3. finite discrete projection operator

imposing the upper bound L on the sum introduces periodicity over the interval $L\Delta Q$

The projection operator

2. discrete projection operator

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3. finite discrete projection operator

imposing the upper bound L on the sum introduces periodicity over the interval $L\Delta Q$

restrict $\hat{Q}$ to a finite interval, and choose L such that

$$L\Delta Q > Q_{\max} - Q_{\min}$$

Projection and TDGCM

$$|\Psi(t)\rangle = \int dq\ f(q,t)\,|\Phi(q)\rangle$$

What is the probability that $\langle\Psi(t)|\,\hat{Q}\,|\Psi(t)\rangle = Q$?

$$\begin{aligned}\Pr(Q) &= \langle\Psi(t)|\,\hat{P}^L_{\hat{Q}}(Q)\,|\Psi(t)\rangle \\ &= \iint dq\,dq'\ f^*(q,t)f(q',t)\,\langle\Phi(q)|\,\hat{P}^L_{\hat{Q}}(Q)\,|\Phi(q')\rangle\end{aligned}$$

Projection and TDGCM

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$$\begin{aligned}\Pr(Q) &= \langle\Psi(t)|\,\hat{P}^{L}_{\hat{Q}}(Q)\,|\Psi(t)\rangle \\ &= \iint dq\,dq'\;\; f^*(q,t) f(q',t) P(Q;q,q')\end{aligned}$$

"probability kernel"

$$\langle\Phi(q)|\,\hat{P}^{L}_{\hat{Q}}(Q)\,|\Phi(q')\rangle$$

Projection and TDGCM

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This allows the projection of mixtures of mean-field states (like the TDGCM ansatz), not only pure HFB states!

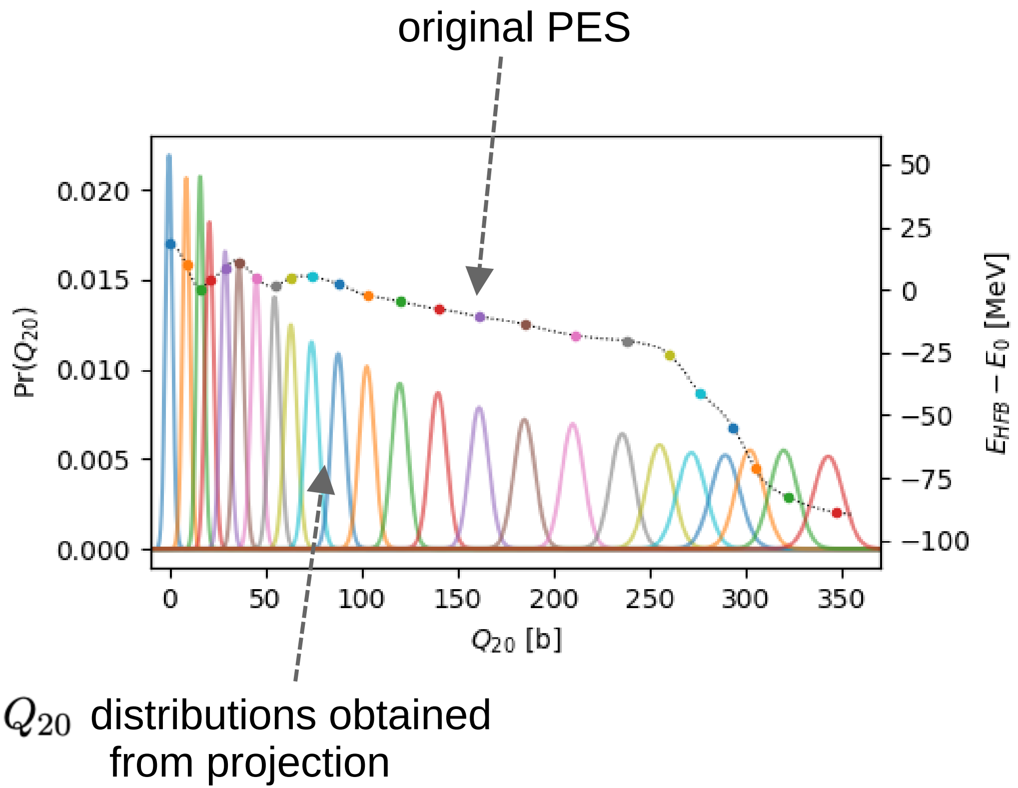
"probability kernel"

$\langle\Phi(q)|\,\hat{P}^L_{\hat{Q}}(Q)\,|\Phi(q')\rangle$

Projection and TDGCM

for pure HFB states:

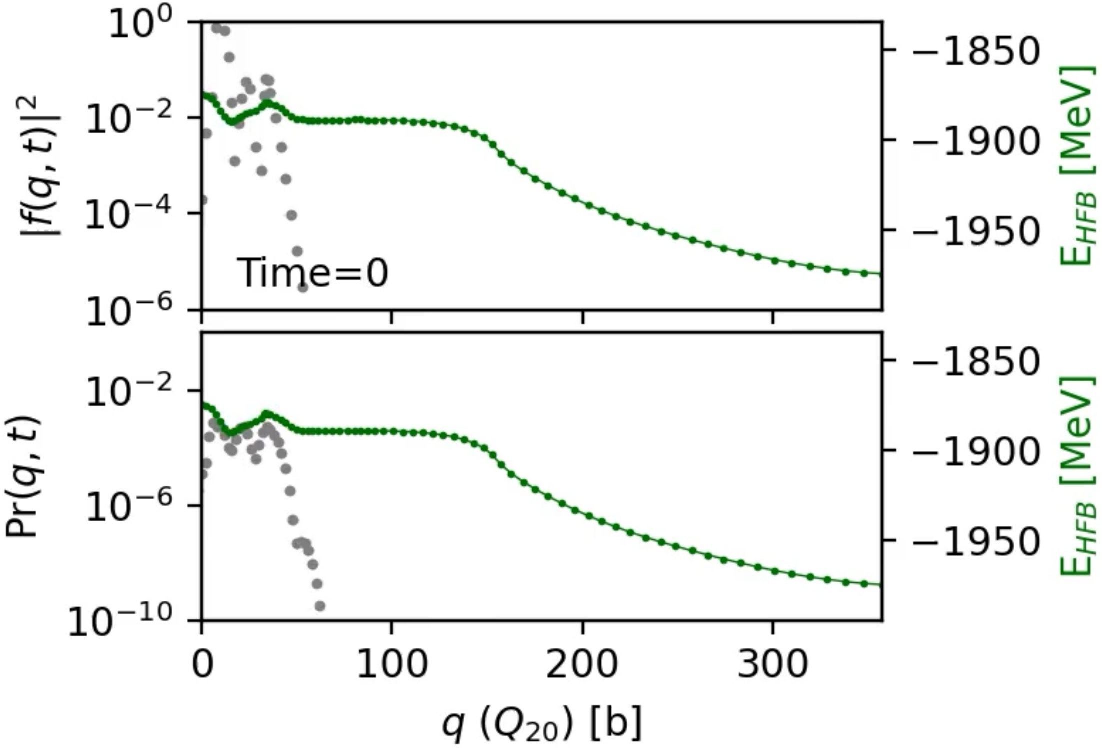
$$\langle\Phi(q)|\,\hat{P}^{L}_{\hat{Q}}(Q)\,|\Phi(q)\rangle = P(Q;q,q)$$



Projection and TDGCM

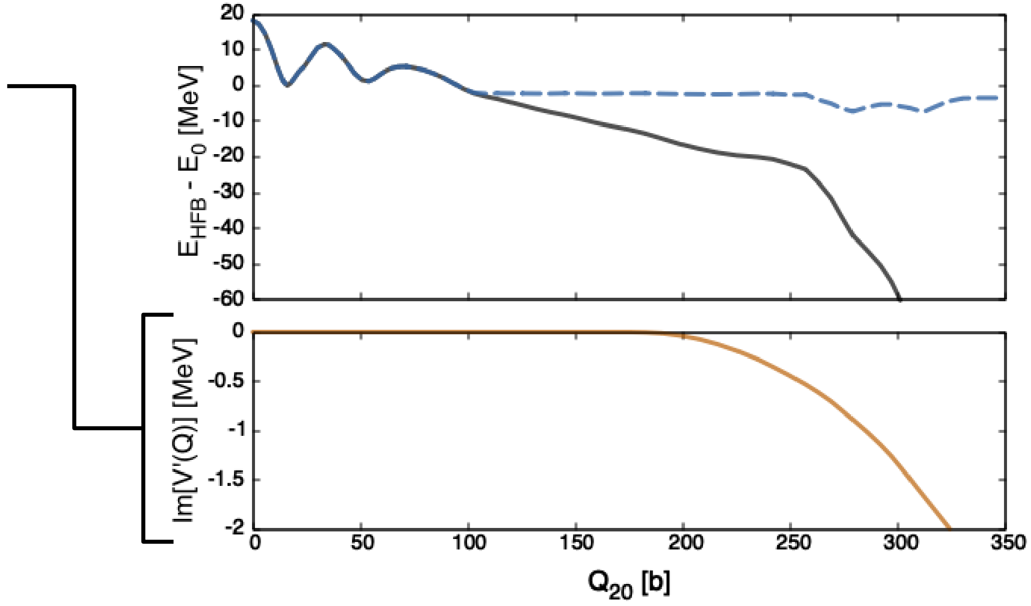
visualisation of the evolving TDGCM state

- without projection
- with projection



The quasistatic approach to spontaneous fission

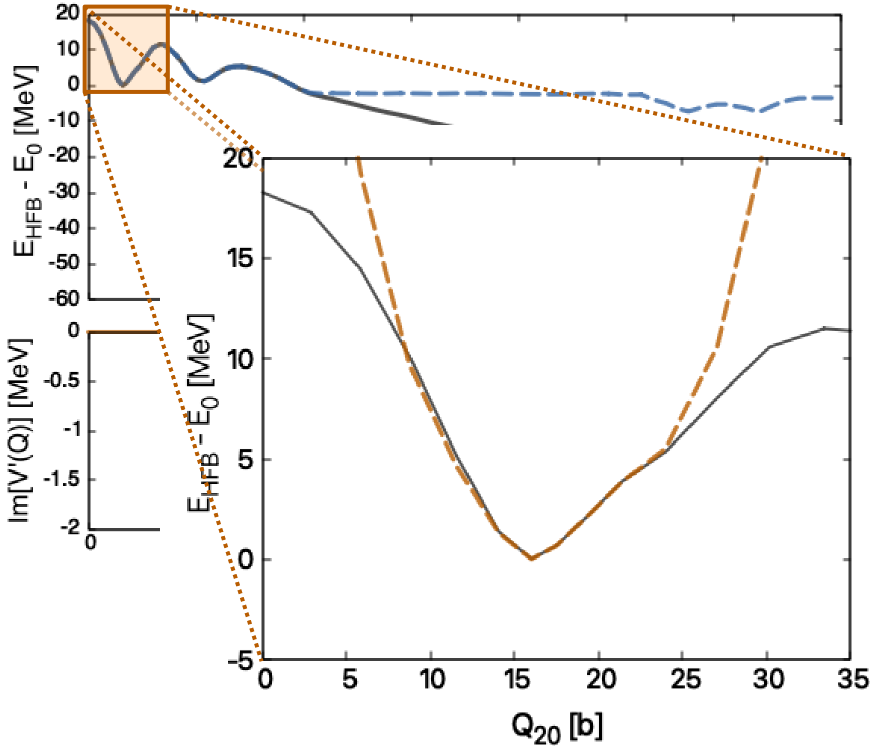
1. Add a complex absorbing potential to the PES



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

The quasistatic approach to spontaneous fission

1. Add a complex absorbing potential to the PES
2. Obtain quasistatic (metastable) eigenstates of the nuclear ground state well



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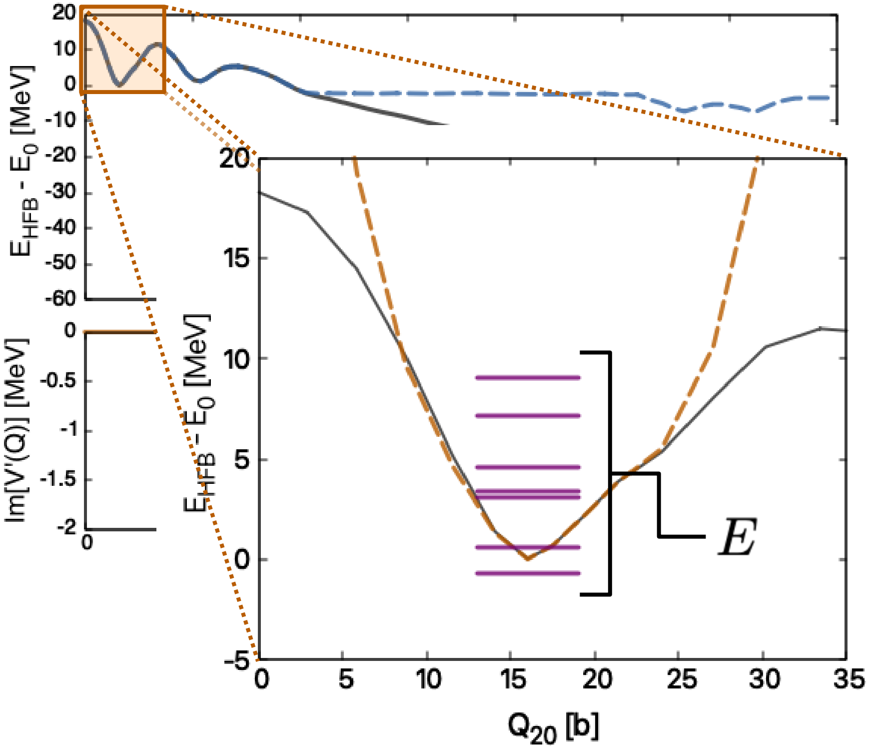
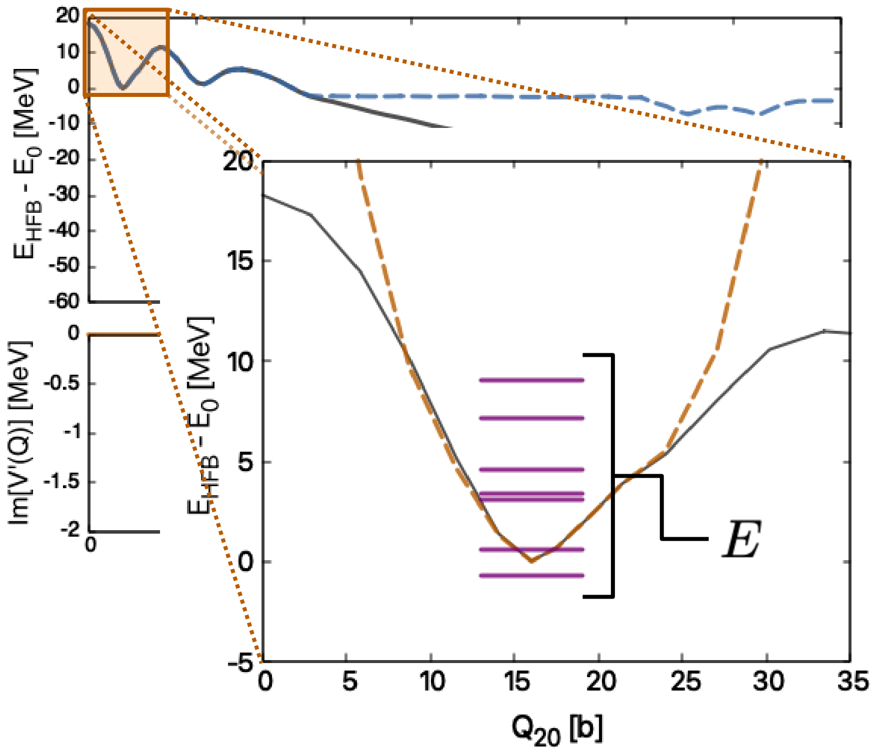


G. Scamps, K. Hagino, *Phys. Rev. C* **91**, 044606 (2015)

The quasistatic approach to spontaneous fission

1. Add a complex absorbing potential to the PES
2. Obtain quasistatic (metastable) eigenstates of the nuclear ground state well
3. Determine SF lifetimes from imaginary components of quasistatic state energies

$$\tau_{\mathrm{SF}} \propto 1/\mathrm{Im}(E)$$



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

Modification of the Hamiltonian kernel

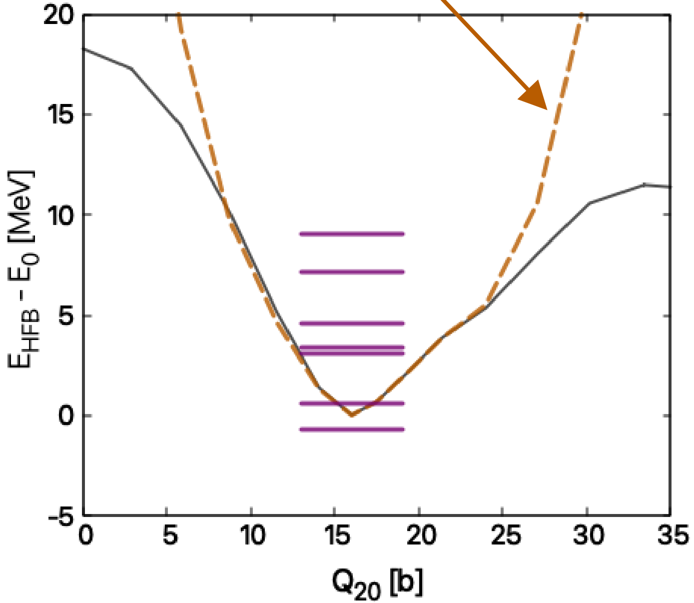
local Schrödinger equation

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

$$H'(q,q') = H(q,q') + V'(q,q')$$

GCM formalism

modified potential to
determine bound states



Modification of the Hamiltonian kernel

local Schrödinger equation

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

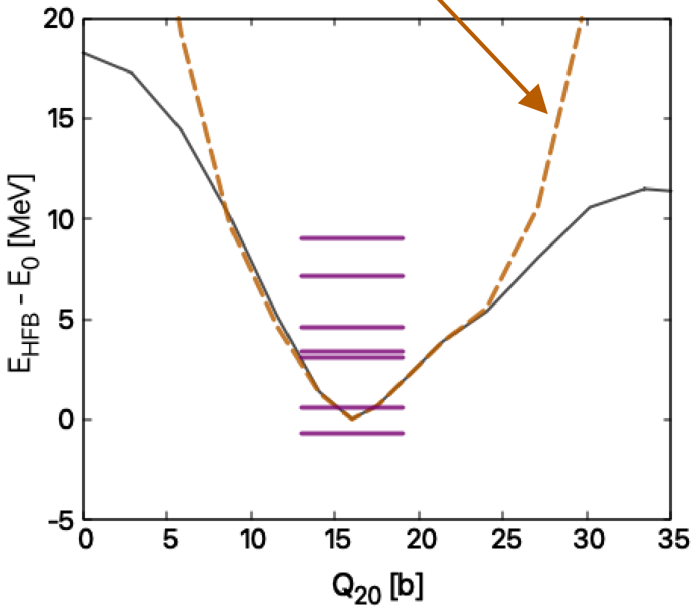
$$H'(q,q') = H(q,q') + V'(q,q')$$

GCM formalism

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

$$V'(q)$$

modified potential to determine bound states



Modification of the Hamiltonian kernel

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

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

Modification of the Hamiltonian kernel

$$H'(q,q') = H(q,q') + V'(q,q')$$

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

$$= \langle \Phi(q) | \left[\int dQ \; \hat{P}_{\hat{Q}}(Q) V'(Q) \right] | \Phi(q') \rangle$$

projection operator

local modification
to potential

Modification of the Hamiltonian kernel

$$H'(q,q') = H(q,q') + V'(q,q')$$

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

$$= \langle \Phi(q) | \left[\int dQ \; \hat{P}_{\hat{Q}}(Q) V'(Q) \right] | \Phi(q') \rangle$$

$$= \int dQ \; V'(Q) \, P(Q; q, q')$$

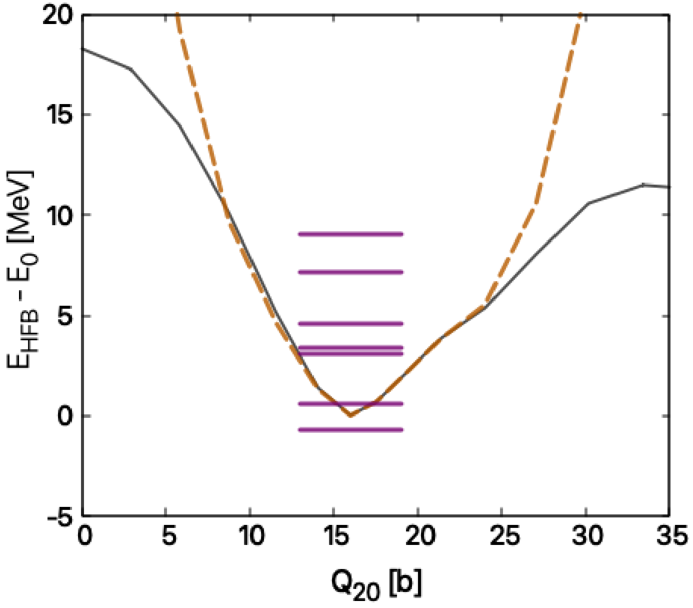
probability kernel

Modification of the Hamiltonian kernel

confining potential

$$V'(Q) = V_c(Q)$$

quadratic extrapolation
around the ground state well
to produce bound states



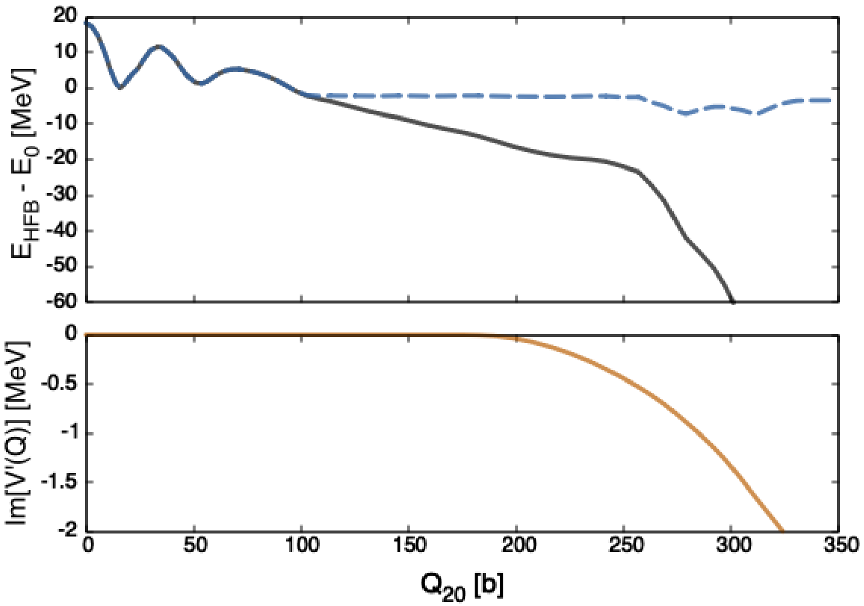
Modification of the Hamiltonian kernel

quasistatic potential

$$V'(Q) = V_q(Q) + iW(Q)$$

real “flattening” potential to hold the post-barrier energy constant

imaginary absorption potential to simulate loss due to spontaneous fission



Eigenstates of the collective Hamiltonian

collective Schrödinger equation

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

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

Eigenstates of the collective Hamiltonian

collective Schrödinger equation

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

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

exact solution

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

Eigenstates of the collective Hamiltonian

$$\mathbf{g}(t) = e^{-iH_C t/\hbar} \cdot \mathbf{g}(0)$$

The eigenvectors of the modified collective Hamiltonian are the energy eigenstates of the system:

confining potential
$V'(Q) = V_c(Q)$

→

bound states with energy eigenvalues $\lambda_i = E_i$

diagonalise H_C

quasistatic potential
$V'(Q) = V_q(Q) + iW(Q)$

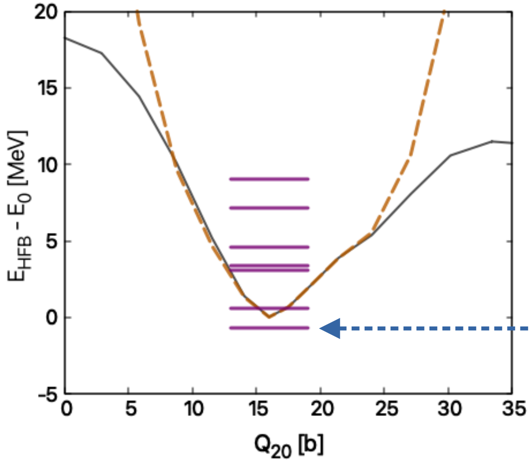
→

quasistatic states with energy eigenvalues $\lambda_i = E_i - \frac{i}{2}\Gamma_i$

Extracting spontaneous fission lifetimes

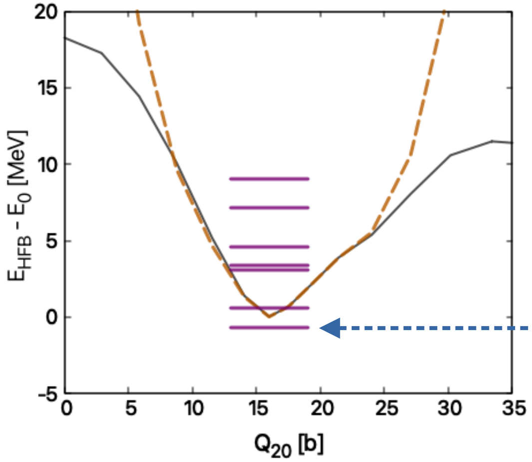
each quasistatic state
is in resonance...

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



with the bound eigenstate that
has the same real energy

Extracting spontaneous fission lifetimes



each quasistatic state
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

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

Extracting spontaneous fission lifetimes

each quasistatic state
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with a lifetime determined by the resonance width

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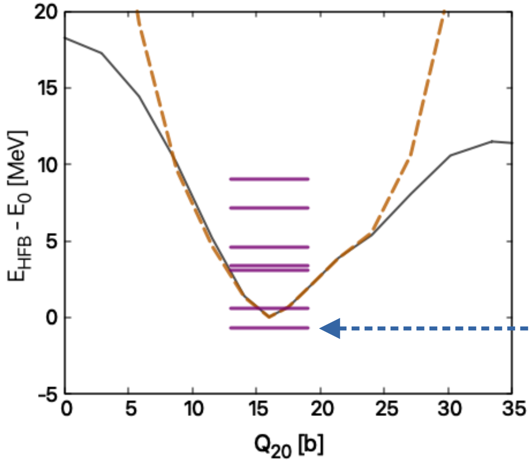

$$\tau_i = \frac{\hbar}{\Gamma_i}$$

spontaneous fission lifetime

Parameter dependence of SF lifetime

Γ_i depends on...

flattening potential

maintain post-barrier energy at

$$E_0 - \Delta$$

flattening gap

absorption potential

quadratic functional form

$$W(Q) = r_{\mathrm{abs}} \Theta(Q - Q_{\mathrm{abs}})(Q - Q_{\mathrm{abs}})^2$$

absorption rate (negative)

absorption threshold

Parameter dependence of SF lifetime

Γ_i depends on...

flattening potential

maintain post-barrier energy at

$$E_0 - \Delta$$

flattening gap (Δ)

absorption potential

quadratic functional form

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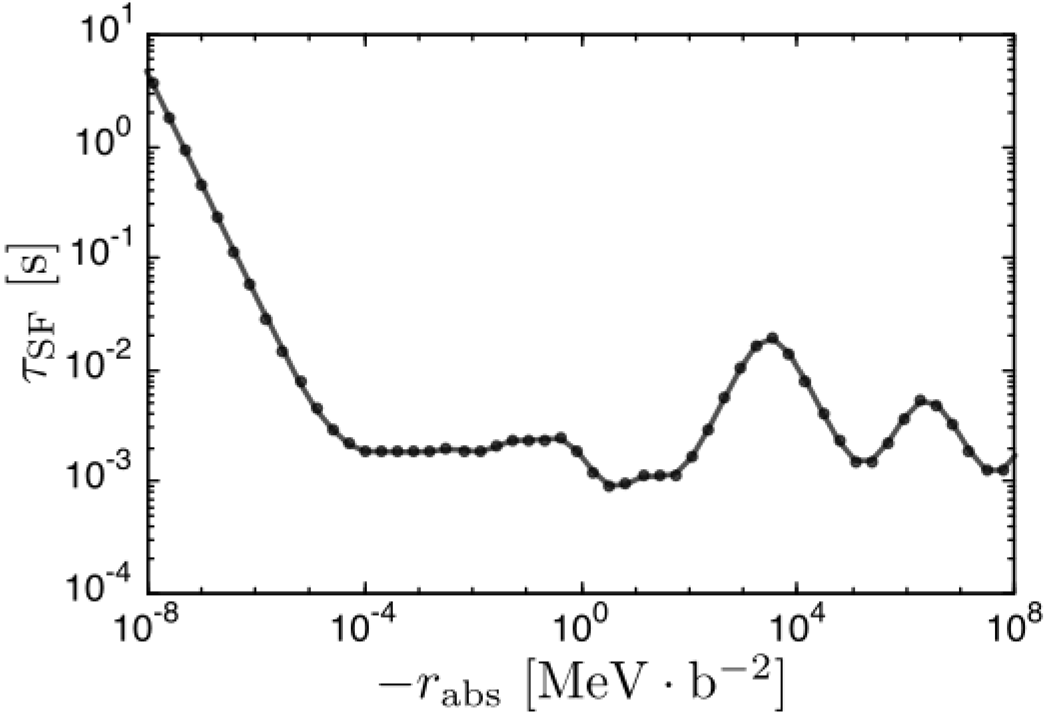
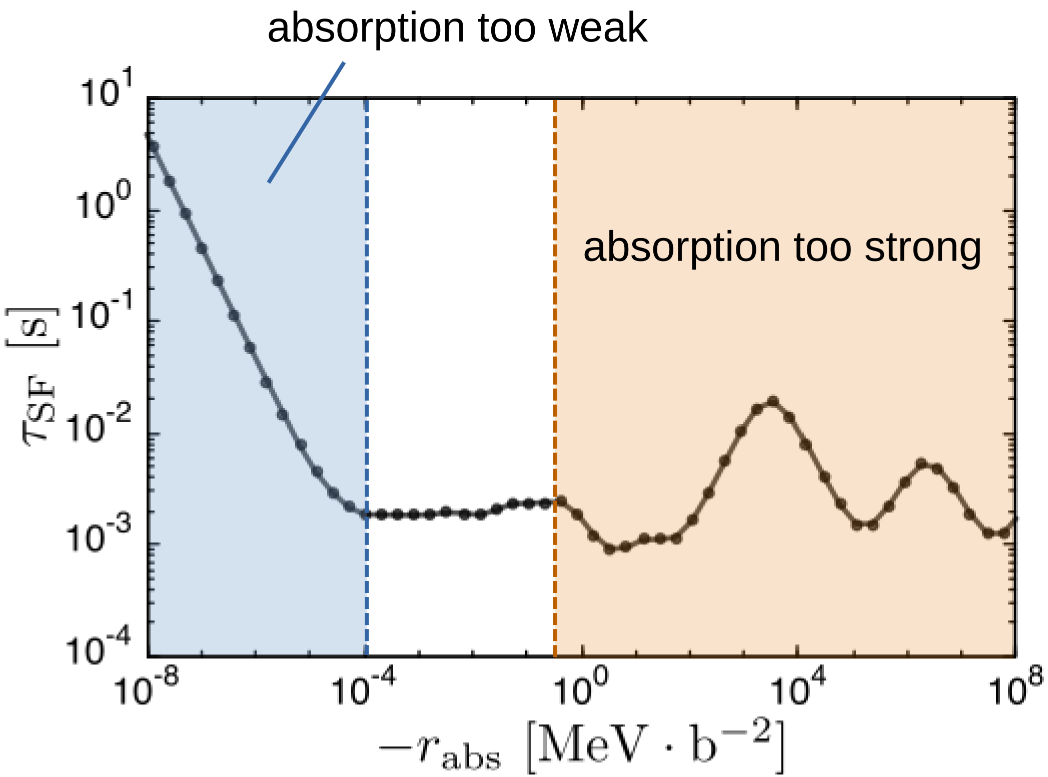
absorption rate (negative) (r_{abs})

absorption threshold (Q_{abs})

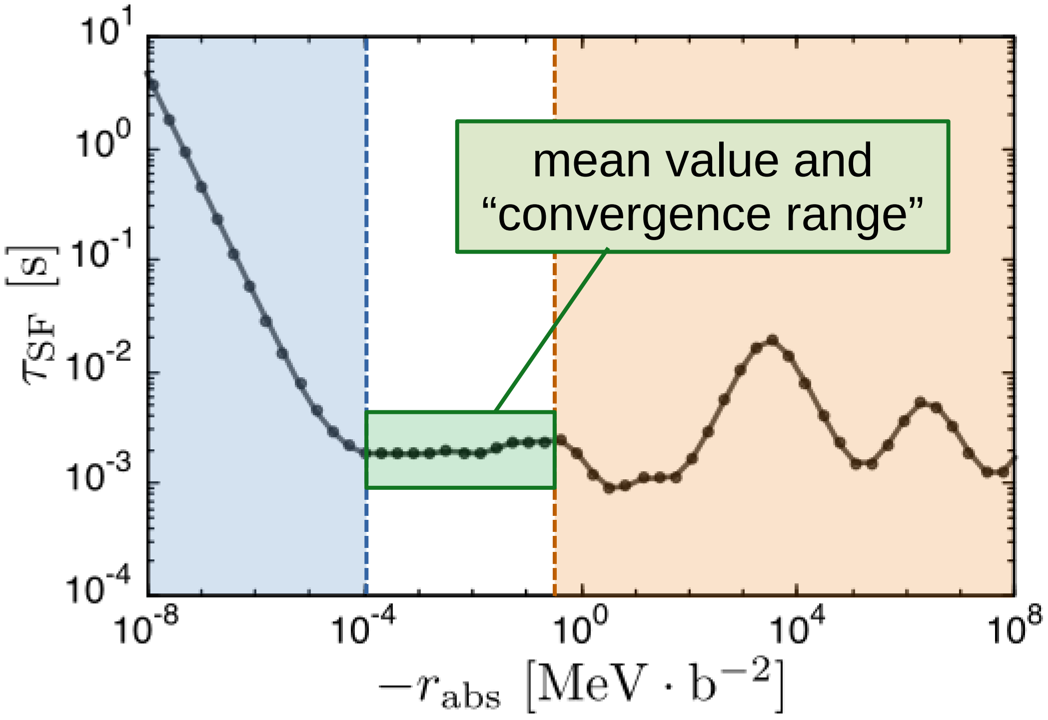
Variation of lifetime with absorption rate



Variation of lifetime with absorption rate

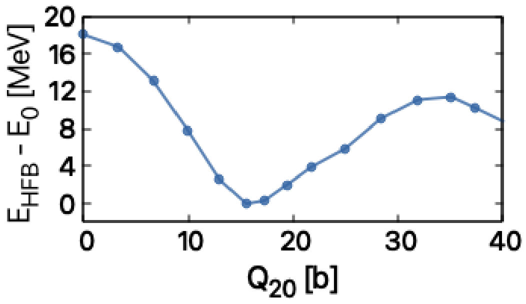


Variation of lifetime with absorption rate

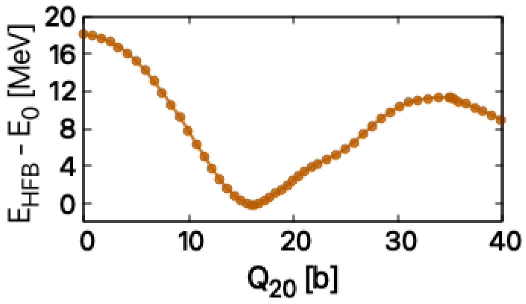


A new unknown: the mesh density

The same PES can be represented by a different number of generator states!



- Rarely considered in previous GCM and TDGCM studies
- Now easily accessible (in 1D) with the link/drop method



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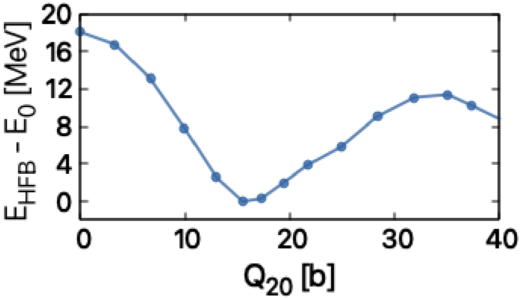


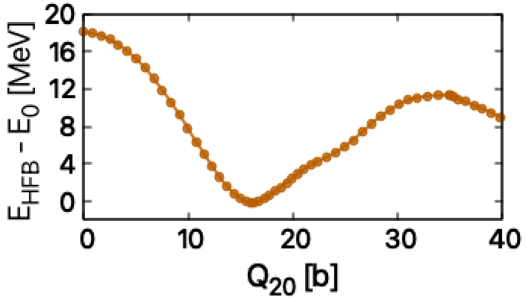
low density

$$\bar{N} \ll 1$$

- Rarely considered in previous GCM and TDGCM studies
- Now easily accessible (in 1D) with the link/drop method

quantified by the average overlap between neighbouring states on the path

$$\bar{N} = \langle N(q_n, q_{n+1}) \rangle$$

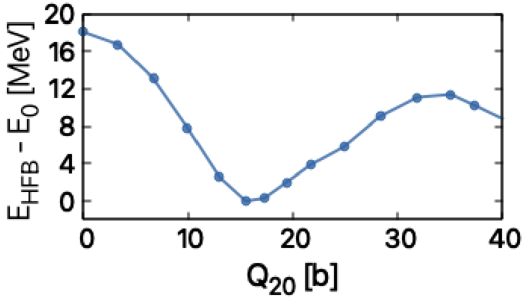


high density

$$\bar{N} \rightarrow 1$$

A new unknown: the mesh density

The same PES can be represented by a
different number of generator states!



low density

$\bar{N} \ll 1$

When the mesh density is too low:

Features of the PES lose their accuracy (e.g. fission barriers)

High-momentum TDGCM states are no longer representable

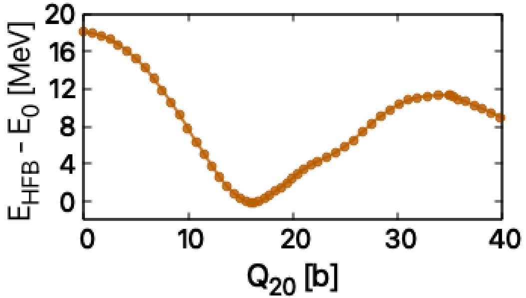
A new unknown: the mesh density

The same PES can be represented by a different number of generator states!

When the mesh density is too high:

Computations are much more expensive due to the large number of generator states

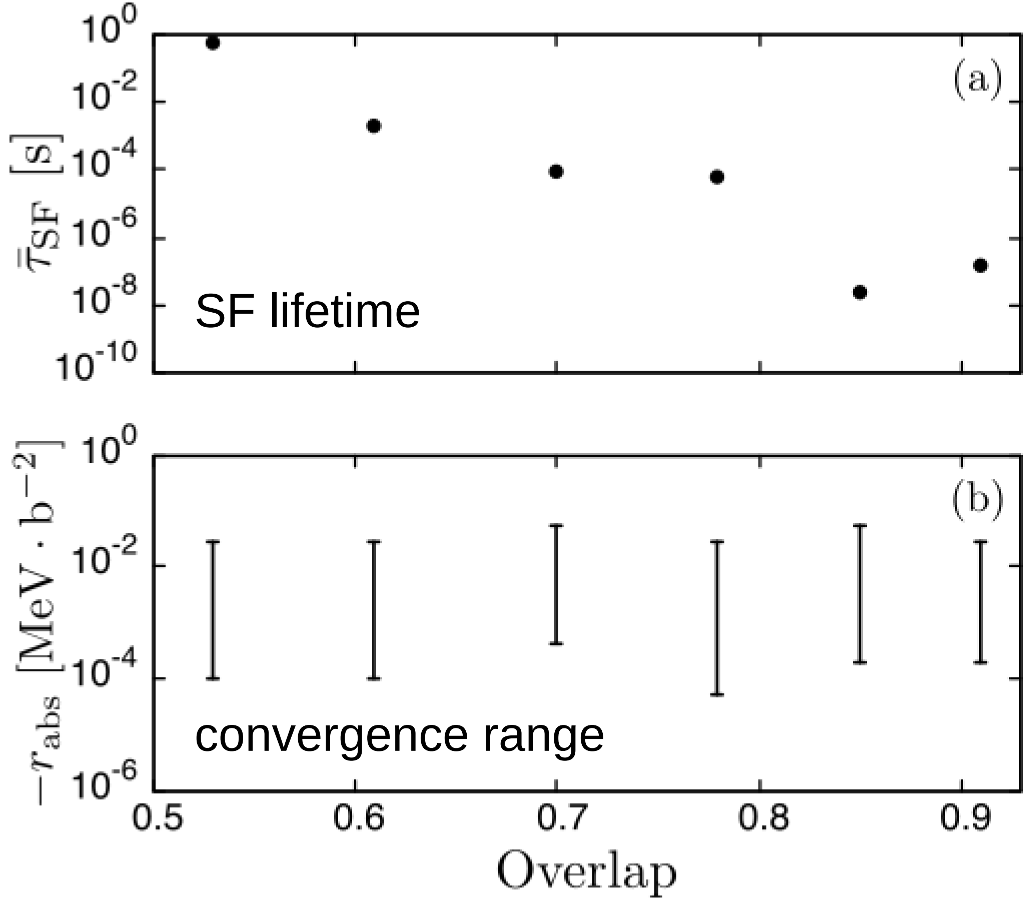
Redundancy in the basis leads to numerical stability issues when inverting the overlap kernel



high density

$\bar{N} \to 1$

Variation of lifetime with mesh density



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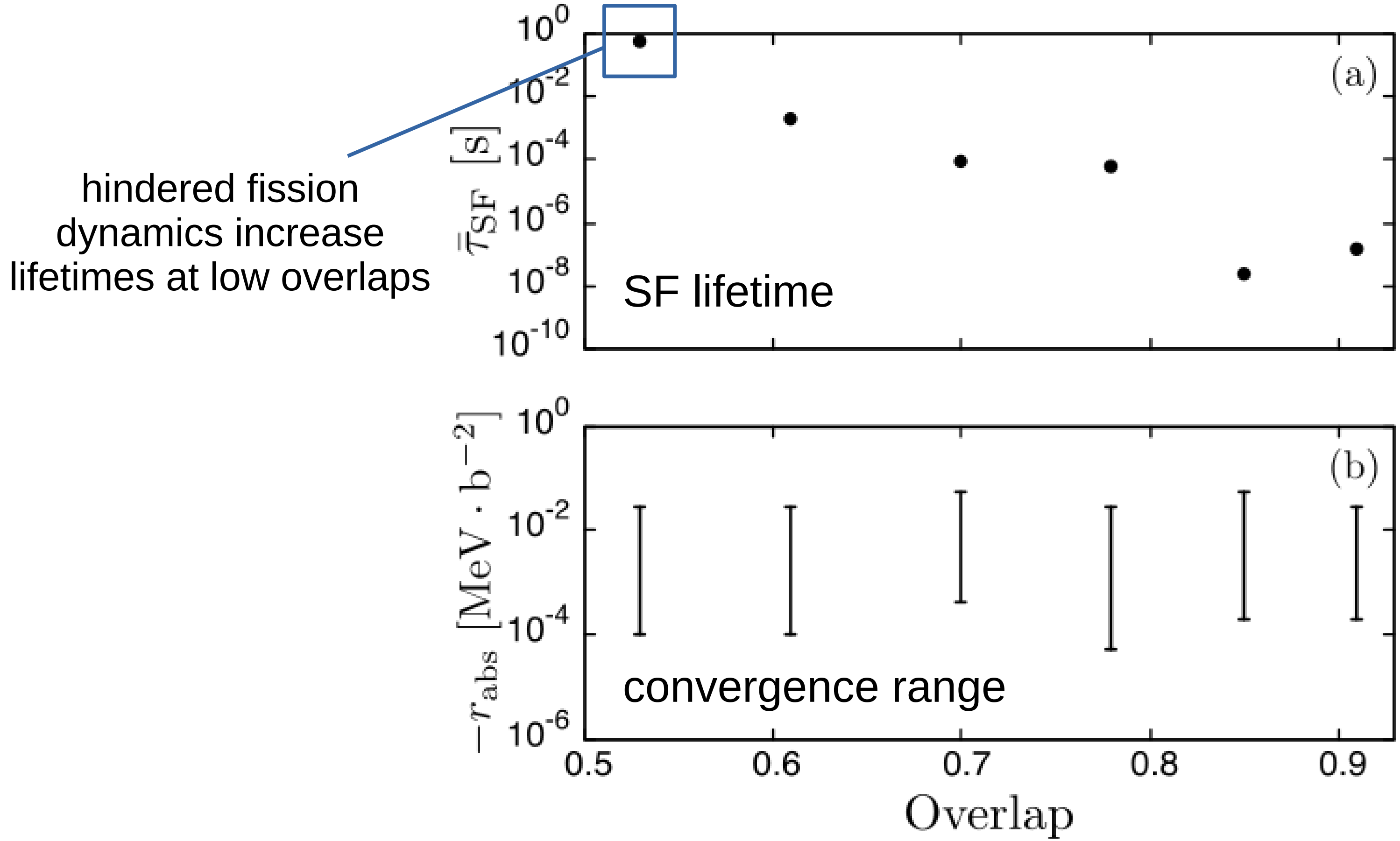

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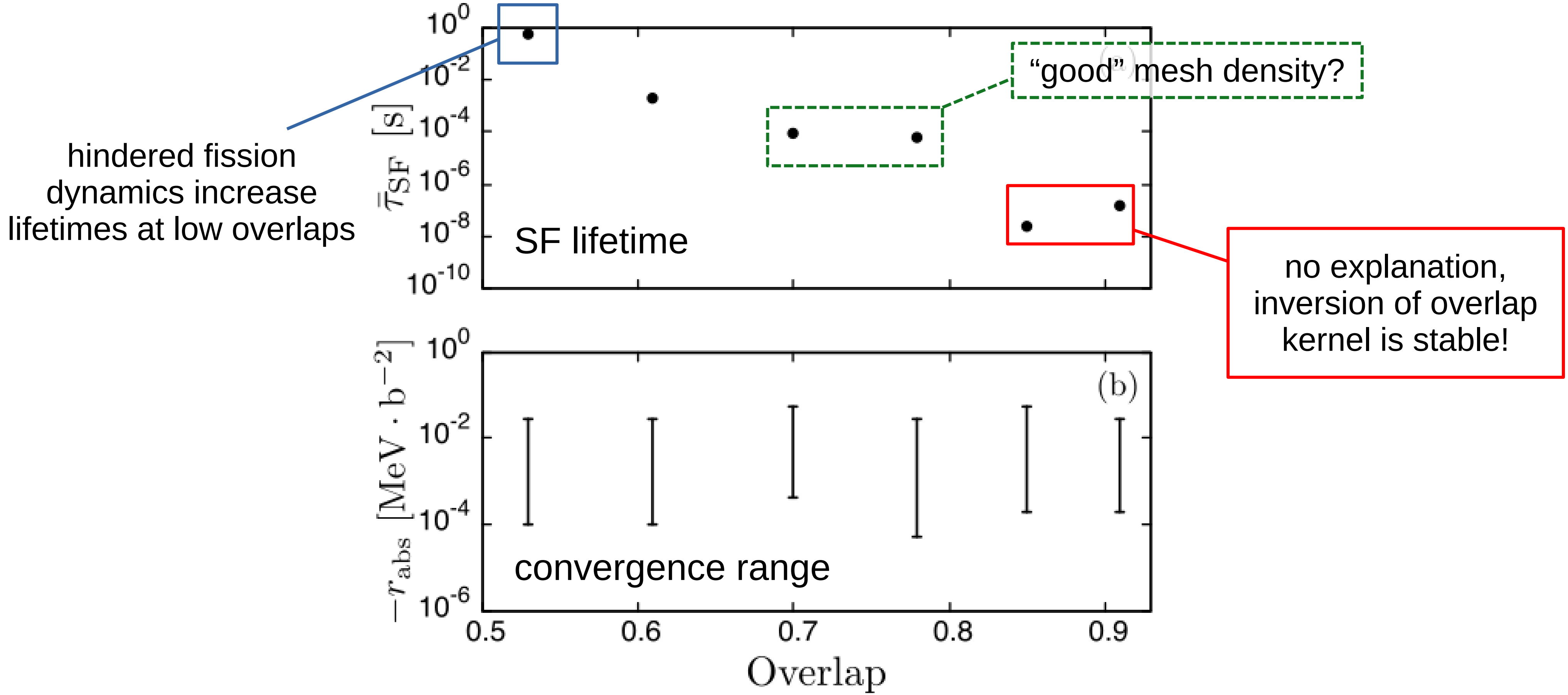
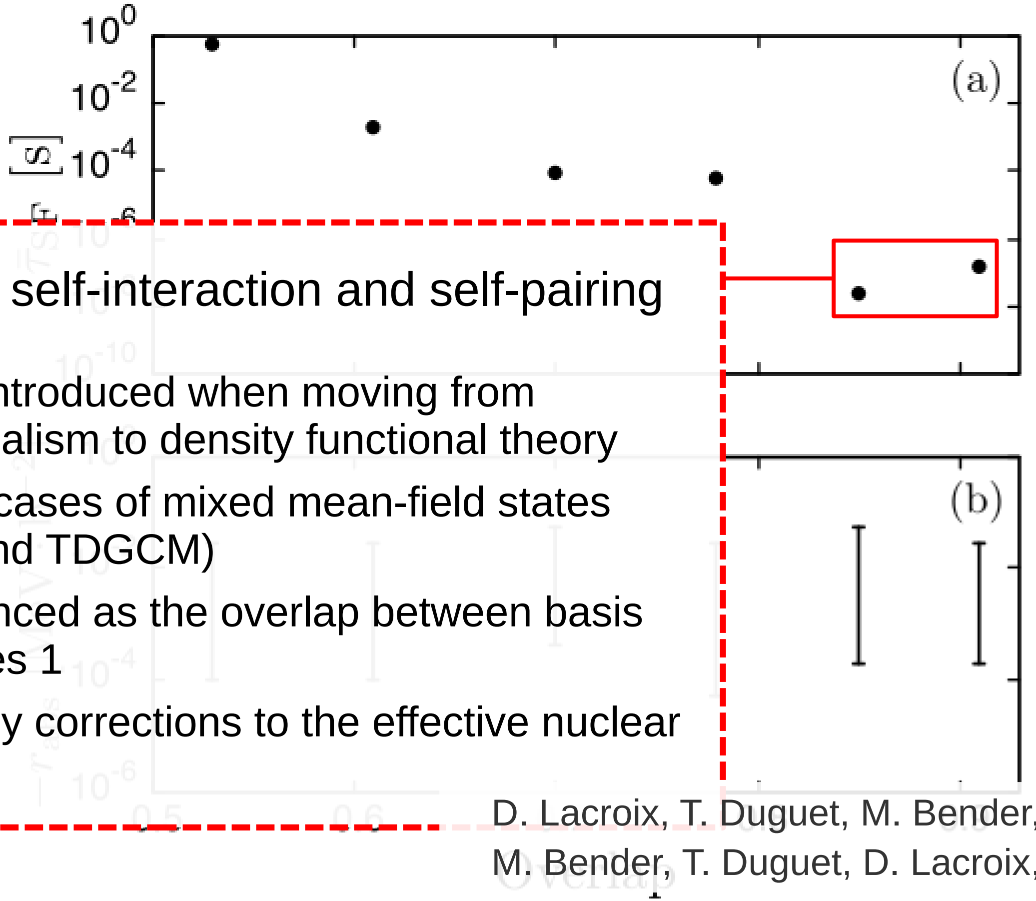


Variation of lifetime with mesh density



possible cause: self-interaction and self-pairing

- Spurious terms introduced when moving from Hamiltonian formalism to density functional theory
- Compounded in cases of mixed mean-field states (such as GCM and TDGCM)
- Effects are enhanced as the overlap between basis states approaches 1
- Must be solved by corrections to the effective nuclear interaction!

D. Lacroix, T. Duguet, M. Bender, *Phys. Rev. C* **79**, 044318 (2009)
M. Bender, T. Duguet, D. Lacroix, *Phys. Rev. C* **79**, 044319 (2009)

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	7.788×10^{-5}	9.426×10^{3}	**8.262×10^{-9}**

*Values taken from https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html, accessed 07/06/2026

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- 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

Could be addressed by introducing the conjugate “momentum” as an additional generator coordinate†

*Values taken from https://www-nds.iaea.org/relnsd/vcharthtml/VChartHTML.html, accessed 07/06/2026

†K. Goeke, P.-G. Reinhard, *Ann. Phys.* **124**, 249–289 (1980)

Summary

exact TDGCM model of fission in one 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 collective coordinate distributions of HFB states and their superpositions (e.g. in GCM)
- 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)

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- Dr. Guillaume Scamps (L2IT)

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

The workshop organisers

You, for listening!