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

Ngee Wein Lau

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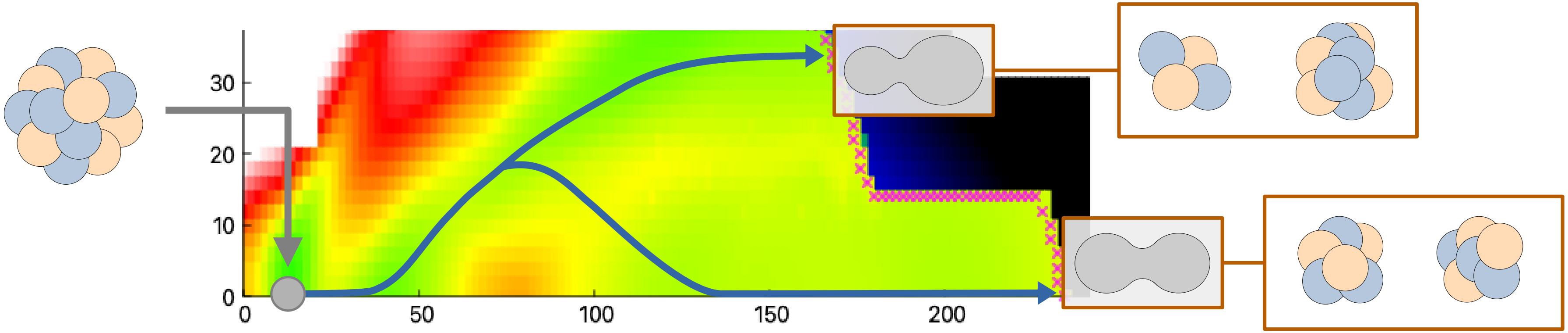


Acknowledgements

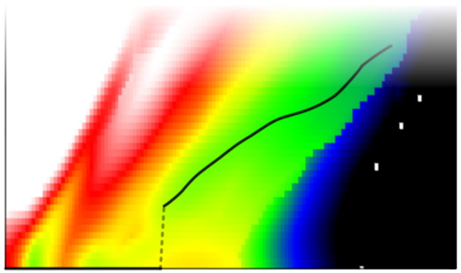
Ph.D. supervisory panel:
- Rémi Bernard – CEA Cadarache
- Cédric Simenel – Australian National University
- Taiki Tanaka – GANIL

Collaborators:
- Luis Robledo – Universidad Autonoma de Madrid

Project goals

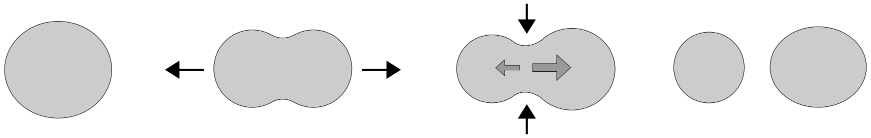
static nuclear model

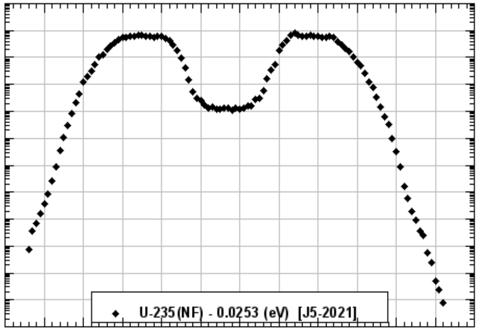
potential energy surfaces (PESs)



TDGCM

time-dependent generator coordinate method





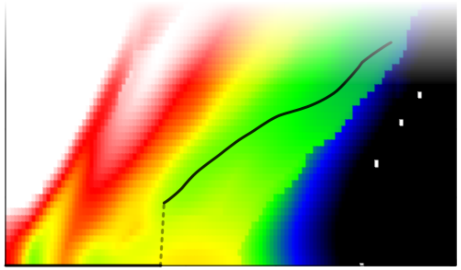
fission observables:

fragment masses
fragment charges
kinetic energies

Project goals

static nuclear model

potential energy surfaces (PESs)

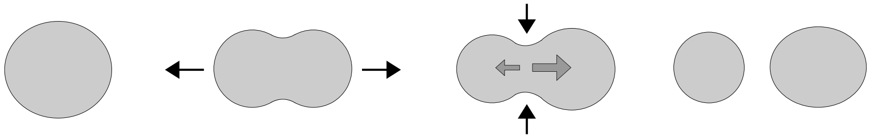


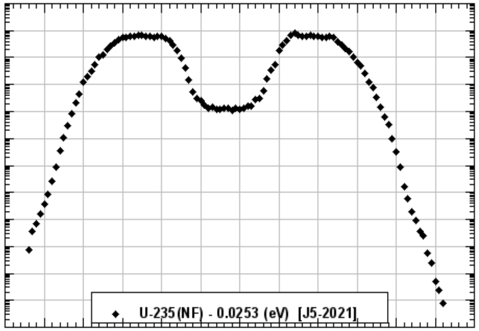
Gaussian overlap approximation

GOA

TDGCM

time-dependent generator coordinate method





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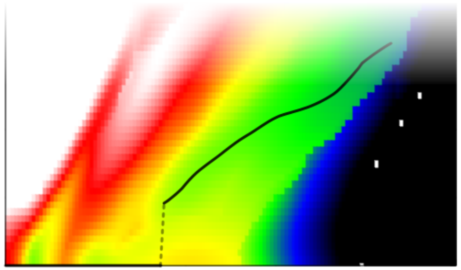
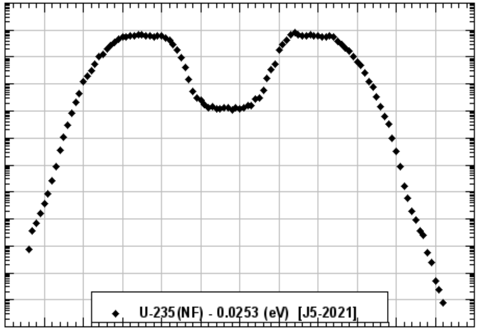


GOA

TDGCM

?



fission observables:

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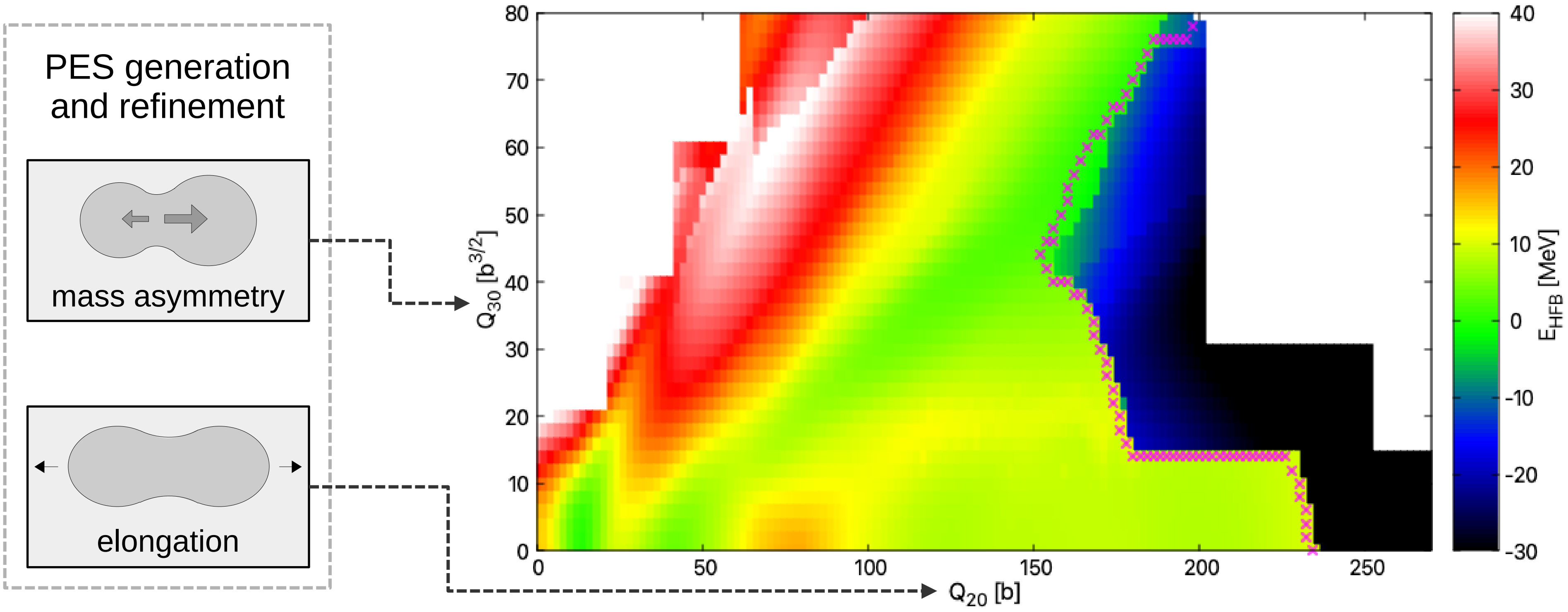
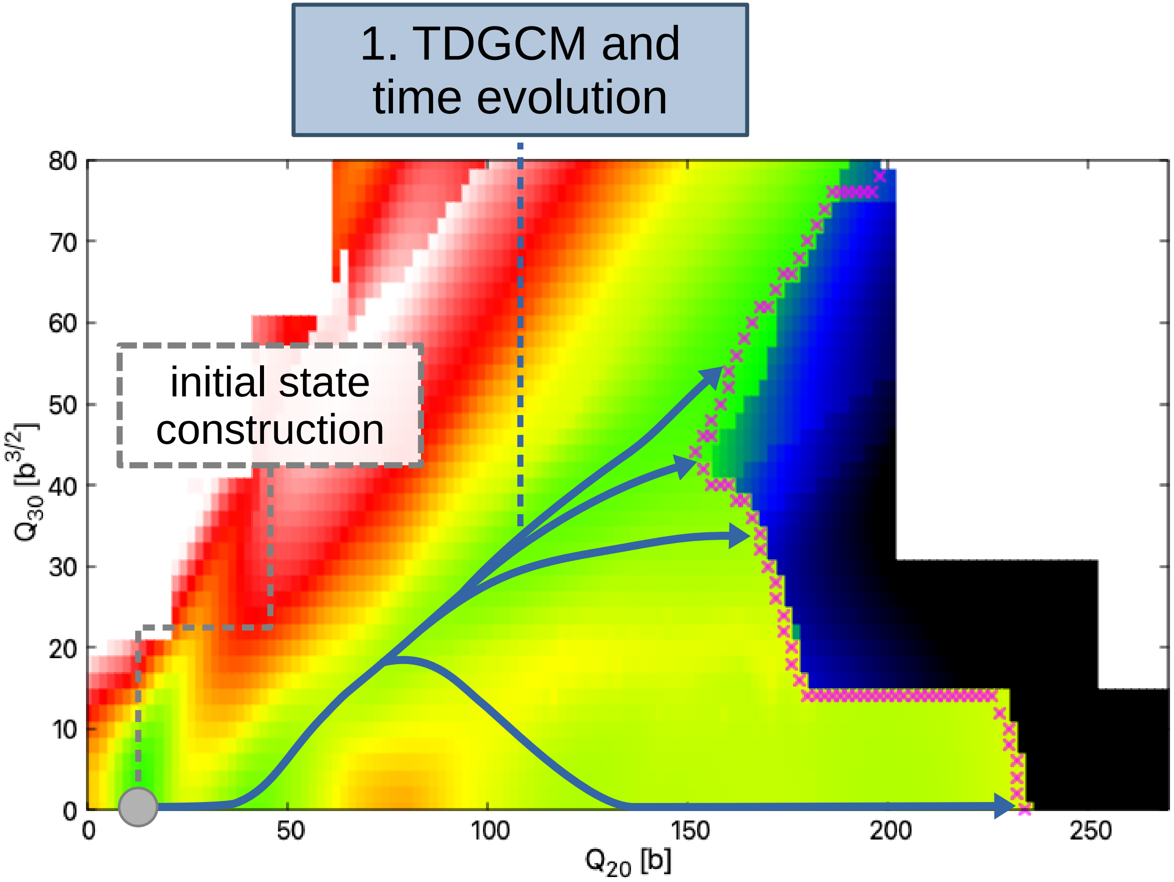
Goal: develop and implement a GOA-free TDGCM to produce an improved model of nuclear fission

A TDGCM description of fission



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

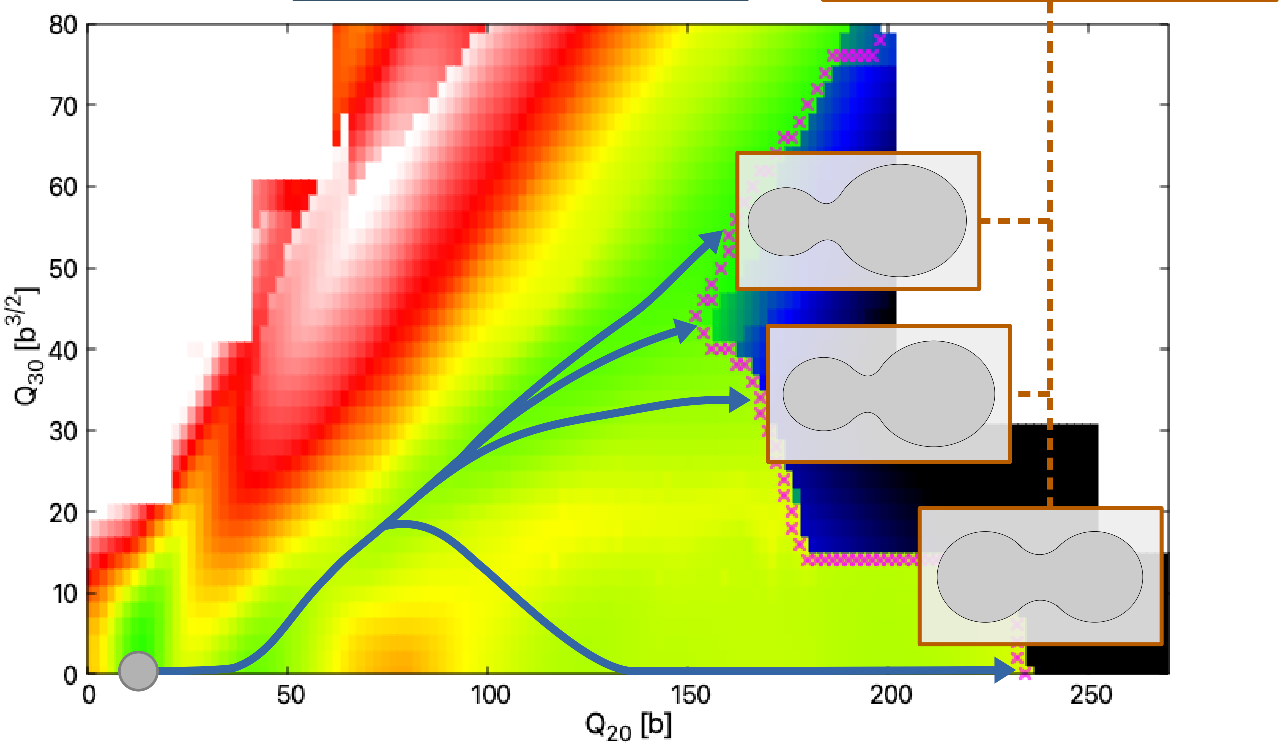
A TDGCM description of fission



A TDGCM description of fission

1. TDGCM and time evolution

2. Extracting fission observables

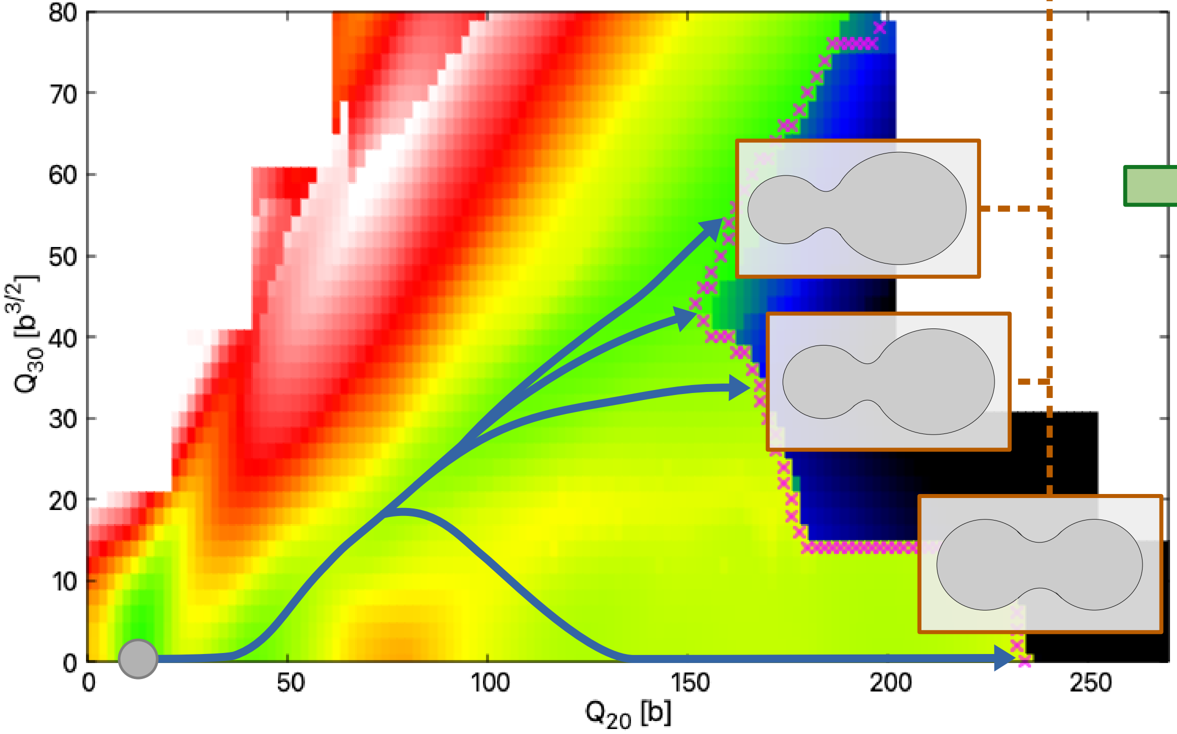


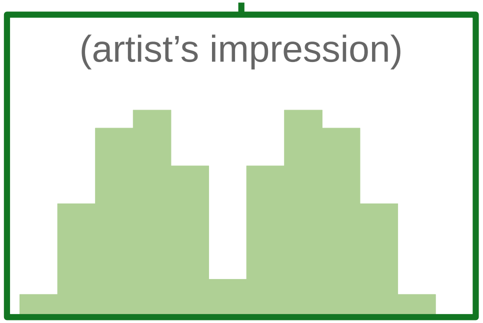
A TDGCM description of fission

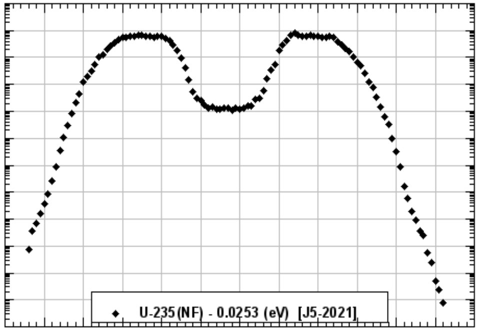
1. TDGCM and time evolution

2. Extracting fission observables

3. Interpreting and improving results



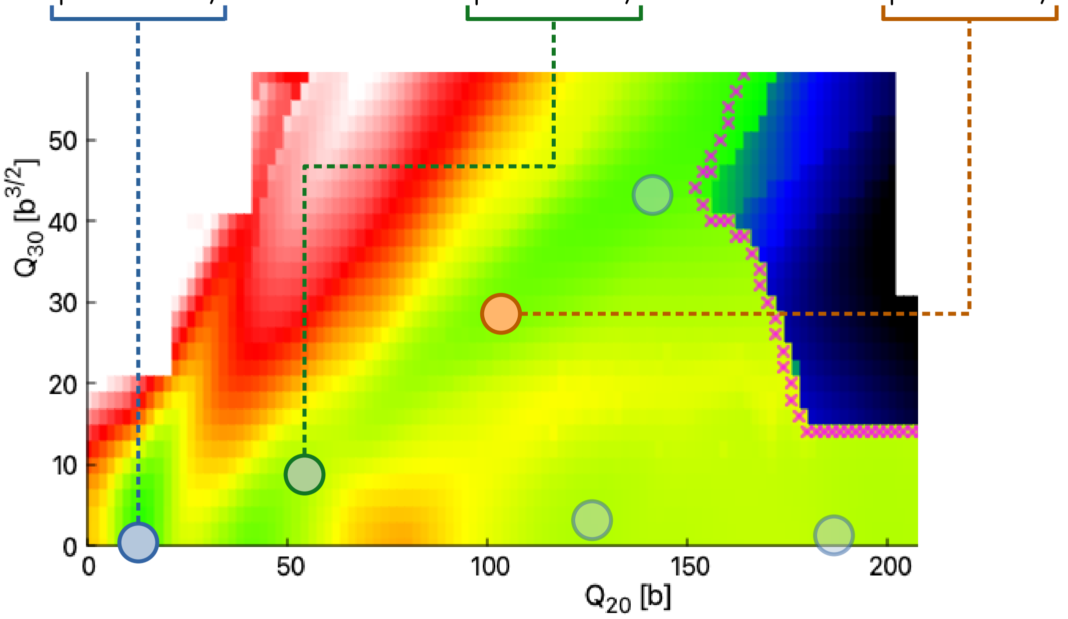




TDGCM

(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)

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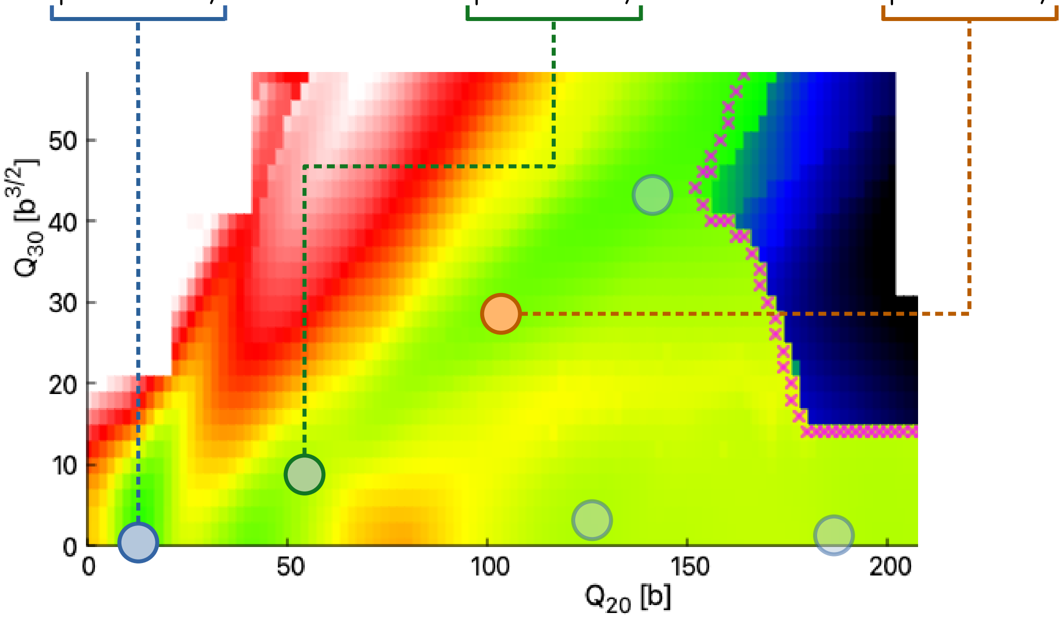
$f(\vec{\mathbf{q}}, t)$

weight function



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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

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

overlap kernel

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

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Exact solution of TDGCM

eigenvalues (positive real)

eigenvectors

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

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

“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

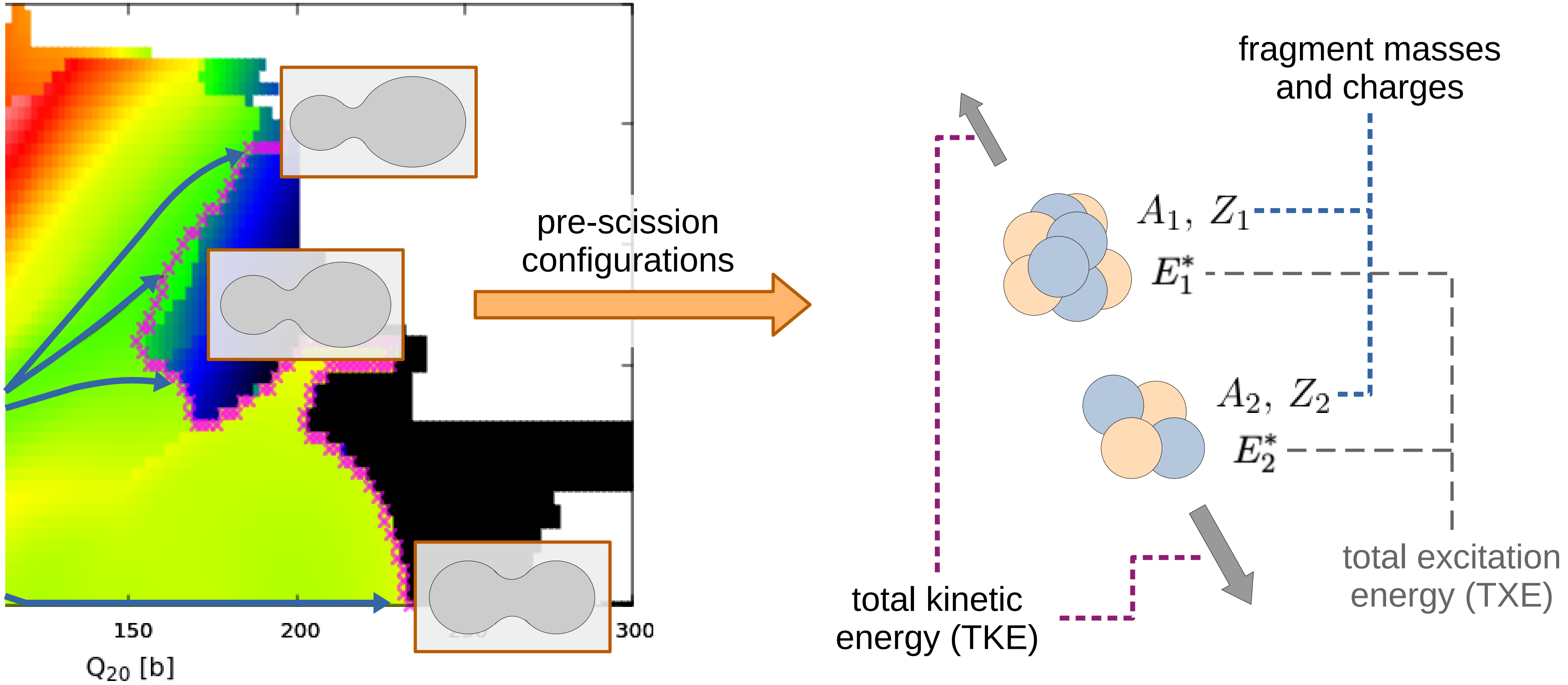
$$\sum_{k'} \left(\tilde{H}_{kk'} - i\hbar \delta_{kk'} \frac{d}{dt} \right) g_{k'}(t) = 0$$

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

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

Nonlocal Collective Schrödinger Equation (CSE)

Observables at the scission line

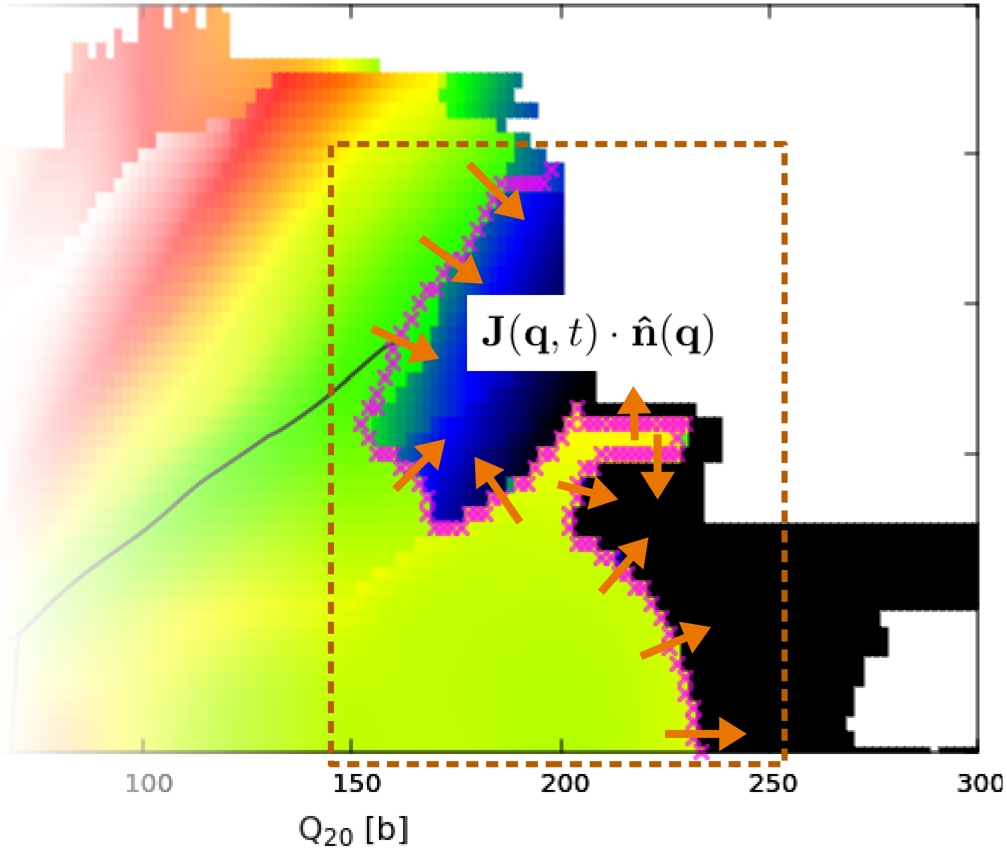


Observables at the scission line

probability flux

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

probability current



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

Observables at the scission line

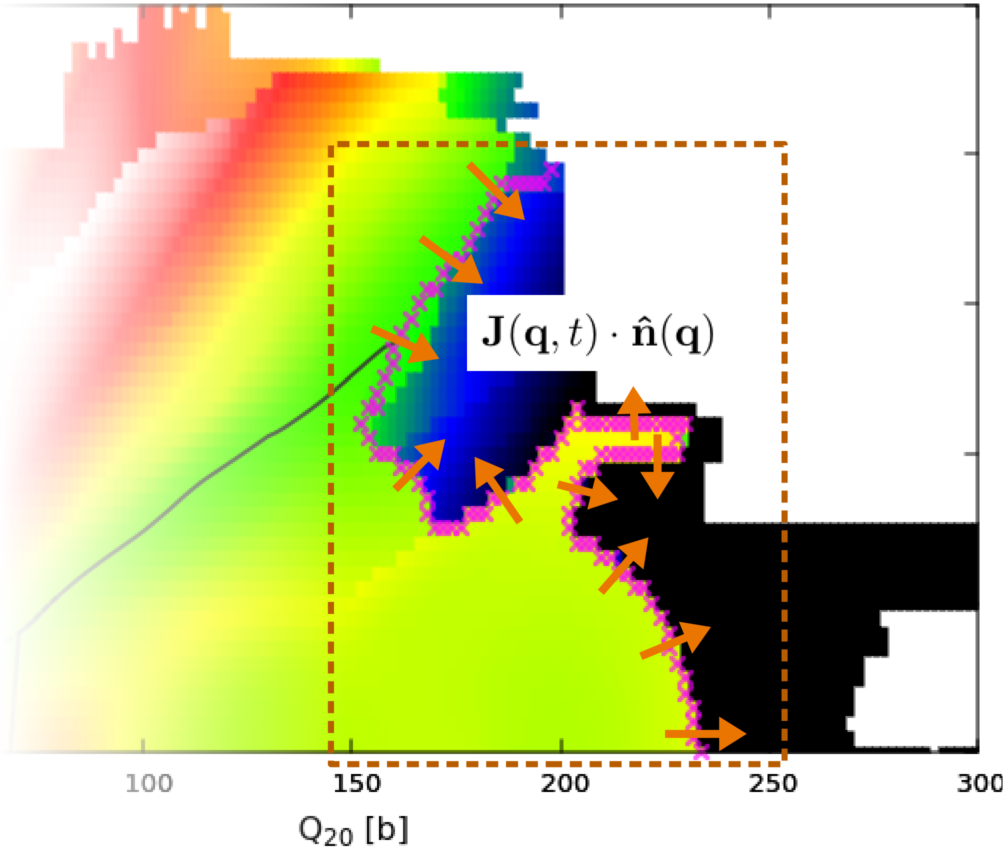
probability flux

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

probability current

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

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 CSE

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

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

probability current

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Observables at the scission line

local continuity equation

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

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

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

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

“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)

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

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

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

2) Rederive a nonlocal CSE

SME basis transformation
change of coordinates
Taylor expansion

3) Use expansion techniques to produce a local CSE

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

symmetrised Hill-Wheeler equation

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

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

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

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

Symmetric Moment Expansion (SME)

symmetrised Hill-Wheeler equation

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

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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

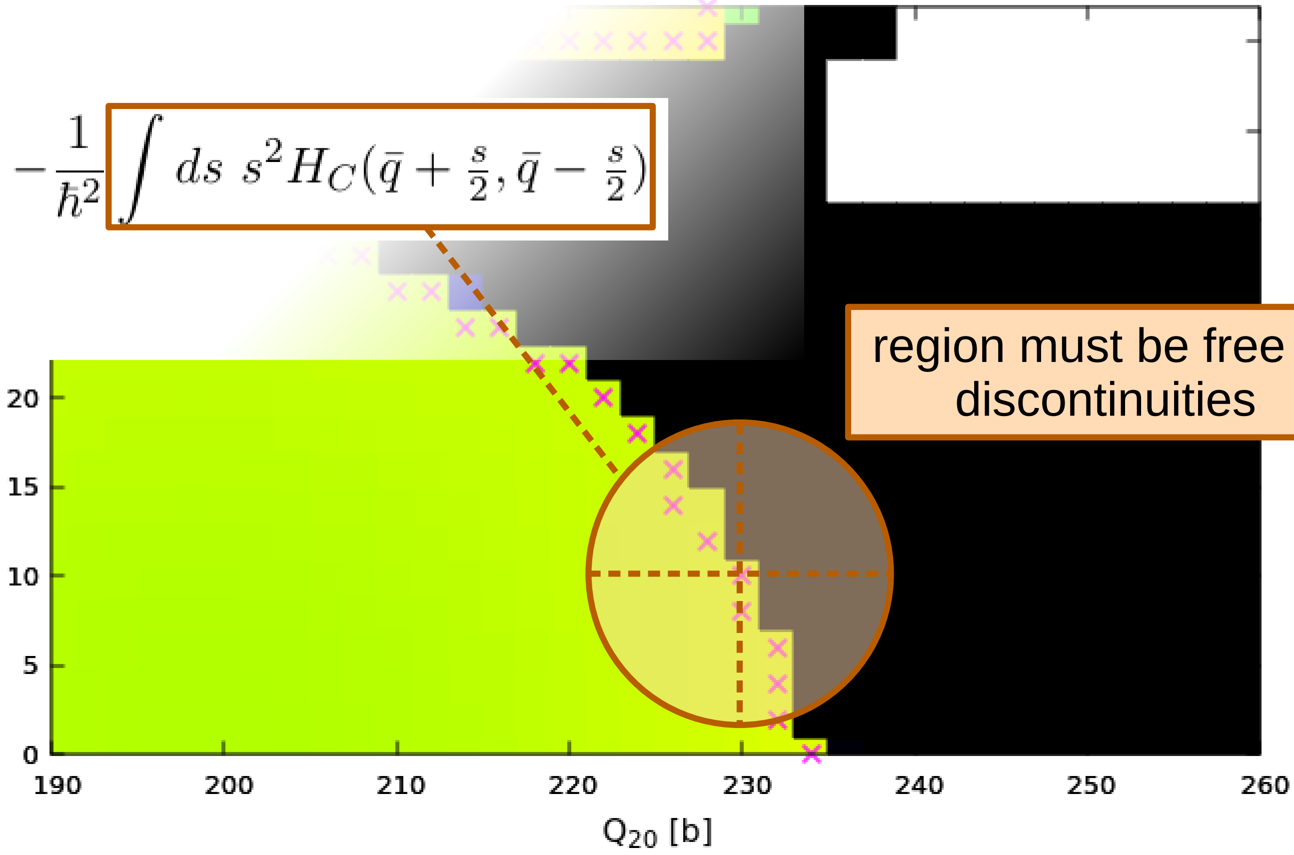
$$\hat{H}_C(\bar{q})G(\bar{q},t) = i\hbar\frac{d}{dt}G(\bar{q},t)$$

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

probability current

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

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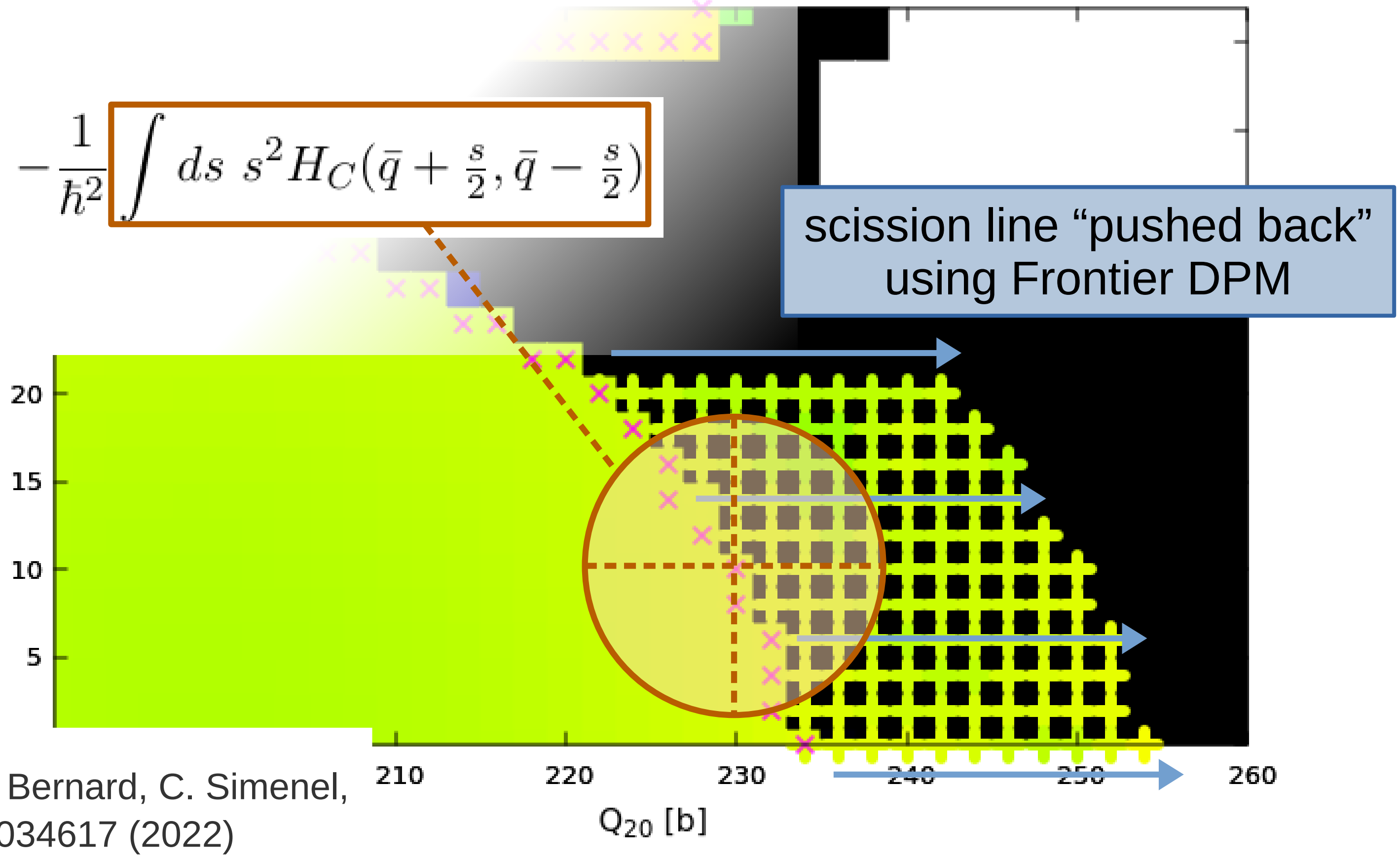

N.-W. T. Lau, R. N. Bernard, C. Simenel, *Phys. Rev. C* **105**, 034617 (2022)

Practicalities of flux calculations

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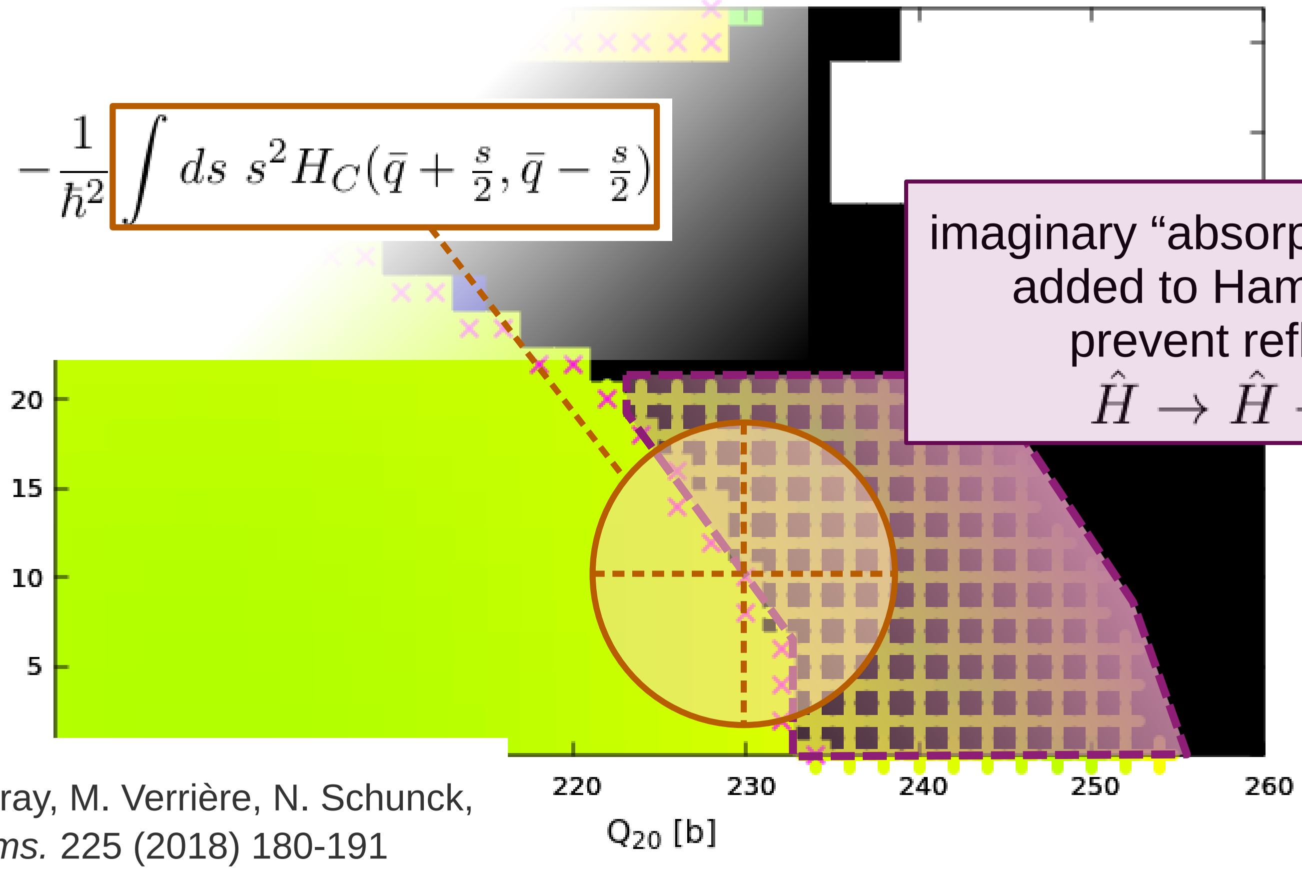

imaginary "absorption potential" added to Hamiltonian to prevent reflections

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

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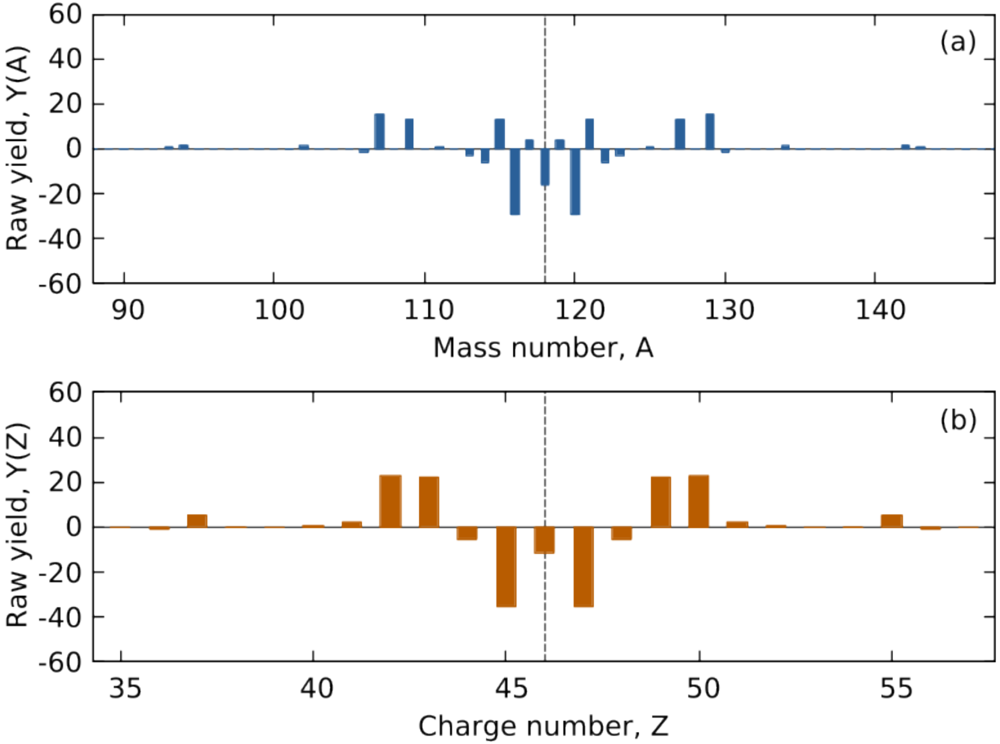
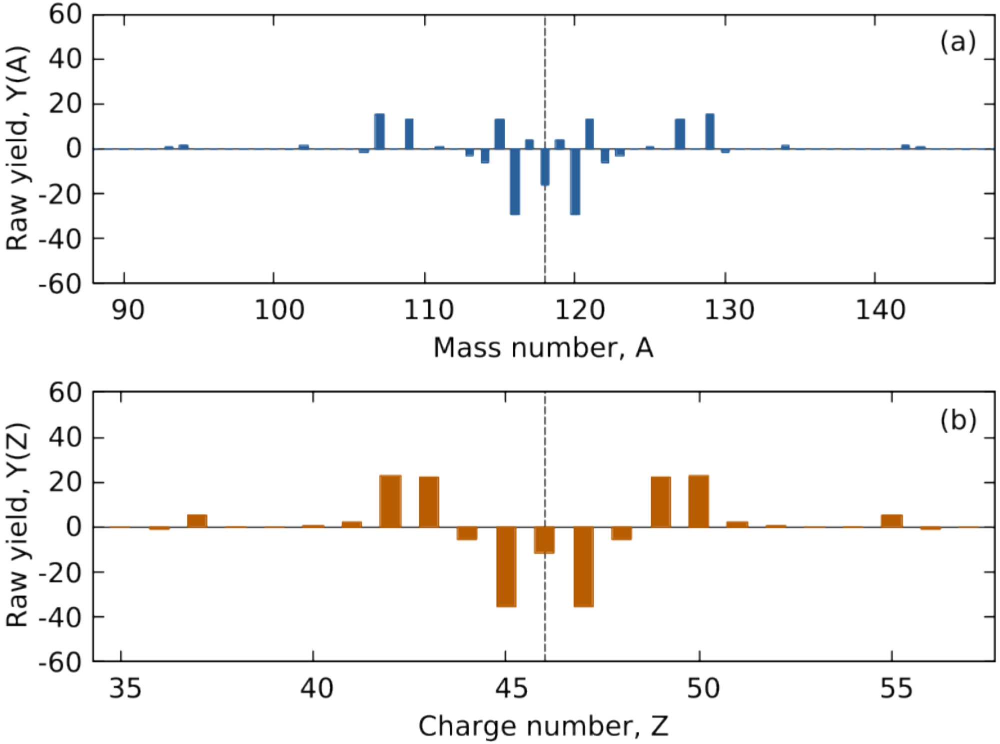
2D fission outcomes – ^{236}U



no absorption field

2D fission outcomes – ^{236}U



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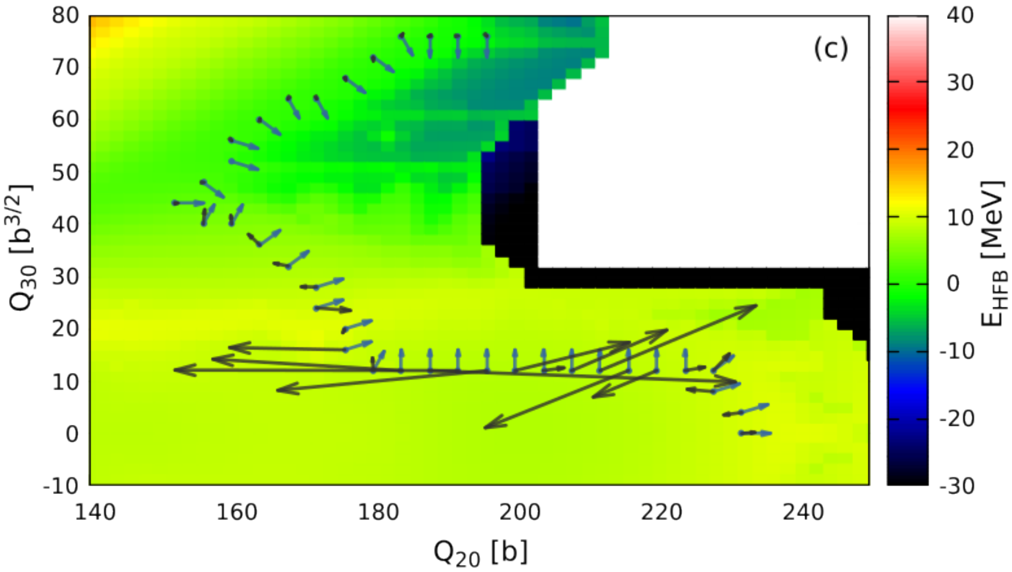
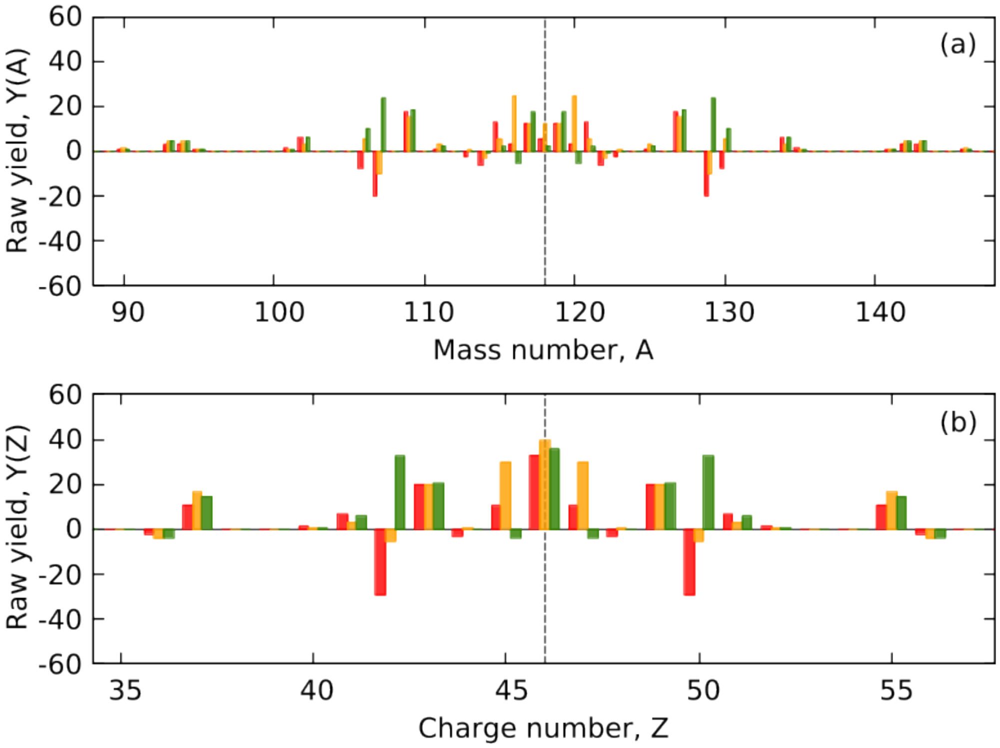
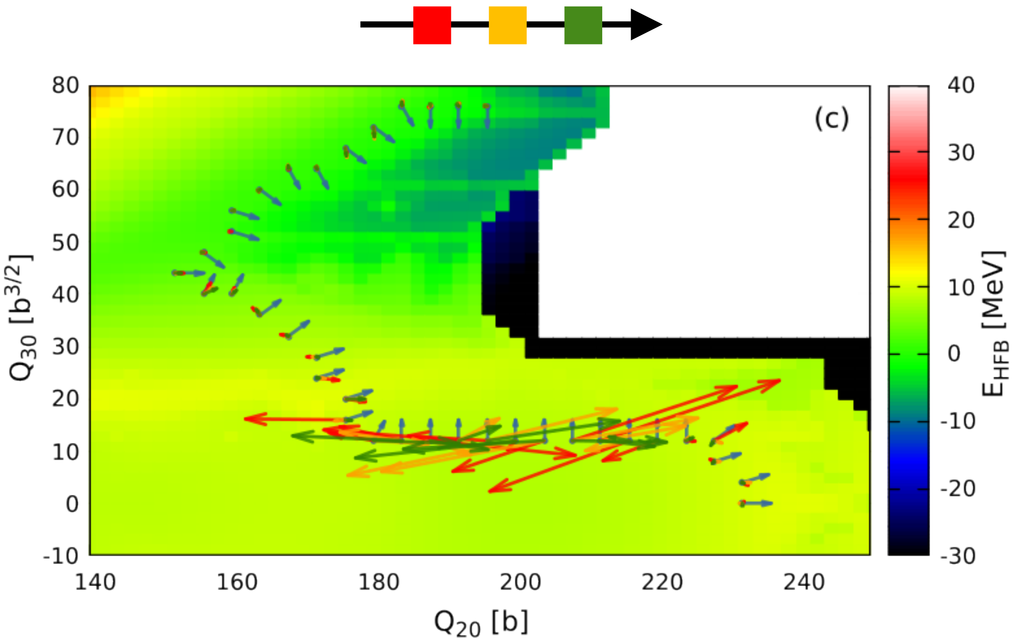


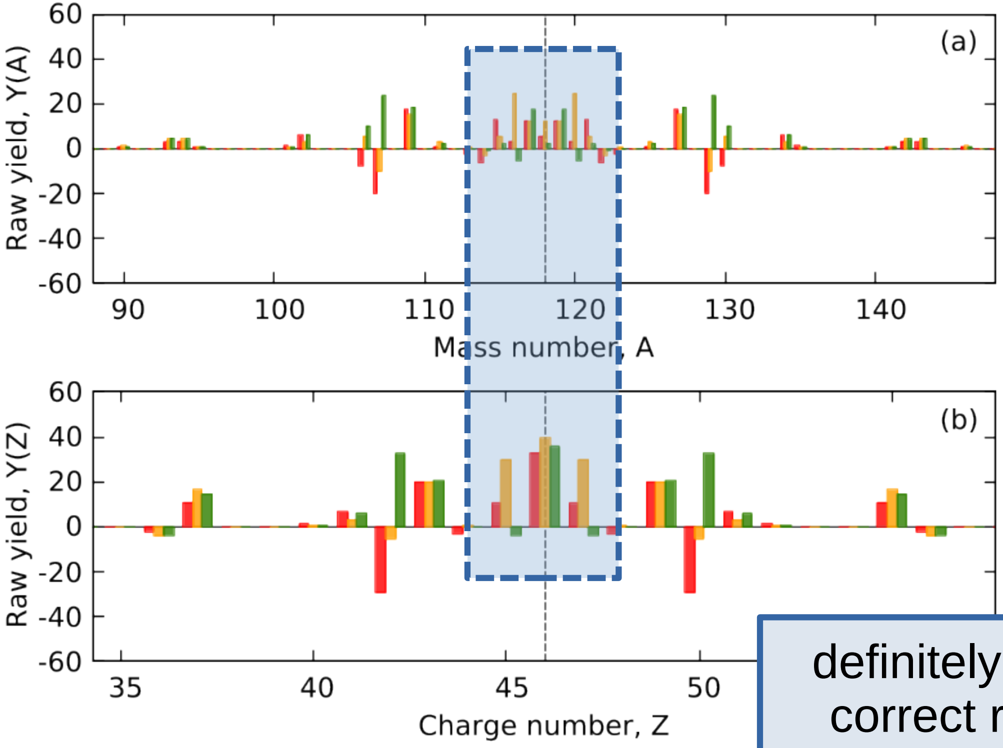
2D fission outcomes – ^{236}U



increasing absorption strength



2D fission outcomes – ^{236}U



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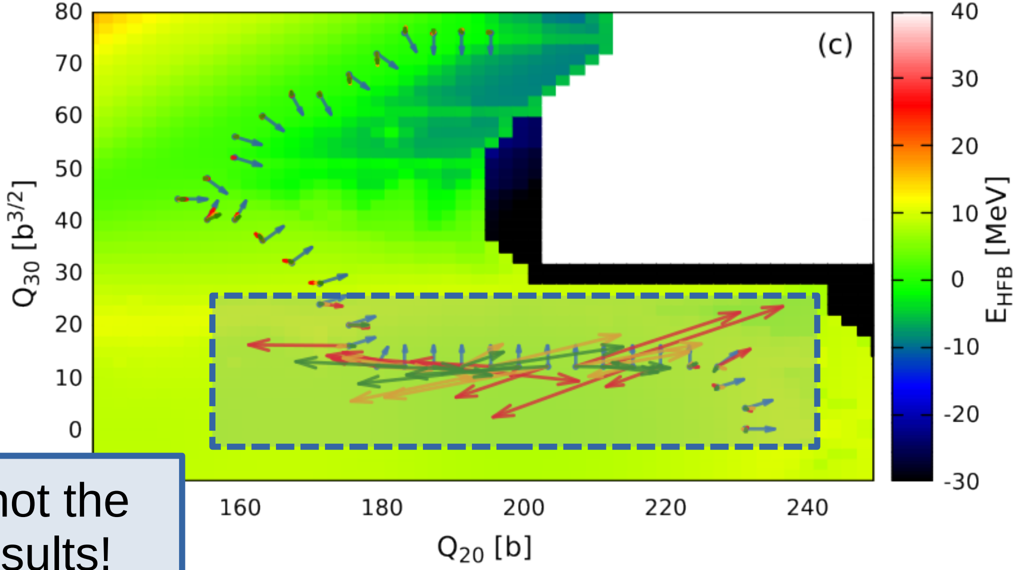
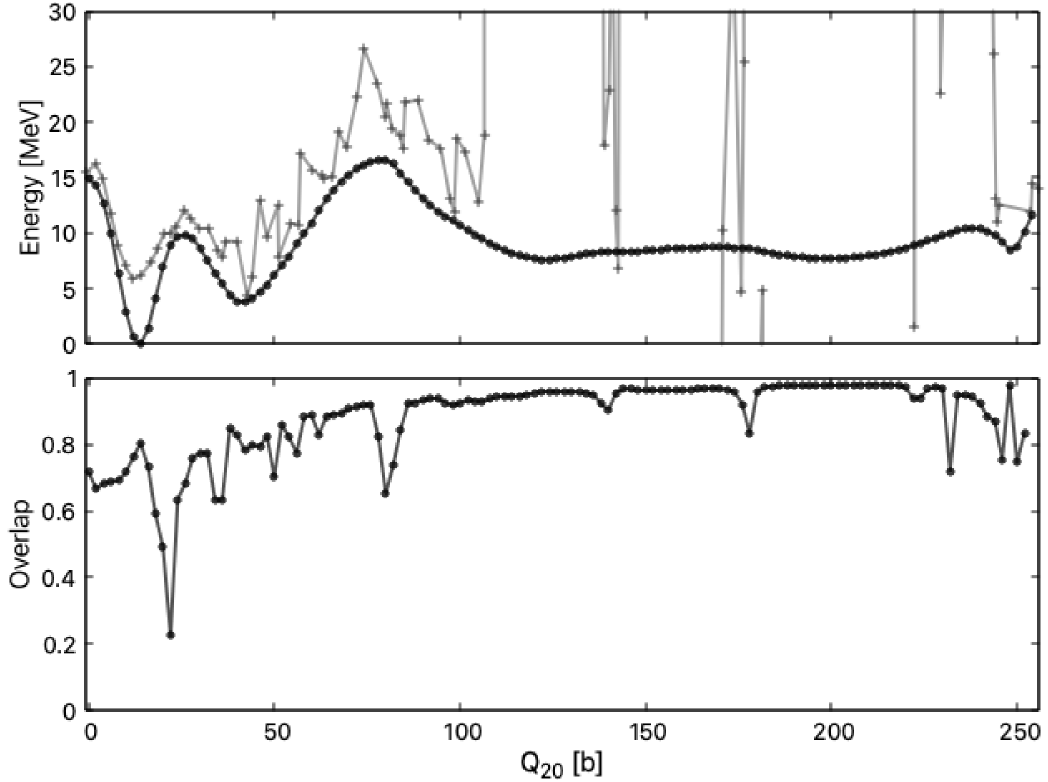


definitely not the correct results!

What now?

Testing behaviour with Gaussian overlaps



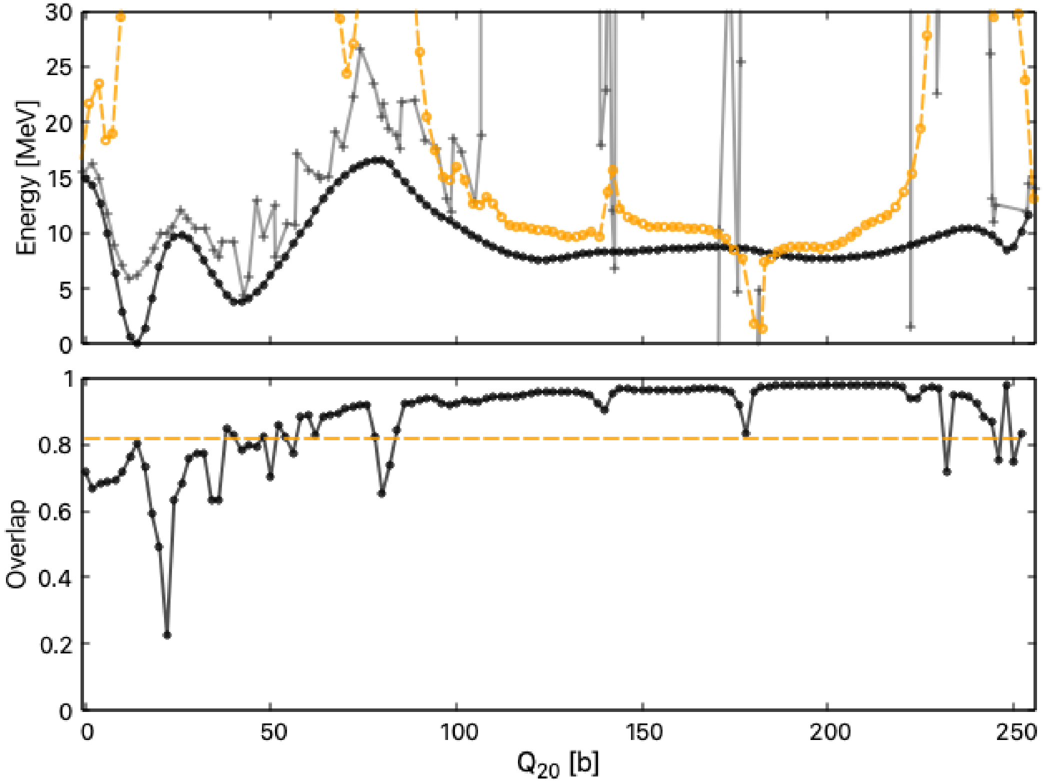
Original PES

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

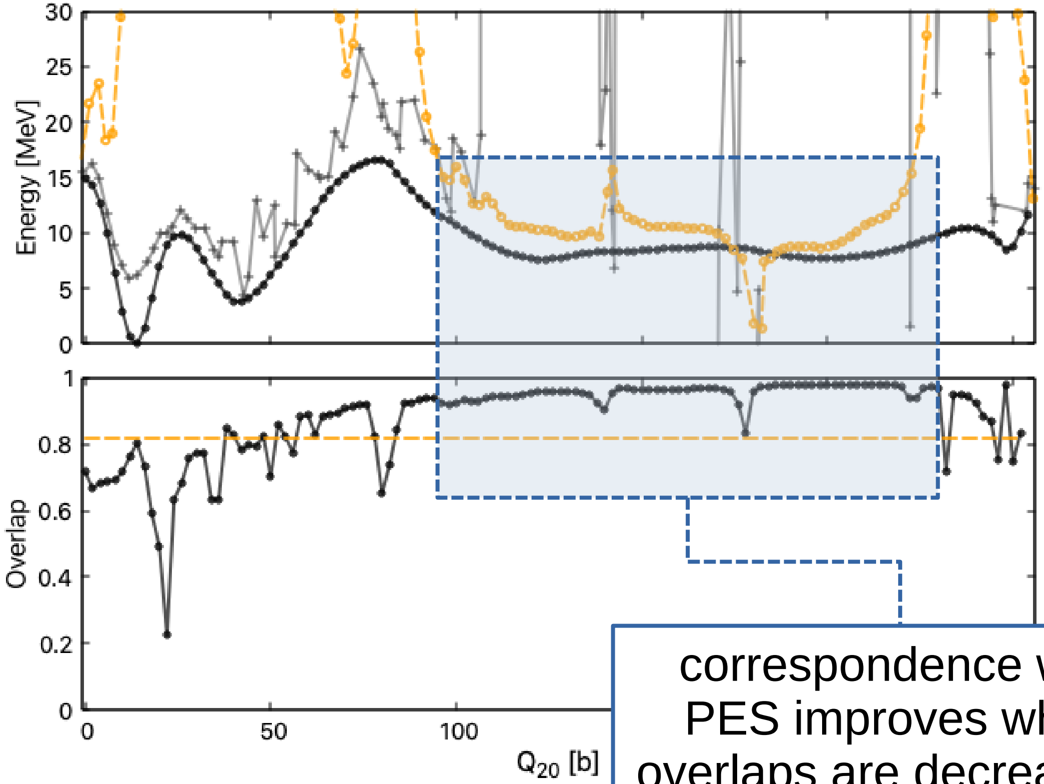
SME states:

■ Full HFB basis (original overlaps)

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

What now?

Testing behaviour with Gaussian overlaps



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

Original PES

SME states:

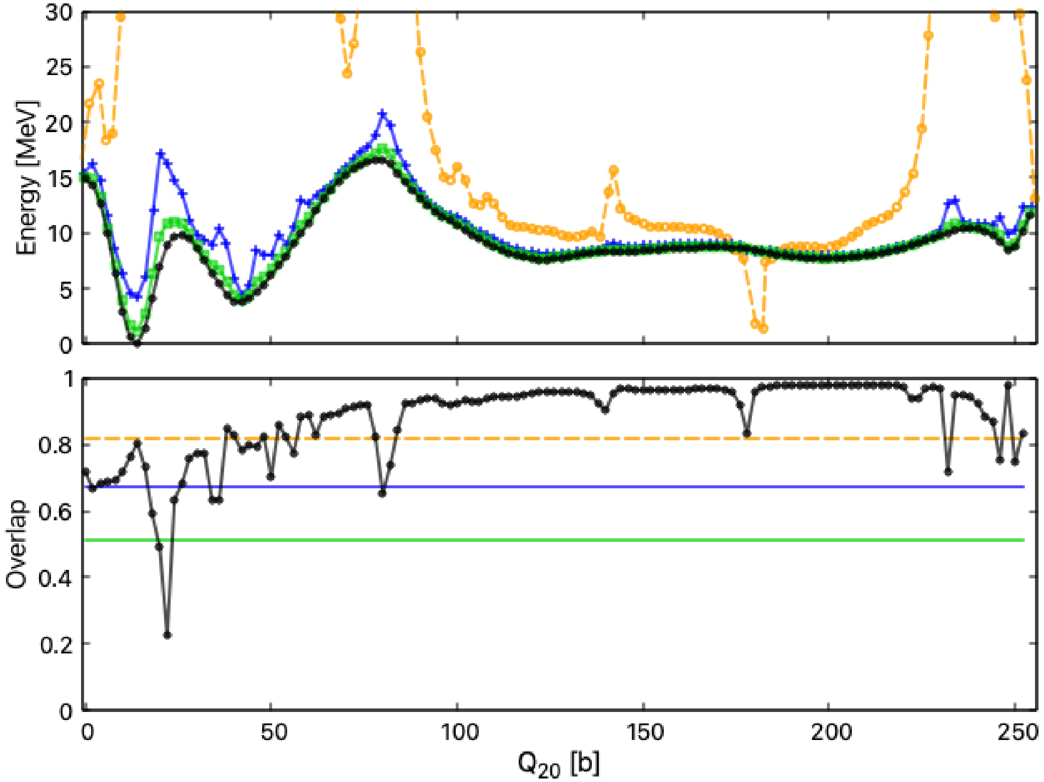
Full HFB basis
(original overlaps)

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

correspondence with
PES improves when
overlaps are decreased?

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?

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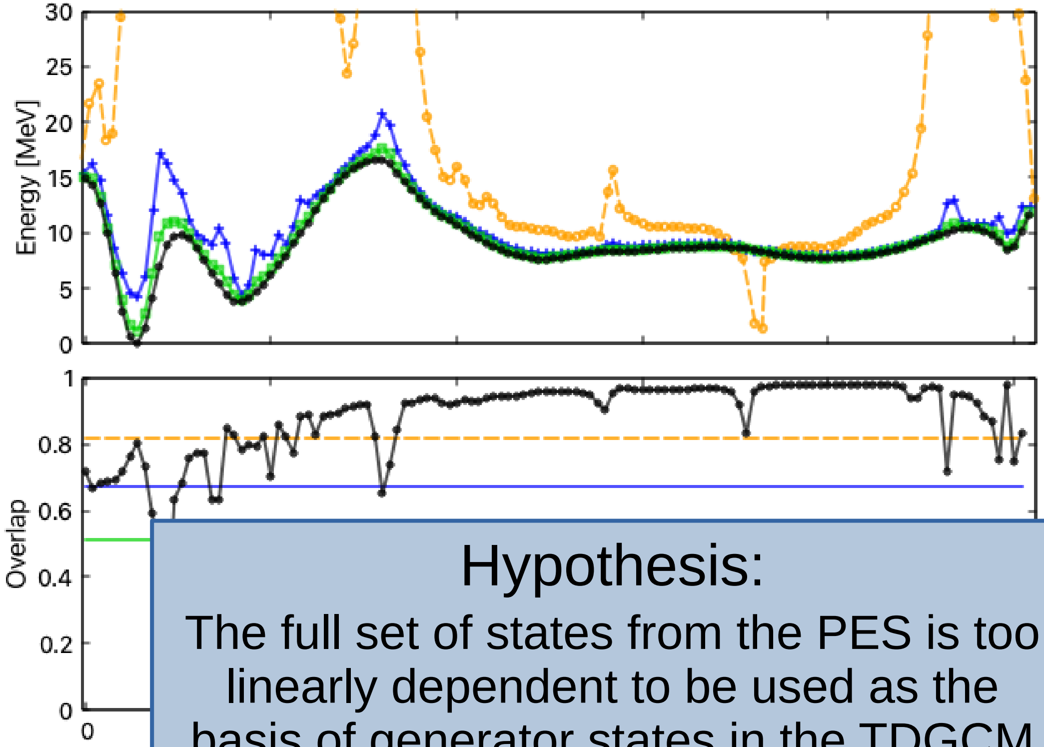

Hypothesis:

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

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

- Original PES

SME states:

- GOA overlaps with width $2\sigma^2 = 20$
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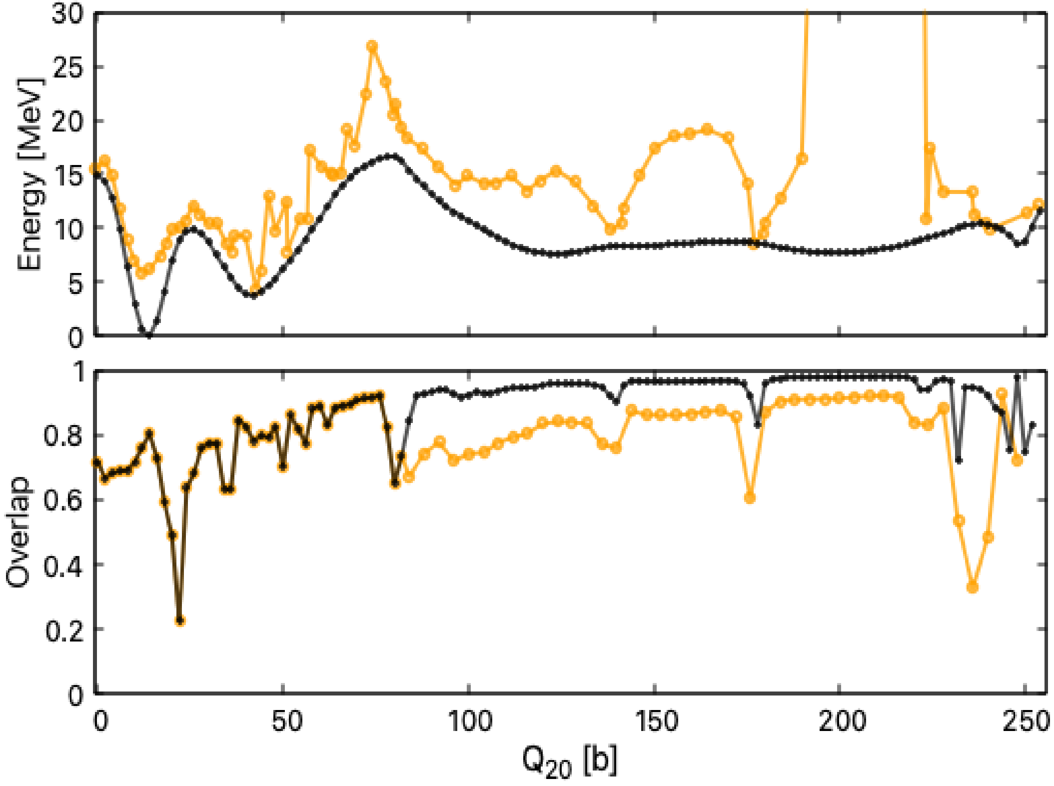
Effects of reducing basis size

1D symmetric fission path of ^{236}U



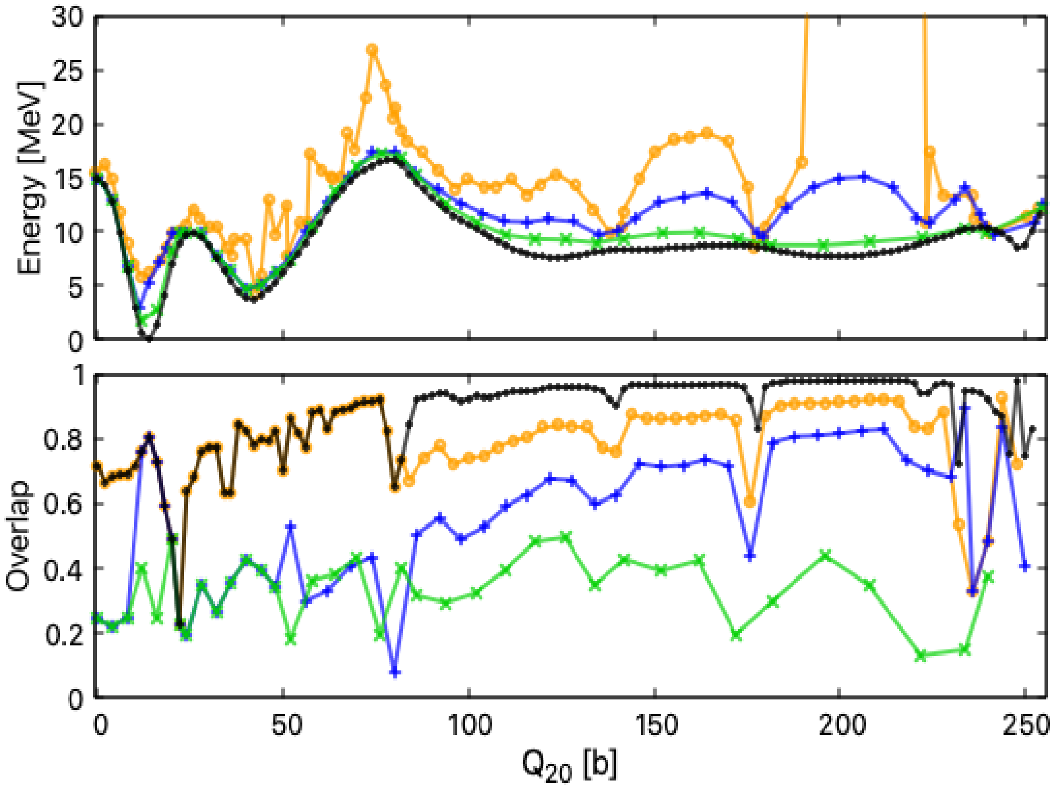
■ Original PES in HFB basis (128 states)

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:

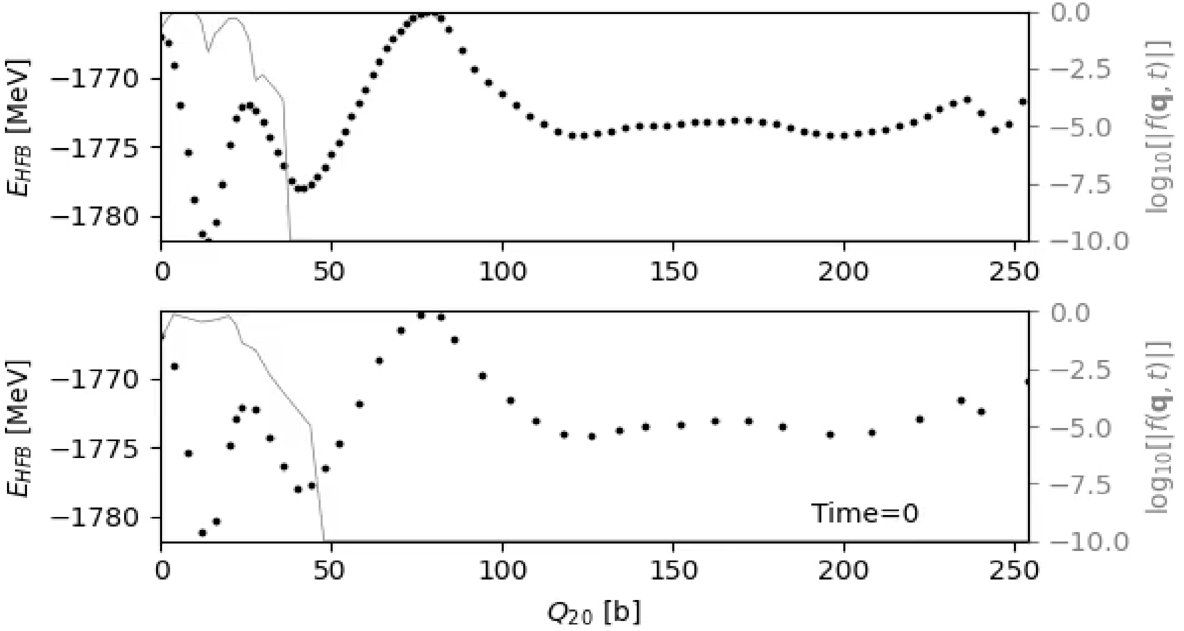
- Doubled mesh after saddle "1s2s" (85 states)
- Manually selected mesh (53 states)
- Manually selected mesh (38 states)

Effects of reducing basis size

1D symmetric fission path of ^{236}U

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

Manually selected mesh
(38 states)



Effects of reducing basis size

1D symmetric fission path of ^{236}U

Doubled mesh after saddle
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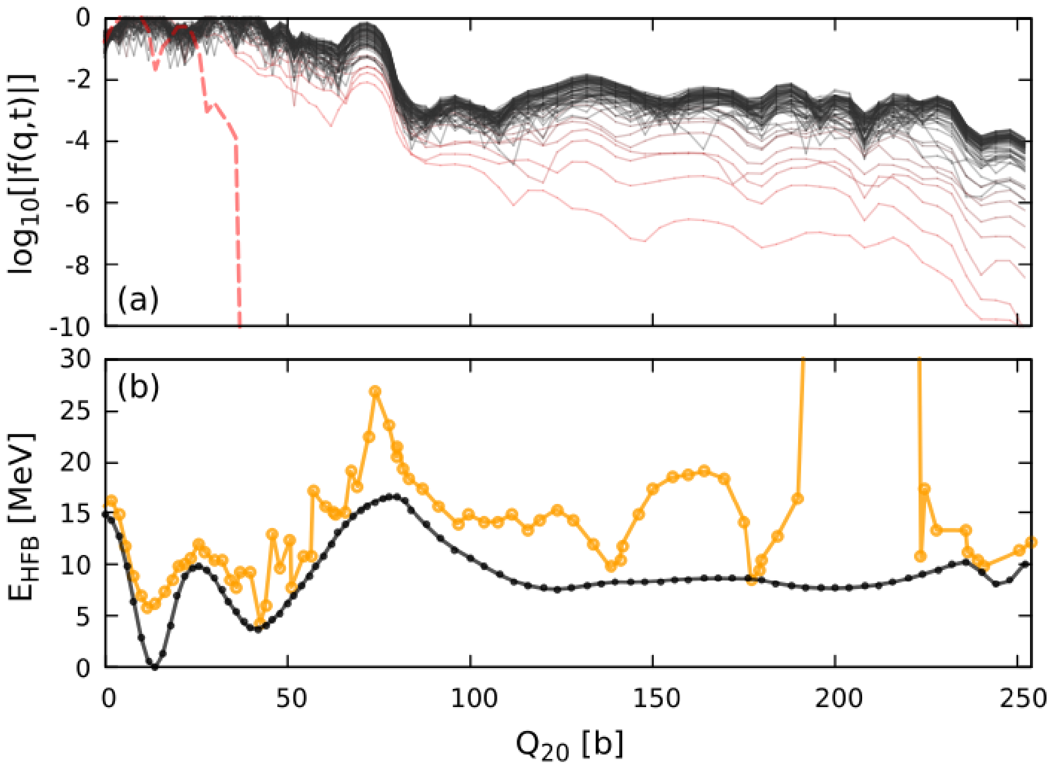
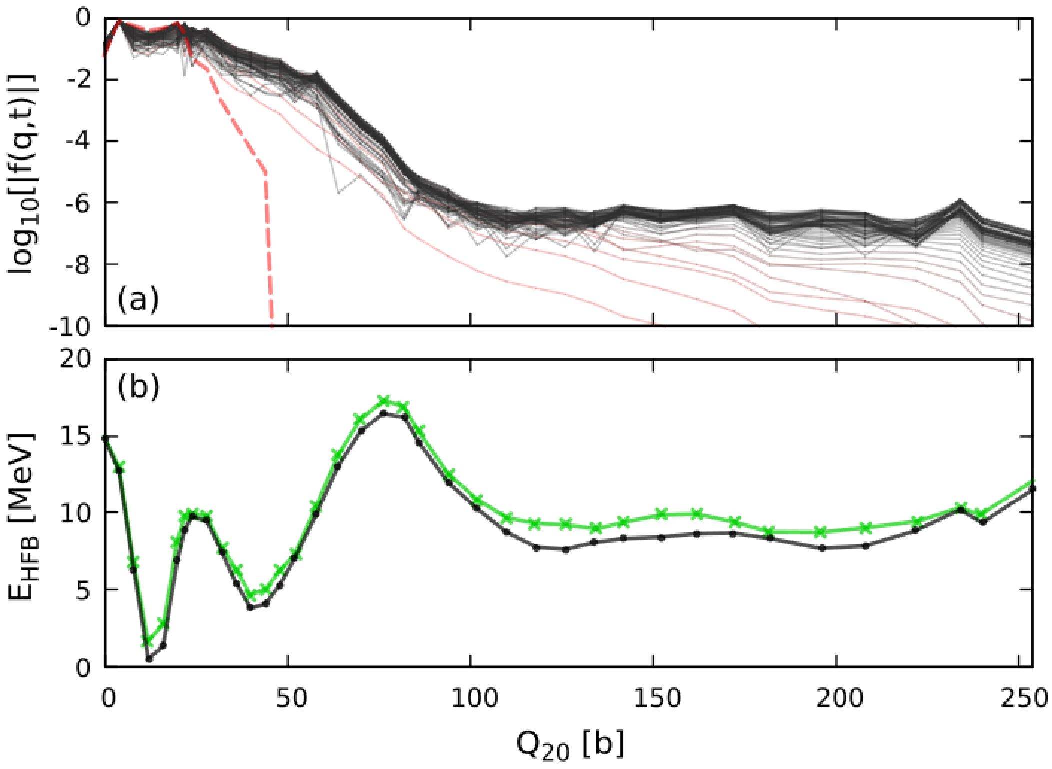


Effects of reducing basis size

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.

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

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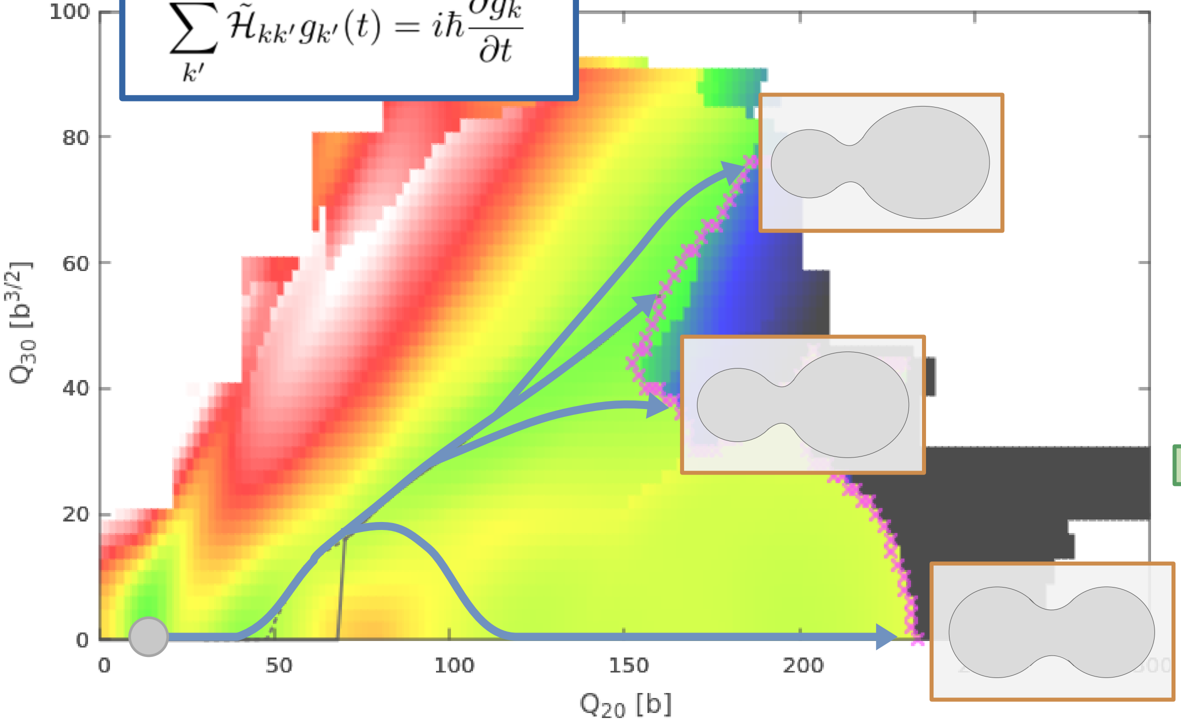
- How can this process be generalised to two dimensions?

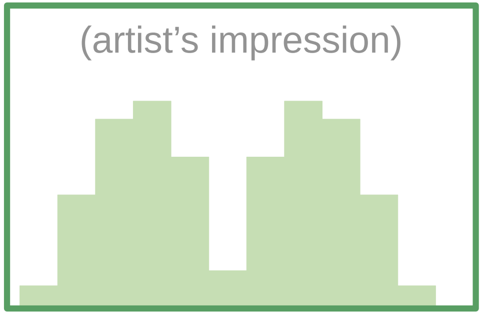
*P. Carpentier, N. Pillet, D. Lacroix, N. Dubray, D. Regnier, *Physical Review Letters* **133**, 152501 (2024)

Summary

dynamics from exact TDGCM formalism

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





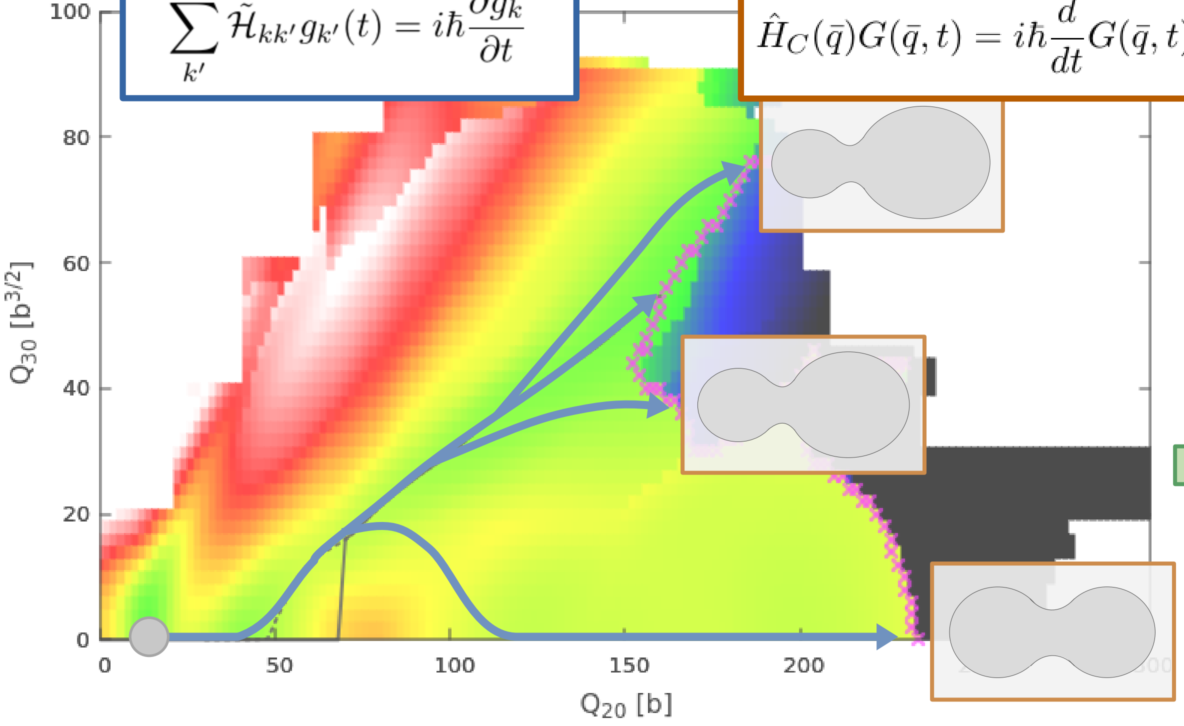
Summary

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

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



(artist's impression)

Summary

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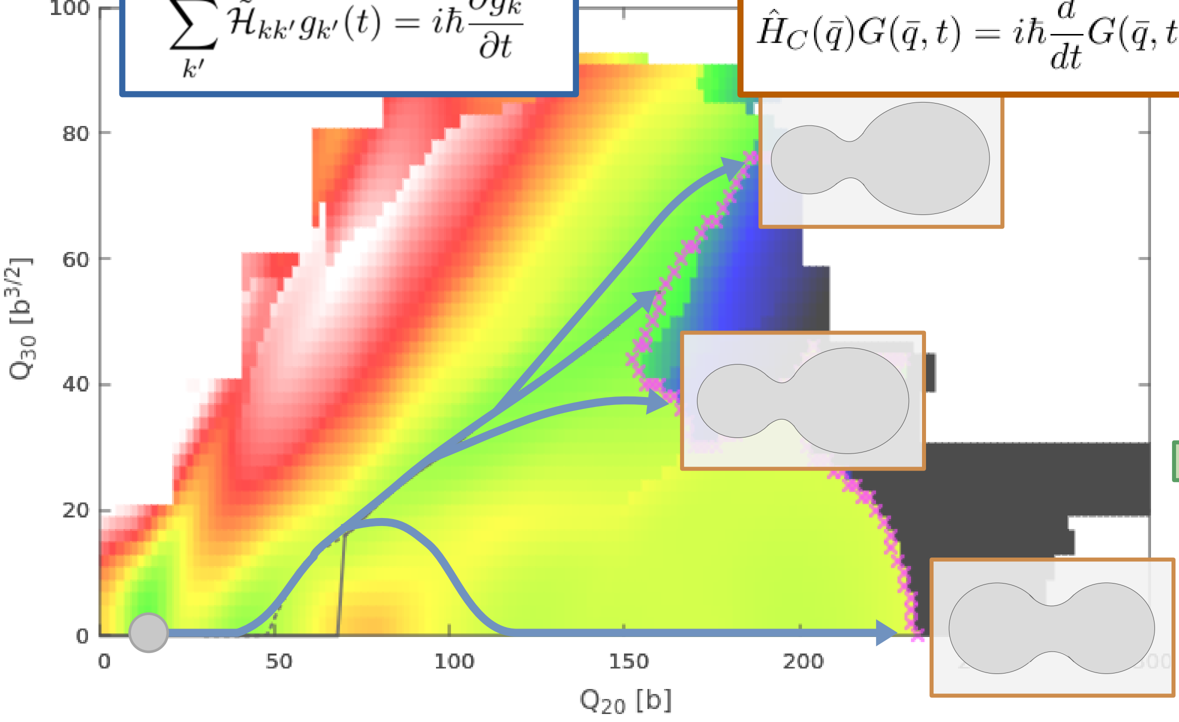
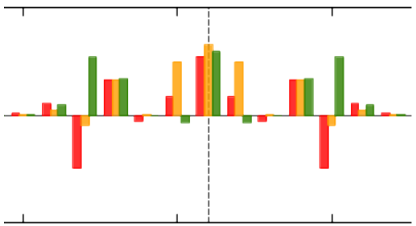


investigate unexpected initial results



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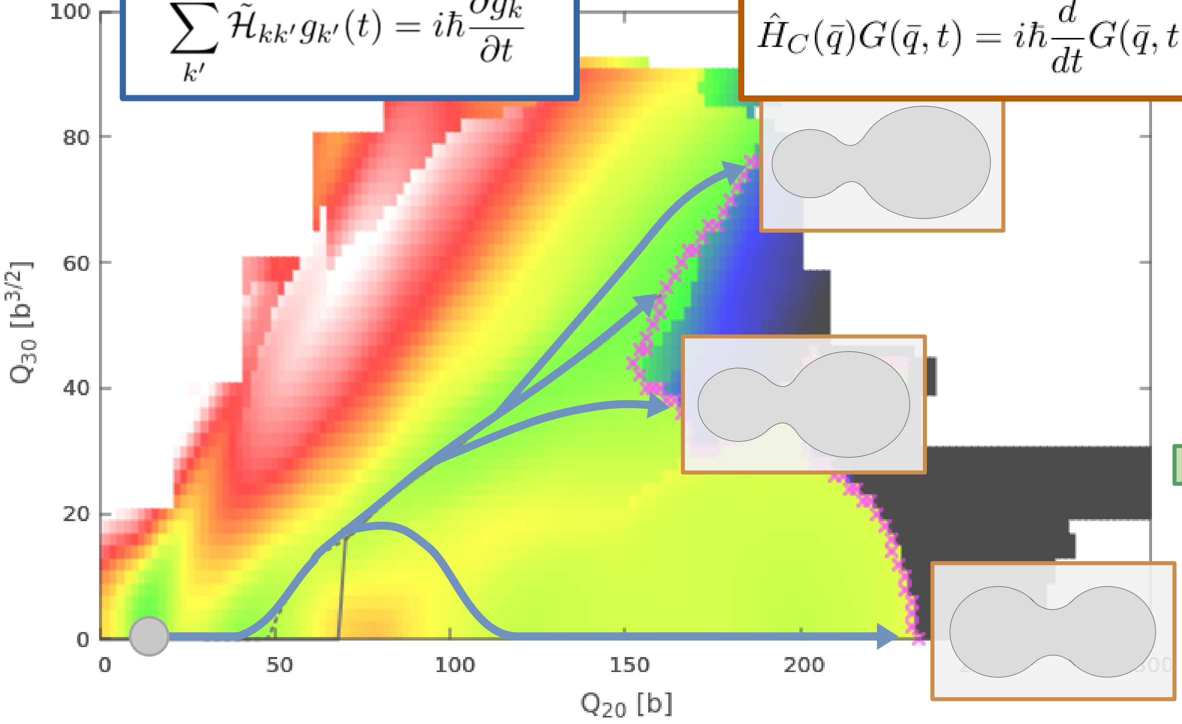
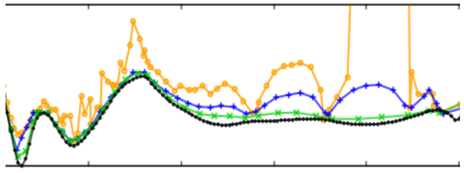


remove redundant basis states to lower overlaps



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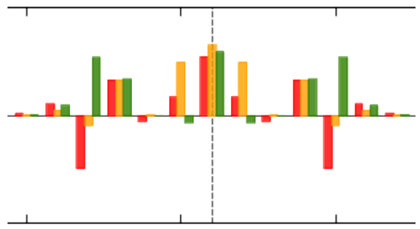
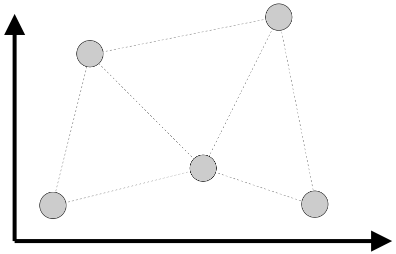
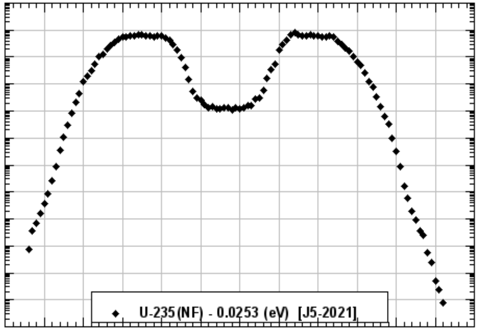


Future research

generation of
sparse 2D PESs



accurate fission yields
(hopefully!)

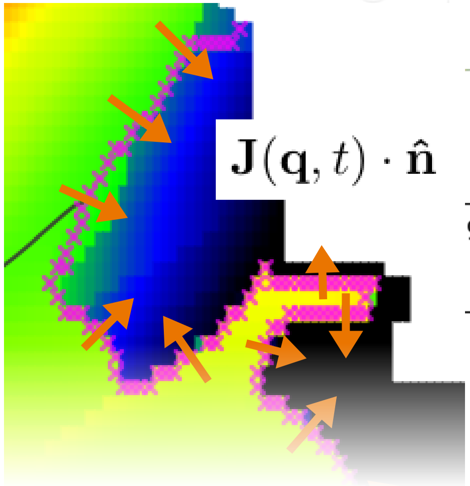


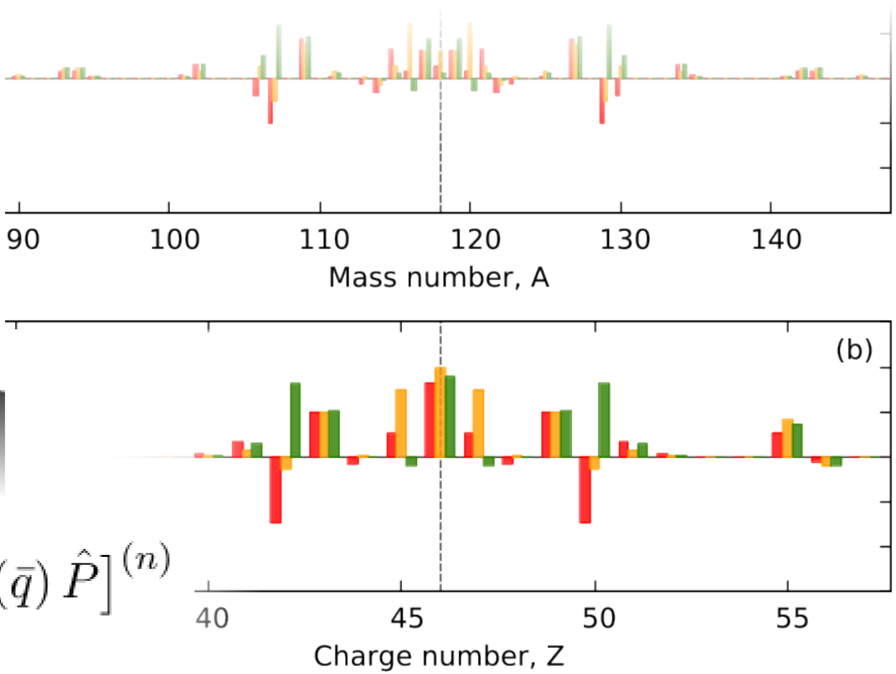
Extensions:

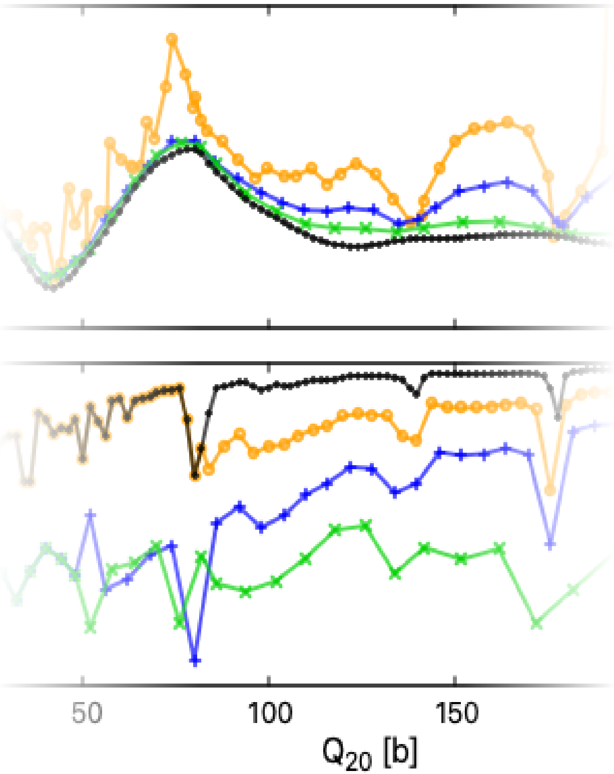
- Restoration of broken symmetries (VAP)
- Generalisation to higher dimensions

Questions?

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







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