Improved modelling of fission dynamics with the time-dependent generator coordinate method

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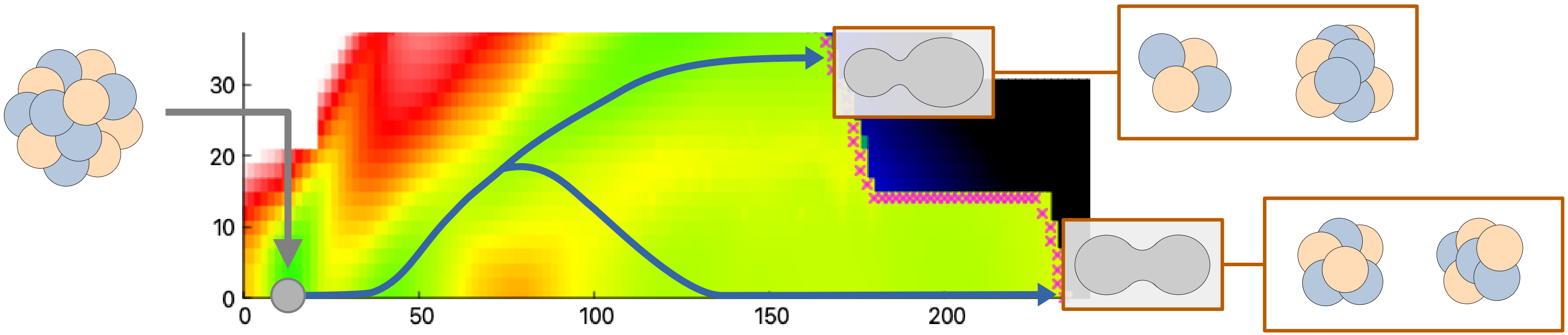
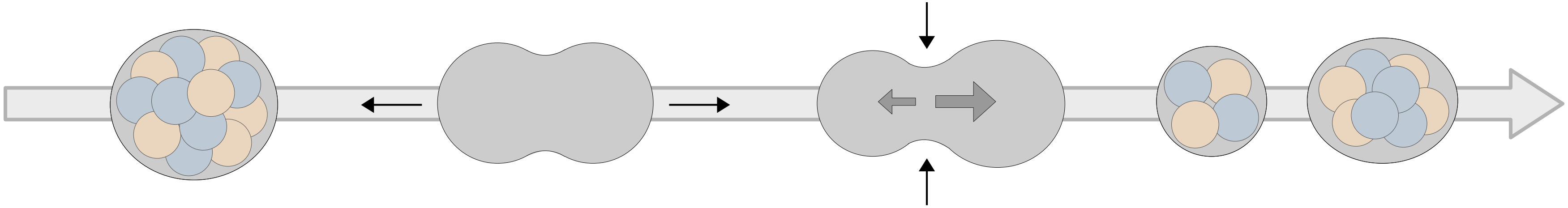
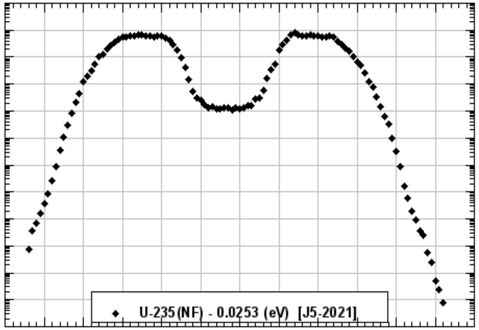
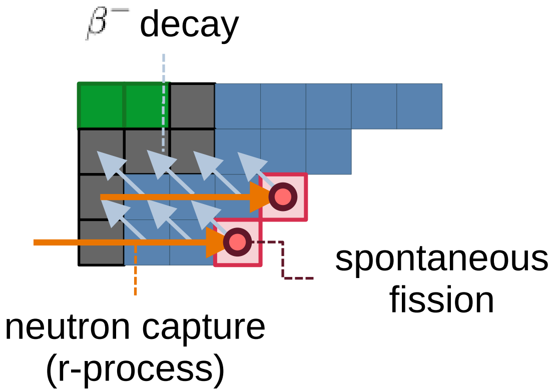


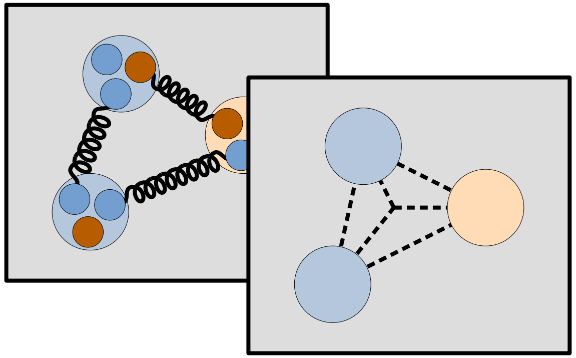
Modelling nuclear fission – why and how?



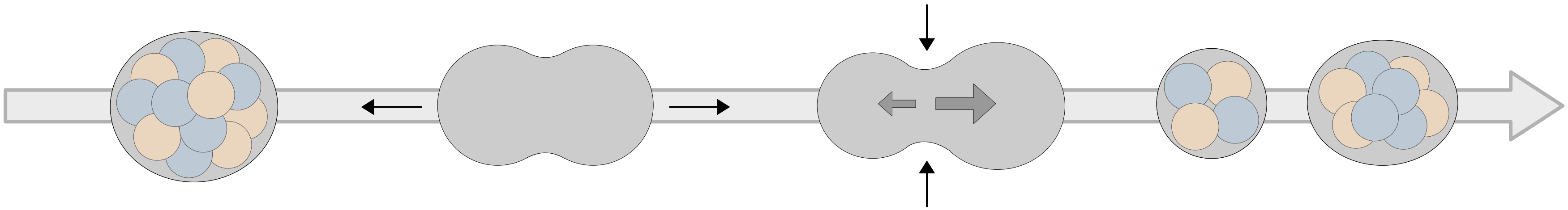


Plot downloaded from *https://wwwndc.jaea.go.jp/cgi-bin/FPYfig?iso=nU235&typ=g1*, accessed 22/04/2024

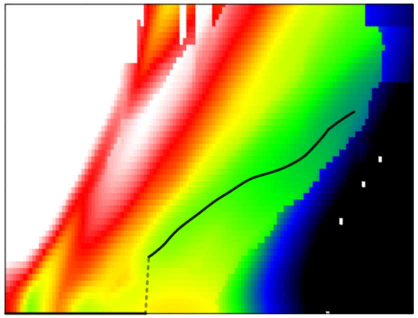




Modelling nuclear fission – why and how?

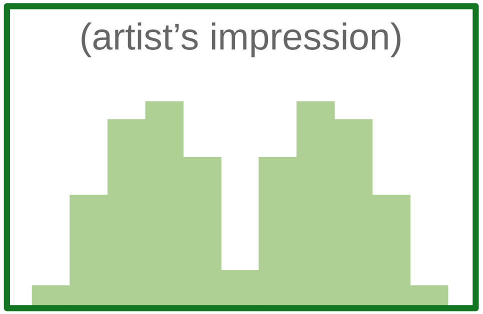


potential energy surfaces (PESs)

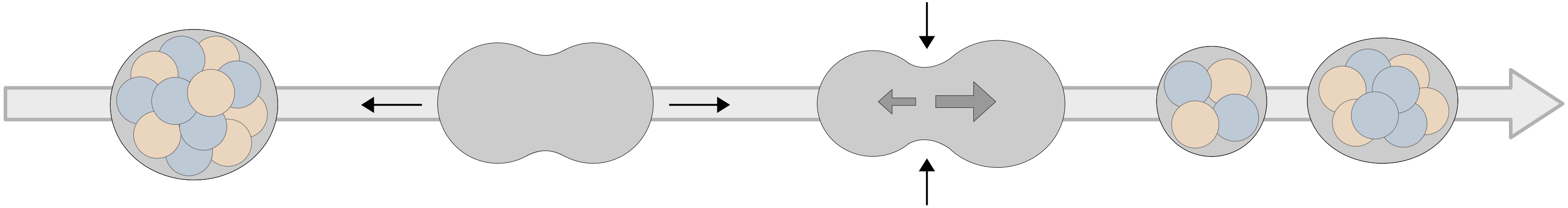


the time-dependent generator coordinate method (TDGCM)

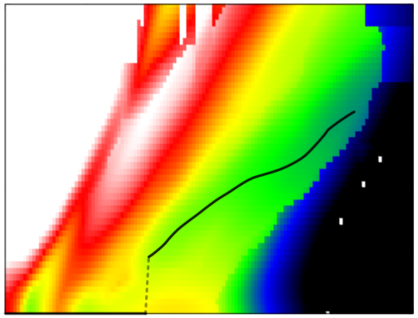
fission observables



Modelling nuclear fission – why and how?



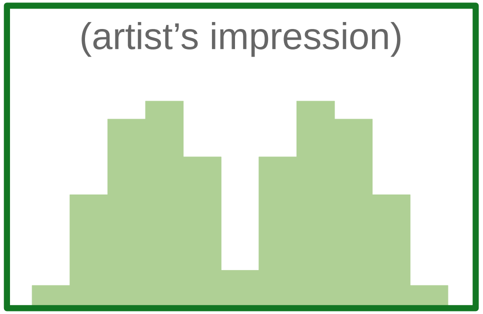
potential energy surfaces (PESs)



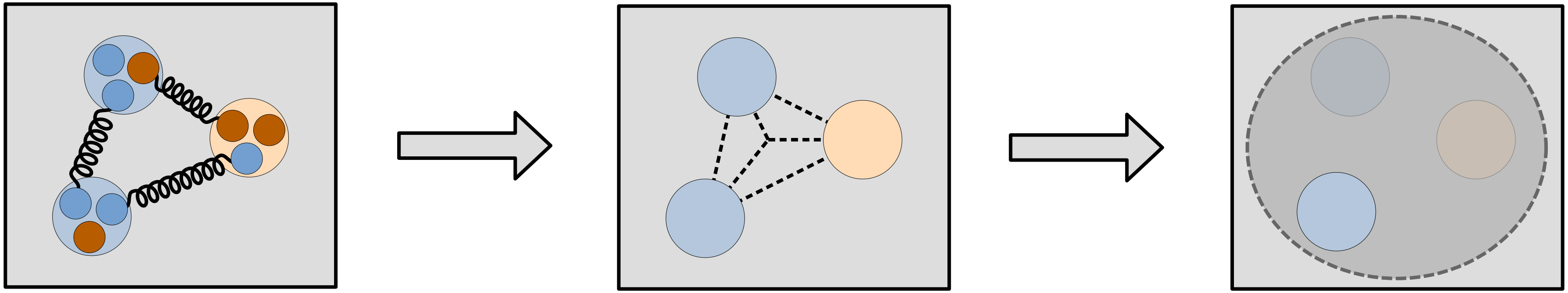
the time-dependent generator coordinate method (TDGCM)

without the GOA!

fission observables



Modelling the nucleus



Standard Model
quantum chromodynamics

Too complicated!

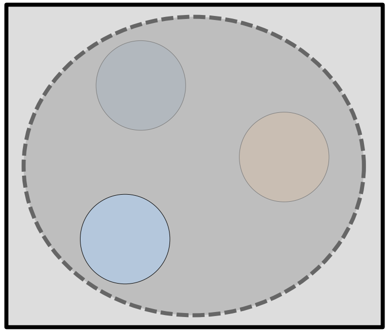
effective interaction
quantum many-body problem
(e.g. Skyrme or Gogny force)

Still too complicated!

mean field interaction

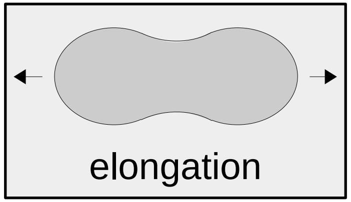
isolated particles in a
density-dependent potential

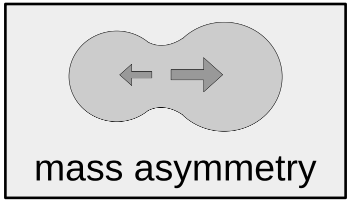
Modelling the nucleus

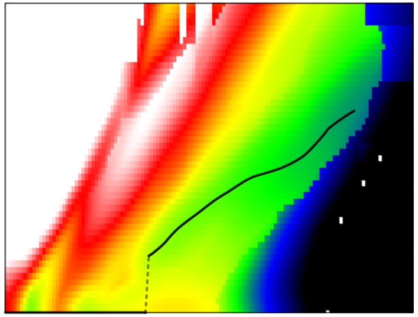


mean field
nuclear interaction

solve across a mesh of
constraints on nuclear shape

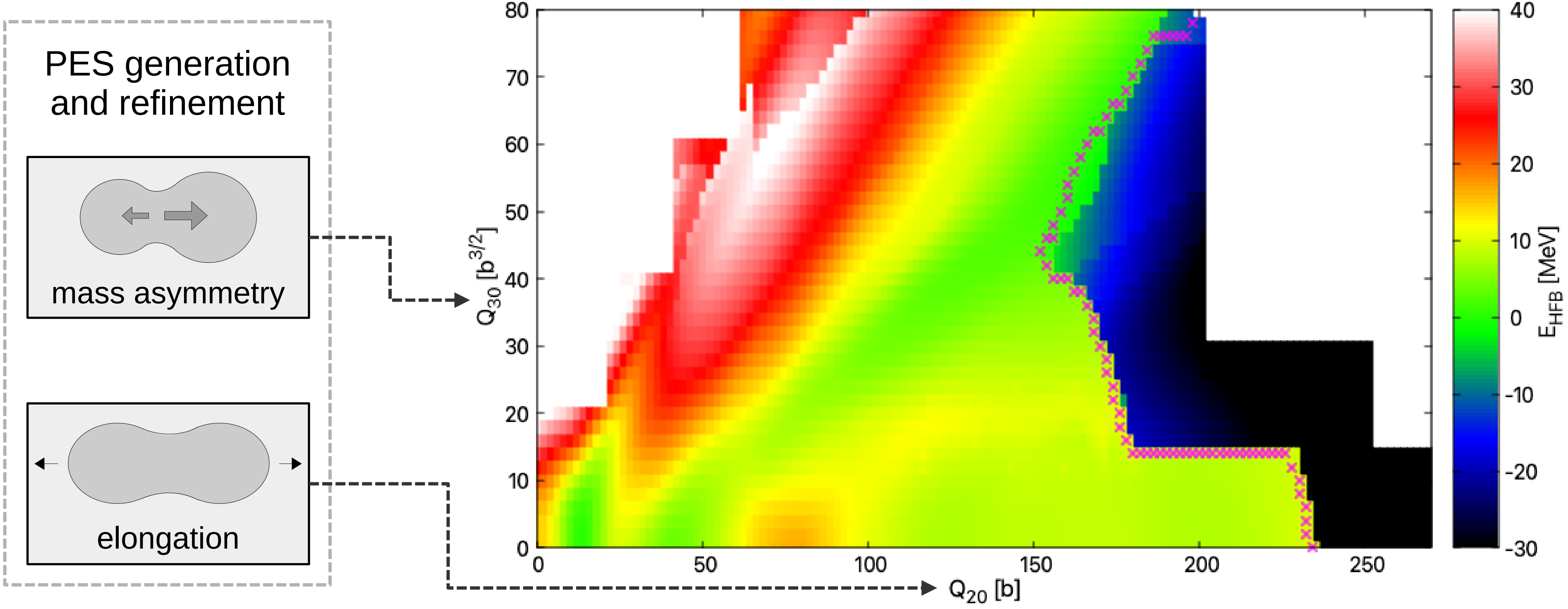






potential energy
surface

Modelling the nucleus

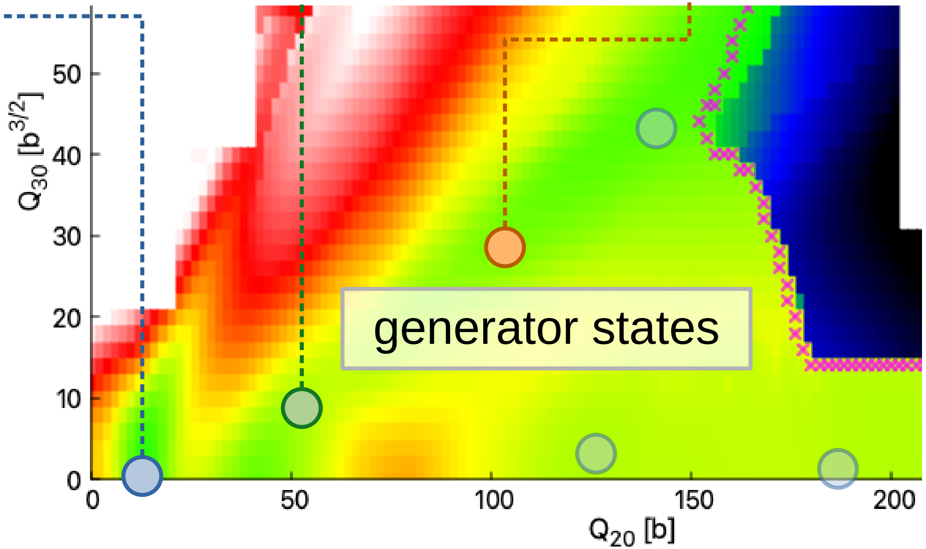


For more details, see:
N.-W. T. Lau, R. N. Bernard, C. Simenel, *Phys. Rev. C* **105**, 034617 (2022)

Dynamics with the TDGCM

(time-dependent generator coordinate method)

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



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)

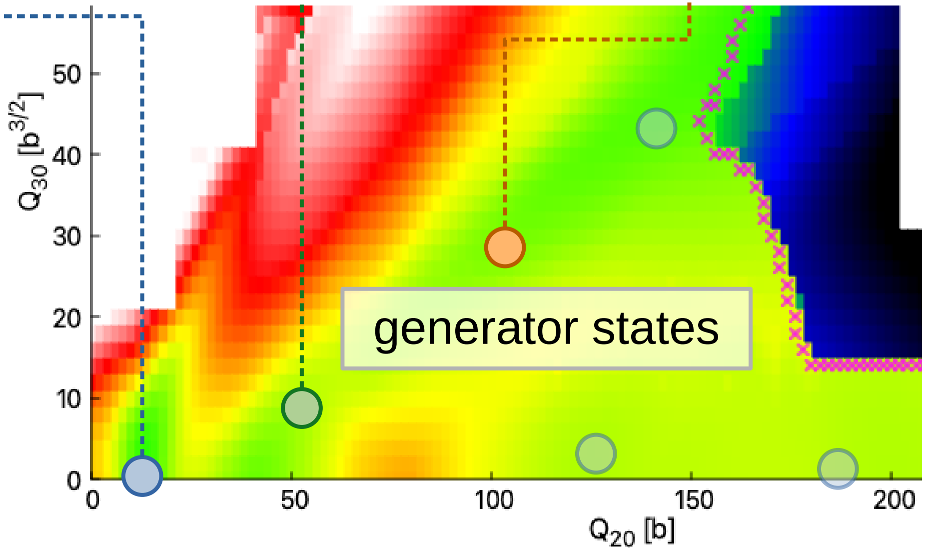
Dynamics with the TDGCM

(time-dependent generator coordinate method)

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

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

weight function



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Dynamics with 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

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

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 the 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 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

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

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

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

Nonlocal Collective Schrödinger Equation (CSE)

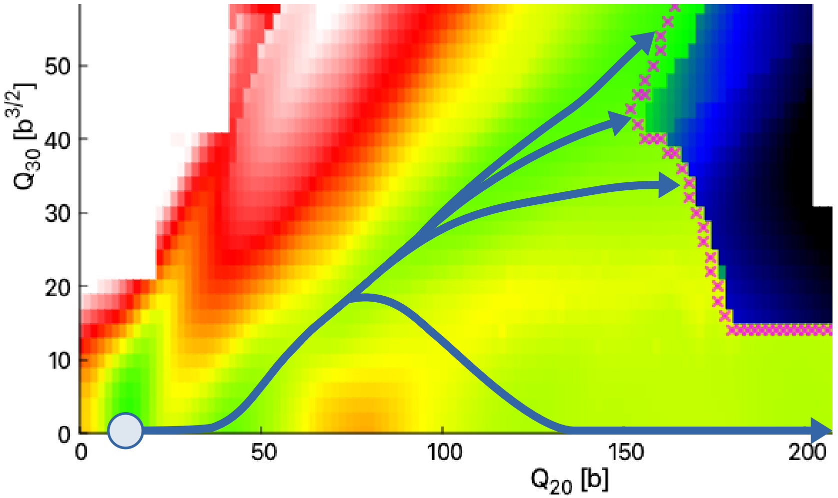
Exact solution of the TDGCM

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

natural basis transformation

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

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



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

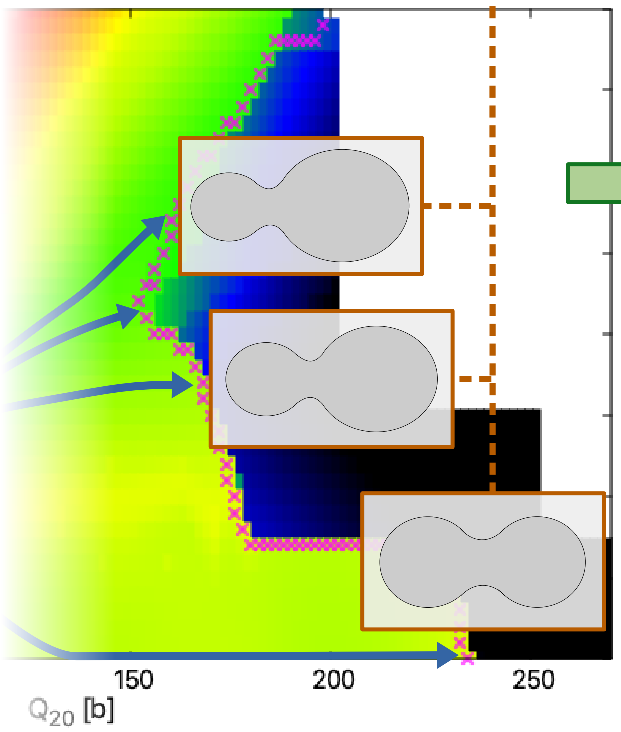
Nonlocal Collective Schrödinger Equation (CSE)

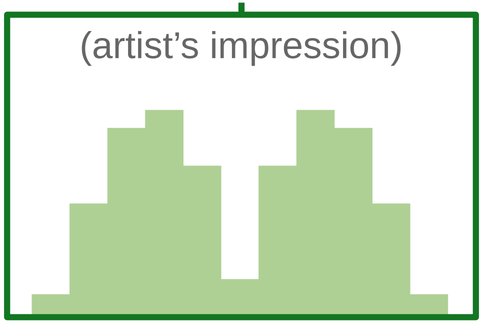
Getting results

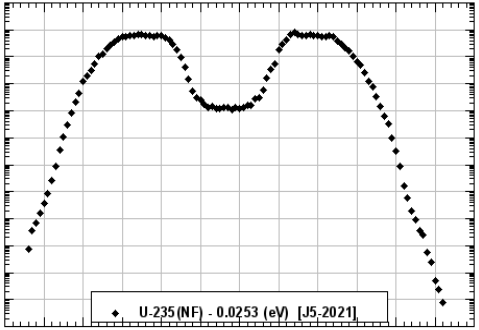
2. Extracting fission observables

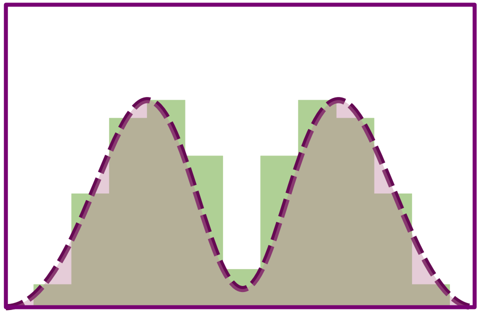
3. Interpreting and improving results

4. Application of projection techniques

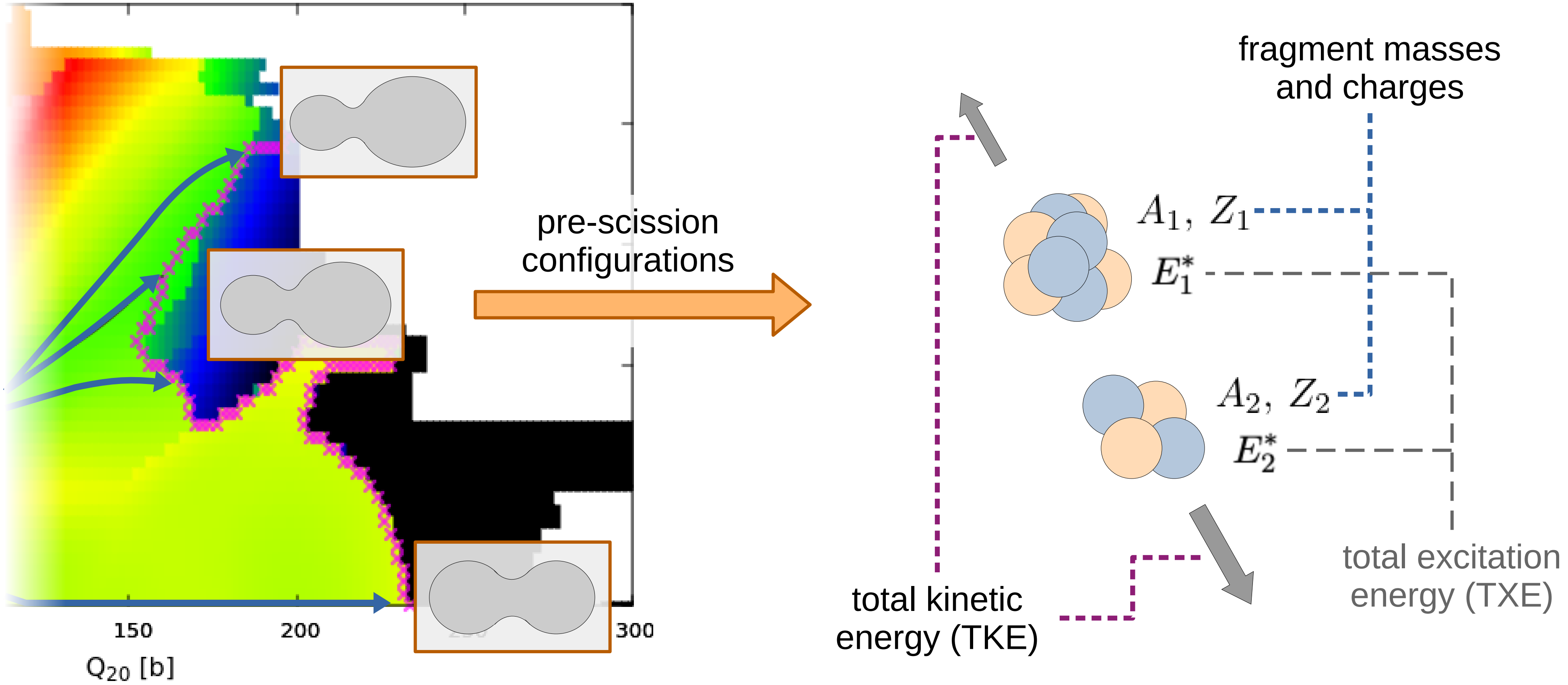








Observables at the scission line

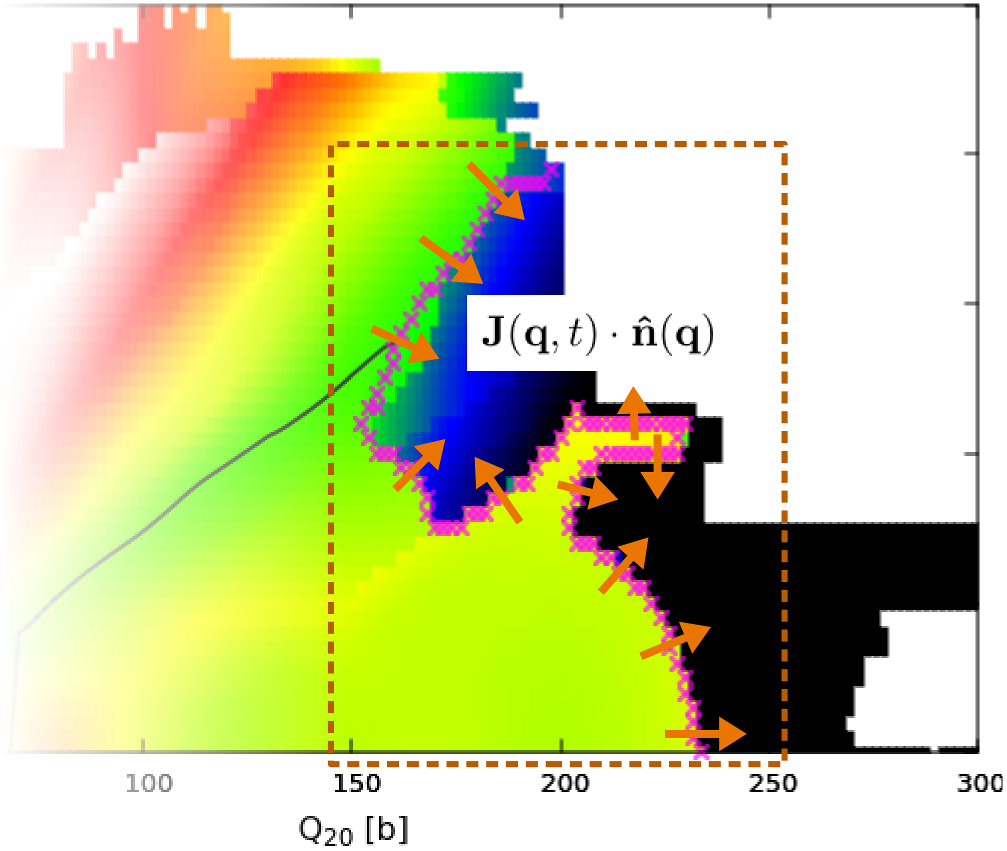


Observables at the scission line

probability flux

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

probability current



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

Observables at the scission line

probability flux

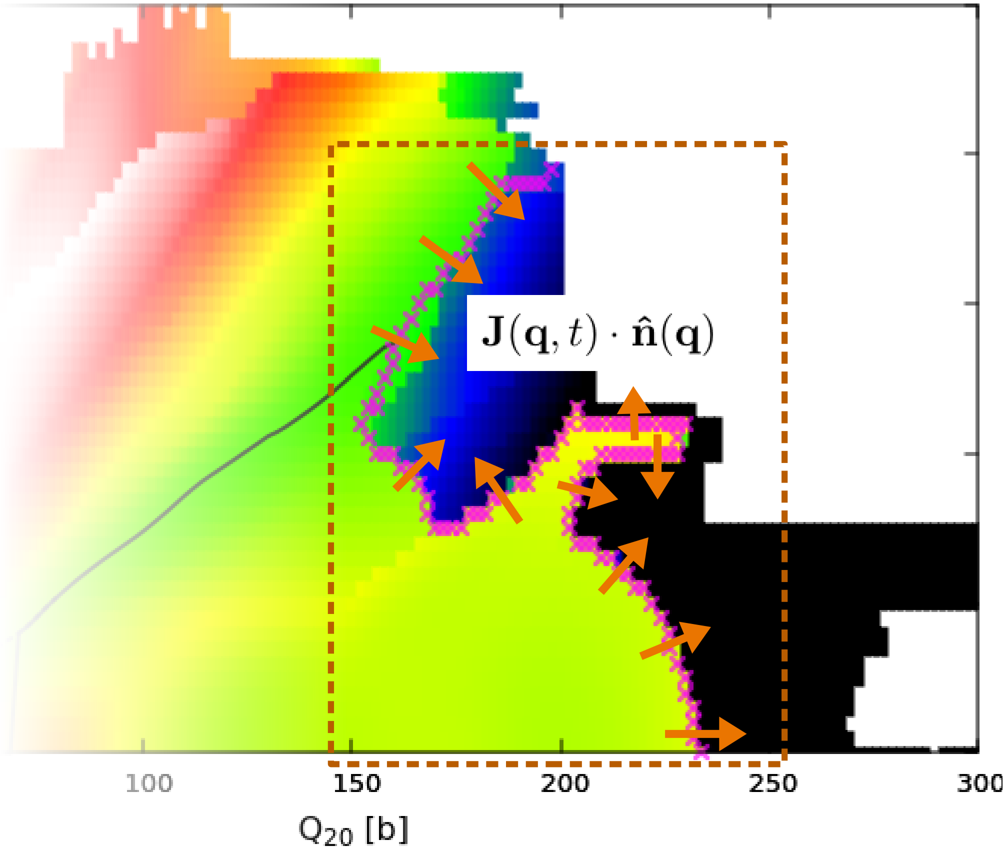
$$F(\mathbf{q}, T) = \int_0^T dt\, \mathbf{J}(\mathbf{q}, t) \cdot \hat{\mathbf{n}}(\mathbf{q})$$

probability current

probability density function

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

local continuity equation



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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 collective Schrödinger equation (CSE)

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

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

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 collective Schrödinger equation (CSE)

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

Symmetric Moment Expansion (SME)

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

alternate orthonormal "SME" basis: $|q\rangle = \int dp \; N^{-1/2}(p,q) \, |\Phi(p)\rangle$

change of coordinates and 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

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)

symmetrised Hill-Wheeler equation

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

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

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

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

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

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

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

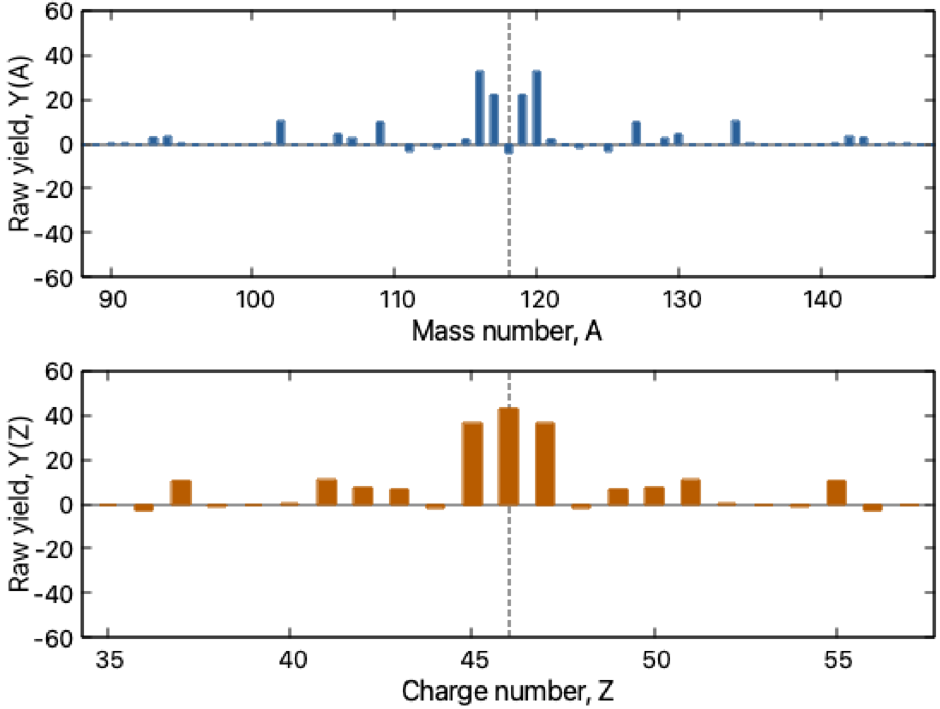
truncate expansion at second order

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

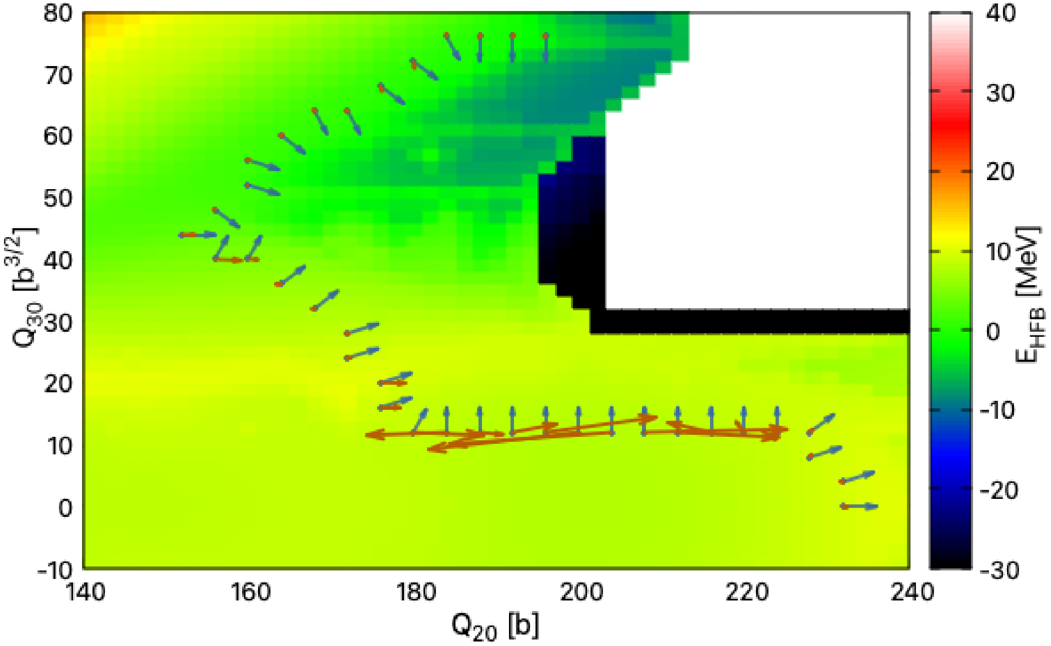
probability current

2D fission outcomes – ^{236}U

primary fission product yields



time-integrated flux at scission line



2D fission outcomes – ^{236}U

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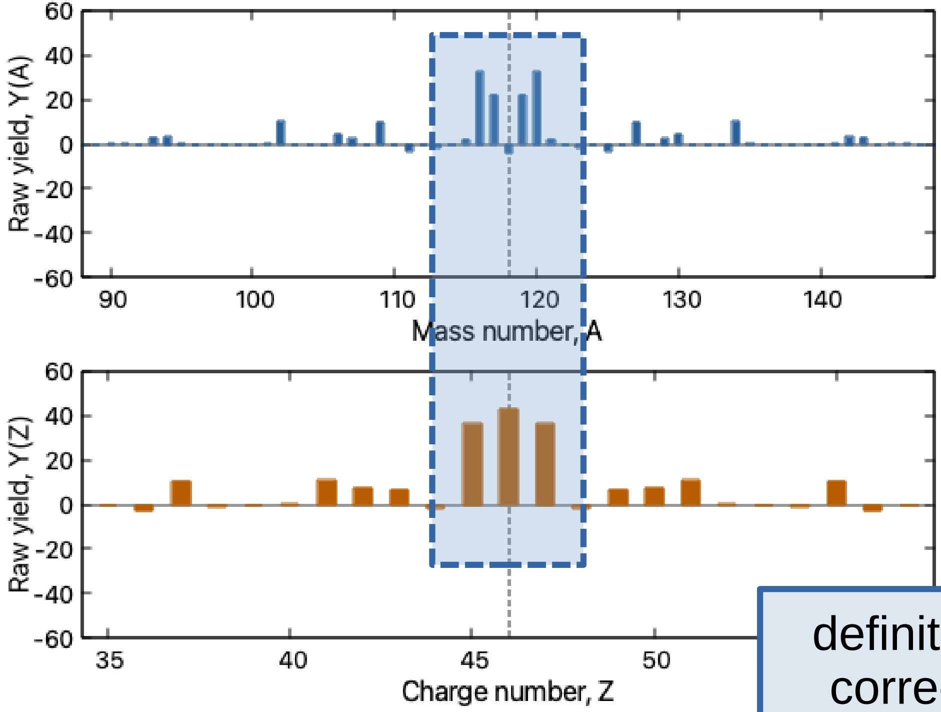
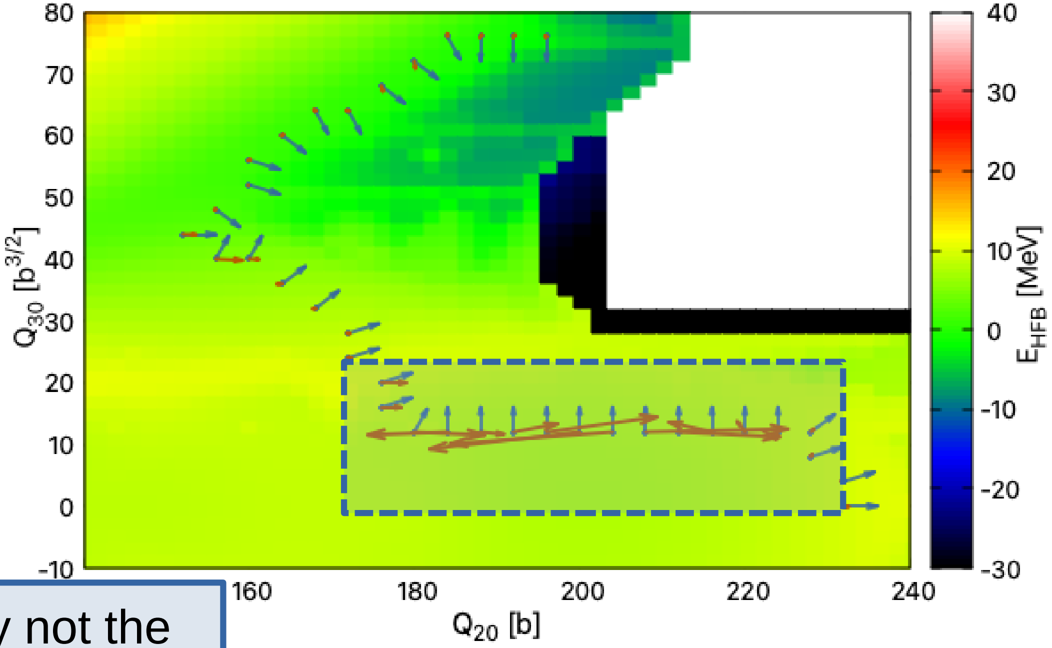


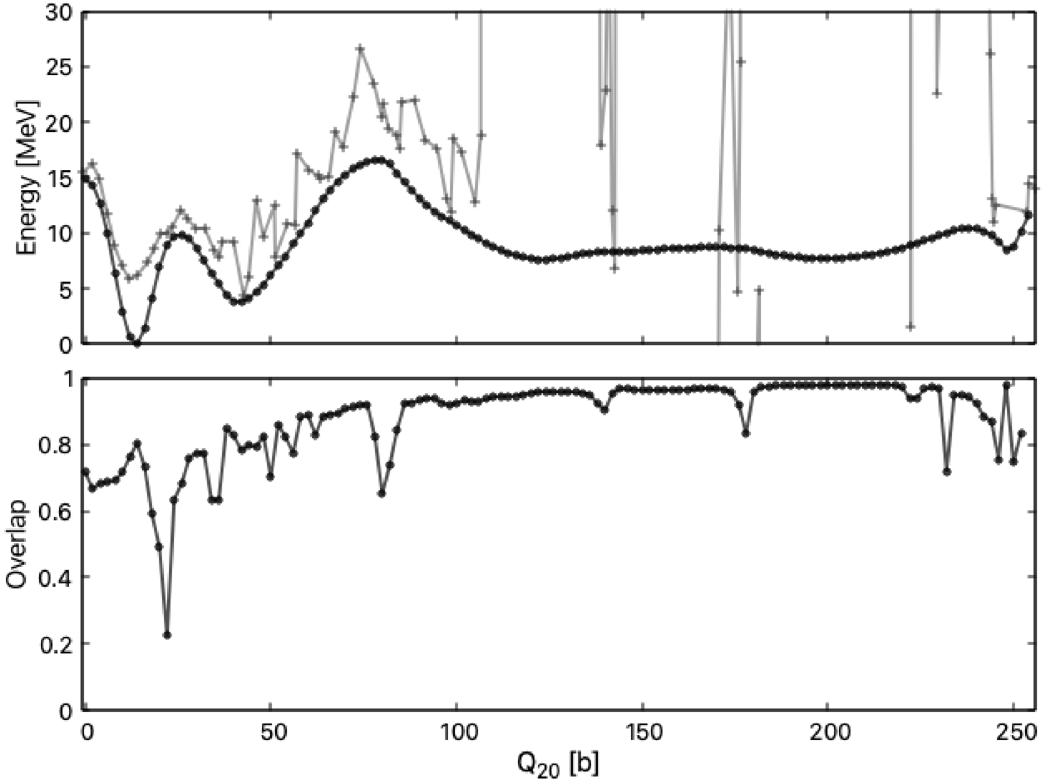
time-integrated flux at scission line



definitely not the correct results!

What now?

Testing behaviour with Gaussian overlaps



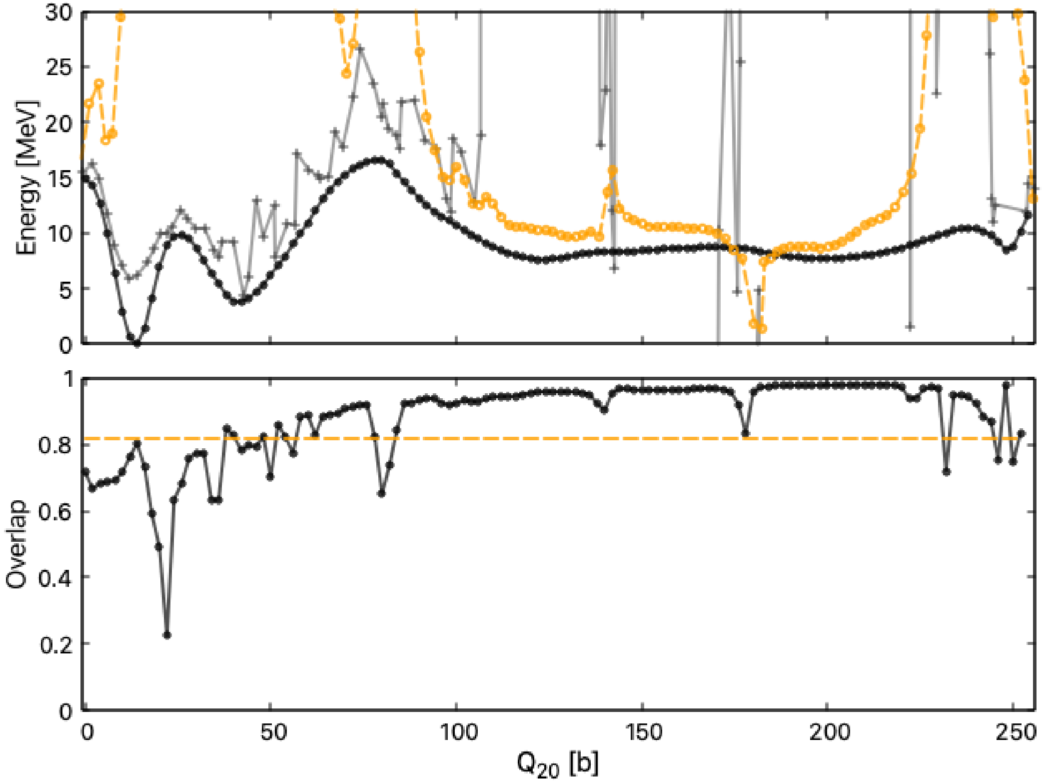
Original PES

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

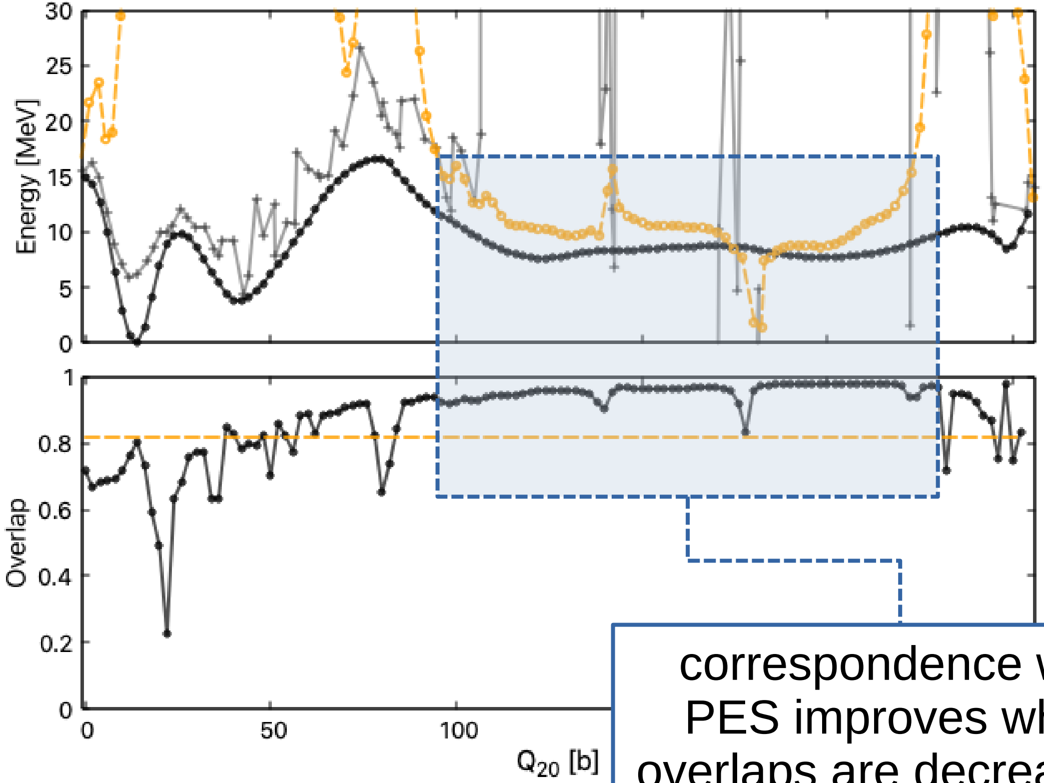
SME states:

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?

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

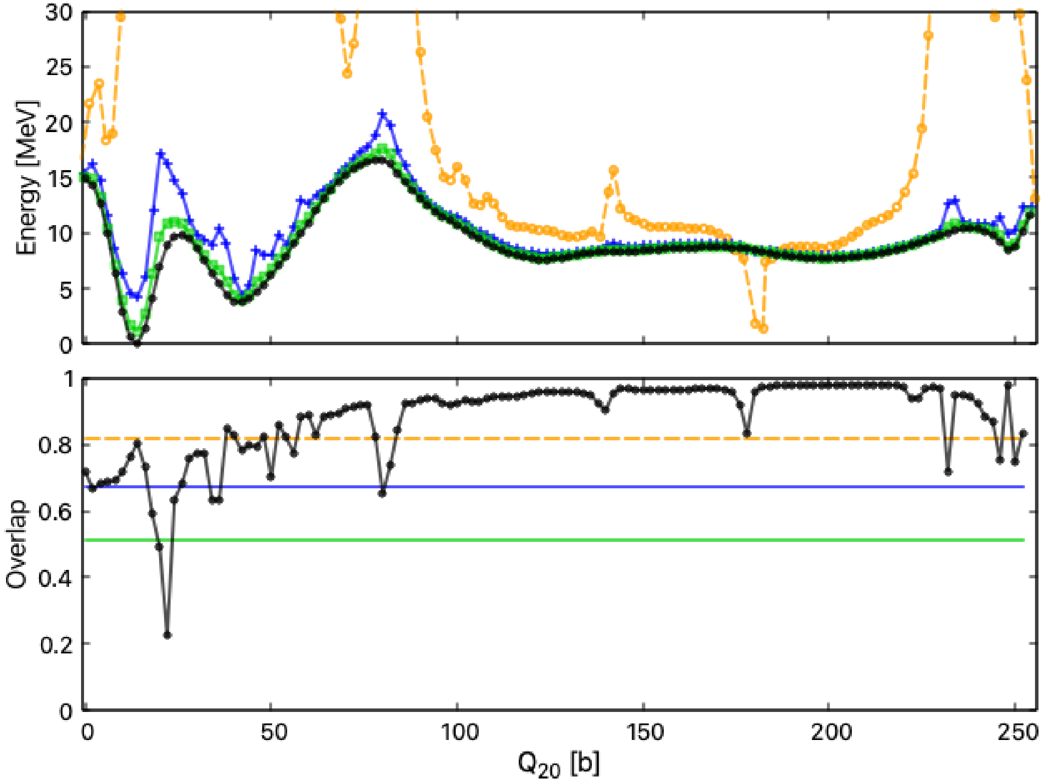
- Original PES

SME states:

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

What now?

Testing behaviour with Gaussian overlaps



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

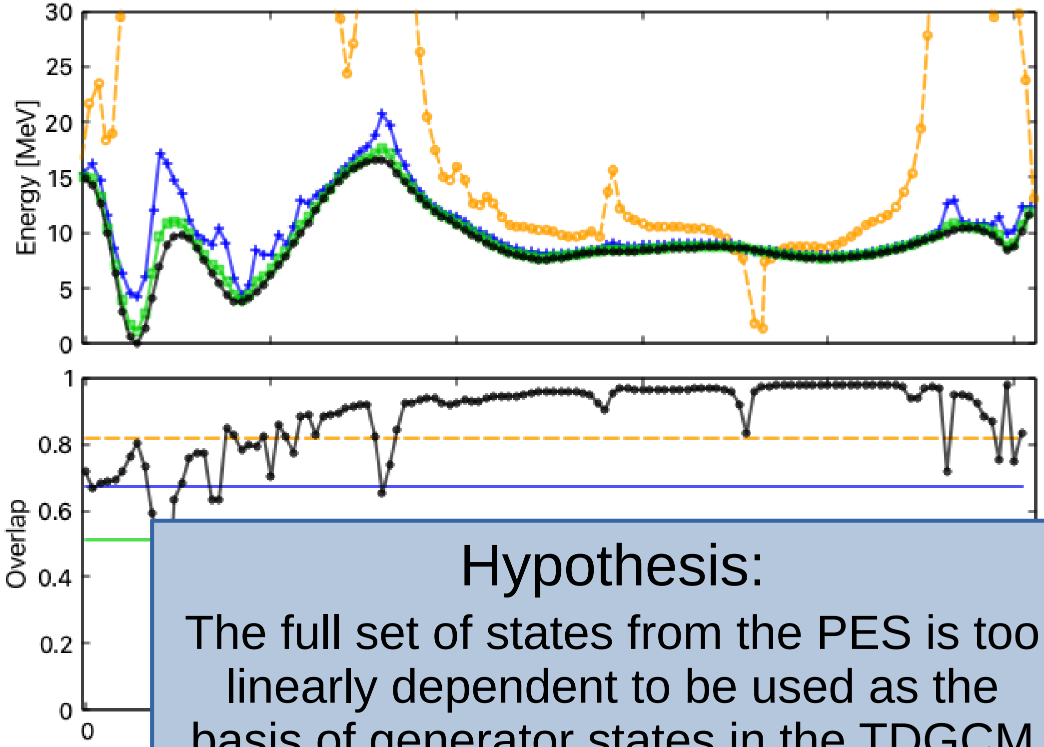
- Original PES

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 $2\sigma^2 = 10$

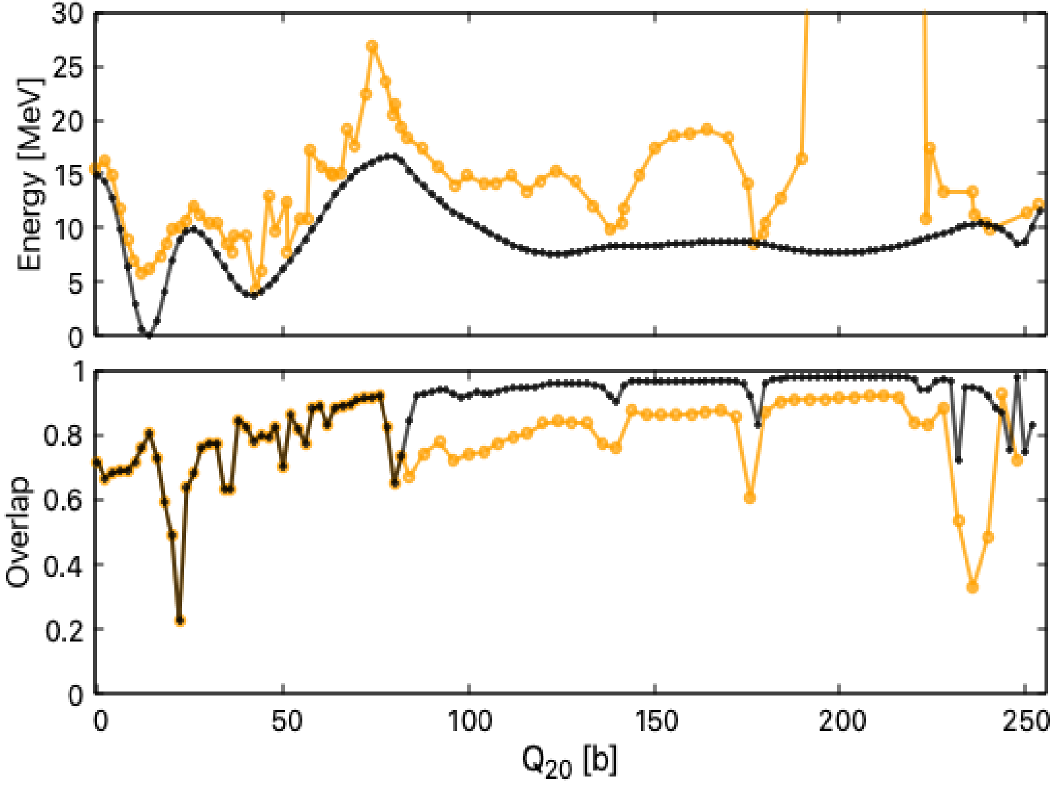
GOA overlaps with width $2\sigma^2 = 6$

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



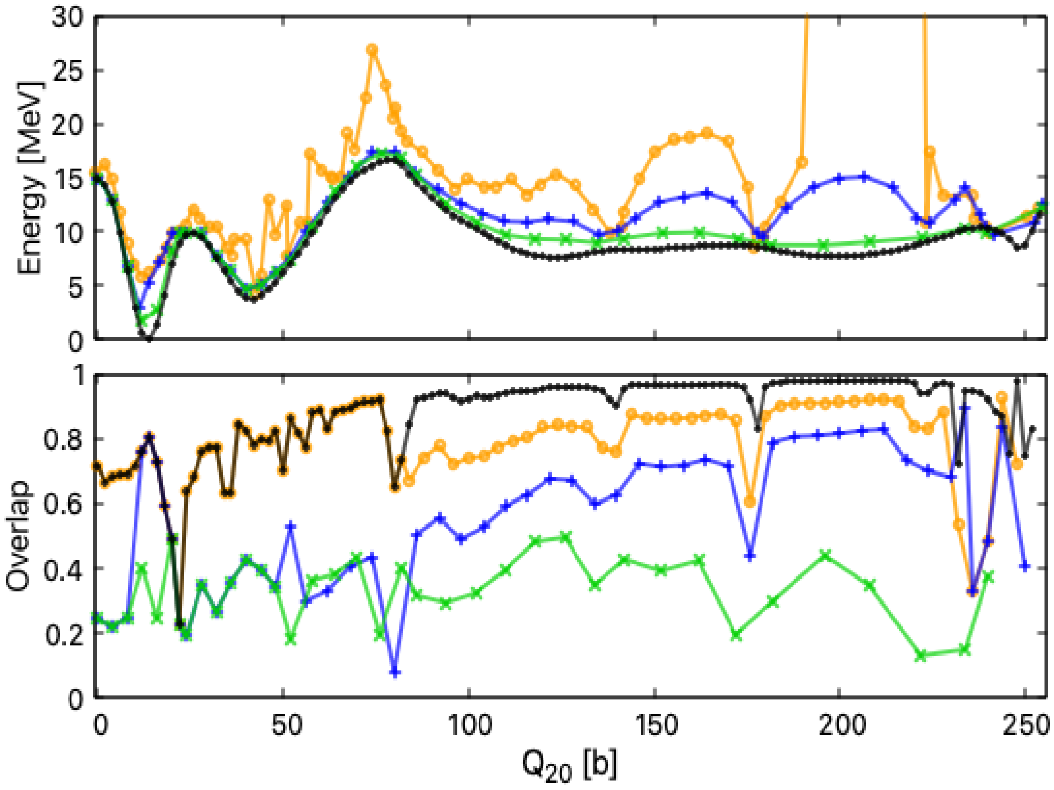
Original PES in HFB basis (128 states)

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)

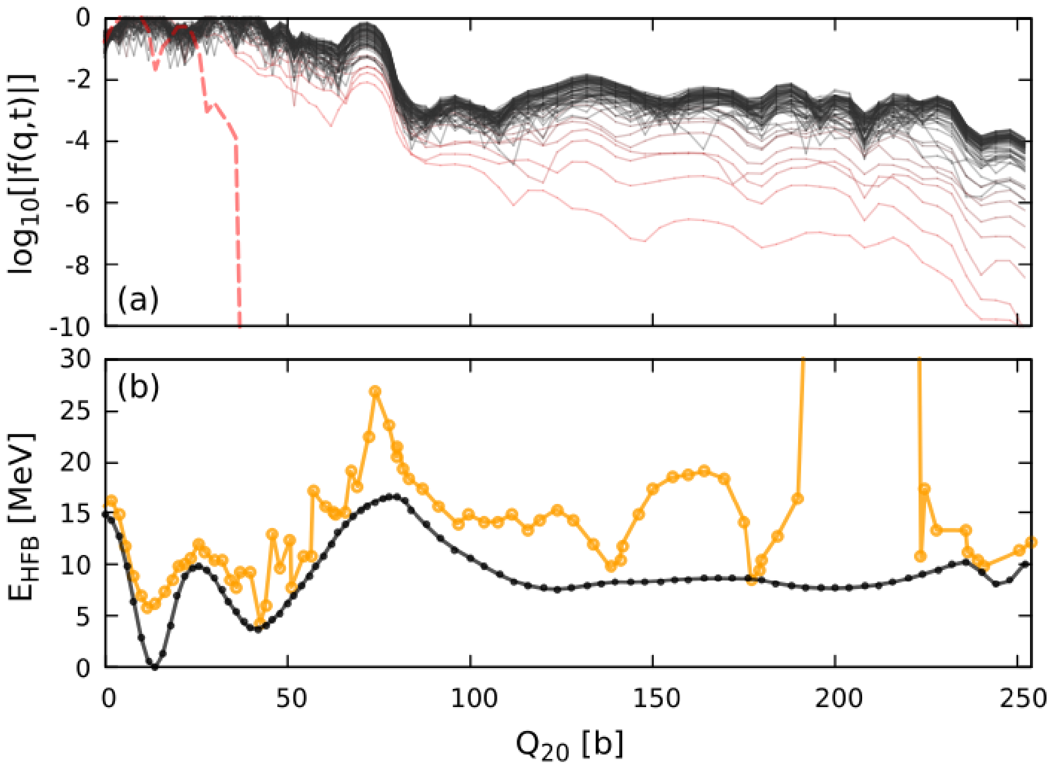
SME states:

- 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

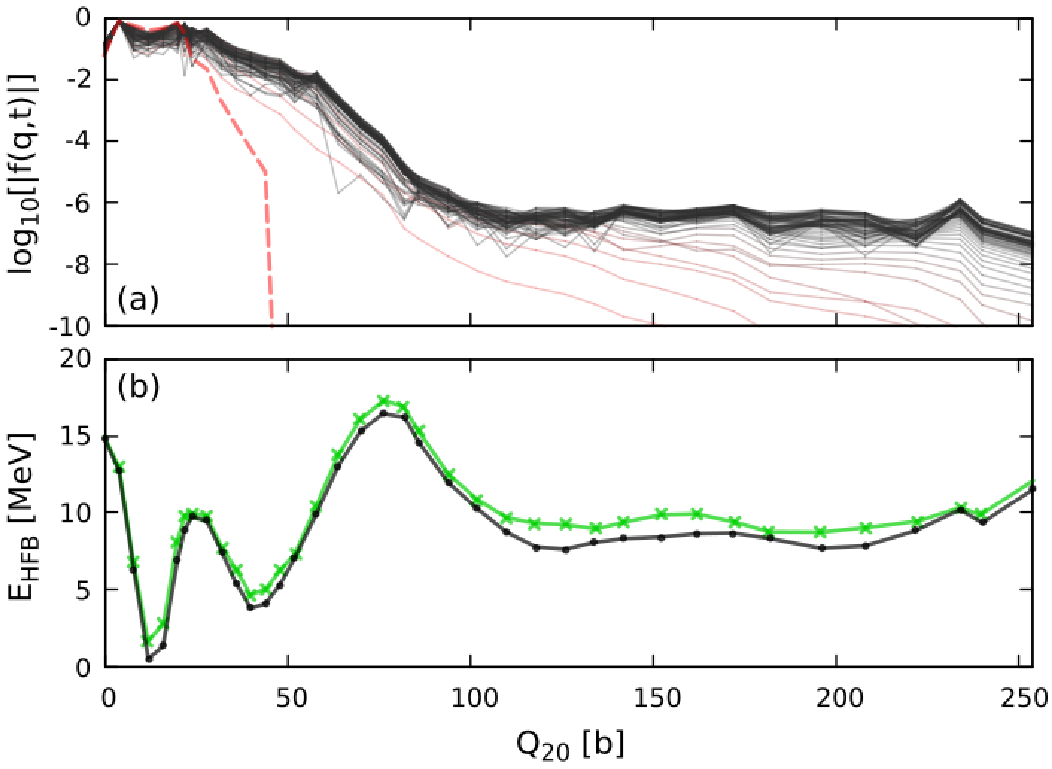
Doubled mesh after saddle
“1s2s” (85 states)



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 natural basis, producing more realistic nuclear dynamics in one dimension.

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

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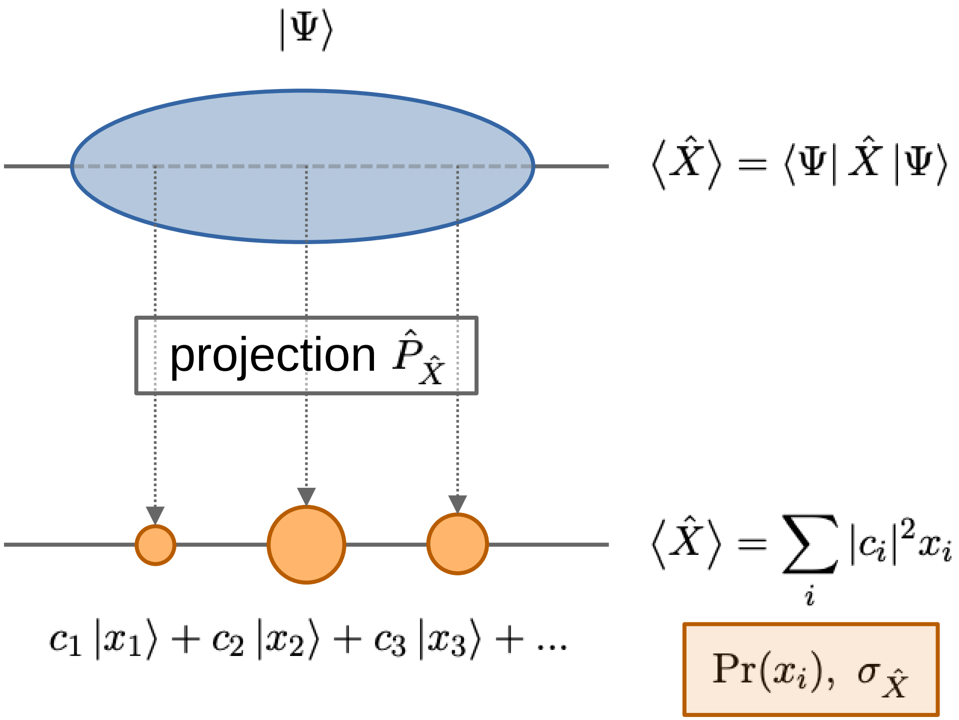
- How can this process be generalised to two dimensions?

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

The role of projection techniques

- Physical symmetries are often broken by nuclear models
- Projection of the wavefunctions can restore the broken symmetries and lost observables



Projection theory for TDGCM

$$\hat{P}_{\hat{X}}(x_i) \sim |\psi(x_i)\rangle\langle\psi(x_i)|$$

$$\hat{P}_{\hat{X}}(x_i)\,|\Psi\rangle = \left\langle \psi(x_i) \middle| \Psi \right\rangle |\psi(x_i)\rangle$$

projection operator

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

TDGCM ansatz

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projection operator

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

TDGCM ansatz

measurement probability

$$\mathrm{Pr}(x_i,t) = \langle\Psi(t)|\,\hat{P}_{\hat{X}}(x_i)\,|\Psi(t)\rangle$$

$$= \int dq\,dq'\;\; f^*(q,t)f(q',t)\;\; \langle\Phi(q)|\,\hat{P}_{\hat{X}}(x_i)\,|\Phi(q')\rangle$$

"probability kernel" $P(x_i;\, q, q')$

Projection theory for TDGCM

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projection operator

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

TDGCM ansatz

one "probability kernel" for each possible eigenvalue x_i !

$$P(x_i;\, q, q')$$

measurement probability

$$\mathrm{Pr}(x_i,t) = \langle\Psi(t)|\,\hat{P}_{\hat{X}}(x_i)\,|\Psi(t)\rangle$$

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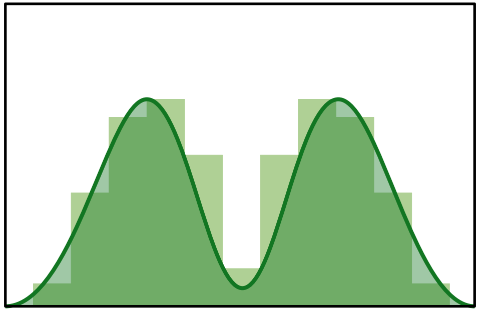
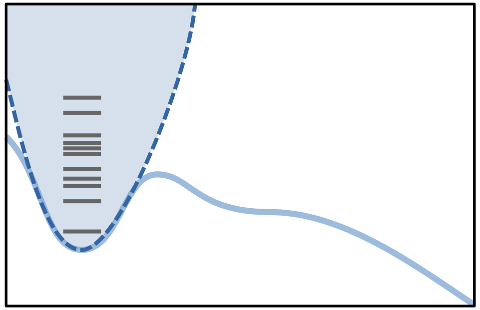
Applications of projection

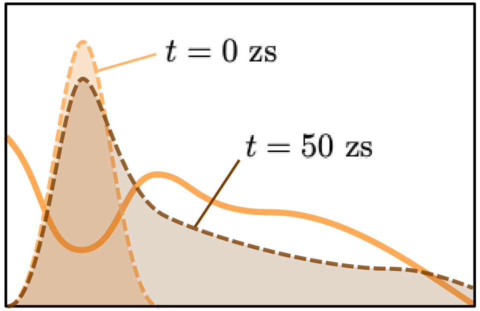
calculation of observable probability distributions



modifications to system (after variational step)



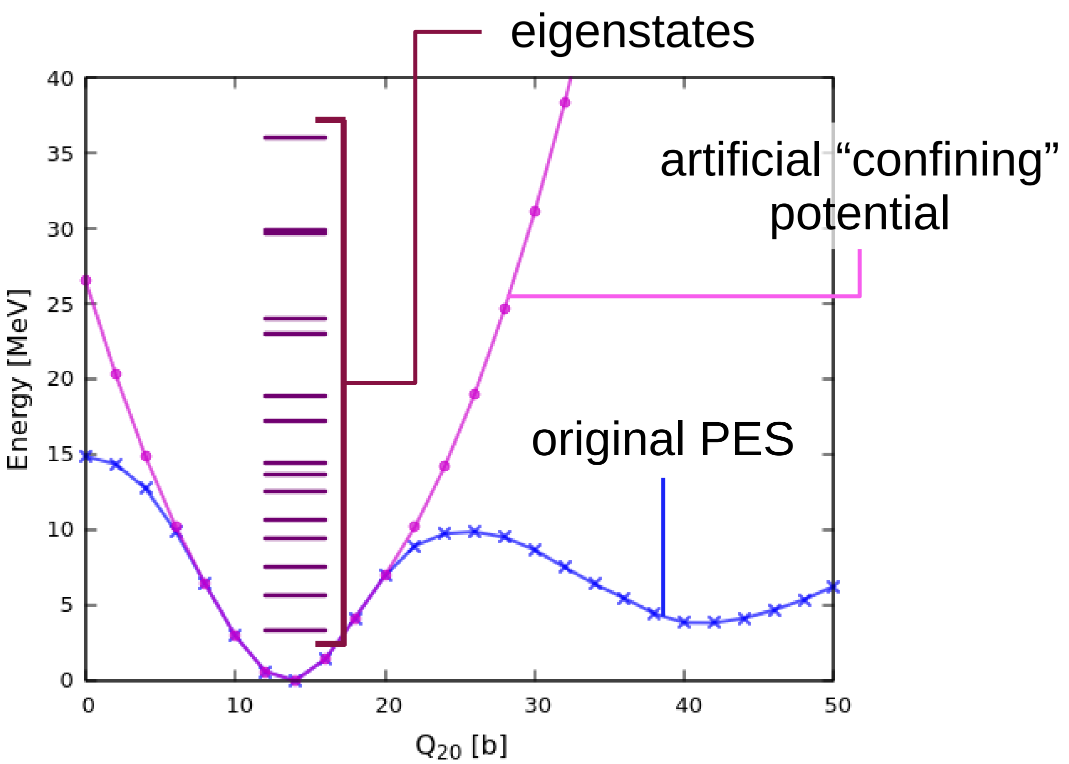
visualisation of dynamic behaviour



the above diagrams do not represent real data

Example: eigenstates in a confined potential

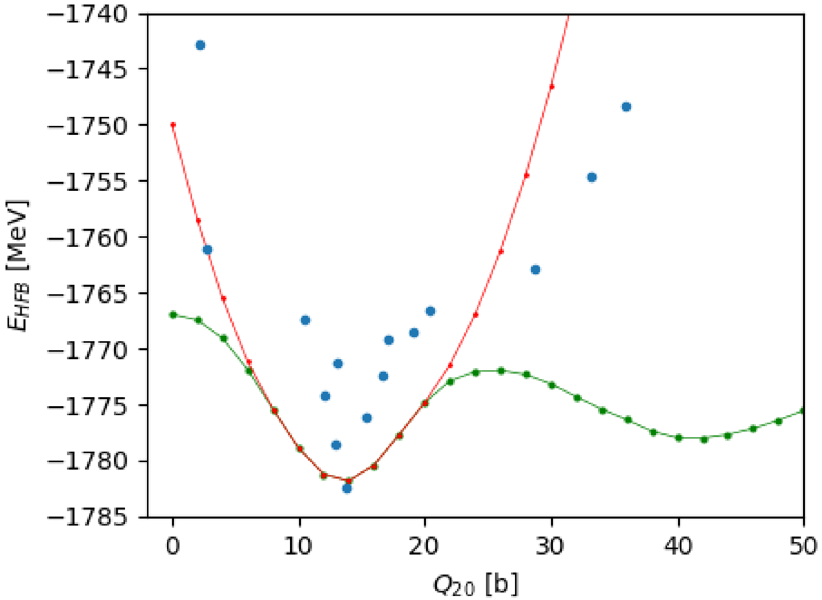
Initial state construction



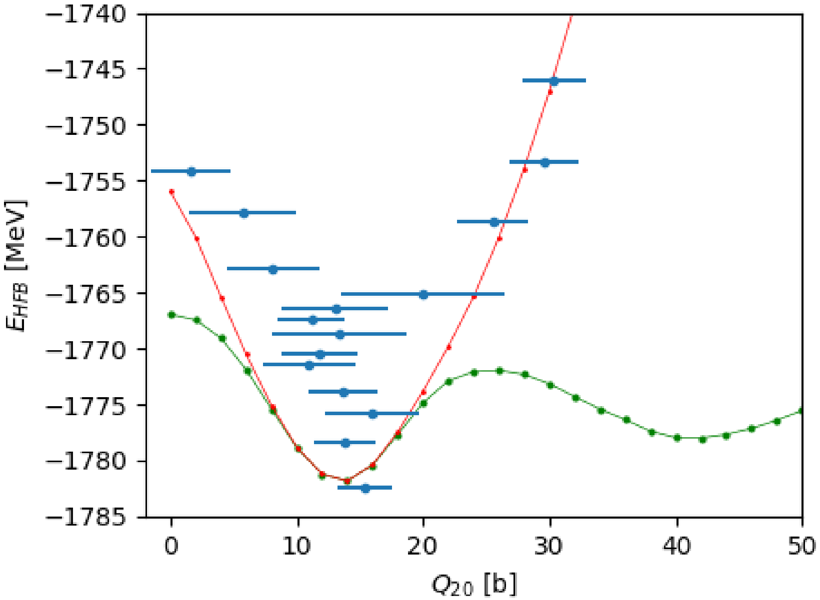
H. Goutte, J. F. Berger, P. Casoli, D. Gogny, *Phys. Rev. C* **71**, 024316 (2005)

Example: eigenstates in a confined potential

Initial state construction

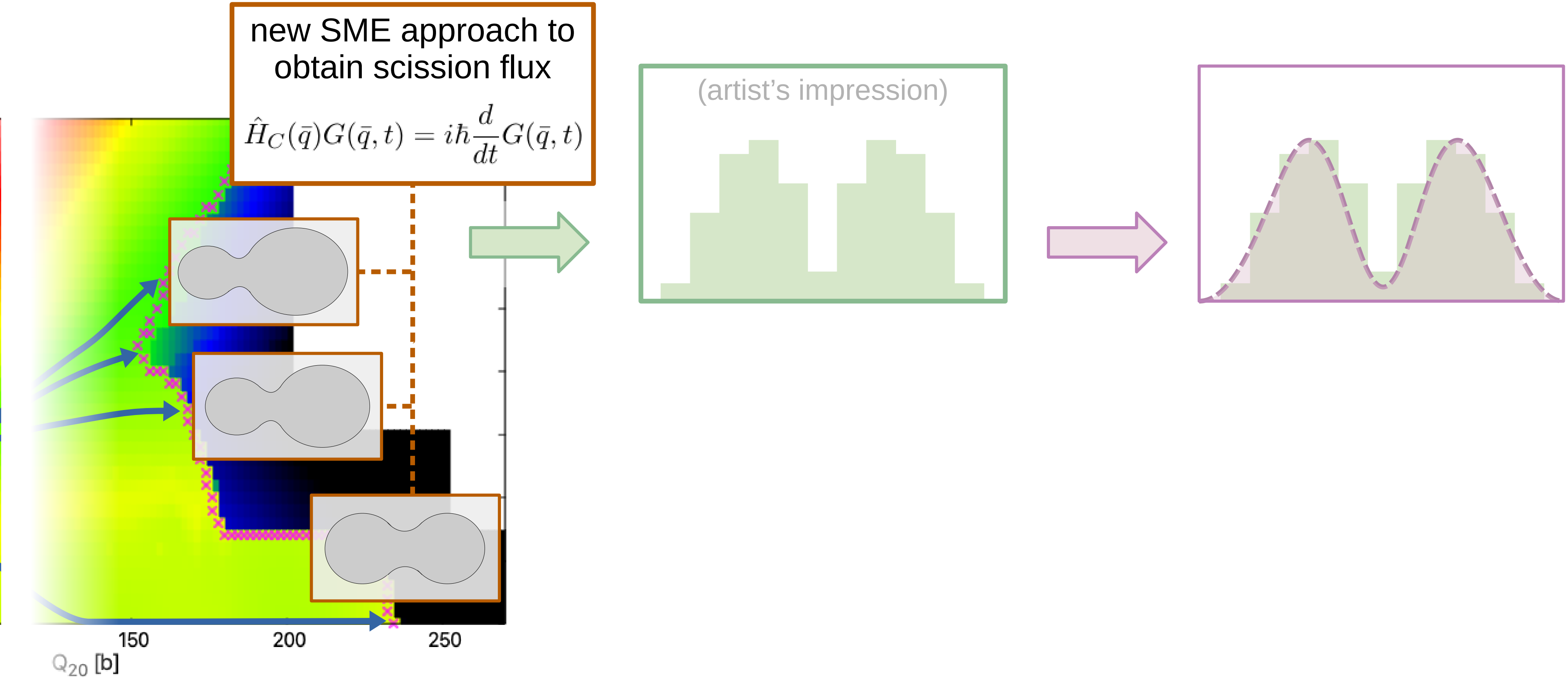


original method
without projection



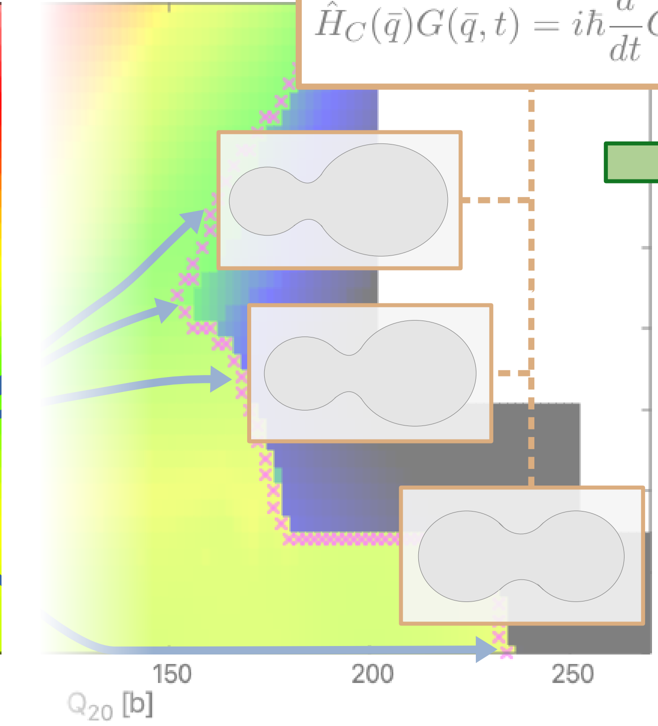
with projection

Summary



new SME approach to obtain scission flux
$\hat{H}_C(\bar{q})G(\bar{q},t) = i\hbar\frac{d}{dt}G(\bar{q},t)$
(artist's impression)
150
200
250
Q_{20} [b]

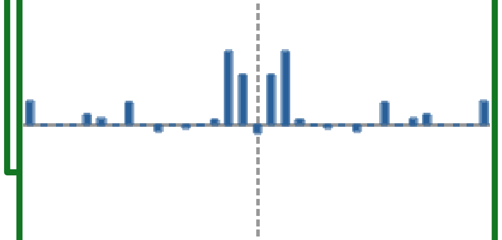
Summary



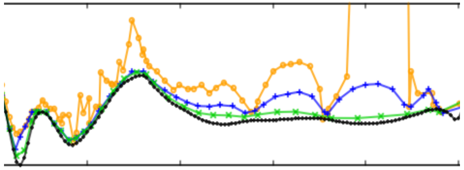
new SME approach to obtain scission flux

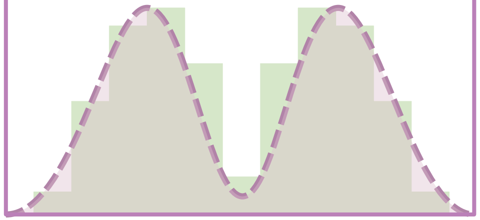
$$\hat{H}_C(\bar{q})G(\bar{q},t) = i\hbar\frac{d}{dt}G(\bar{q},t)$$

investigate unexpected initial results

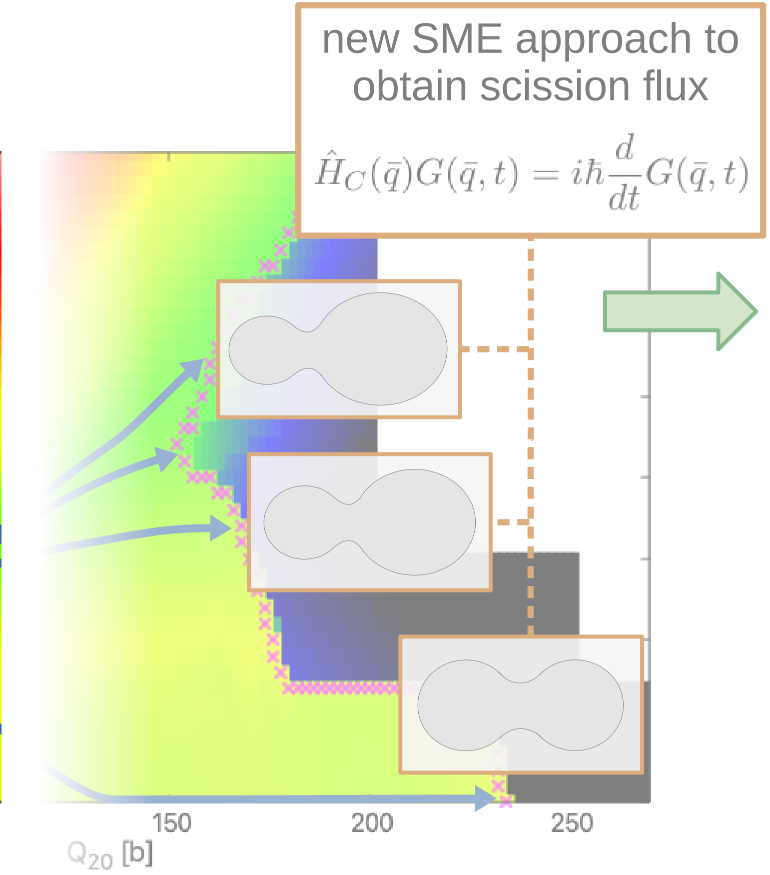


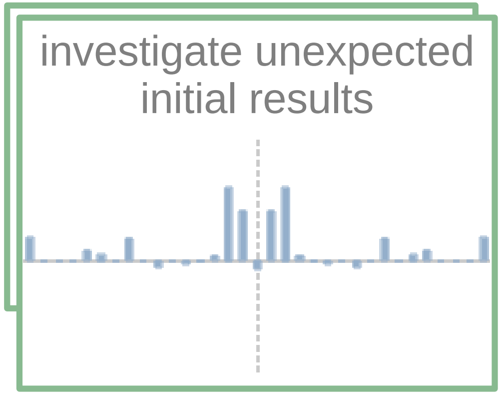
remove redundant basis states to lower overlaps

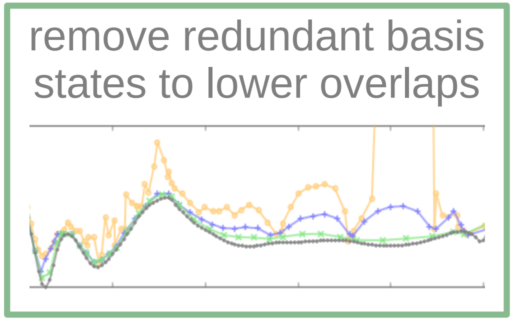


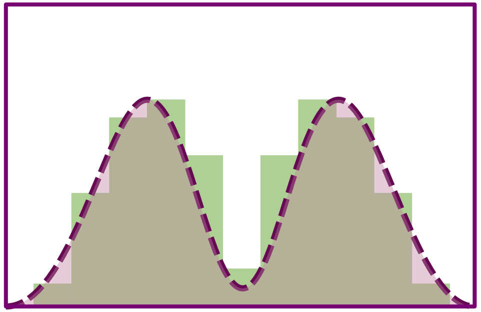


Summary

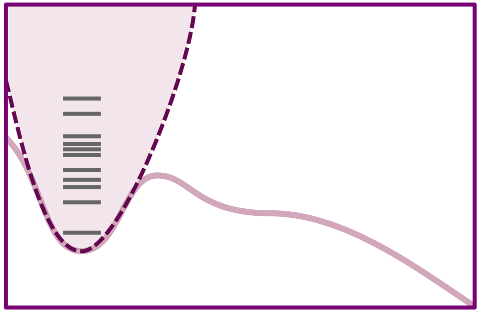






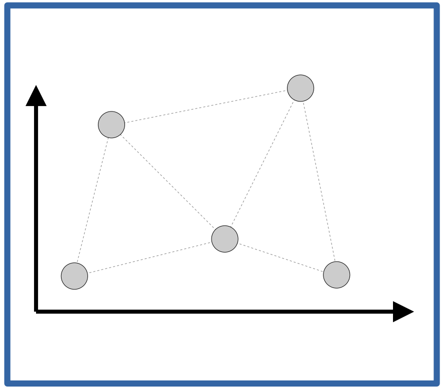


improvements with
projection techniques



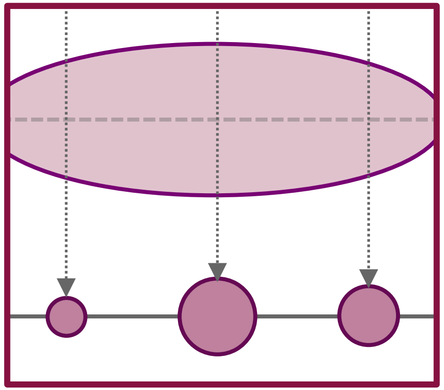
Future work

“Exact” TDGCM



- Realistic fission dynamics in 2D
- Generation of “sparse” 2D PESs

projection techniques



- Application to scission dynamics
- Description of spontaneous fission?*

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

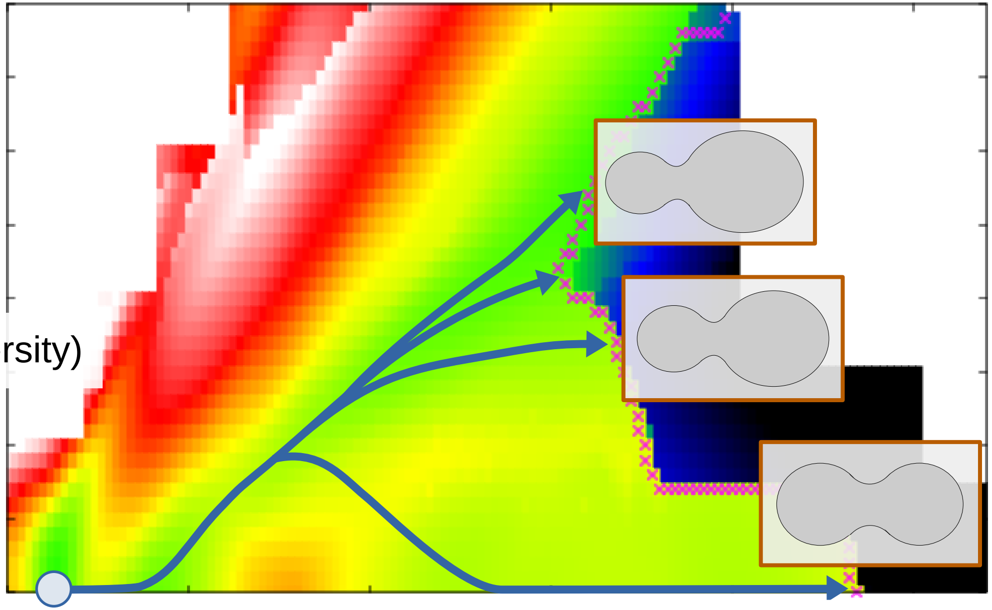
Thank you!

Postdoctoral supervisor (2024 –):

- Dr Guillaume Scamps (L2IT – IN2P3/CNRS)

Ph.D. supervisors (2021 – 2024):

- Prof. Cédric Simenel (Australian National University)
- Dr Rémi Bernard (CEA Cadarache)
- Dr Taiki Tanaka (GANIL)



Additional thanks to Prof. Luis Robledo (Universidad Autonoma de Madrid) for the use of HFBaxial and associated code