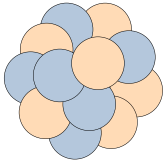
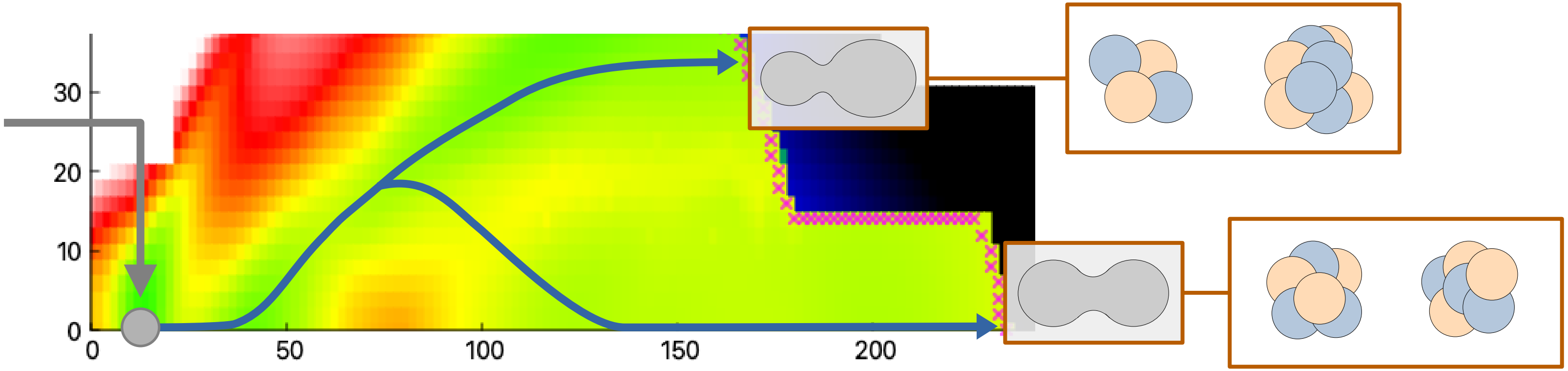
Towards an improved description of nuclear fission using the TDGCM without the GOA

Ngee Wein Lau

L2IT IN2P3 – Université Toulouse III / CNRS
(previously RSPhys, Australian National University)





Acknowledgements

Ph.D. supervisory panel:

- Rémi Bernard – CEA Cadarache
- Cédric Simenel – Australian National University
- Taiki Tanaka – GANIL

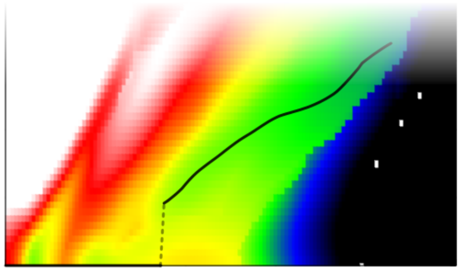
Collaborators:

- Luis Robledo – Universidad Autonoma de Madrid

Project goals

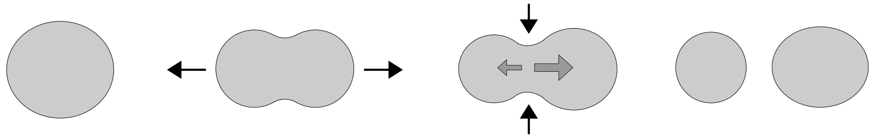
static nuclear model

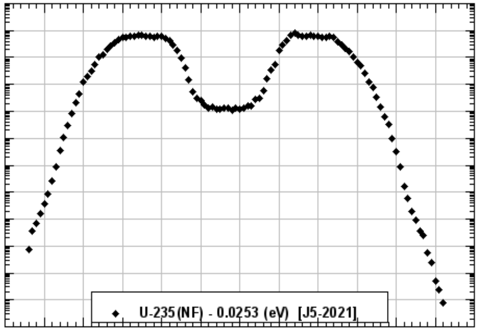
potential energy surfaces (PESs)



TDGCM

time-dependent generator coordinate method

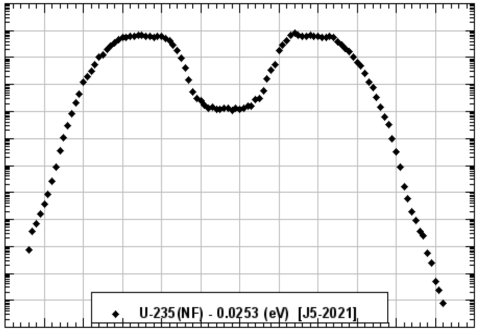




fission observables:

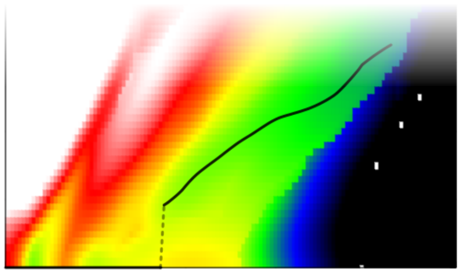
fragment masses
fragment charges
kinetic energies

Project goals



static nuclear model

potential energy surfaces (PESs)

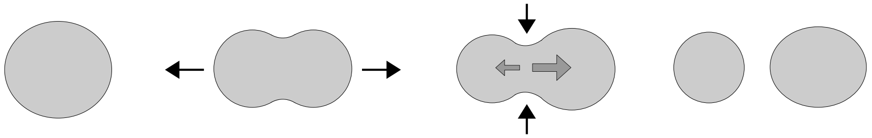


Gaussian overlap approximation

GOA

TDGCM

time-dependent generator coordinate method



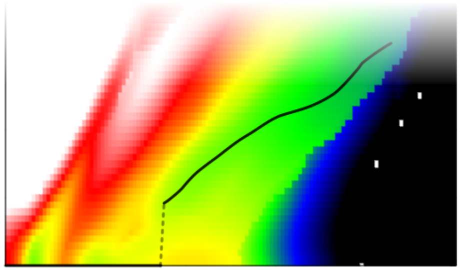
fission observables:

fragment masses
fragment charges
kinetic energies

Project goals

static nuclear model

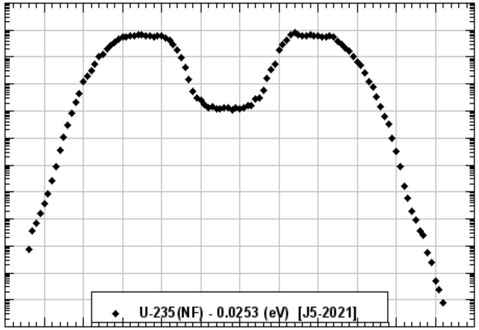
potential energy surfaces (PESs)



GOA

TDGCM

?

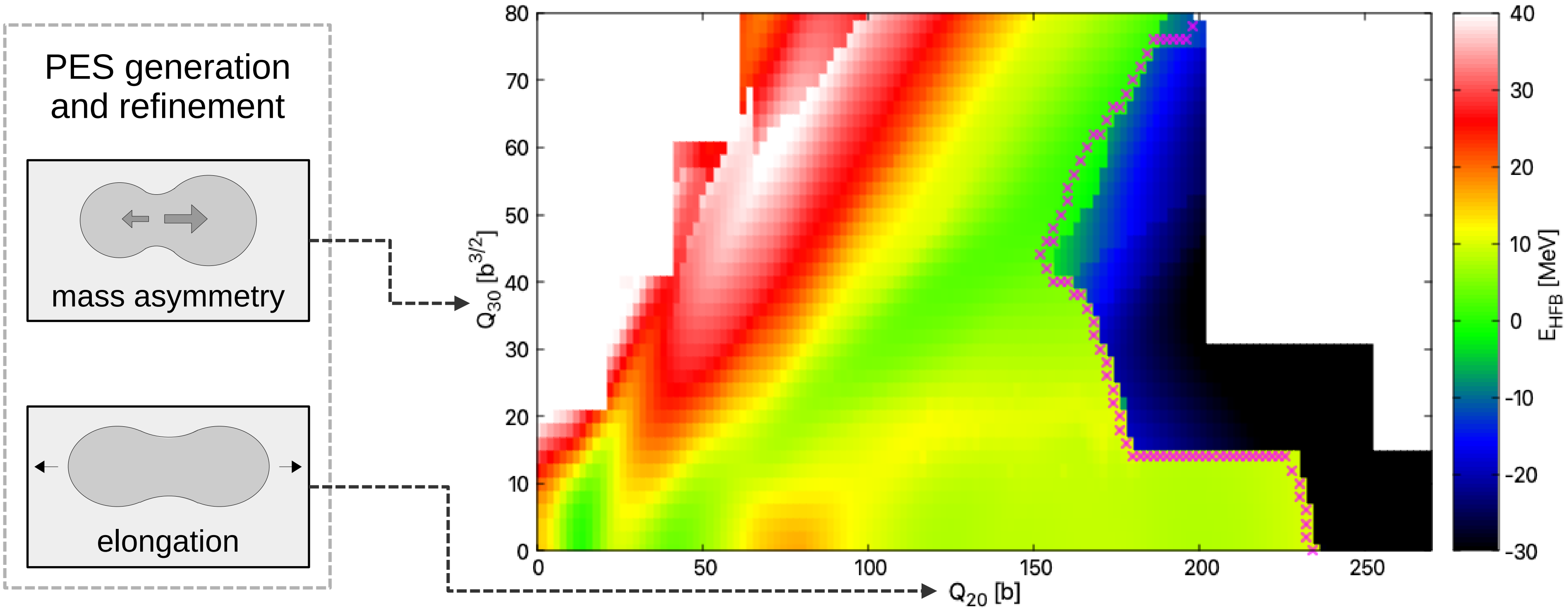


fission observables:

fragment masses
fragment charges
kinetic energies

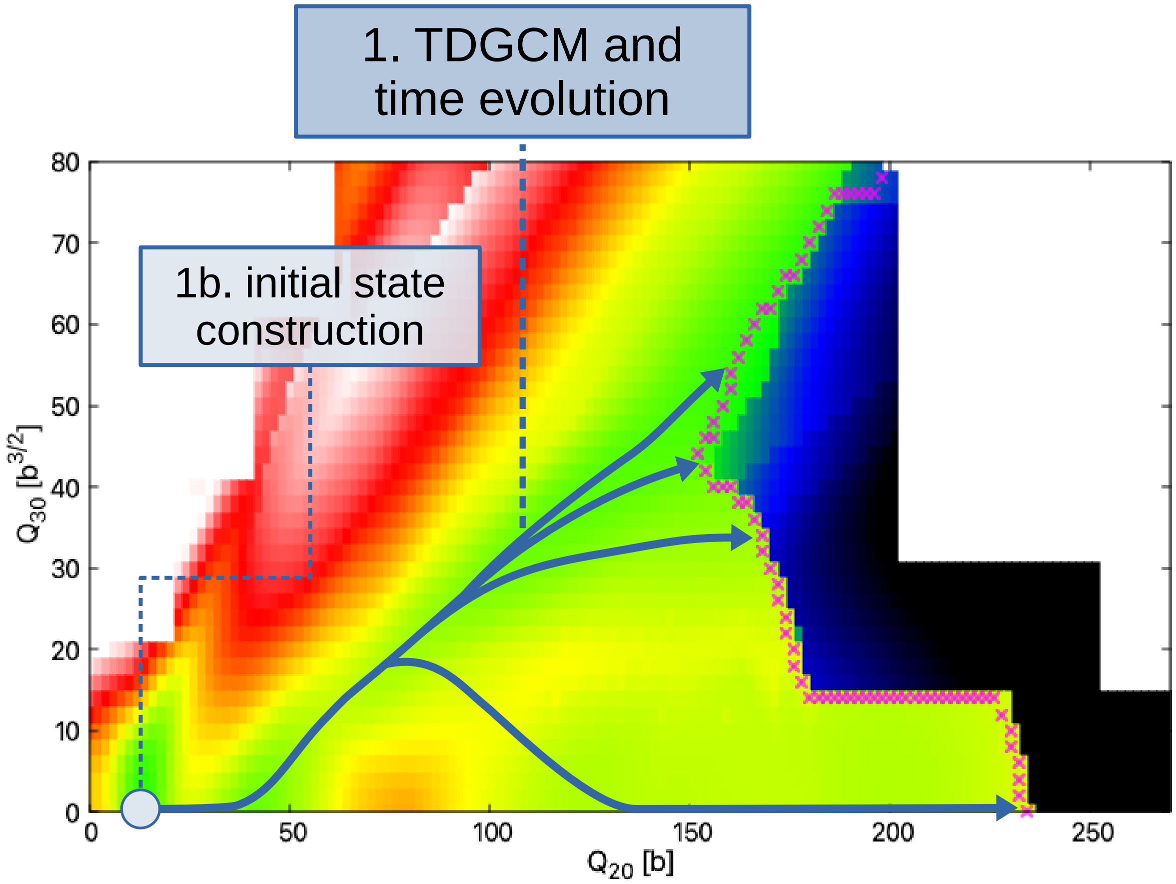
Goal: develop and implement a GOA-free TDGCM to produce an improved model of nuclear fission

A TDGCM description of fission



For more details, see:
N.-W. T. Lau, R. N. Bernard, C. Simenel, *Phys. Rev. C* **105**, 034617 (2022)

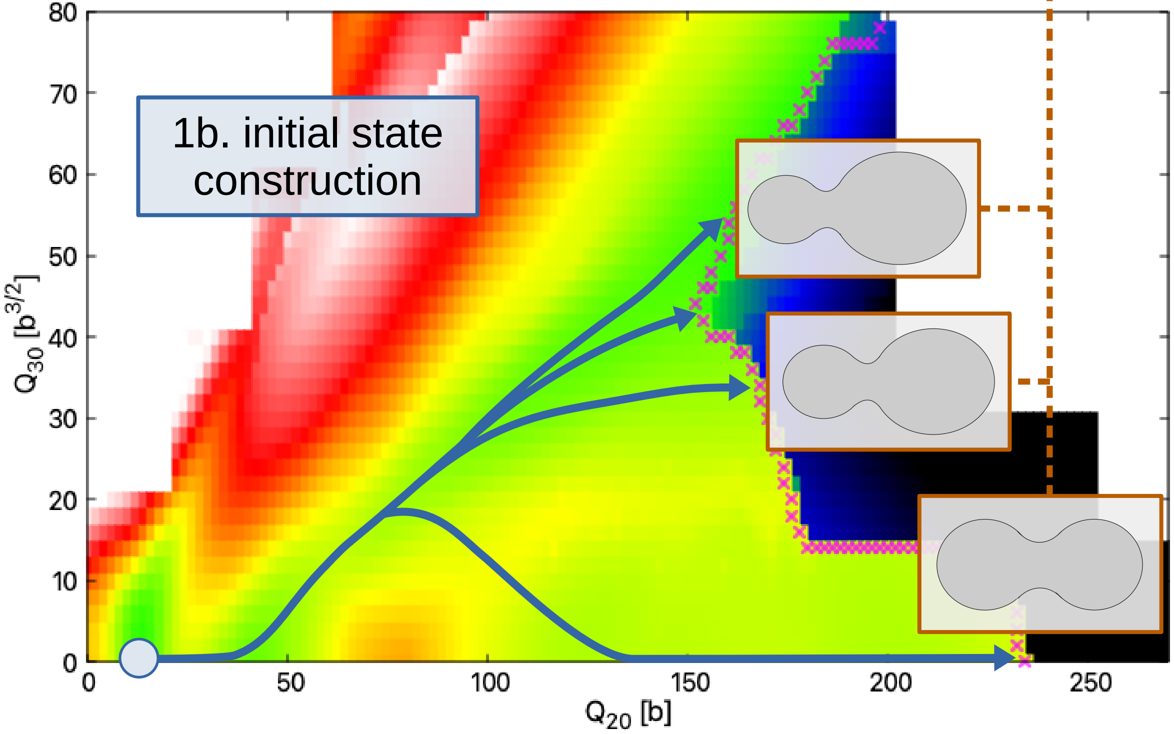
A TDGCM description of fission



A TDGCM description of fission

1. TDGCM and time evolution

2. Extracting fission observables

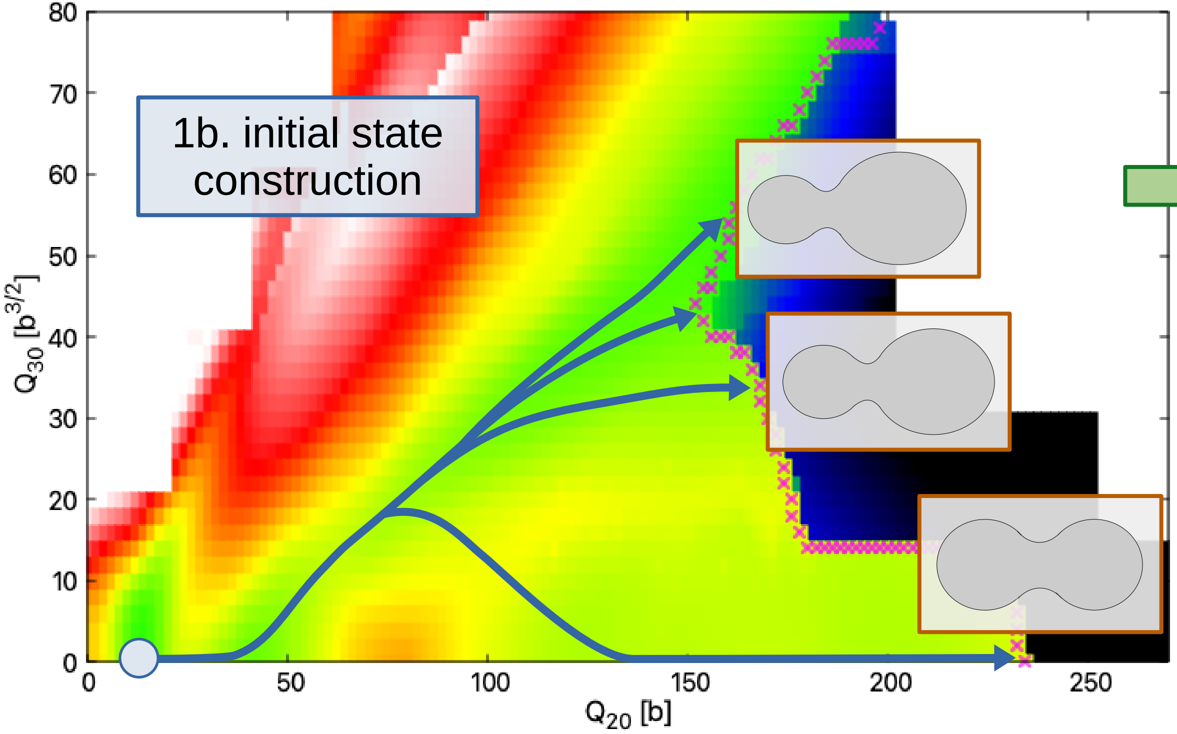


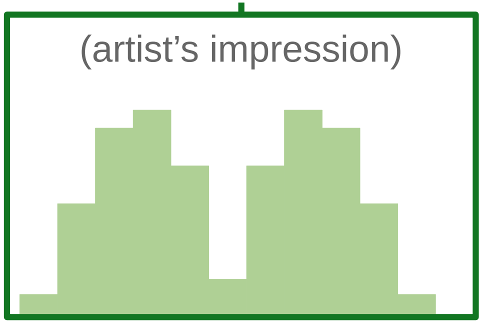
A TDGCM description of fission

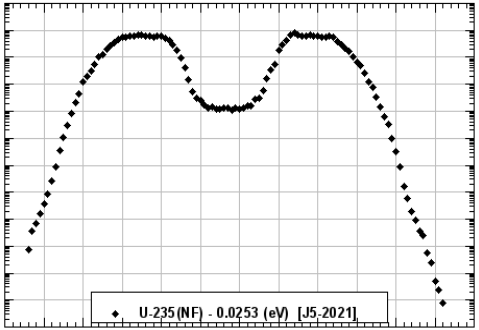
1. TDGCM and time evolution

2. Extracting fission observables

3. Interpreting and improving results



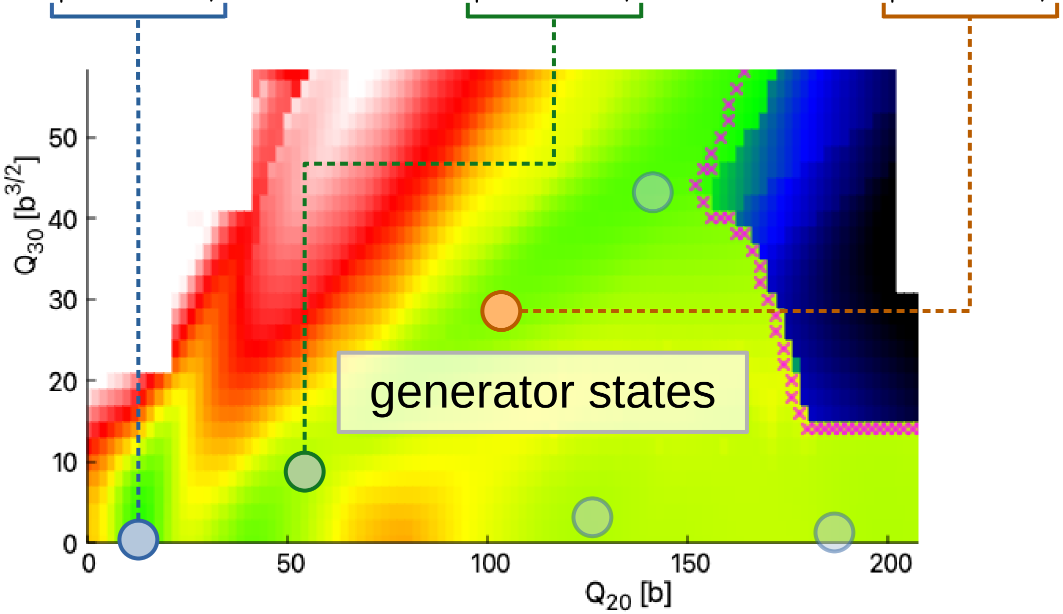




TDGCM

(Time-dependent generator coordinate method)

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



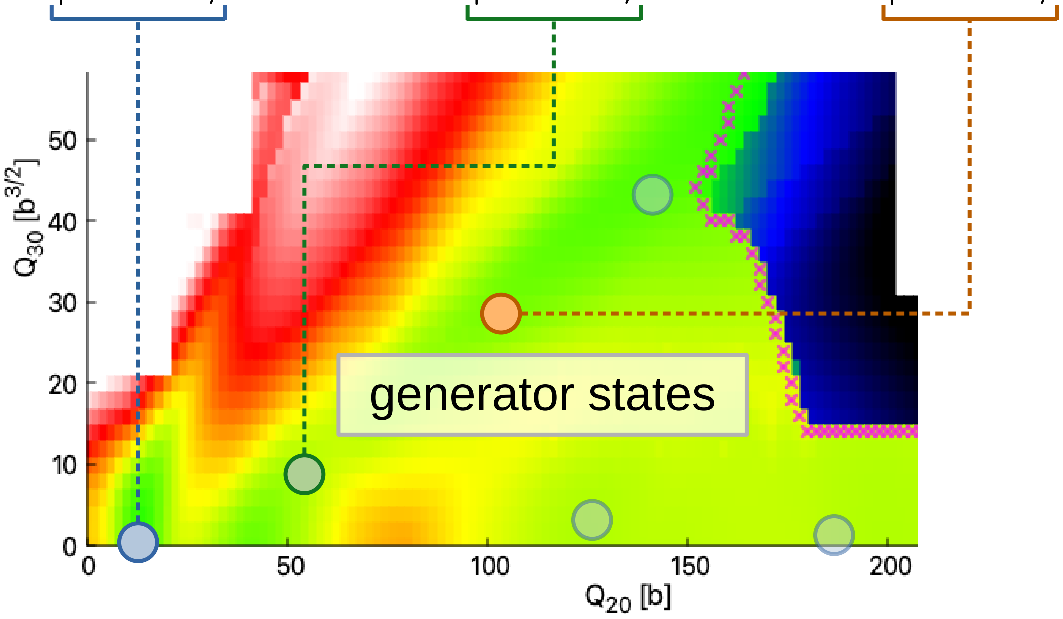
P. Ring, P. Schuck, *The Nuclear Many-Body Problem (Ch. 10),* Springer, Berlin (2004)
P.-G. Reinhard, R. Cusson, K. Goeke, *Nucl. Phys. A* **398**, 141 (1983)

TDGCM
(Time-dependent generator coordinate method)

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

$f(\vec{\mathbf{q}},t)$

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)

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

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

overlap kernel

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

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 TDGCM

eigenvalues
(positive real)

eigenvectors

$$N(\mathbf{q}, \mathbf{q}') \to n_k, \; u_k(\mathbf{q})$$

$$|k\rangle = \frac{1}{\sqrt{n_k}} \int d\mathbf{q} \; u_k(\mathbf{q}) |\Phi(\mathbf{q})\rangle, \; \langle k|k'\rangle = \delta_{kk'}$$

“natural” basis of orthonormal states

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

Exact solution of 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

$$\sum_{k'} \left(\tilde{H}_{kk'} - i\hbar \delta_{kk'} \frac{d}{dt} \right) g_{k'}(t) = 0$$

$$\langle k | \hat{H} | k' \rangle$$

$$\sum_{k'} \tilde{H}_{kk'} g_{k'}(t) = i\hbar \frac{dg_k}{dt}$$

Nonlocal Collective Schrödinger Equation (CSE)

The Gaussian overlap approximation

$$\mathcal{N}(\mathbf{q},\mathbf{q}') \approx \exp\left(-\frac{1}{2}\mathbf{s}\cdot\Gamma(\bar{\mathbf{q}})\cdot\mathbf{s}\right)$$

Gaussian approximation of overlap kernel

$$\bar{\mathbf{q}} = \frac{1}{2}(\mathbf{q}+\mathbf{q}')$$

$$\mathbf{s} = \mathbf{q}-\mathbf{q}'$$

$$\mathcal{H}(\mathbf{q},\mathbf{q}') \approx \mathcal{N}(\mathbf{q},\mathbf{q}')\left[h_0(\bar{\mathbf{q}}) \ + \ \mathbf{h}_1(\bar{\mathbf{q}})\cdot\bar{\mathbf{q}} \ + \ \bar{\mathbf{q}}\cdot H_2(\bar{\mathbf{q}})\cdot\bar{\mathbf{q}} \ + \ \mathcal{O}(\bar{\mathbf{q}}^3)\right]$$

quadratic approximation for Hamiltonian (and other) kernels

P. Ring, P. Schuck, *The Nuclear Many-Body Problem (Ch. 10.7.4),* Springer, Berlin (2004)
P. -G. Reinhard, K. Goeke, *Rep. Prog. Phys.* **50** 1 (1987)

The Gaussian overlap approximation

Local Collective Schrödinger Equation (CSE)

$$\left[-\frac{\hbar^2}{2}\nabla\cdot B(\mathbf{q})\cdot\nabla + V(\mathbf{q})\right] g(\mathbf{q},t) = i\hbar\frac{\partial}{\partial t}g(\mathbf{q},t)$$

$B(\mathbf{q})$: Collective inertia tensor

$$V(\mathbf{q}) = E_{\mathrm{HFB}}(\mathbf{q}) - \epsilon_{\mathrm{ZPE}}(\mathbf{q})$$

$E_{\mathrm{HFB}}(\mathbf{q})$: Energy from PES

$\epsilon_{\mathrm{ZPE}}(\mathbf{q})$: Zero-point energy correction

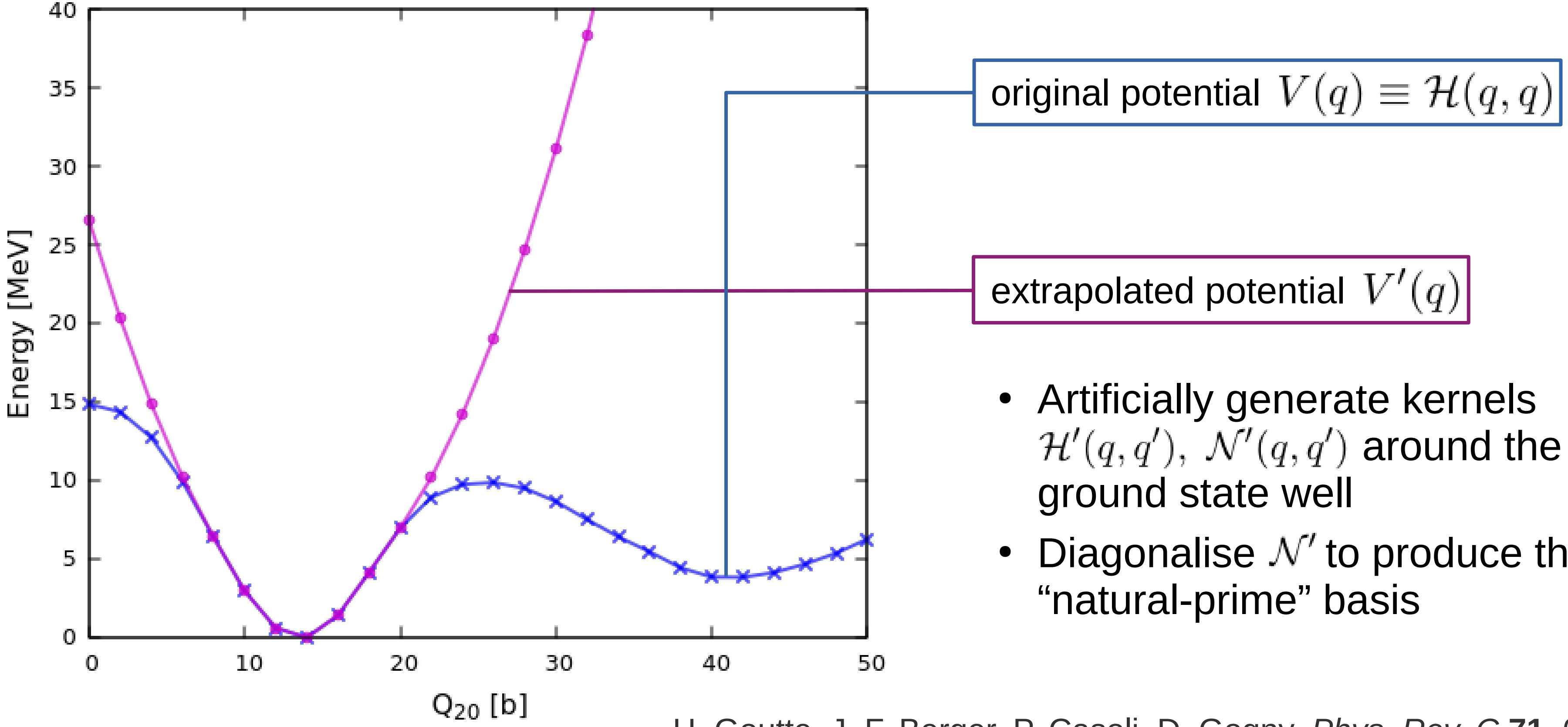
The Gaussian overlap approximation

Local Collective Schrödinger Equation (CSE)

$$\left[-\frac{\hbar^2}{2}\nabla\cdot B(\mathbf{q})\cdot\nabla + V(\mathbf{q})\right] g(\mathbf{q},t) = i\hbar\frac{\partial}{\partial t}g(\mathbf{q},t)$$

- Smooths out natural variations in overlap across the PES
- Validity of assumptions should be checked before use
- Not suitable to handle pairing correlations or dissipative effects
- Cannot support symmetry restoration via projections

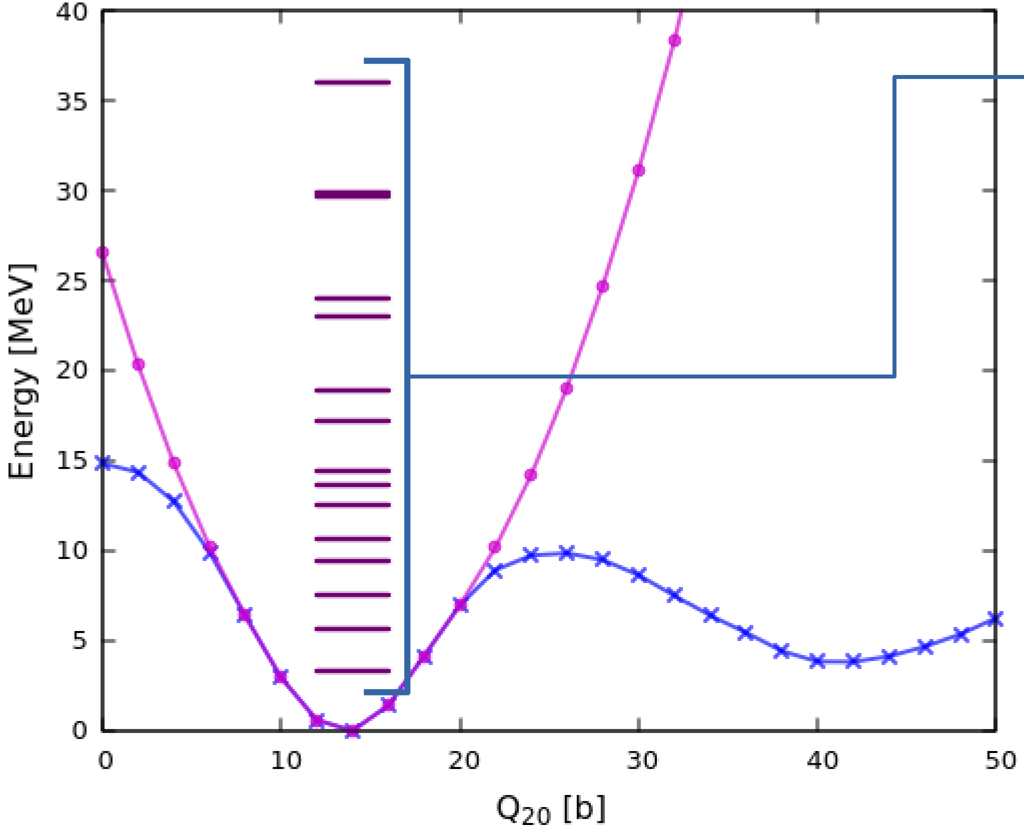
Initial state construction



- Artificially generate kernels $\mathcal{H}'(q,q'),\ \mathcal{N}'(q,q')$ around the ground state well
- Diagonalise $\mathcal{N}'$ to produce the "natural-prime" basis

H. Goutte, J. F. Berger, P. Casoli, D. Gogny, *Phys. Rev. C* **71**, 024316 (2005)

Initial state construction

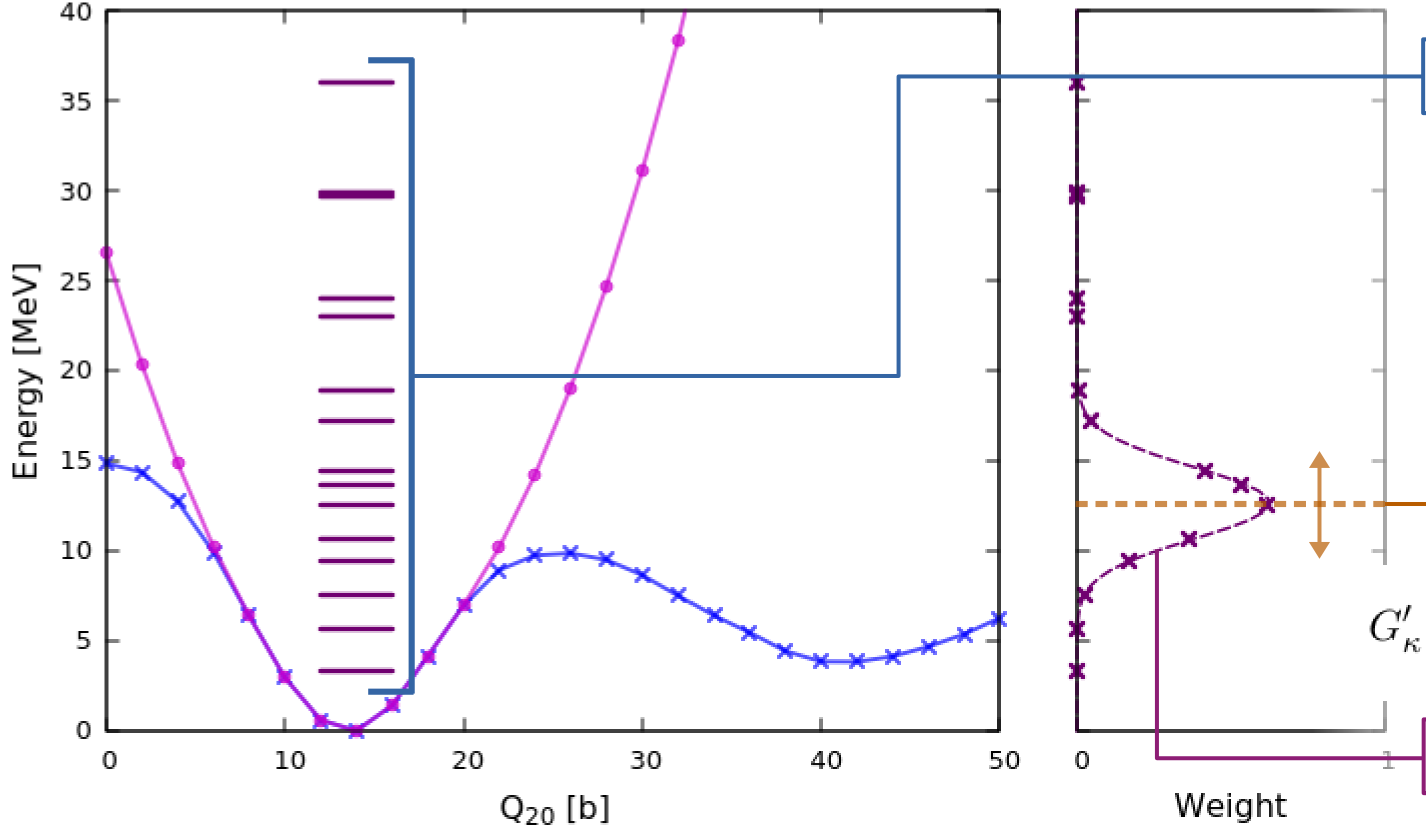


eigenstates $h_{\kappa\kappa'}$ of $\tilde{\mathcal{H}}'_{\kappa\kappa'}$

$$\sum_{\kappa'} \tilde{\mathcal{H}}'_{\kappa\kappa'} h_{\kappa'\lambda} = \varepsilon_\lambda h_{\kappa\lambda}$$

from exact time-independent GCM

Initial state construction



eigenstates $h_{\kappa\kappa'}$ of $\tilde{\mathcal{H}}'_{\kappa\kappa'}$

$$\sum_{\kappa'} \tilde{\mathcal{H}}'_{\kappa\kappa'} h_{\kappa'\lambda} = \varepsilon_\lambda h_{\kappa\lambda}$$

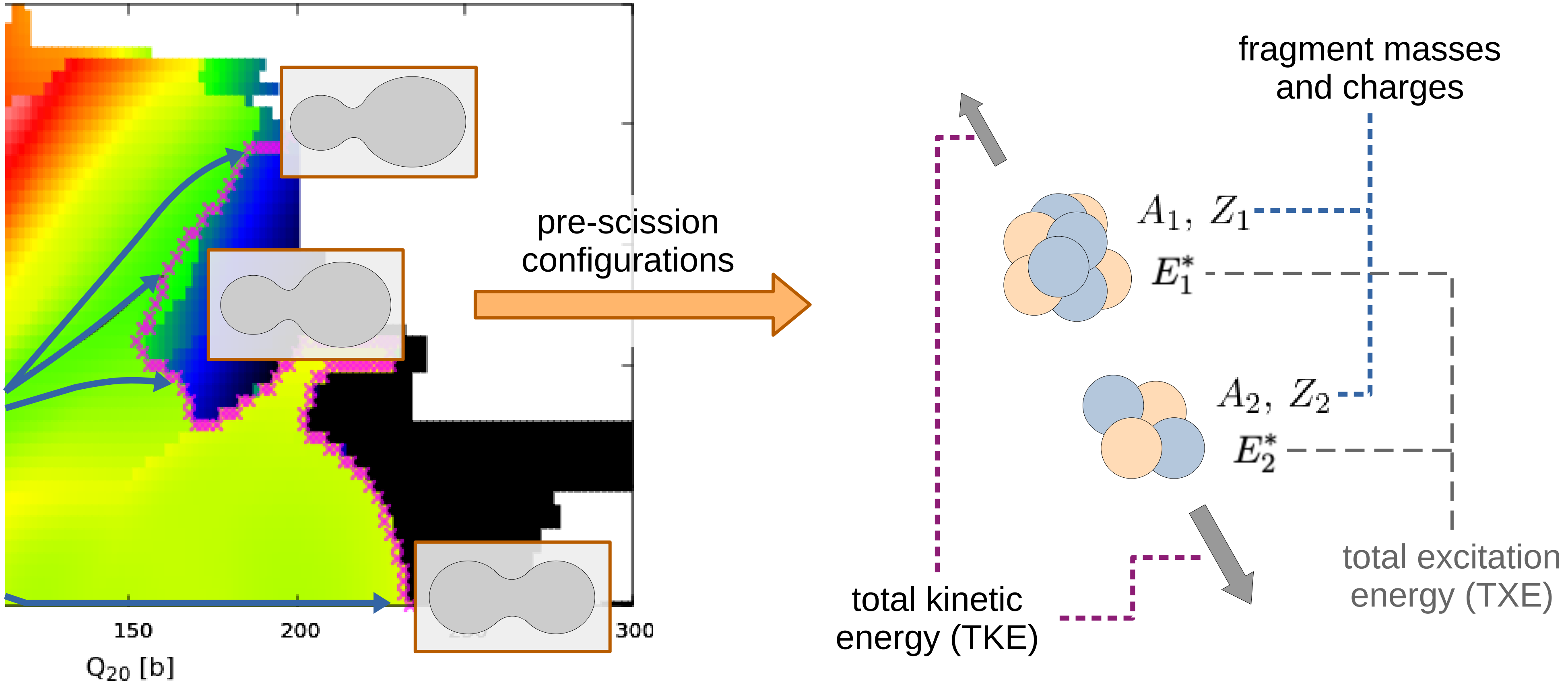
from exact time-independent GCM

adjusted to produce desired (real) energy

$$G'_\kappa \propto \sum_{\kappa'} \exp\left(-\frac{(\varepsilon_{\kappa'} - \bar{E})^2}{2\sigma^2}\right) h_{\kappa\kappa'}$$

Gaussian-like initial state

Observables at the scission line

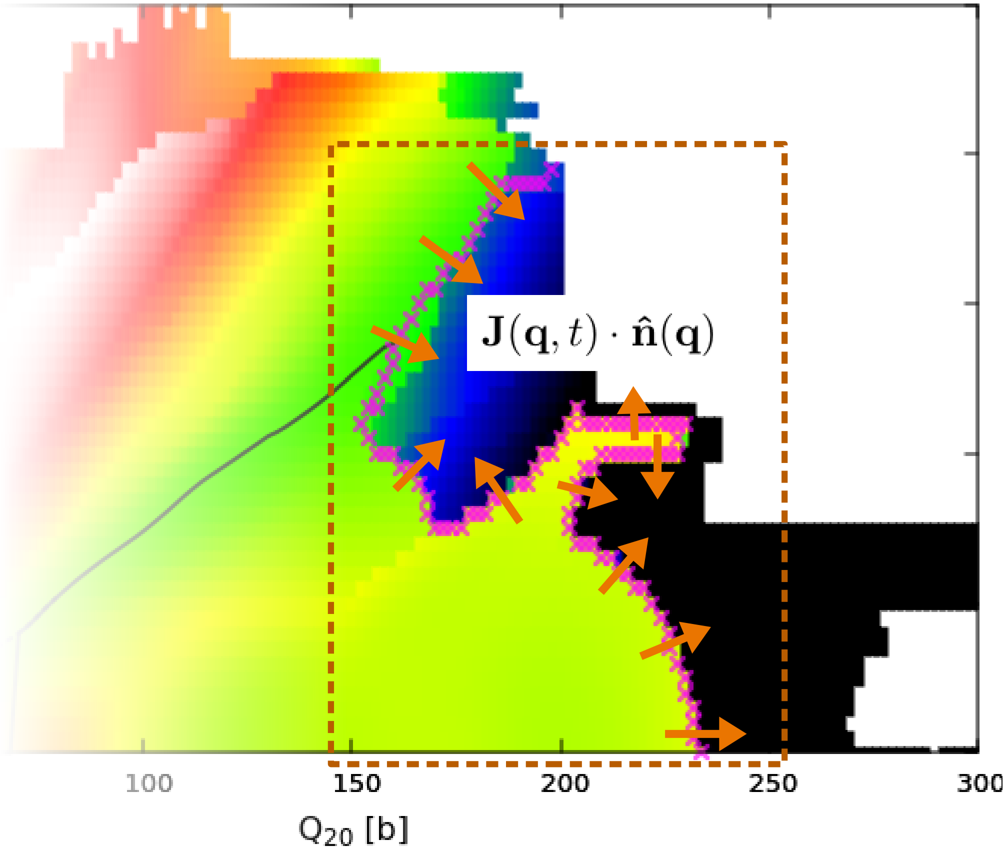


Observables at the scission line

probability flux

$$F(\mathbf{q}, T) = \int_0^T dt\, \underbrace{\mathbf{J}(\mathbf{q}, t) \cdot \hat{\mathbf{n}}(\mathbf{q})}$$

probability current



D. Regnier, M. Verrière, N. Dubray, N. Schunck,
Comp. Phys. Commun. 200 (2016) 350-363

Observables at the scission line

probability flux

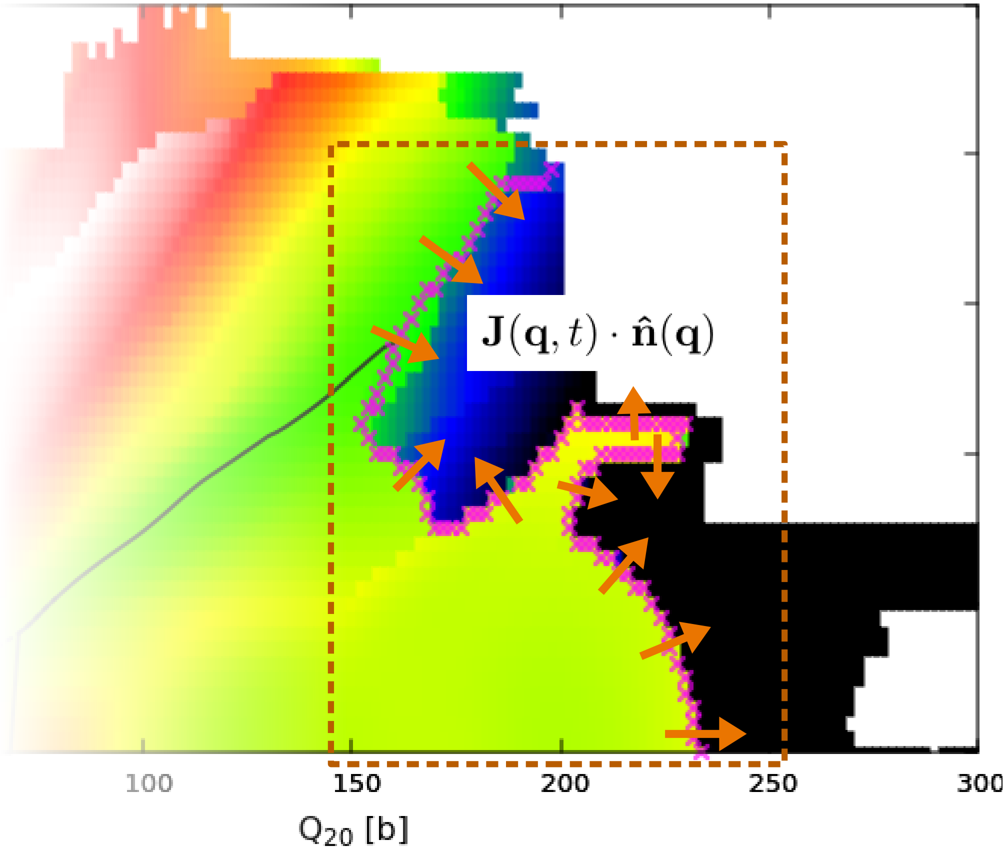
$$F(\mathbf{q}, T) = \int_0^T dt\, \mathbf{J}(\mathbf{q}, t) \cdot \hat{\mathbf{n}}(\mathbf{q})$$

probability current

probability density function

$$\frac{\partial}{\partial t}|g(\mathbf{q}, t)|^2 = -\nabla \cdot \mathbf{J}(\mathbf{q}, t)$$

local continuity equation



D. Regnier, M. Verrière, N. Dubray, N. Schunck, *Comp. Phys. Commun.* 200 (2016) 350-363

Observables at the scission line

local continuity equation

$$\frac{\partial}{\partial t}\left|g(\mathbf{q},t)\right|^2 = -\nabla \cdot \mathbf{J}(\mathbf{q},t)$$
$$= \frac{\partial g^*}{\partial t} g + g^* \frac{\partial g}{\partial t}$$

TDGCM+GOA: local CSE

$$\left[-\frac{\hbar^2}{2}\nabla \cdot B(\mathbf{q}) \cdot \nabla + V(\mathbf{q})\right] g(\mathbf{q},t) = i\hbar \frac{\partial}{\partial t} g(\mathbf{q},t)$$

$$\mathbf{J}(\mathbf{q},t) = -\frac{i\hbar}{2} B(\mathbf{q})\left[g^*(\nabla g) - g(\nabla g^*)\right]$$

probability current

D. Regnier, M. Verrière, N. Dubray, N. Schunck,
Comp. Phys. Commun. 200 (2016) 350-363

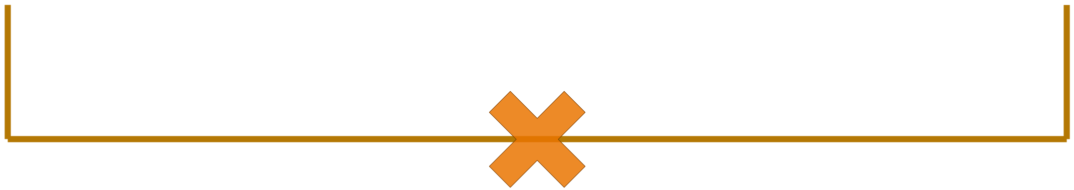
Observables at the scission line

local continuity equation

$$\frac{\partial}{\partial t}\left|g(\mathbf{q},t)\right|^2 = -\nabla \cdot \mathbf{J}(\mathbf{q},t)$$
$$= \frac{\partial g^*}{\partial t} g + g^* \frac{\partial g}{\partial t}$$

exact TDGCM: nonlocal CSE

$$\sum_{k'} \tilde{\mathcal{H}}_{kk'} g_{k'}(t) = i\hbar \frac{\partial g_k}{\partial t}$$



Symmetric Moment Expansion (SME)

1) Define a new orthonormal basis with “spatial” coordinates

2) Rederive a nonlocal CSE

3) Use expansion techniques to produce a local CSE

Symmetric Moment Expansion (SME)

1) Define a new orthonormal basis with “spatial” coordinates
2) Rederive a nonlocal CSE
3) Use expansion techniques to produce a local CSE

eigenvalues (positive real)

eigenvectors

$$N^{\pm 1/2}(q, q') = \sum_k u_k(q) n_k^{\pm 1/2} u_k^*(q')$$

$$|q\rangle = \int dp \, N^{-1/2}(p, q) \big|\Phi(p)\big\rangle, \; \big\langle q \big| q' \big\rangle = \delta(q - q')$$

“SME” basis of orthonormal states

R. Bernard, H. Goutte, D. Gogny, W. Younes, *Phys. Rev. C* **84**, 044308 (2011)
P. Ring, P. Schuck, *The Nuclear Many-Body Problem (Ch. 10.7.2),* Springer, Berlin (2004)

Symmetric Moment Expansion (SME)

1) Define a new orthonormal basis with “spatial” coordinates

2) Rederive a nonlocal CSE

3) Use expansion techniques to produce a local CSE

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

SME basis transformation

Nonlocal CSE (SME basis)

$$\int dq' \; \underbrace{H_C(q,q')}_{\text{nonlocal collective Hamiltonian}} G(q',t) = i\hbar \frac{d}{dt} G(q,t)$$

nonlocal collective Hamiltonian

Symmetric Moment Expansion (SME)

1) Define a new orthonormal basis with "spatial" coordinates

2) Rederive a nonlocal CSE

3) Use expansion techniques to produce a local CSE

$$\bar{q} = \frac{1}{2}(q + q')$$

$$s = q - q'$$

change to central coordinates

$$G(\bar{q} \pm \tfrac{s}{2}, t) = e^{\pm is\hat{P}/2\hbar} G(\bar{q}, t), \;\; \hat{P} = -i\hbar\nabla$$

Taylor expansion of weight function around s = 0

Symmetric Moment Expansion (SME)

1) Define a new orthonormal basis with "spatial" coordinates

2) Rederive a nonlocal CSE

3) Use expansion techniques to produce a local CSE

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

SME basis transformation
change of coordinates
Taylor expansion

$$\int ds\ e^{-is\hat{P}/2\hbar} H_C(\bar{q} + \tfrac{s}{2}, \bar{q} - \tfrac{s}{2}) e^{-is\hat{P}/2\hbar}\ G(\bar{q}, t) = i\hbar \frac{d}{dt} G(\bar{q}, t)$$

symmetrised Hill-Wheeler equation

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

$$\int ds\ e^{-is\hat{P}/2\hbar} H_C(\bar{q} + \tfrac{s}{2}, \bar{q} - \tfrac{s}{2}) e^{-is\hat{P}/2\hbar}\, G(\bar{q}, t) = i\hbar \frac{d}{dt} G(\bar{q}, t)$$

$$\hat{H}_C(\bar{q}) = \text{?}$$

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

$$\int ds\ e^{-is\hat{P}/2\hbar} H_C(\bar{q} + \tfrac{s}{2}, \bar{q} - \tfrac{s}{2}) e^{-is\hat{P}/2\hbar}\, G(\bar{q}, t) = i\hbar \frac{d}{dt} G(\bar{q}, t)$$

$$\hat{H}_C(\bar{q}) = \ ?$$

$$h_C^{(n)}(\bar{q}) = \left(-\frac{i}{\hbar}\right)^n \int ds\ s^n H_C(\bar{q} + \tfrac{s}{2}, \bar{q} - \tfrac{s}{2})$$

moments of the collective Hamiltonian

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

$$\int ds\; e^{-is\hat{P}/2\hbar} H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2}) e^{-is\hat{P}/2\hbar} G(\bar{q},t) = i\hbar \frac{d}{dt} G(\bar{q},t)$$

$$\hat{H}_C(\bar{q}) = \text{?}$$

$$h_C^{(n)}(\bar{q}) = \left(-\frac{i}{\hbar}\right)^n \int ds\; s^n H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2})$$

moments of the collective Hamiltonian

$$[A\,\hat{P}]^{(n)} = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\hat{P}^k A \hat{P}^{n-k}$$

symmetric ordered product of operators (SOPO)

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

$$\int ds\ e^{-is\hat{P}/2\hbar} H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2}) e^{-is\hat{P}/2\hbar}\, G(\bar{q},t) = i\hbar \frac{d}{dt} G(\bar{q},t)$$

$$\hat{H}_C(\bar{q}) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[h_C^{(n)}(\bar{q})\,\hat{P}\right]^{(n)}$$

local collective Hamiltonian

$$h_C^{(n)}(\bar{q}) = \left(-\frac{i}{\hbar}\right)^n \int ds\ s^n H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2})$$

moments of the collective Hamiltonian

$$\left[A\,\hat{P}\right]^{(n)} = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} \hat{P}^k A \hat{P}^{n-k}$$

symmetric ordered product of operators (SOPO)

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

$$\int ds\; e^{-is\hat{P}/2\hbar} H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2}) e^{-is\hat{P}/2\hbar}\; G(\bar{q},t) = i\hbar\frac{d}{dt}G(\bar{q},t)$$

$$\hat{H}_C(\bar{q}) = \sum_{n=0}^{\infty}\frac{1}{n!}\left[h_C^{(n)}(\bar{q})\,\hat{P}\right]^{(n)}$$

local collective Hamiltonian

$$\hat{H}_C(\bar{q})G(\bar{q},t) = i\hbar\frac{d}{dt}G(\bar{q},t)$$

local collective Schrödinger equation

still exact!
(when summed to infinite order)

Symmetric Moment Expansion (SME)

local continuity equation

$$\frac{d}{dt}\left|G(\bar{q},t)\right|^2 = -\nabla J(\bar{q},t)$$

SME: local CSE

$$\hat{H}_C(\bar{q})G(\bar{q},t) = i\hbar\frac{d}{dt}G(\bar{q},t)$$

$$J(\bar{q},t) = \frac{i\hbar}{2}\Big(G(\bar{q},t)h_C^{(2)}(\bar{q})\nabla G^*(\bar{q},t) - G^*(\bar{q},t)h_C^{(2)}(\bar{q})\nabla G(\bar{q},t)\Big)$$

probability current

The finite element basis

to continuously interpolate a function with a discrete domain

$$J(\bar{q},t) = \frac{i\hbar}{2}\Big(G(\bar{q},t)h_C^{(2)}(\bar{q})\nabla G^*(\bar{q},t) - G^*(\bar{q},t)h_C^{(2)}(\bar{q})\nabla G(\bar{q},t)\Big)$$

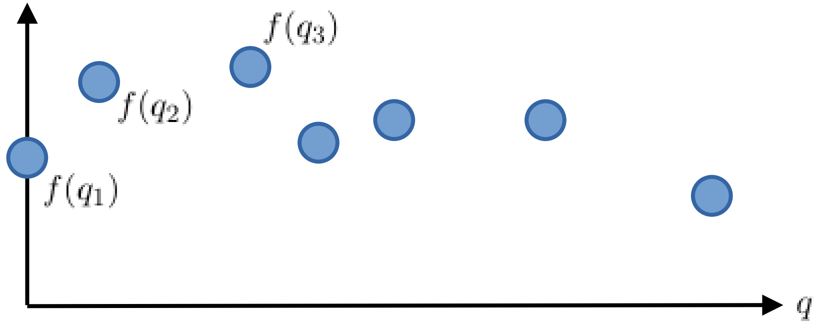
$$-\frac{8\Delta s}{\hbar^2}\sum_{n=0}^{\infty}(n\Delta s)^2 H_C(\bar{q}+n\Delta s, \bar{q}-n\Delta s)$$

$$\frac{G(\bar{q}+\Delta s,t) - G(\bar{q}-\Delta s,t)}{2\Delta s}$$

require a regular mesh of points Δs in the SME coordinate space $\bar{q}$

The finite element basis

to continuously interpolate a function with a discrete domain

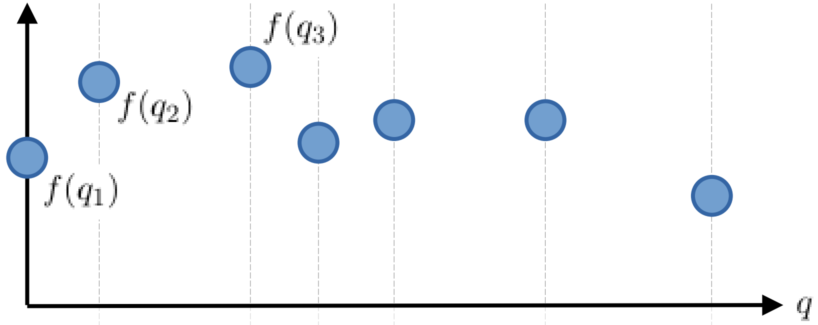


function with discrete domain

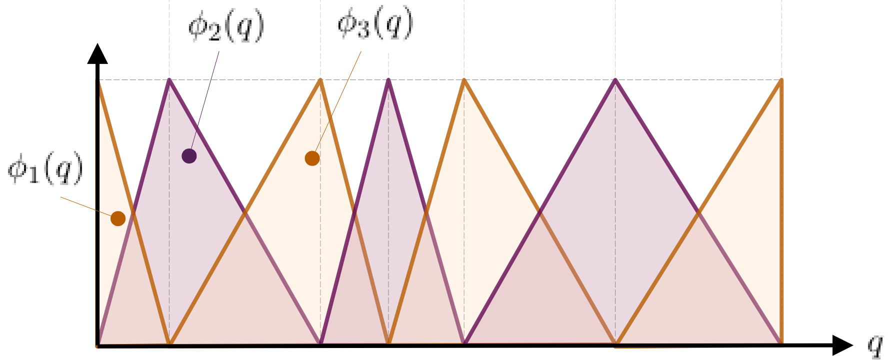
D. Axelsson, V. A. Barker, *Finite Element Solution of Boundary Value Problems (Ch. 5),* Academic Press, Inc. (1984)

The finite element basis

to continuously interpolate a function with a discrete domain



function with discrete domain

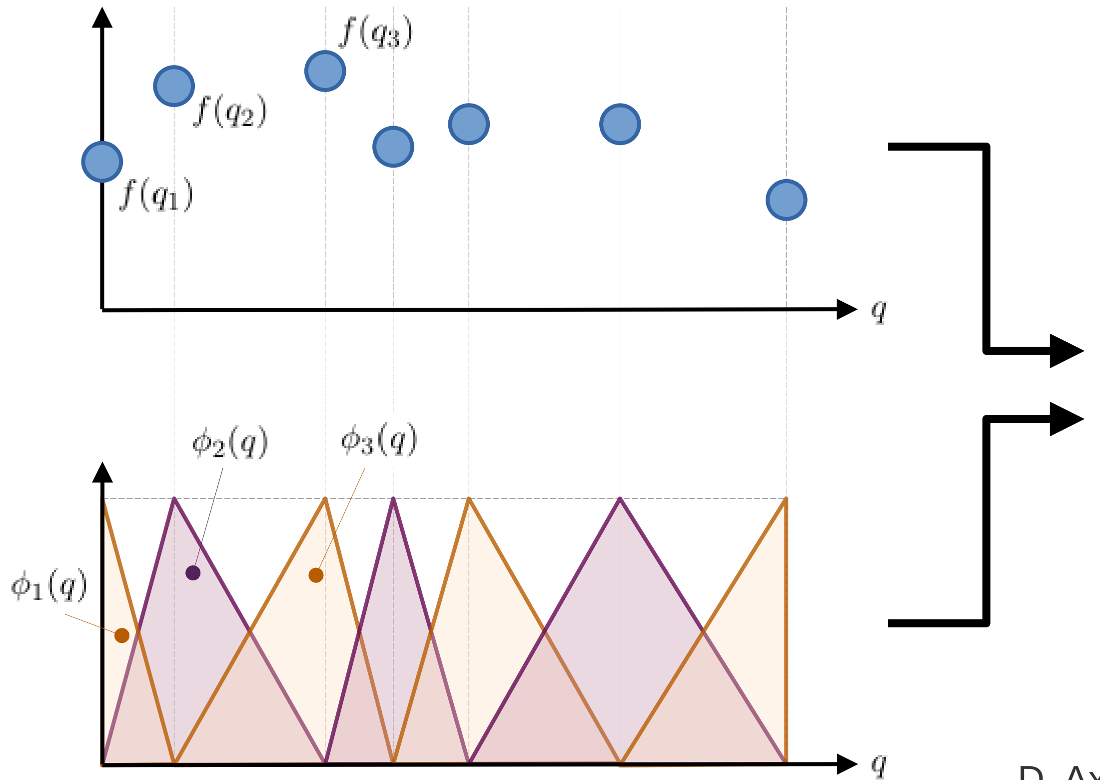


finite element basis functions
(interpolating polynomials)

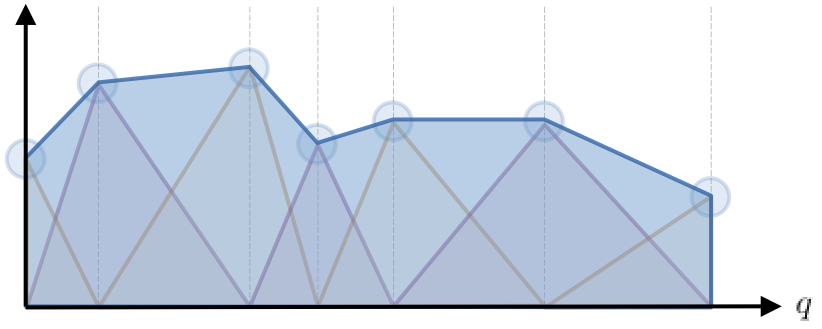
D. Axelsson, V. A. Barker, *Finite Element Solution of Boundary Value Problems (Ch. 5),* Academic Press, Inc. (1984)

The finite element basis

to continuously interpolate a function with a discrete domain



$$f_I(q) = \sum_i f(q_i)\phi_i(q)$$

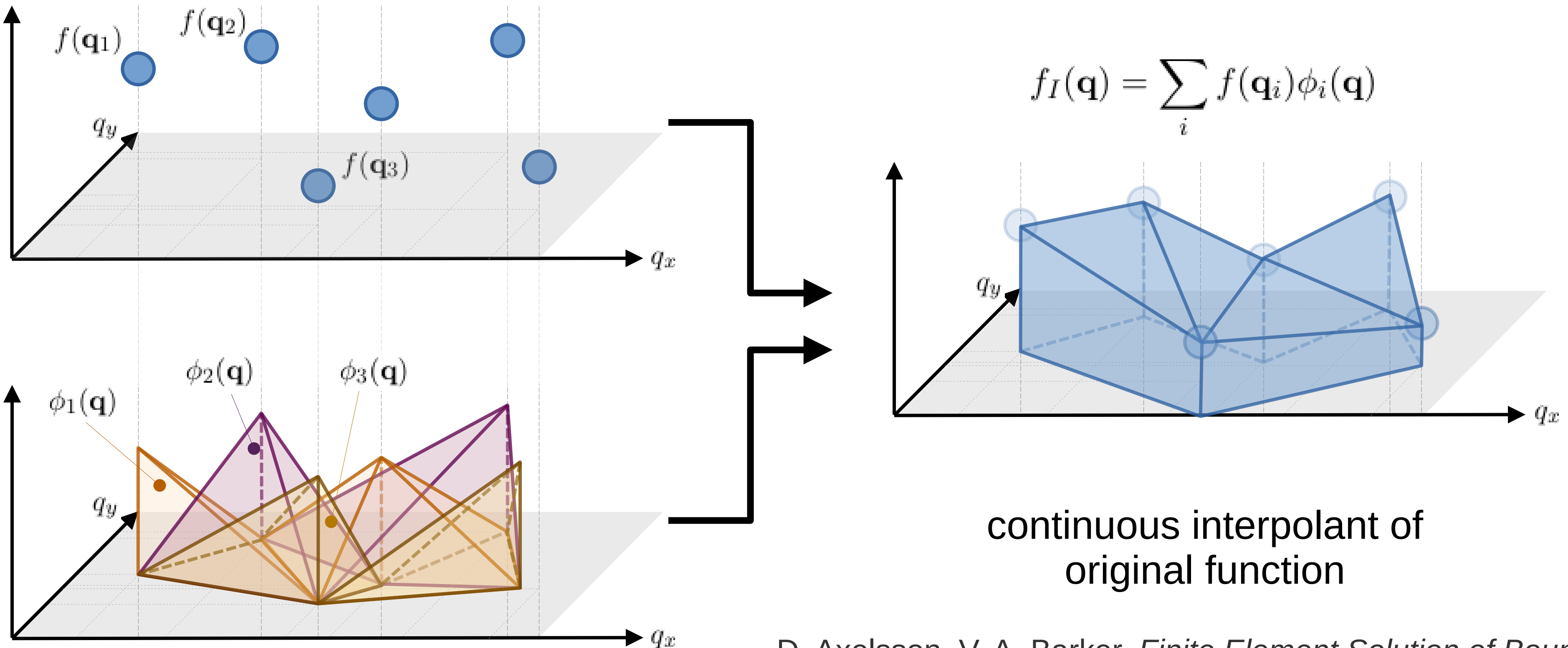


continuous interpolant of original function

D. Axelsson, V. A. Barker, *Finite Element Solution of Boundary Value Problems (Ch. 5),* Academic Press, Inc. (1984)

The finite element basis

to continuously interpolate a function with a discrete domain



continuous interpolant of original function

D. Axelsson, V. A. Barker, *Finite Element Solution of Boundary Value Problems (Ch. 5),* Academic Press, Inc. (1984)

The finite element basis

to continuously interpolate a function with a discrete domain

$$G_I(\bar{\mathbf{q}}, t) = \sum_{k=1}^{K} G(\bar{\mathbf{q}}_k, t)\phi_k(\bar{\mathbf{q}})$$

interpolant of the weight function

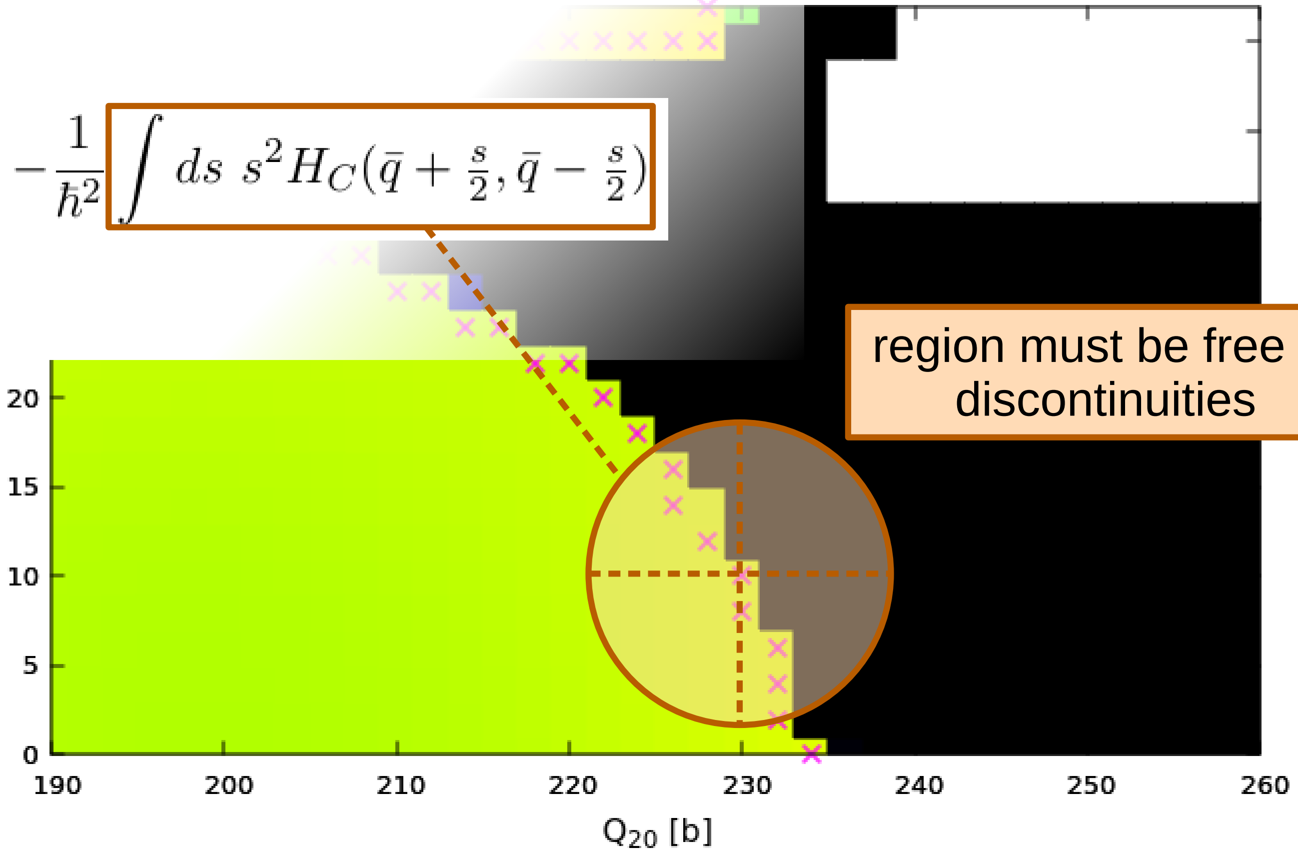
$$H_{C,I}(\bar{\mathbf{q}}, \bar{\mathbf{q}}') = \sum_{k=1}^{K} \sum_{k'=1}^{K} \phi_k(\bar{\mathbf{q}}) H_C(\bar{\mathbf{q}}_k, \bar{\mathbf{q}}_{k'}) \phi_{k'}(\bar{\mathbf{q}}')$$

interpolant of the nonlocal collective Hamiltonian

(error estimation or reformulation needed!)

Practicalities of flux calculations

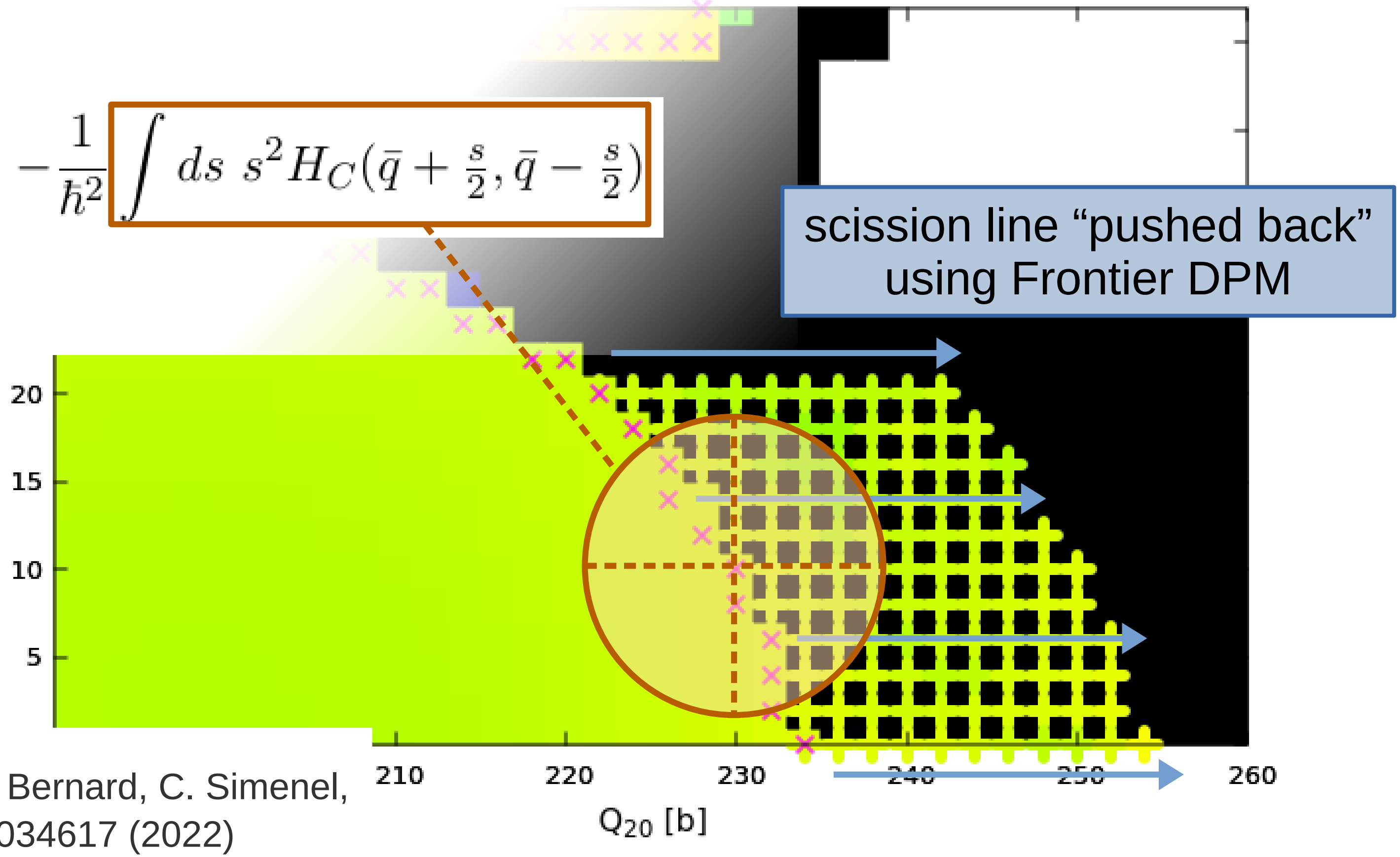
$$h_C^{(2)}(\bar{q}) = -\frac{1}{\hbar^2}\int ds\; s^2 H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2})$$



region must be free of discontinuities

Practicalities of flux calculations

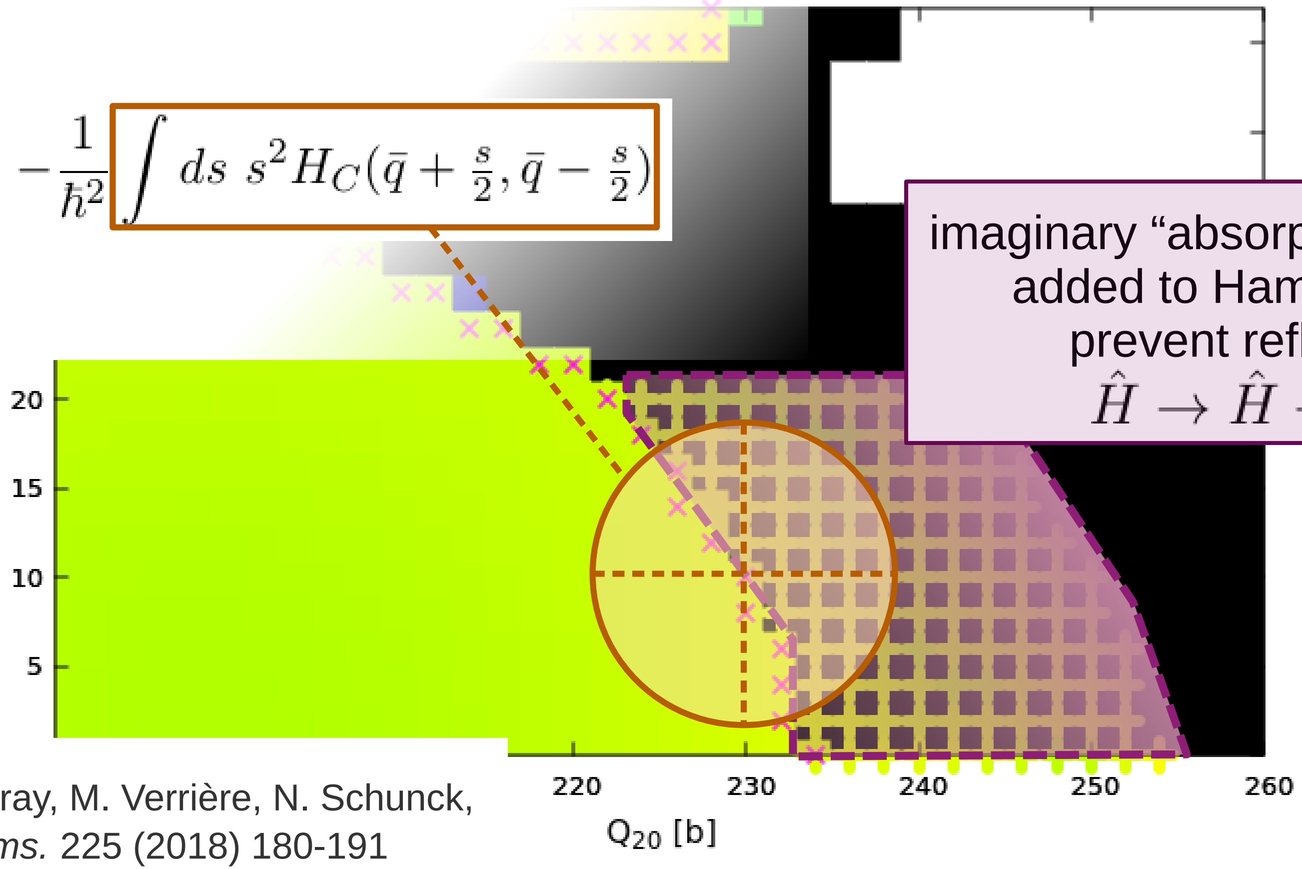
$$h_C^{(2)}(\bar{q}) = -\frac{1}{\hbar^2}\int ds\ s^2 H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2})$$



N.-W. T. Lau, R. N. Bernard, C. Simenel, *Phys. Rev. C* **105**, 034617 (2022)

Practicalities of flux calculations

$$h_C^{(2)}(\bar{q}) = -\frac{1}{\hbar^2}\int ds\; s^2 H_C(\bar{q}+\tfrac{s}{2},\bar{q}-\tfrac{s}{2})$$

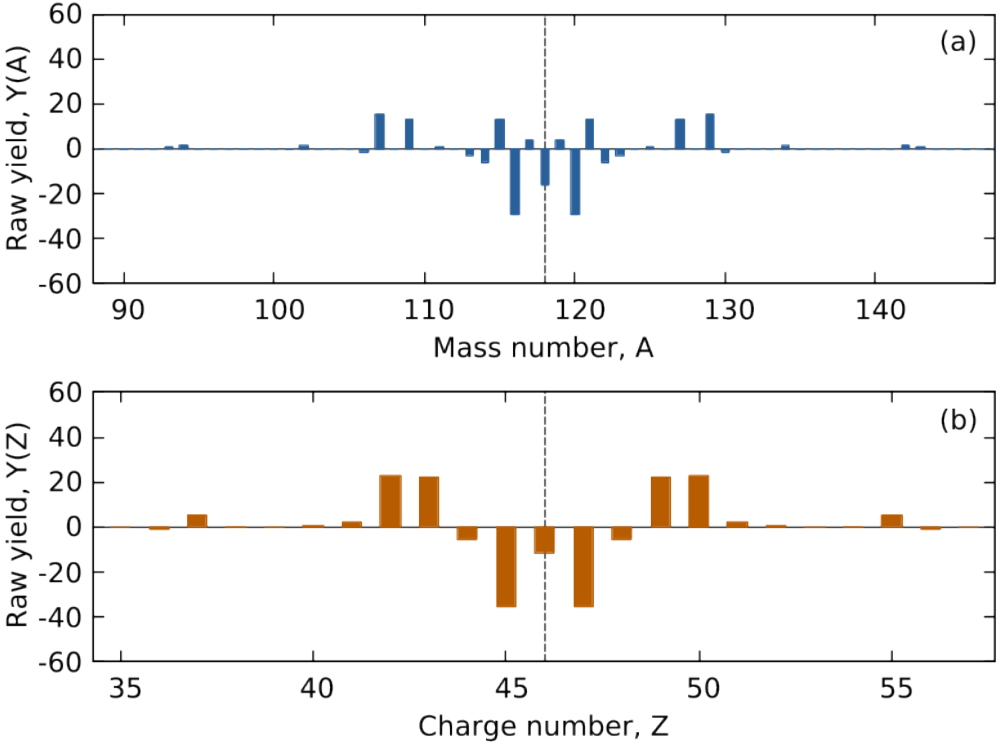


imaginary “absorption potential” added to Hamiltonian to prevent reflections

$$\hat{H} \rightarrow \hat{H} - i\hbar A$$

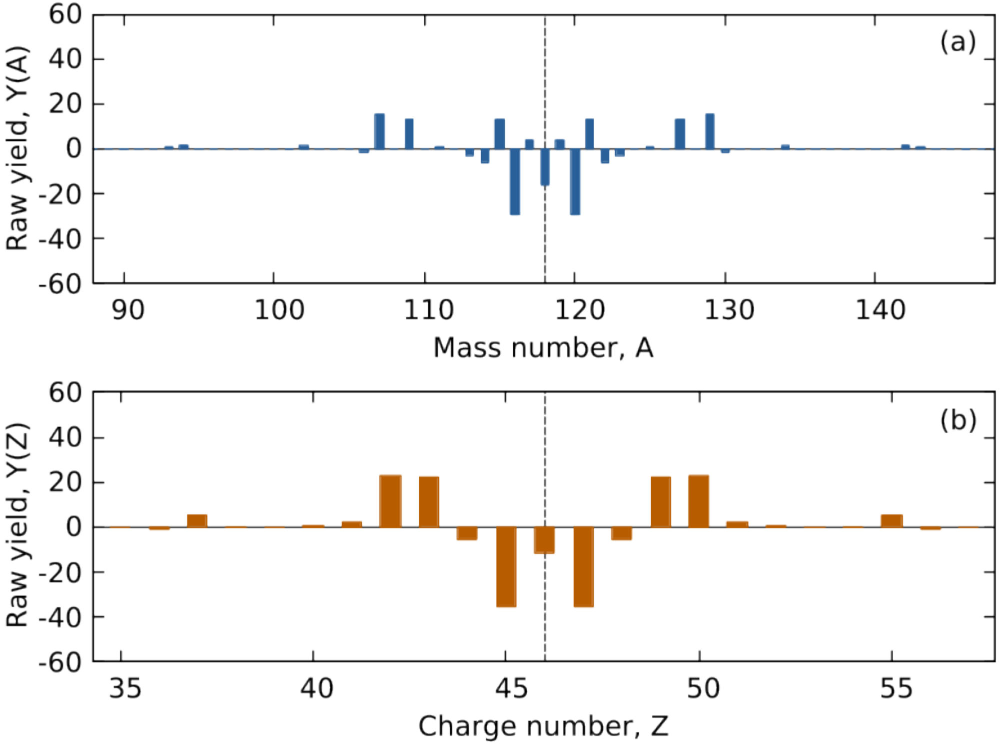
D. Regnier, N. Dubray, M. Verrière, N. Schunck, *Comp. Phys. Comms.* 225 (2018) 180-191

2D fission outcomes – ^{236}U

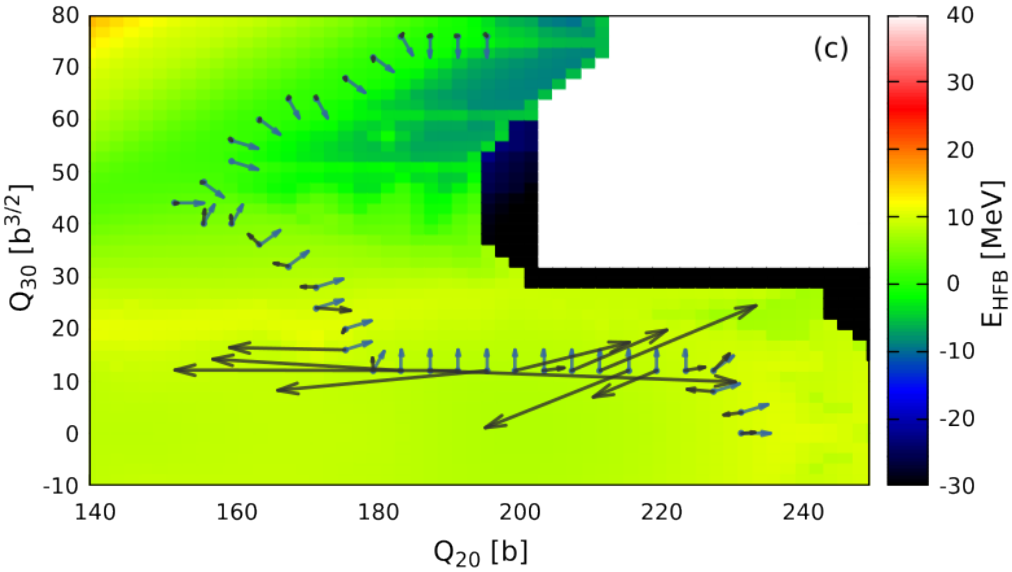


no absorption field

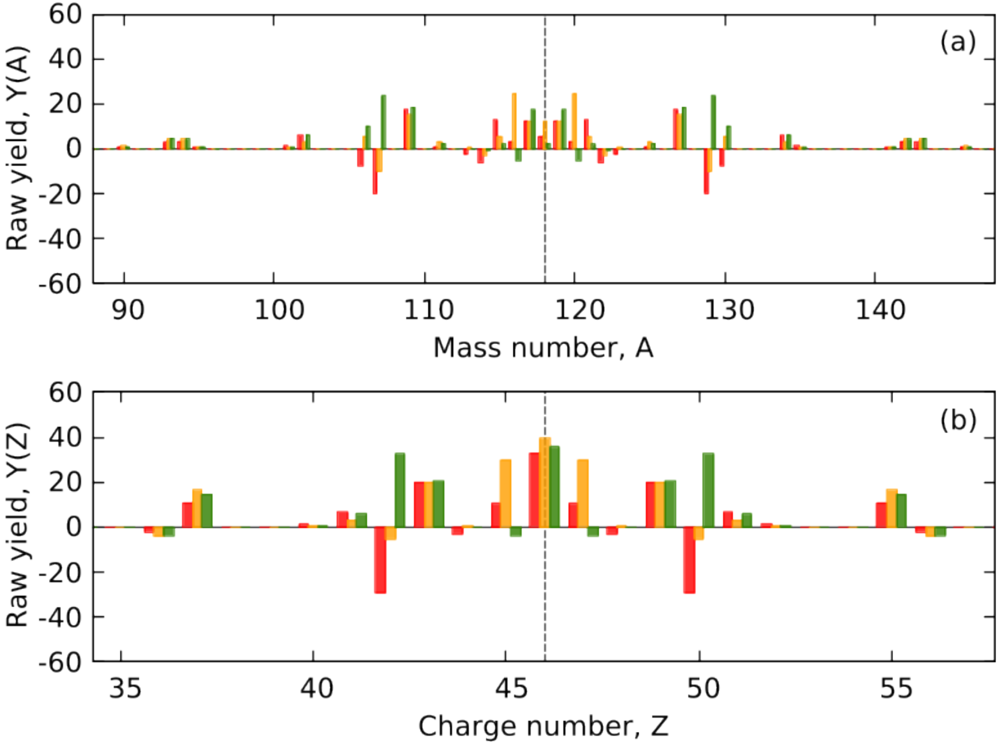
2D fission outcomes – ^{236}U



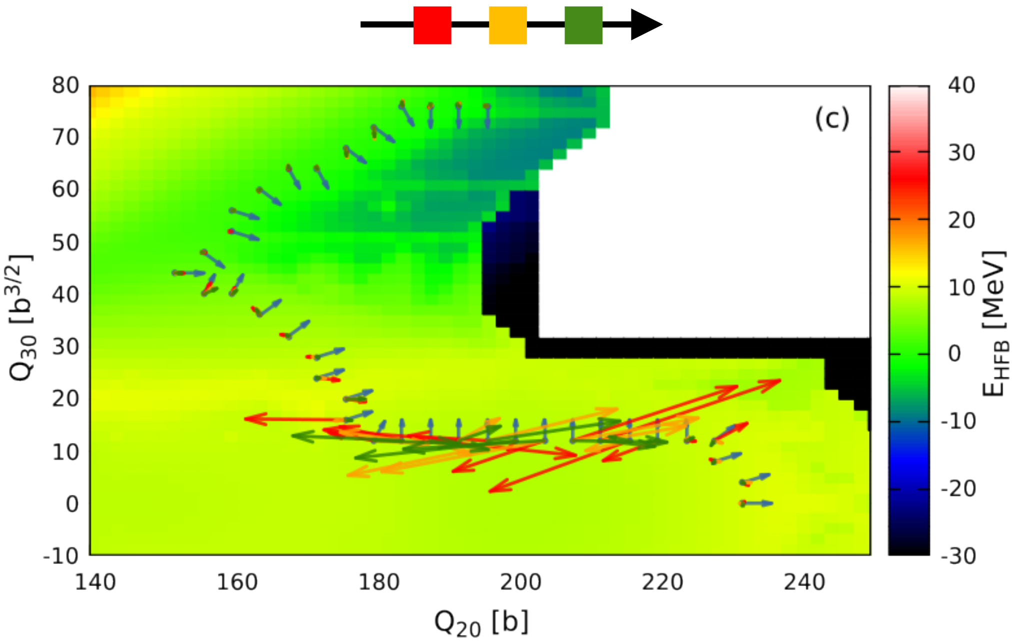
no absorption field



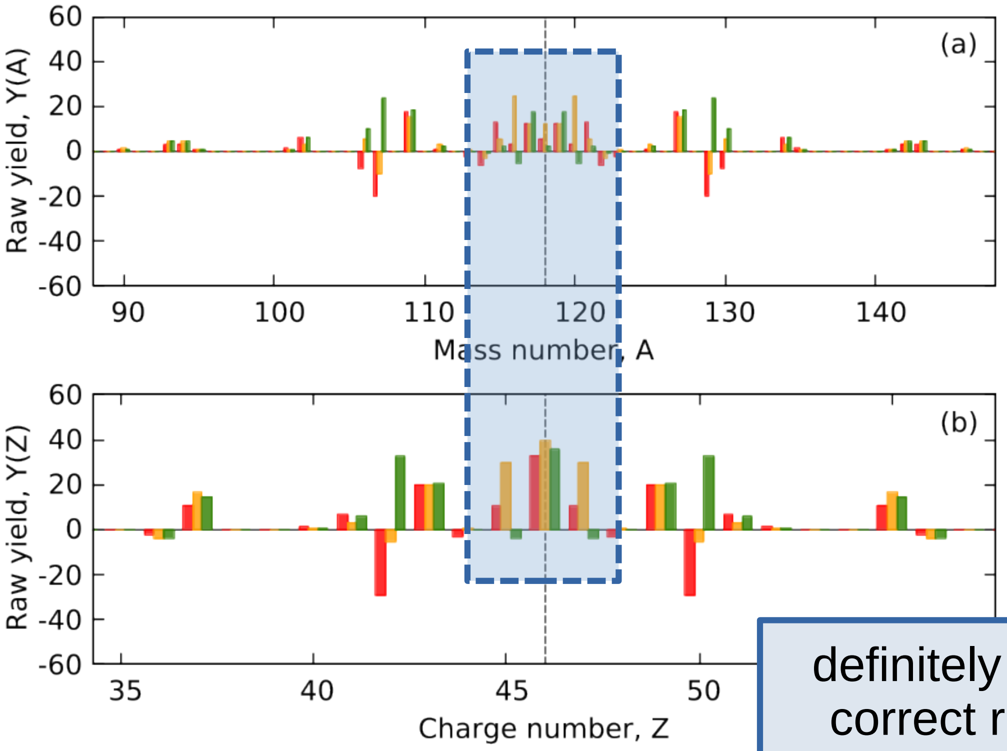
2D fission outcomes – ^{236}U



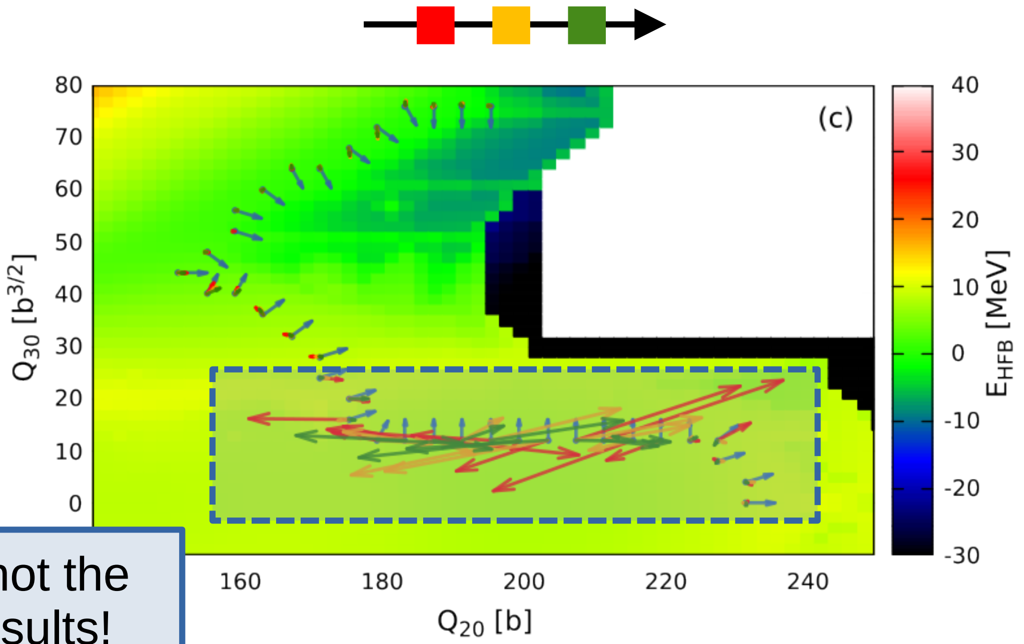
increasing absorption strength



2D fission outcomes – ^{236}U



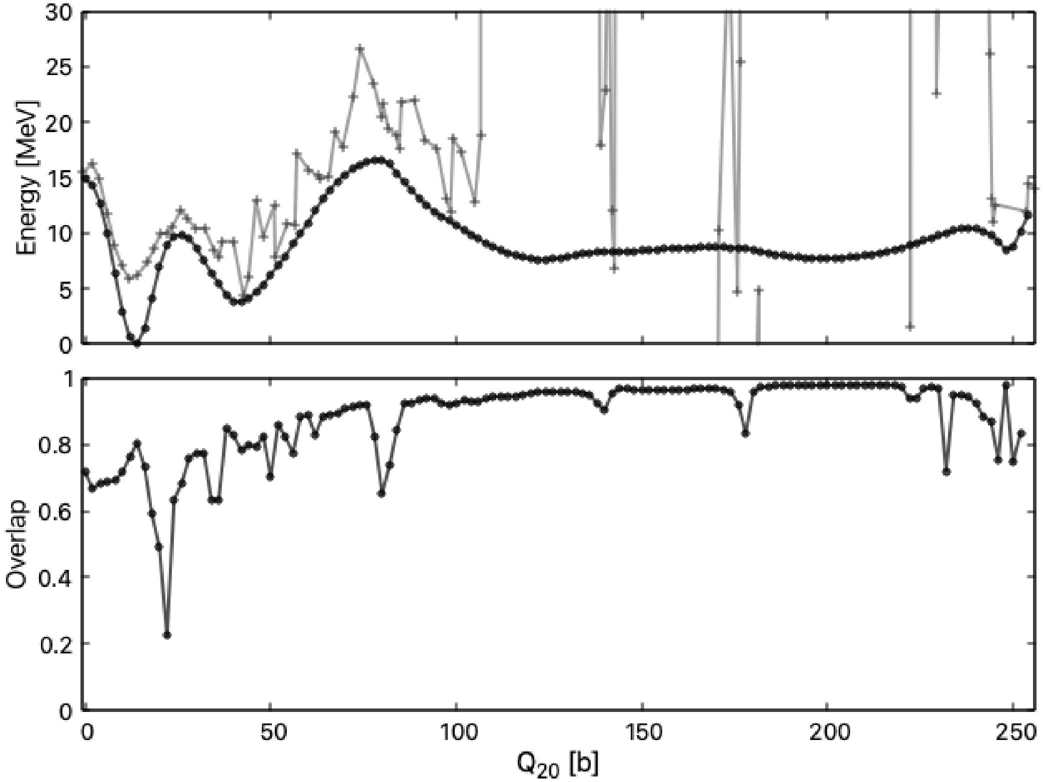
increasing absorption strength



definitely not the correct results!

What now?

Testing behaviour with Gaussian overlaps



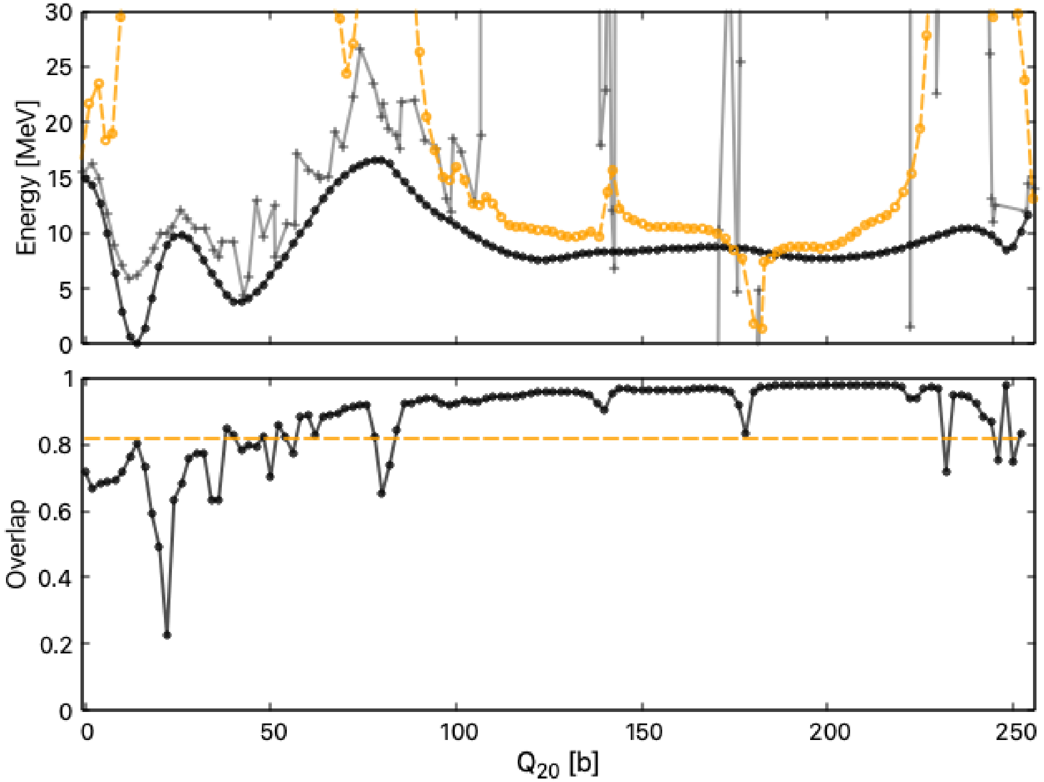
Original PES

SME states:

Full HFB basis
(original overlaps)

What now?

Testing behaviour with Gaussian overlaps



$$\mathcal{N}(q,q') \approx \exp\left(-\frac{(q-q')^2}{2\sigma^2}\right)$$

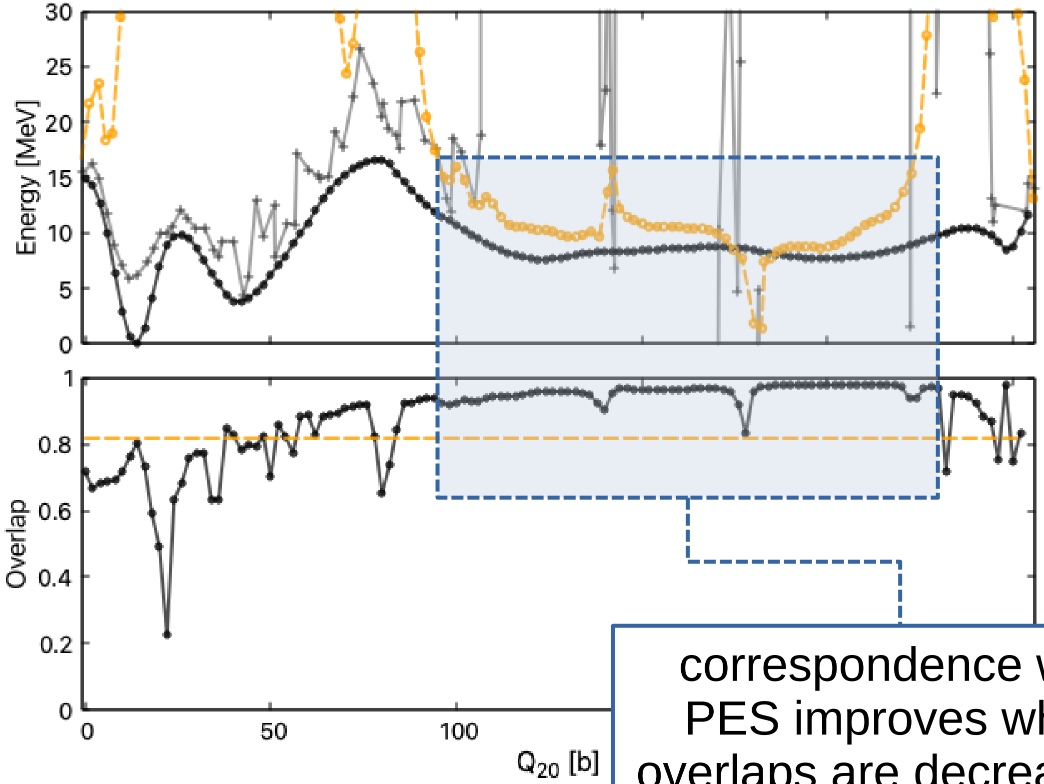
- Original PES

SME states:

- Full HFB basis (original overlaps)
- GOA overlaps with width $2\sigma^2 = 20$

What now?

Testing behaviour with Gaussian overlaps



correspondence with PES improves when overlaps are decreased?

$$\mathcal{N}(q,q') \approx \exp\left(-\frac{(q-q')^2}{2\sigma^2}\right)$$

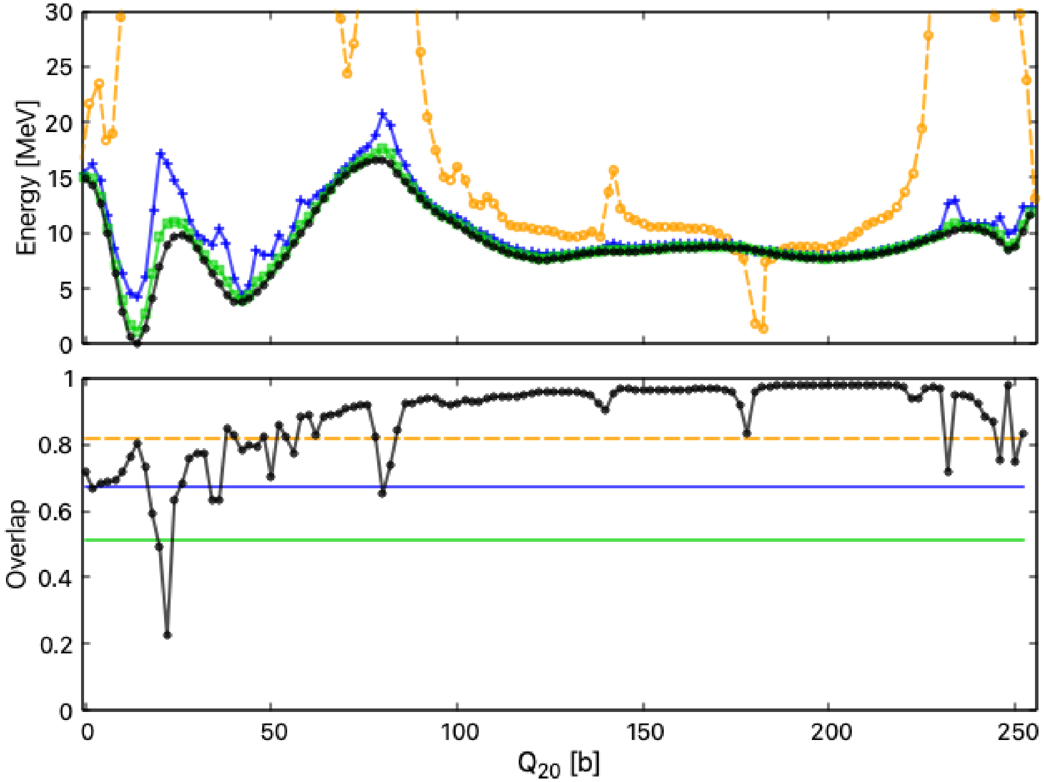
- Original PES

SME states:

- Full HFB basis (original overlaps)
- GOA overlaps with width $2\sigma^2 = 20$

What now?

Testing behaviour with Gaussian overlaps



$$\mathcal{N}(q,q') \approx \exp\left(-\frac{(q-q')^2}{2\sigma^2}\right)$$

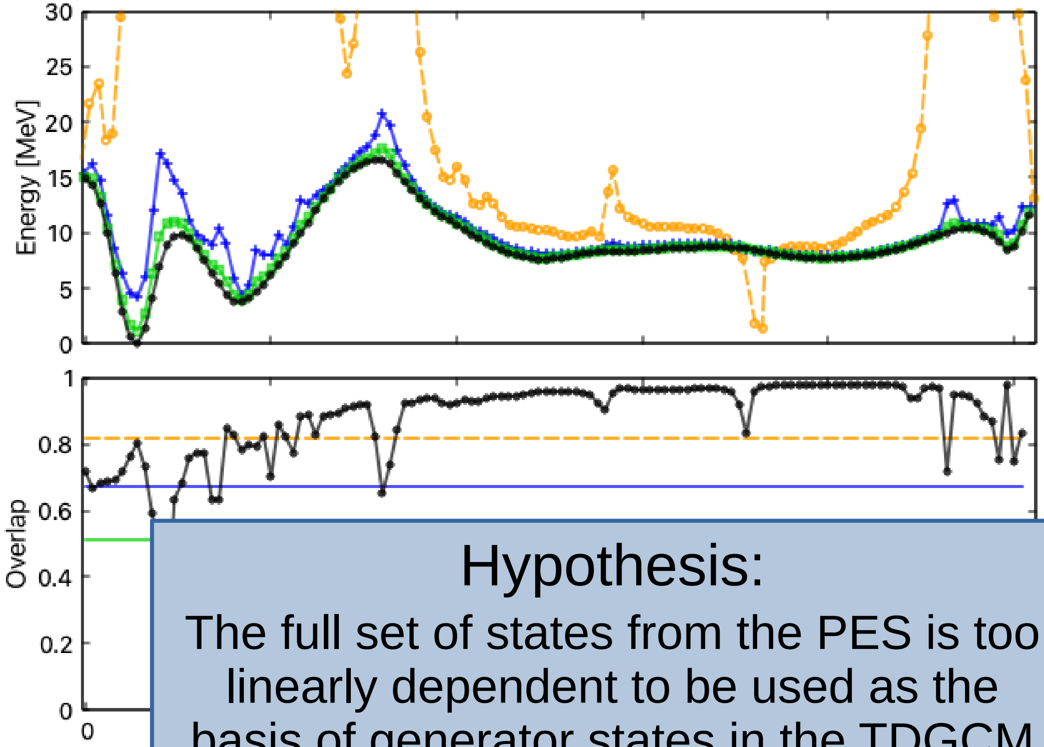
- Original PES

SME states:

- GOA overlaps with width $2\sigma^2 = 20$
- GOA overlaps with width $2\sigma^2 = 10$
- GOA overlaps with width $2\sigma^2 = 6$

What now?

Testing behaviour with Gaussian overlaps



$$\mathcal{N}(q,q') \approx \exp\left(-\frac{(q-q')^2}{2\sigma^2}\right)$$

■ Original PES

SME states:

■ GOA overlaps with width $2\sigma^2 = 20$

■ GOA overlaps with width $2\sigma^2 = 10$

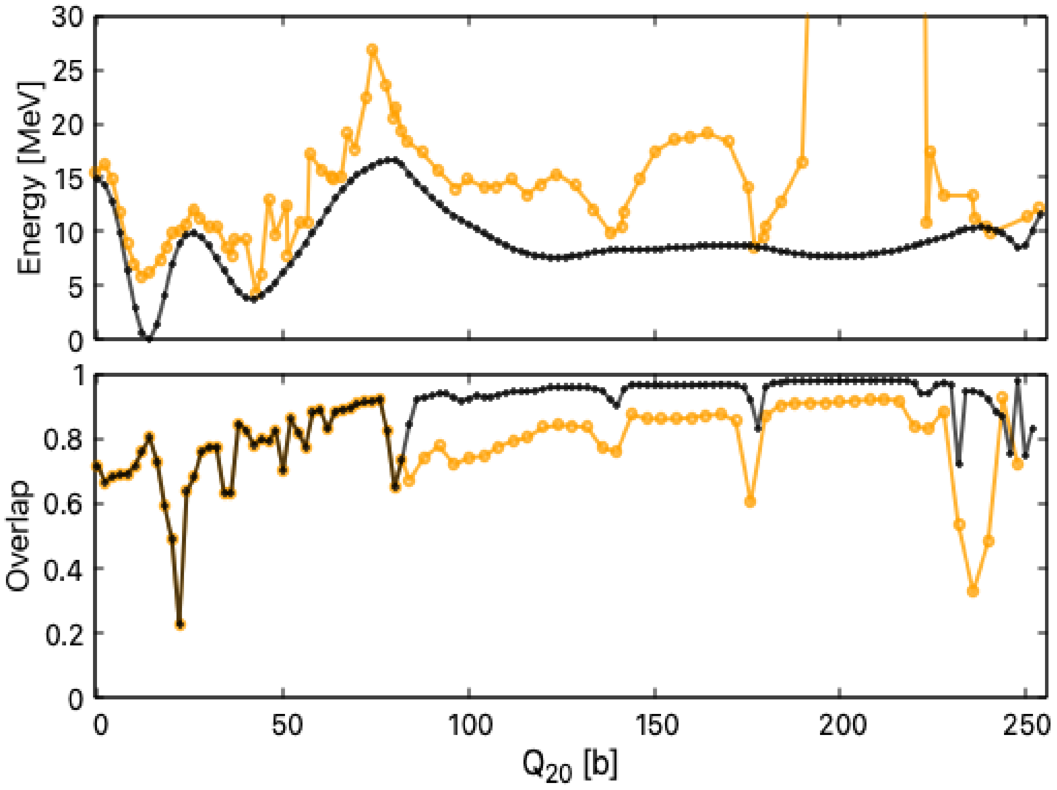
■ GOA overlaps with width $2\sigma^2 = 6$

Hypothesis:

The full set of states from the PES is too linearly dependent to be used as the basis of generator states in the TDGCM

Effects of reducing basis size

1D symmetric fission path of ^{236}U



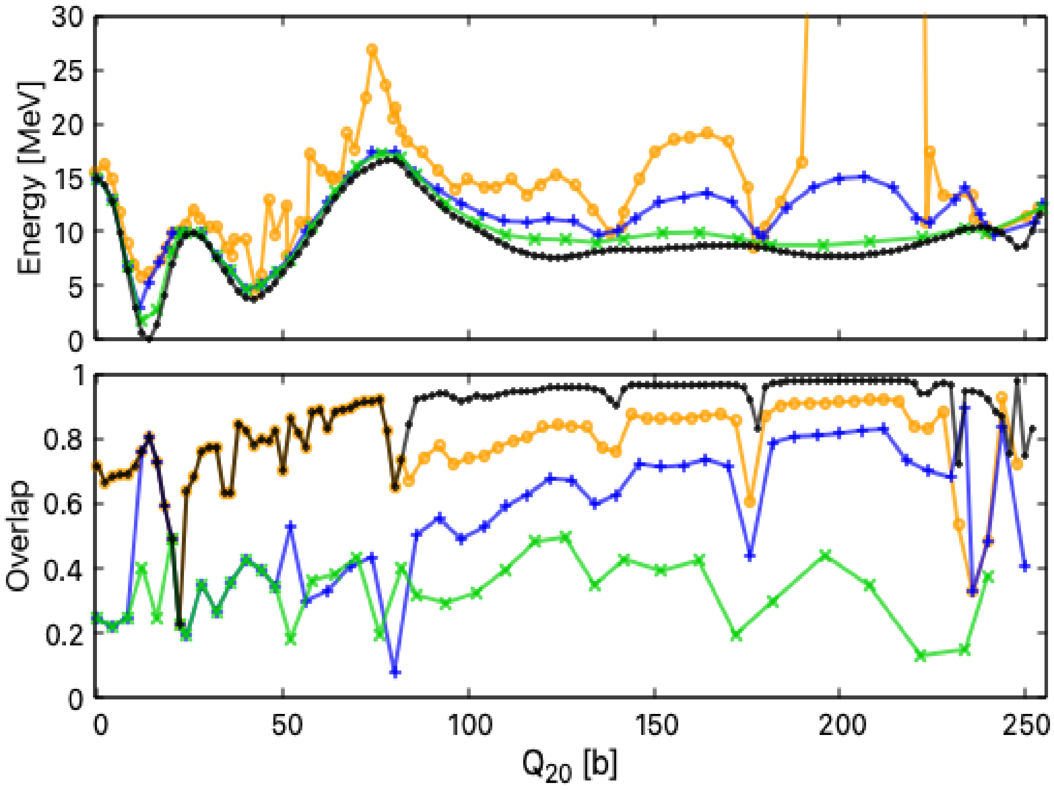
■ Original PES in HFB basis (128 states)

SME states:

■ Doubled mesh after saddle "1s2s" (85 states)

Effects of reducing basis size

1D symmetric fission path of ^{236}U



- Original PES in HFB basis (128 states)

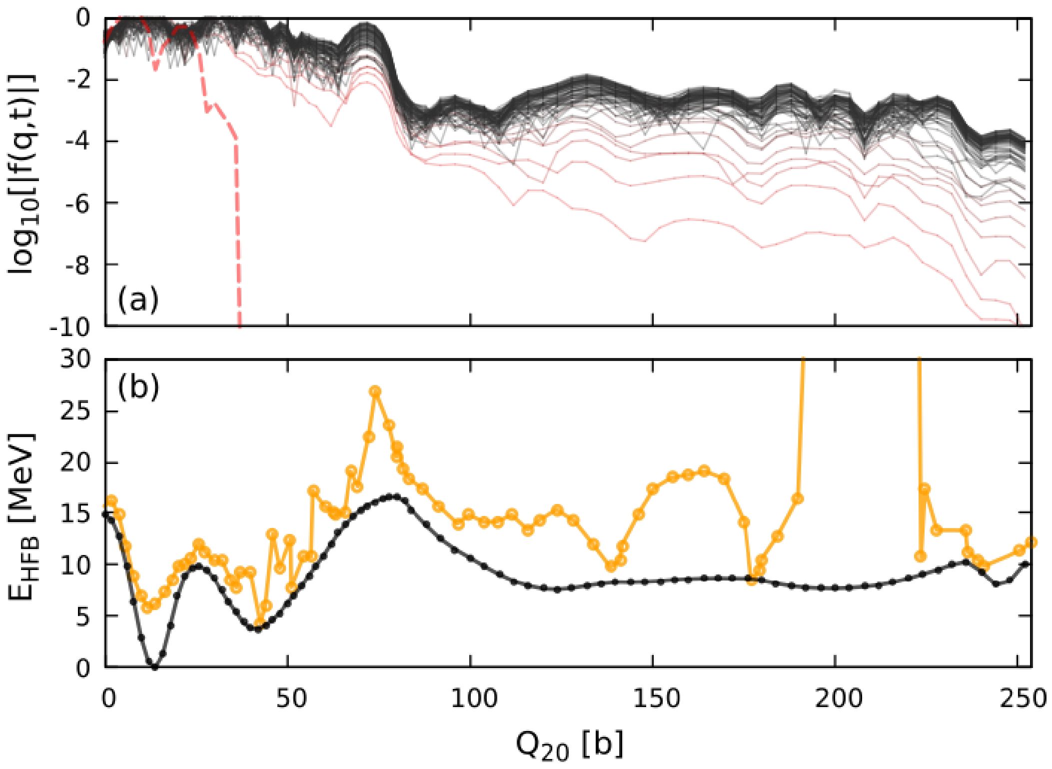
SME states:

- Doubled mesh after saddle "1s2s" (85 states)
- Manually selected mesh (53 states)
- Manually selected mesh (38 states)

Effects of reducing basis size

1D symmetric fission path of ^{236}U

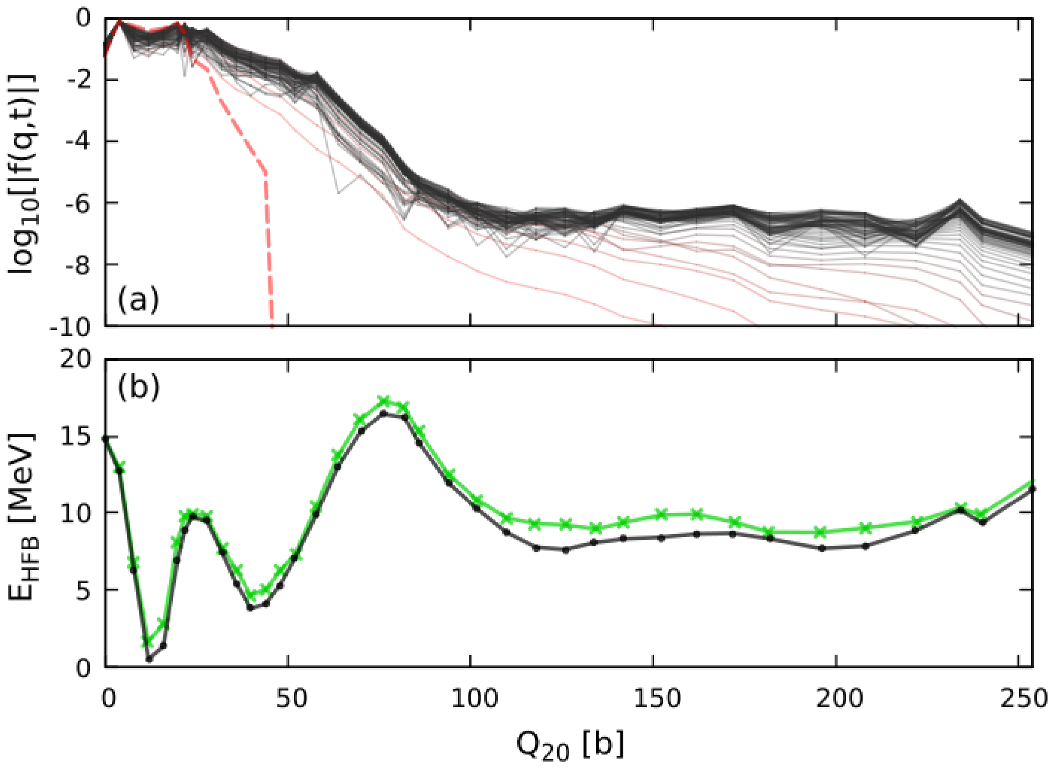
Doubled mesh after saddle
“1s2s” (85 states)



Effects of reducing basis size

1D symmetric fission path of ^{236}U

Manually selected mesh
(38 states)



What have we learned?

A significantly smaller set of HFB basis states with low overlaps leads to a much better representation in the SME basis, producing more realistic nuclear dynamics in one dimension.

What have we learned?

A significantly smaller set of HFB basis states with low overlaps leads to a much better representation in the SME basis, producing more realistic nuclear dynamics in one dimension.

- Manual selection only useful as a proof of concept
- Requires a method to produce a fission path (1D PES) with uniform, low overlaps between adjacent points*

*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Physical Review Letters* **133**, 152501 (2024)

What have we learned?

A significantly smaller set of HFB basis states with low overlaps leads to a much better representation in the SME basis, producing more realistic nuclear dynamics in one dimension.

- Manual selection only useful as a proof of concept
- Requires a method to produce a fission path (1D PES) with uniform, low overlaps between adjacent points*

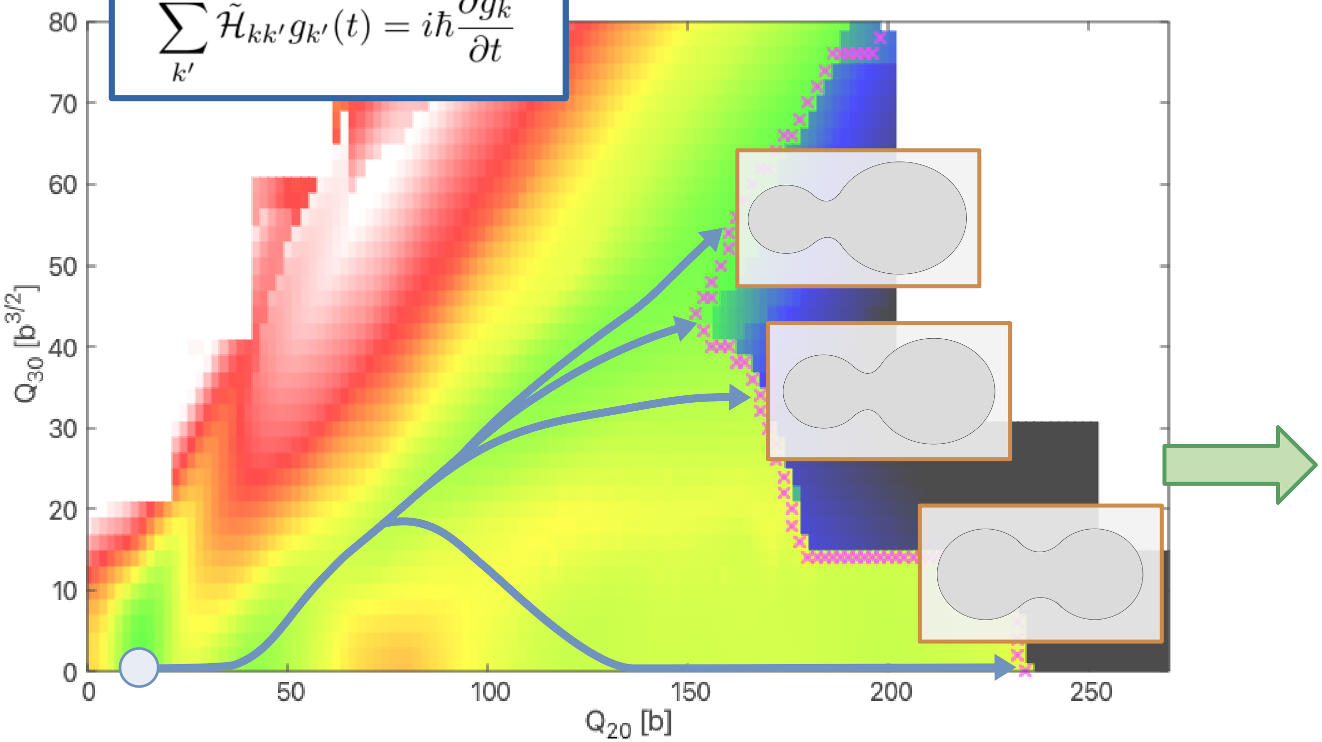
- How can this process be generalised to two dimensions?

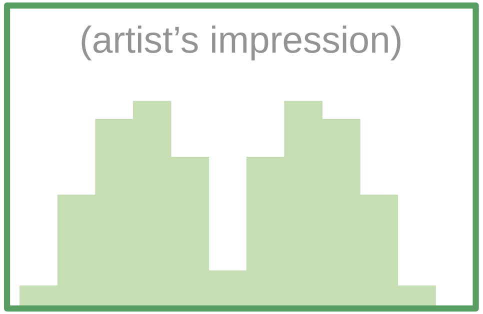
*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Physical Review Letters* **133**, 152501 (2024)

Summary

dynamics from exact TDGCM formalism

$$\sum_{k'} \tilde{\mathcal{H}}_{kk'} g_{k'}(t) = i\hbar \frac{\partial g_k}{\partial t}$$





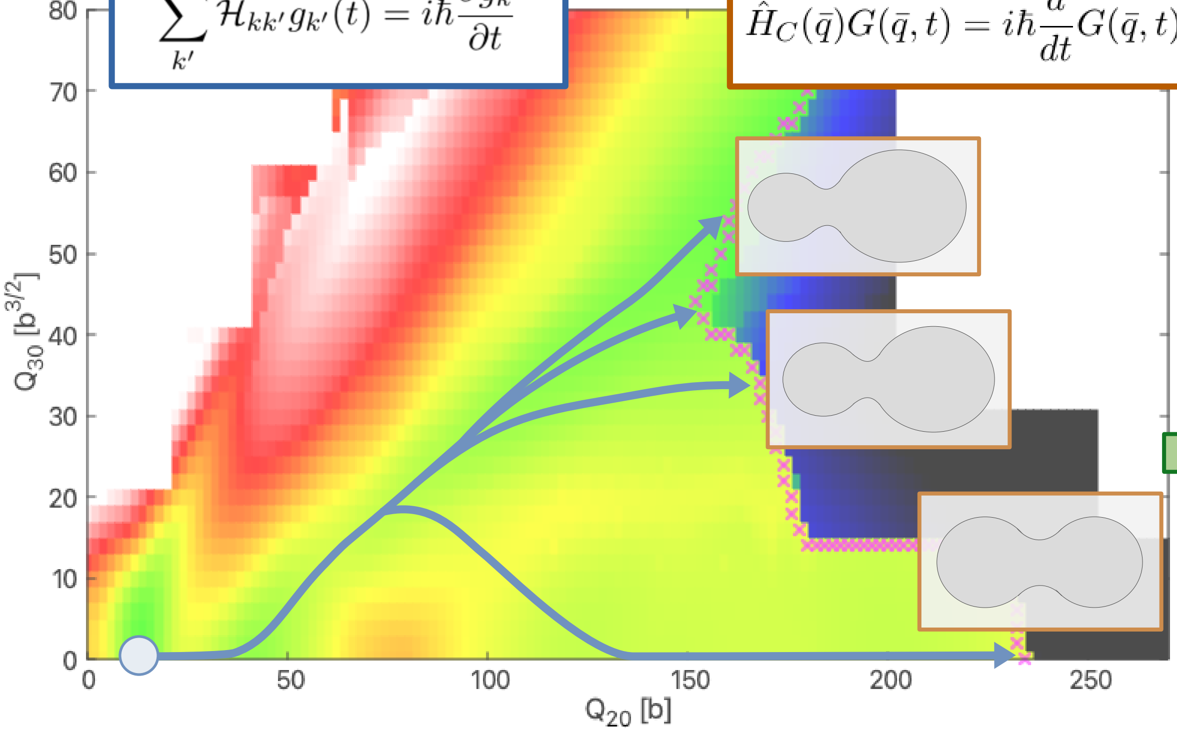
Summary

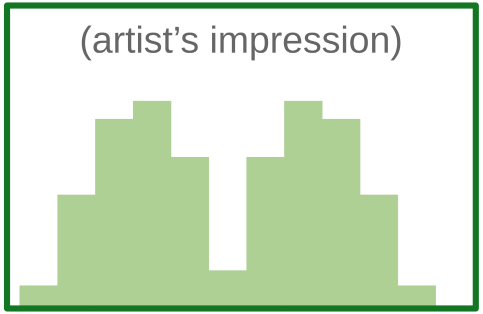
dynamics from exact TDGCM formalism

$$\sum_{k'} \tilde{\mathcal{H}}_{kk'} g_{k'}(t) = i\hbar \frac{\partial g_k}{\partial t}$$

new SME approach to obtain scission flux

$$\hat{H}_C(\bar{q}) G(\bar{q}, t) = i\hbar \frac{d}{dt} G(\bar{q}, t)$$





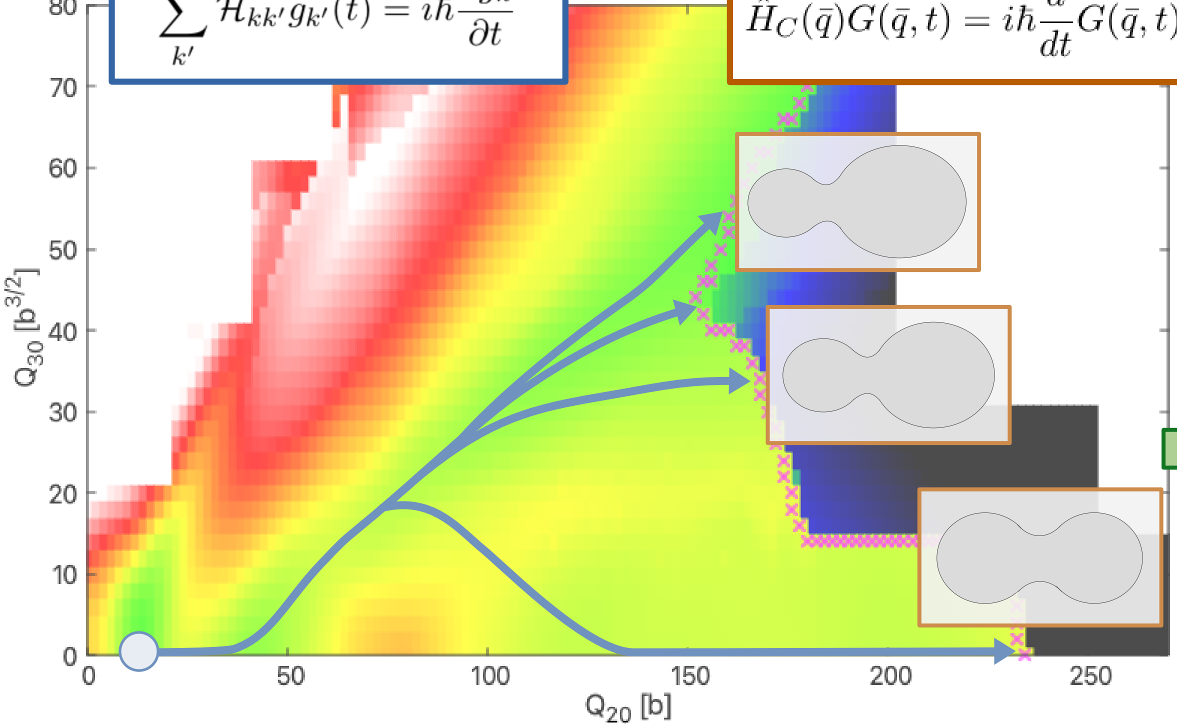
Summary

dynamics from exact TDGCM formalism

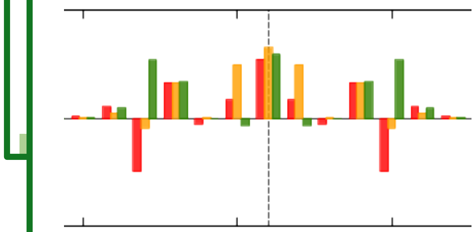
$$\sum_{k'} \tilde{\mathcal{H}}_{kk'} g_{k'}(t) = i\hbar \frac{\partial g_k}{\partial t}$$

new SME approach to obtain scission flux

$$\hat{H}_C(\bar{q}) G(\bar{q}, t) = i\hbar \frac{d}{dt} G(\bar{q}, t)$$



investigate unexpected initial results



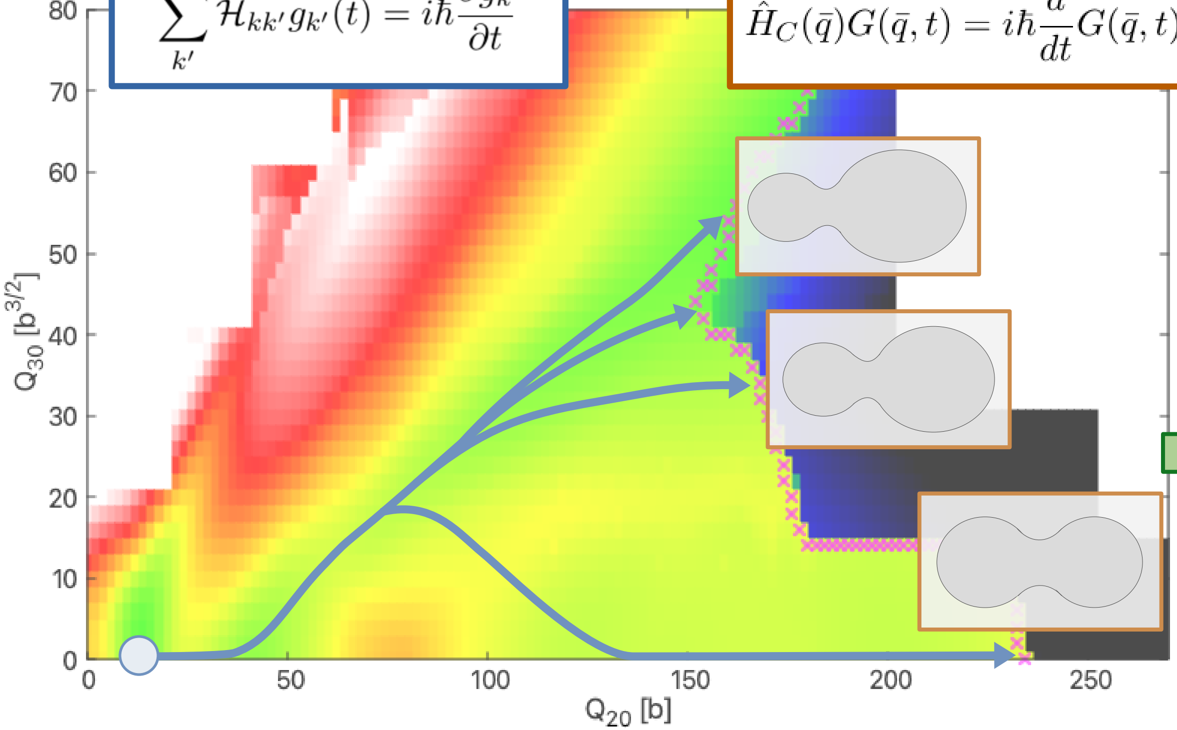
Summary

dynamics from exact TDGCM formalism

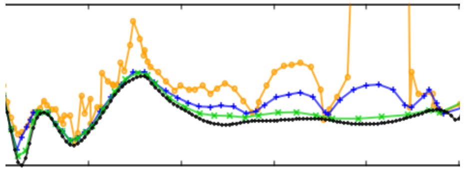
$$\sum_{k'} \tilde{\mathcal{H}}_{kk'} g_{k'}(t) = i\hbar \frac{\partial g_k}{\partial t}$$

new SME approach to obtain scission flux

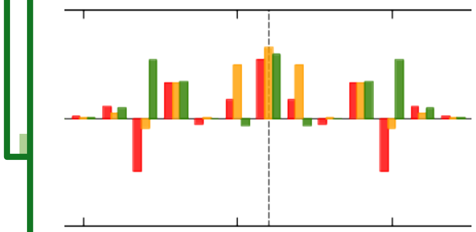
$$\hat{H}_C(\bar{q})G(\bar{q},t) = i\hbar \frac{d}{dt} G(\bar{q},t)$$



remove redundant basis states to lower overlaps

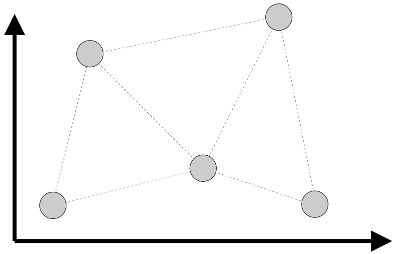


investigate unexpected initial results

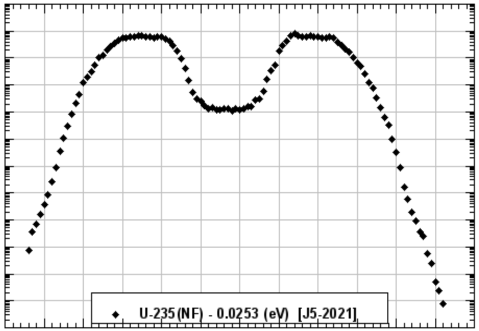


Future research

generation of
sparse 2D PESs



accurate fission yields
(hopefully!)



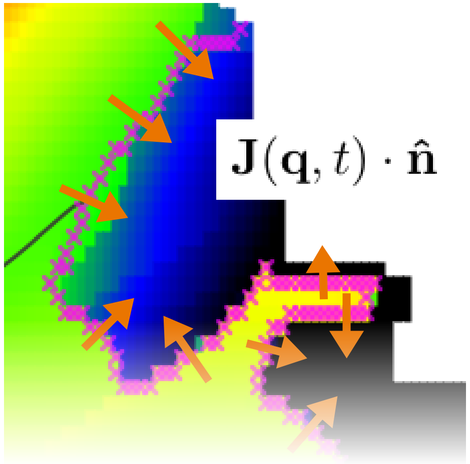
Extensions:

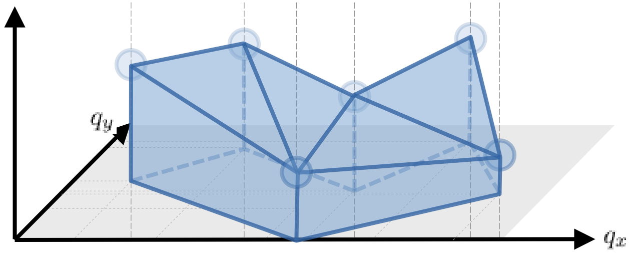
- Restoration of broken symmetries (VAP)
- Generalisation to higher dimensions

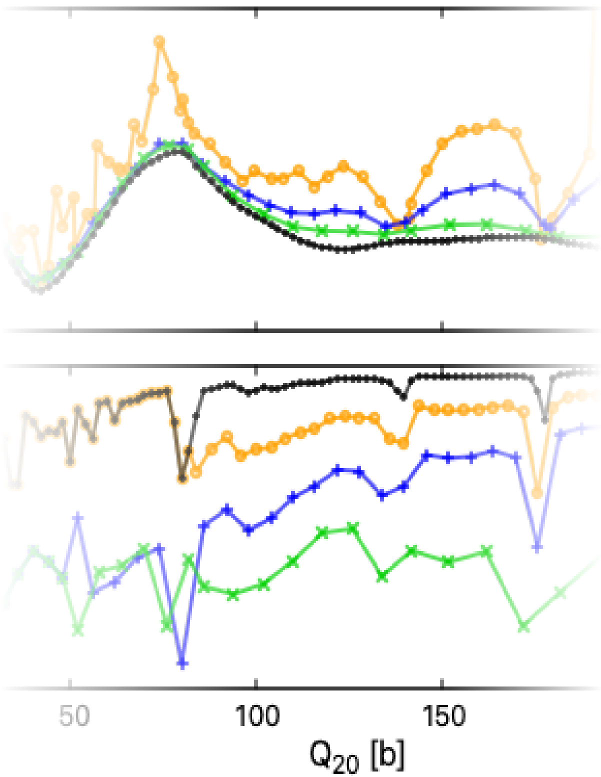
Questions?

Feel free to email me:
ngee_wein.lau@l2it.in2p3.fr

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







$$\hat{H}_C(\bar{q}) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[h_C^{(n)}(\bar{q})\, \hat{P} \right]^{(n)}$$