Probing the fluctuation of fission observables

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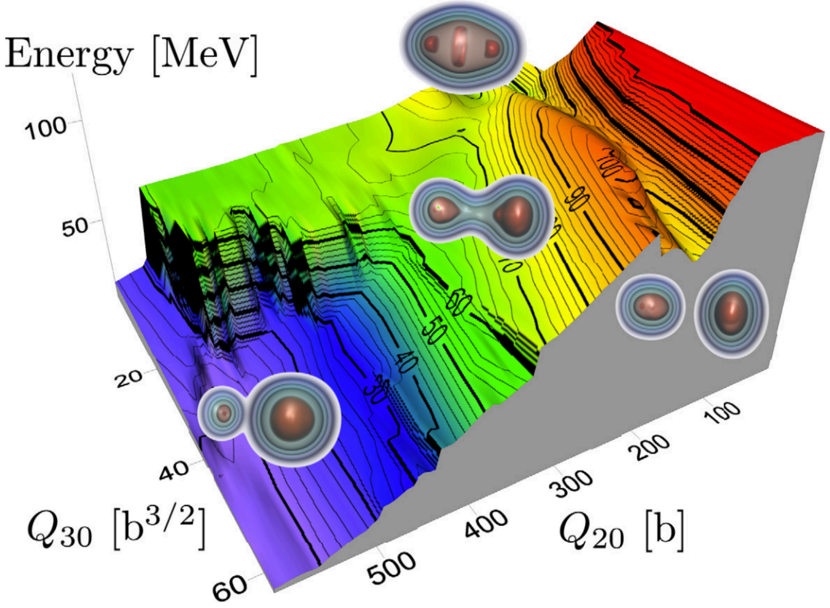
Fission dynamics with energy density functionals

Core concepts

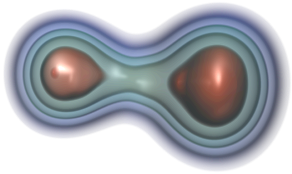
- Nucleons degrees of freedom $r = (\boldsymbol{r}, \sigma)$
- Nucleus described by $\psi(r_1, \cdots, r_A)$
- Hartree-Fock-Bogoliubov approximation (HFB)



N. Schunck, *et al.* Prog. Part. Nucl. Phys. 125 (2022)

Interpretation / Vizualisation

- Local one-body density
  $\rho(\boldsymbol{r}) \propto$ probability to measure **one nucleon** at $\boldsymbol{r}$



- Deformations determined from multipole moments
  $$Q_{20} = \langle\psi|\hat{Q}_{20}|\psi\rangle$$

Fission from energy density functional

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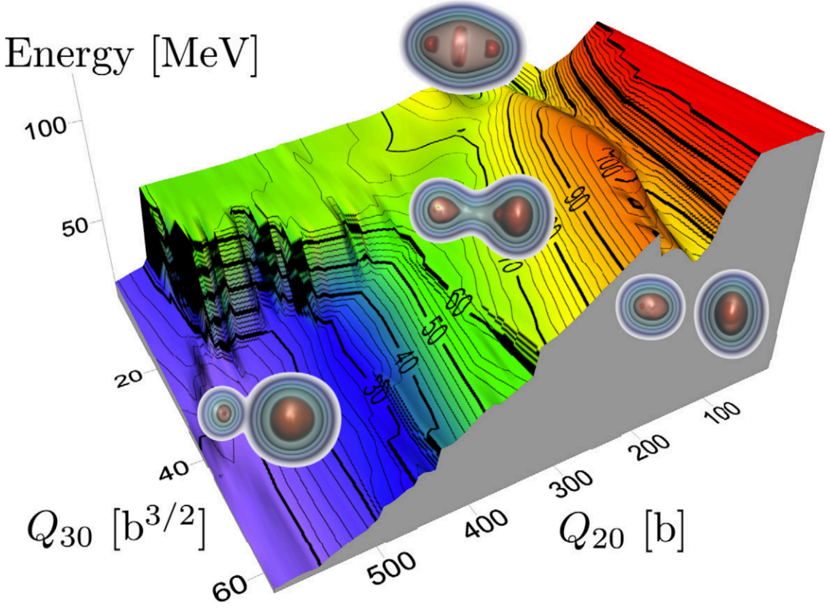

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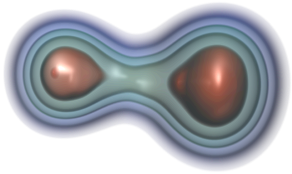


- Deformations determined from multipole moments

$$Q_{20} = \langle \psi | \hat{Q}_{20} | \psi \rangle$$

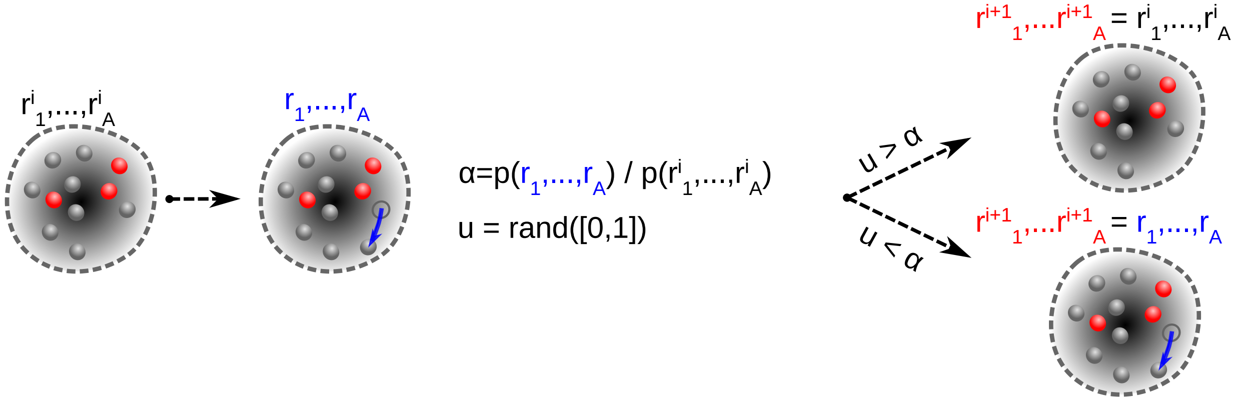
The nucleons are randomly distributed with
$$p(r_1, \cdots, r_A) \propto |\psi(r_1, \cdots, r_N)|^2$$

How to picture this probability distribution ?

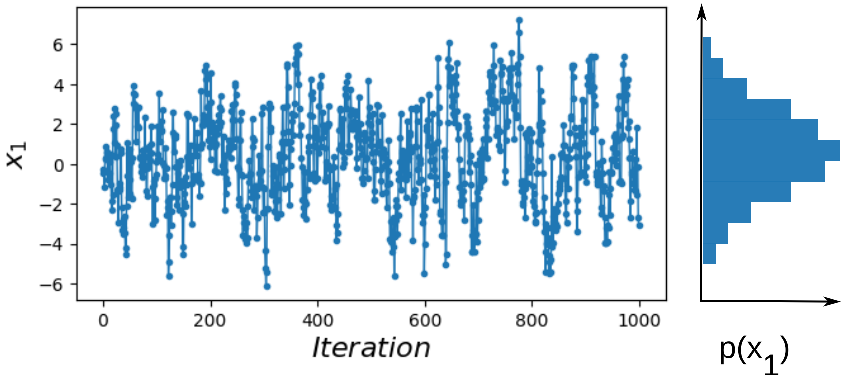
Table of contents

Markov chains to sample from $p(r_1, \cdots, r_A)$

Principle of the Metropolis algorithm, an iterative algorithm

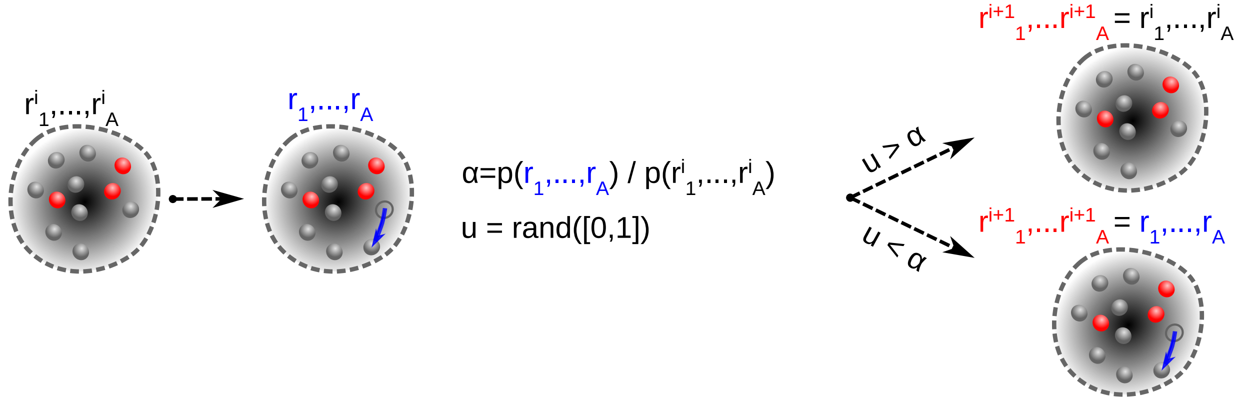


Outcome of the method: $\{r^i_1, \cdots, r^i_A | \, i \in [1, N_{iterations}]\}$



Markov chains to sample from $p(r_1, \cdots, r_A)$

Principle of the **Metropolis algorithm**, an iterative algorithm



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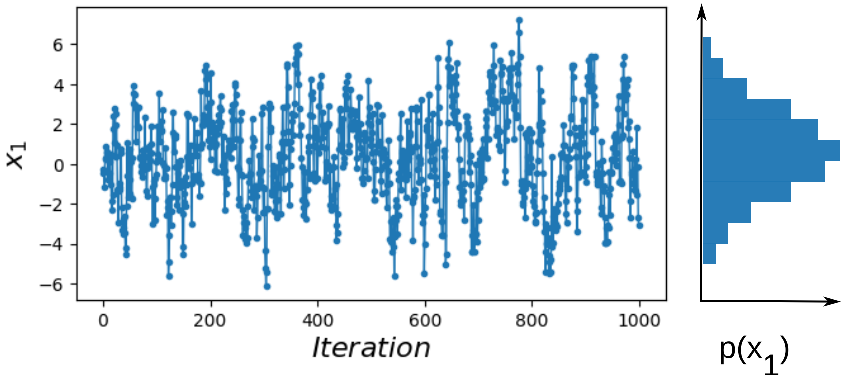


✅ Simple
✅ Needs 'only' evaluations of ratios

$$p(r_1, \cdots, r_A)/p(r'_1, \cdots, r'_A)$$

❌ Converge only after some iterations (burn-in)
❌ Autocorrelation between samples (jump)

Evaluating probablities $p(r_1, \cdots, r_A)$

We stick to wavefunctions that are

- Bogoliubov vacua,
- projected on the good number of protons and neutrons.

$$|\psi_n\rangle = \hat{P}_N \hat{P}_Z \prod_{k=1}^{N/2} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|0\rangle.$$

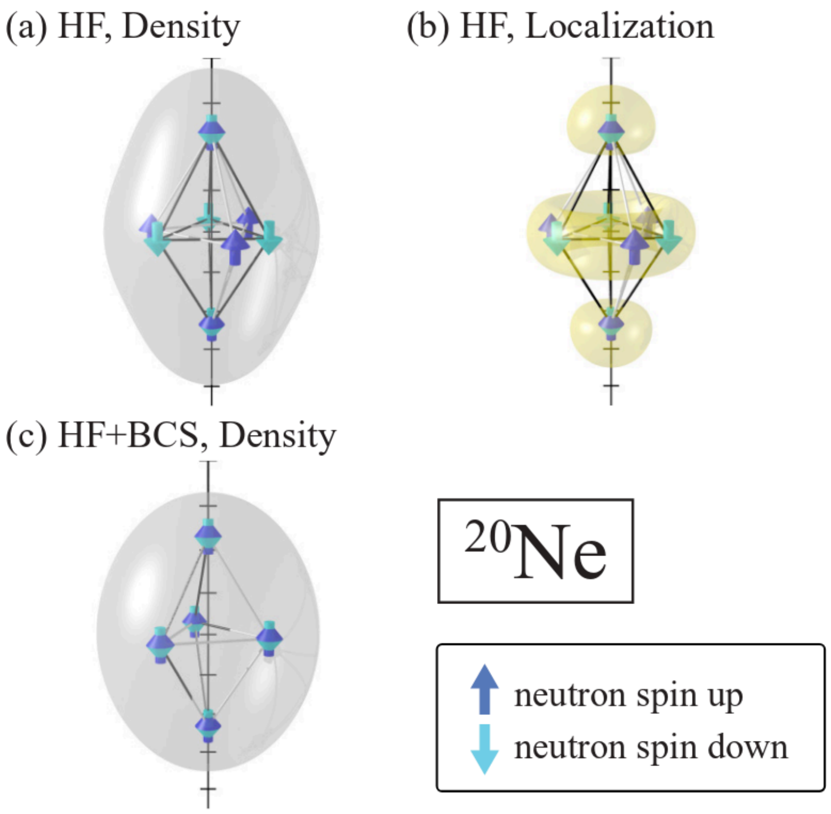
In this case:

$$p(r_1 \cdots r_A) \propto |det(Z - Z^t)|,$$

with

$$Z_{ij} = \sum_{k=1}^{N/2} \frac{v_k}{u_k} \varphi_k(r_i)\varphi_{\bar{k}}(r_j),$$

$$\varphi_k(r) = \langle r|a_k^\dagger|0\rangle.$$



Most probable configuration of ^{20}Ne

M. Matsumoto, Y. Tanimura, Phys. Rev. C **106** (2022)

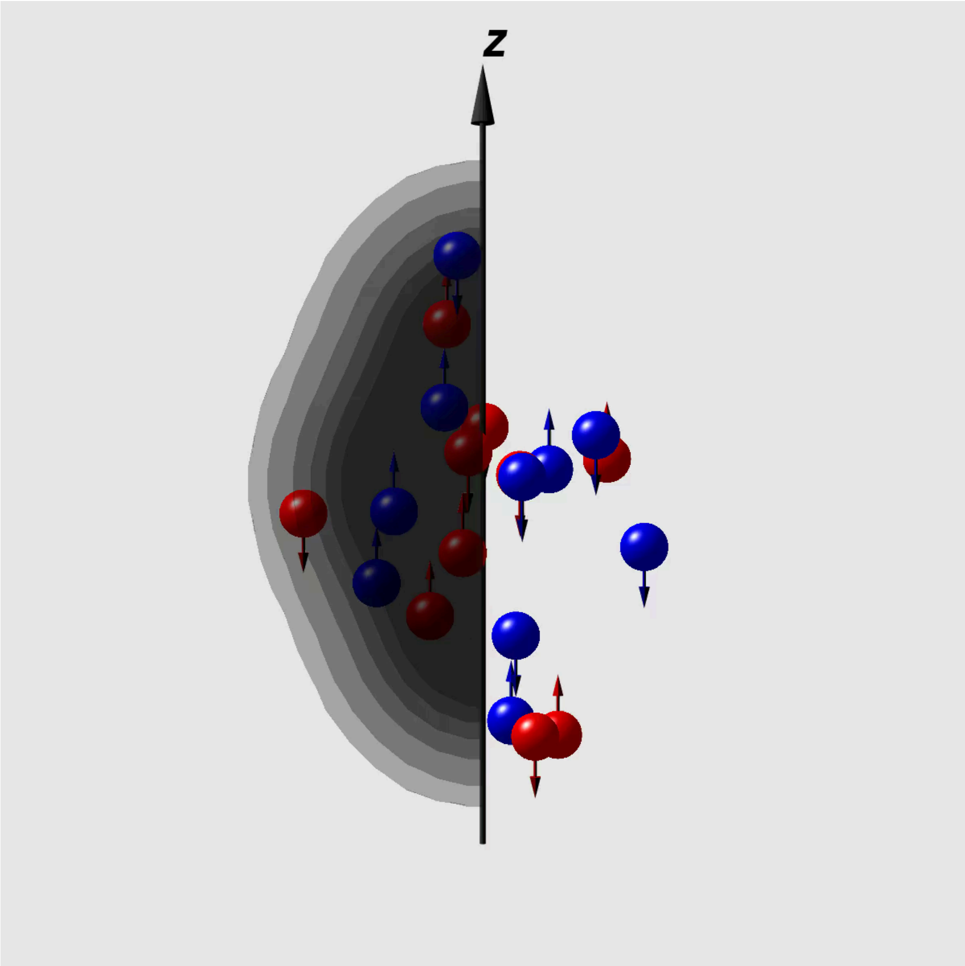
Sampling the nucleons positions in a ^{20}Ne

Wavefunction

- ^{20}Ne ground state
- projected Hartree-Fock-Bogoliubov solution
- Gogny D1S effective interaction

Color code

- Grey: local one-body density
- Red: protons
- Blue: neutrons



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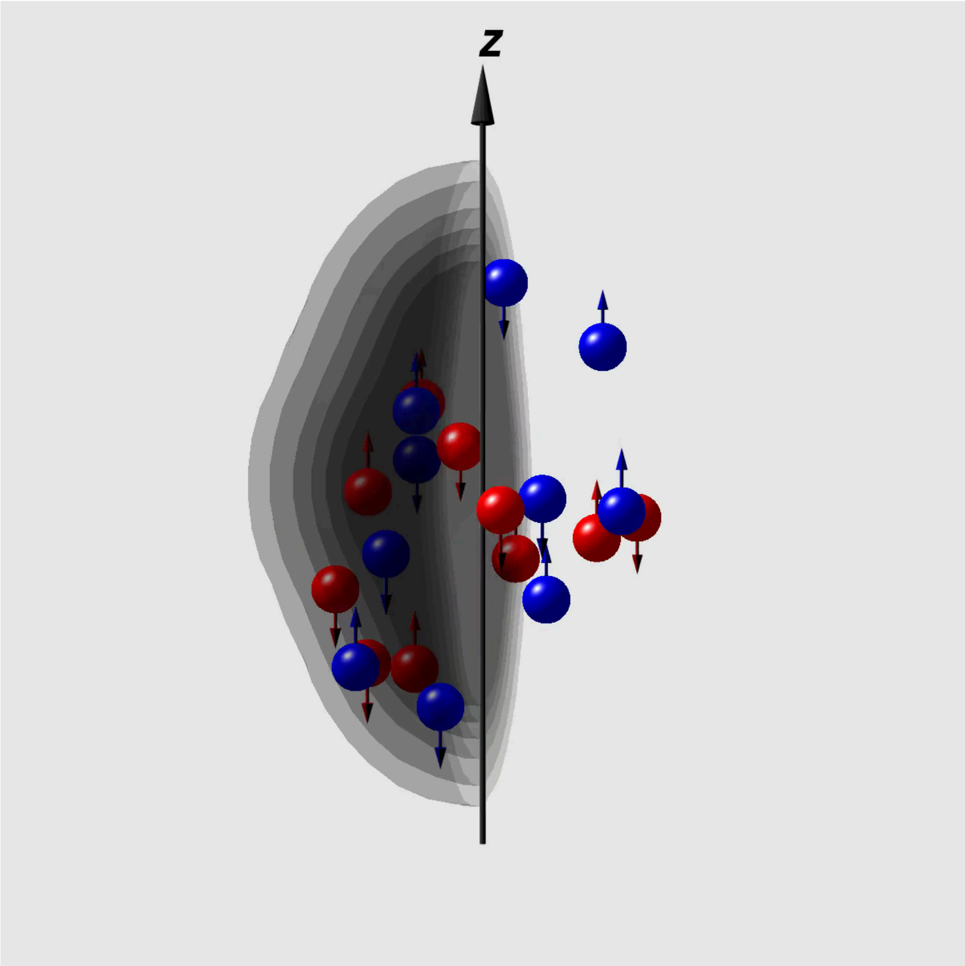

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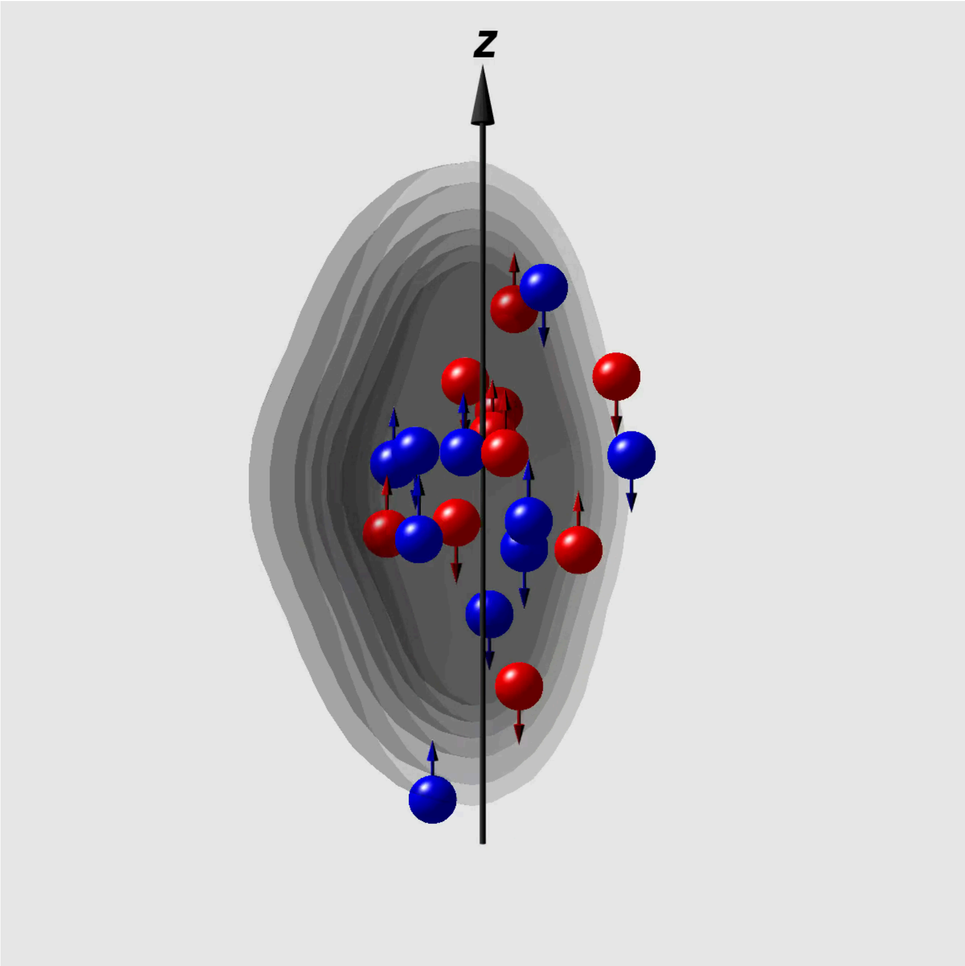

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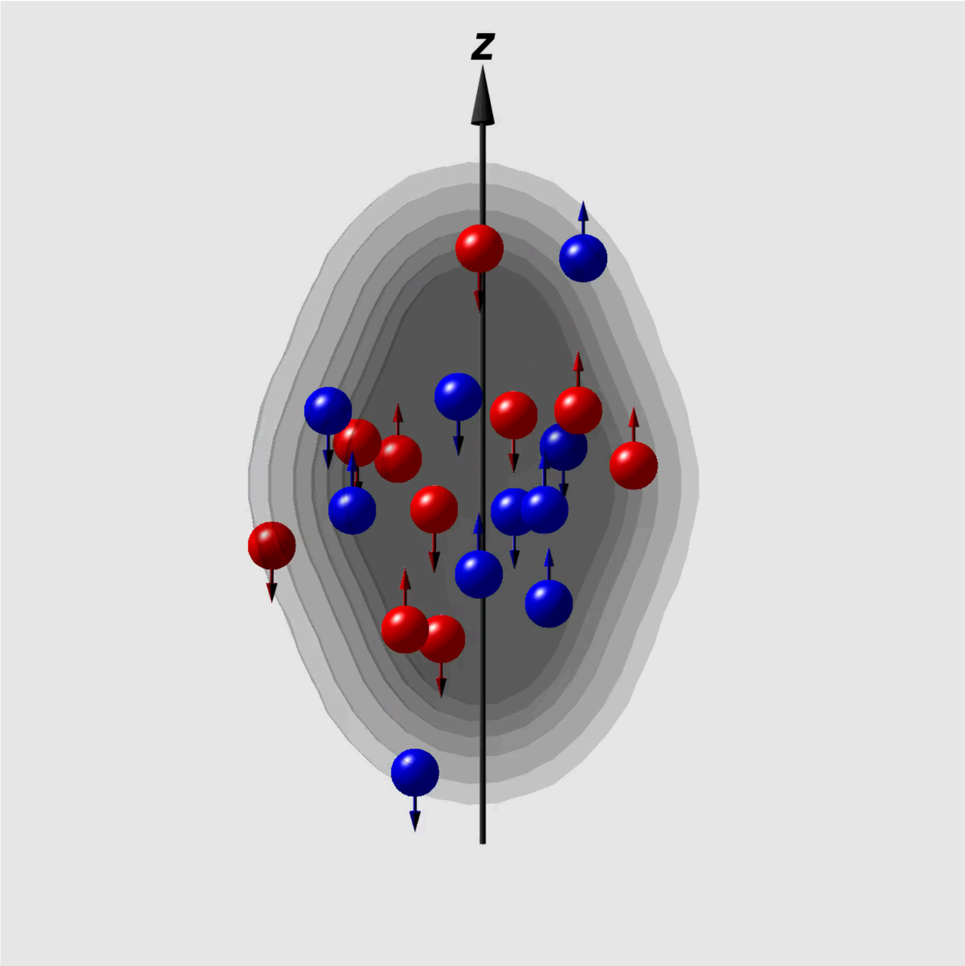

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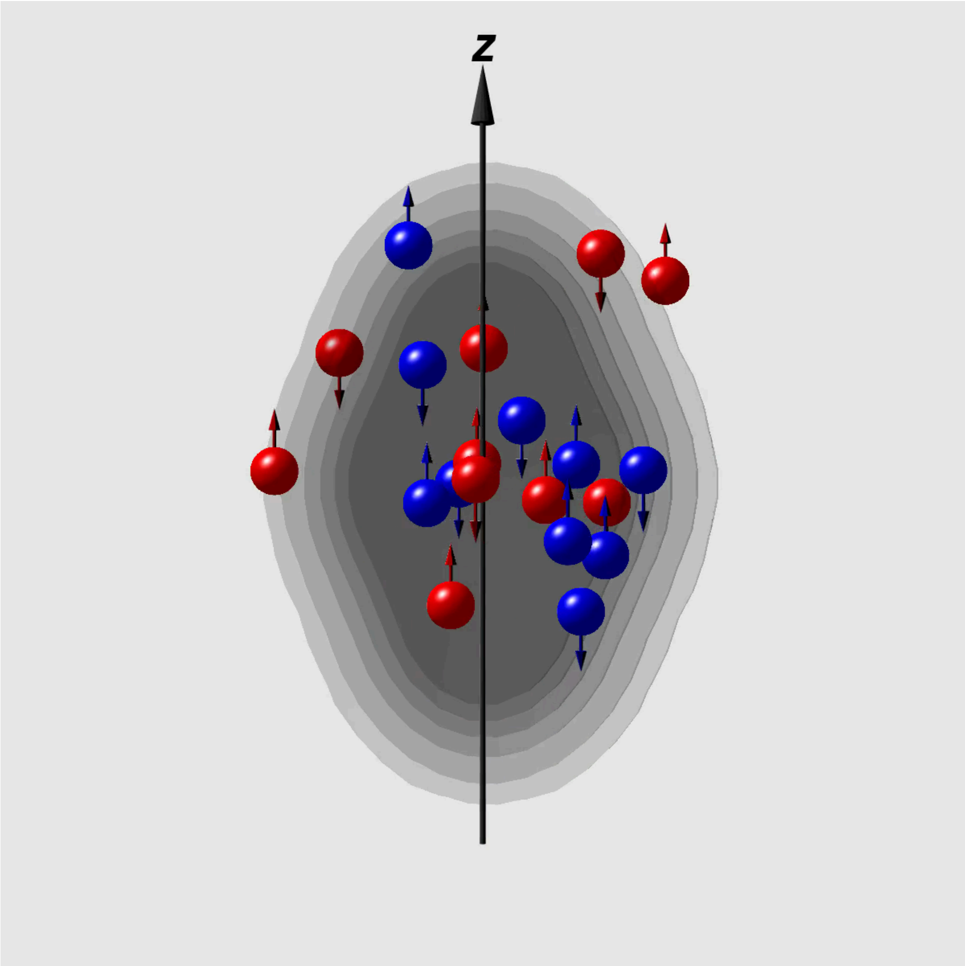

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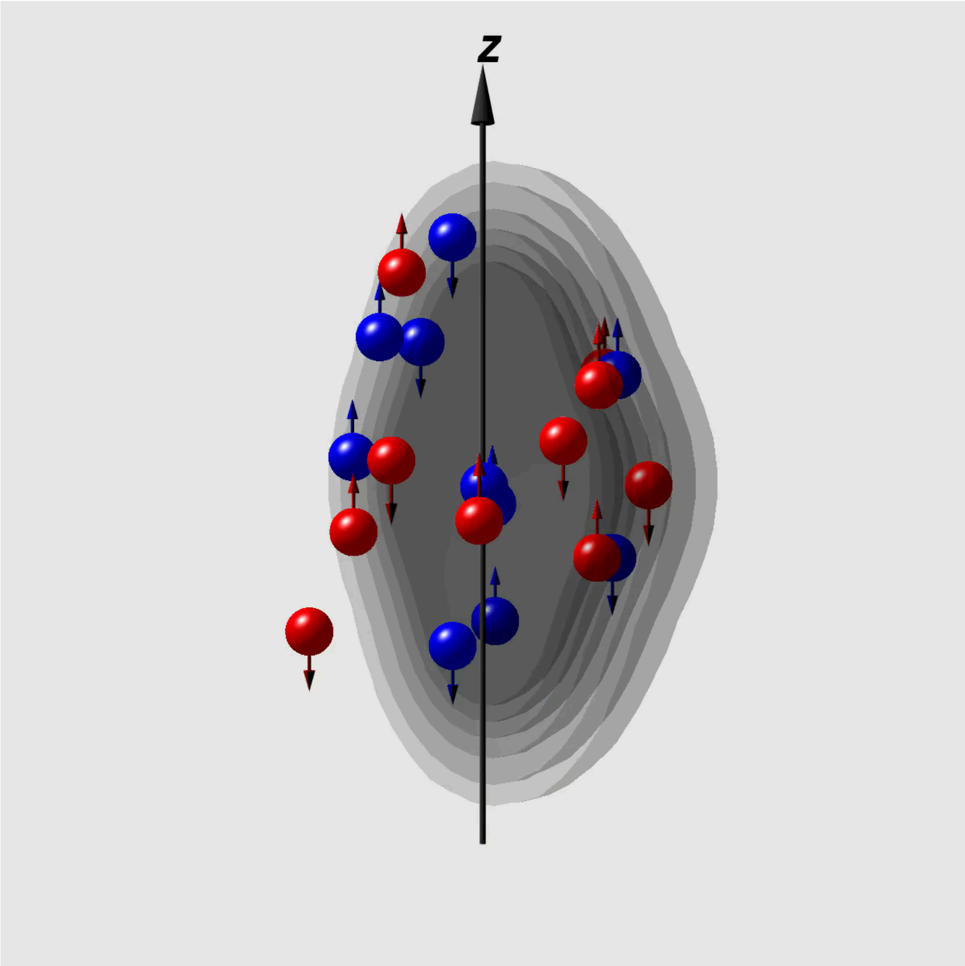

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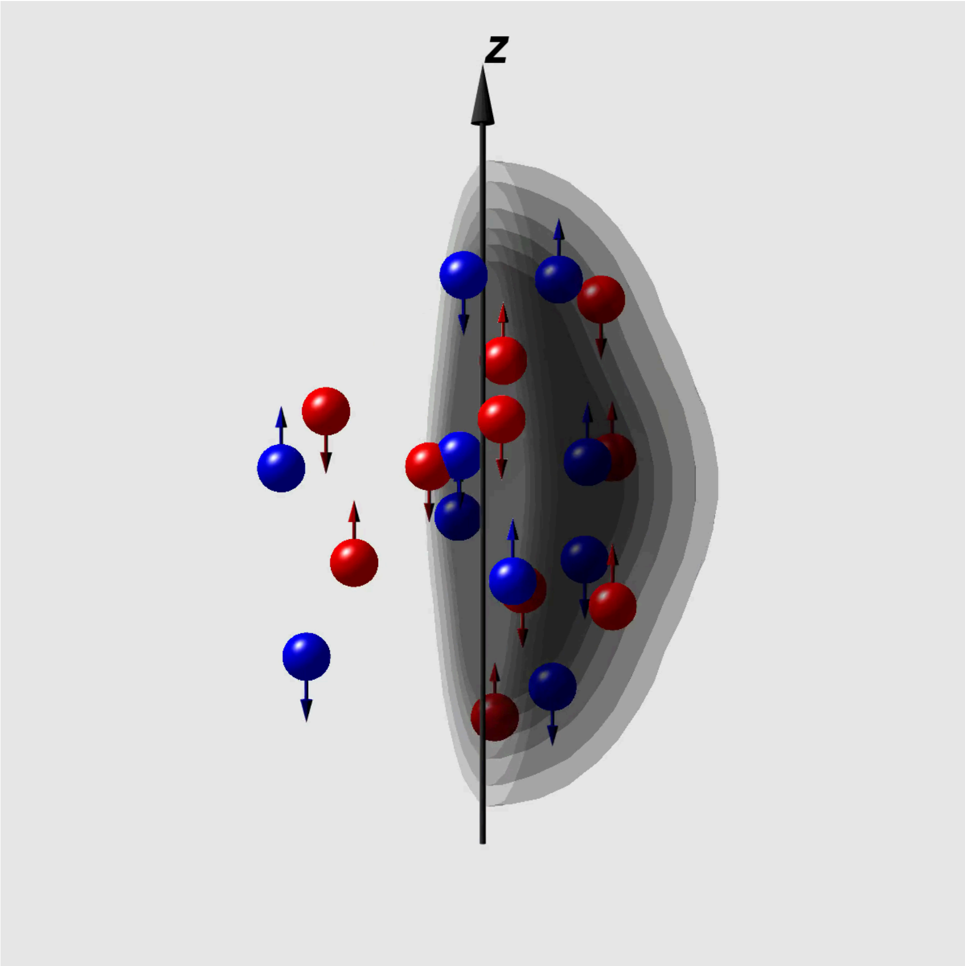


Distribution of some observables

Spatial observables

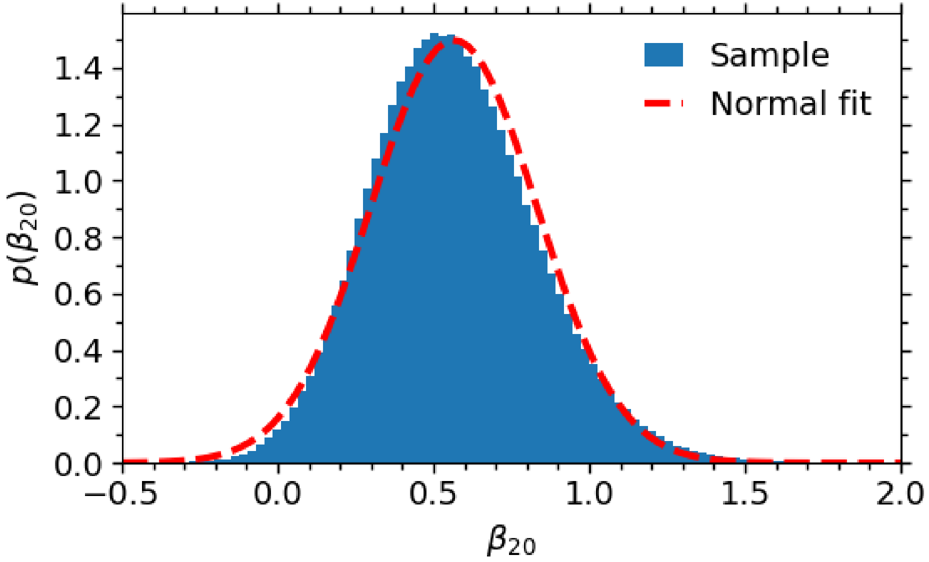
Observables that 'depend only' on the spatial and spin coordinates of the nucleons

- Center of mass
- Multipole moments
- $\cdots$

Sampling spatial observables

We build a representative sample with

$$O^i = O(r_1^i, \cdots, r_A^i)$$



Distribution of the quadrupole moment β_{20} (elongation) for the ^{20}Ne ground state

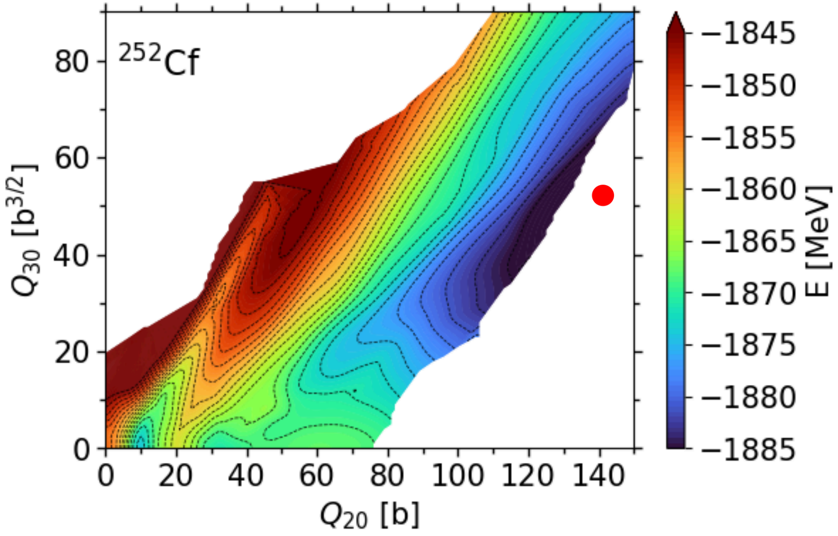
$$\langle \beta_{20} \rangle = 0.56$$

$$\sigma(\beta_{20}) = 0.26$$

Table of contents

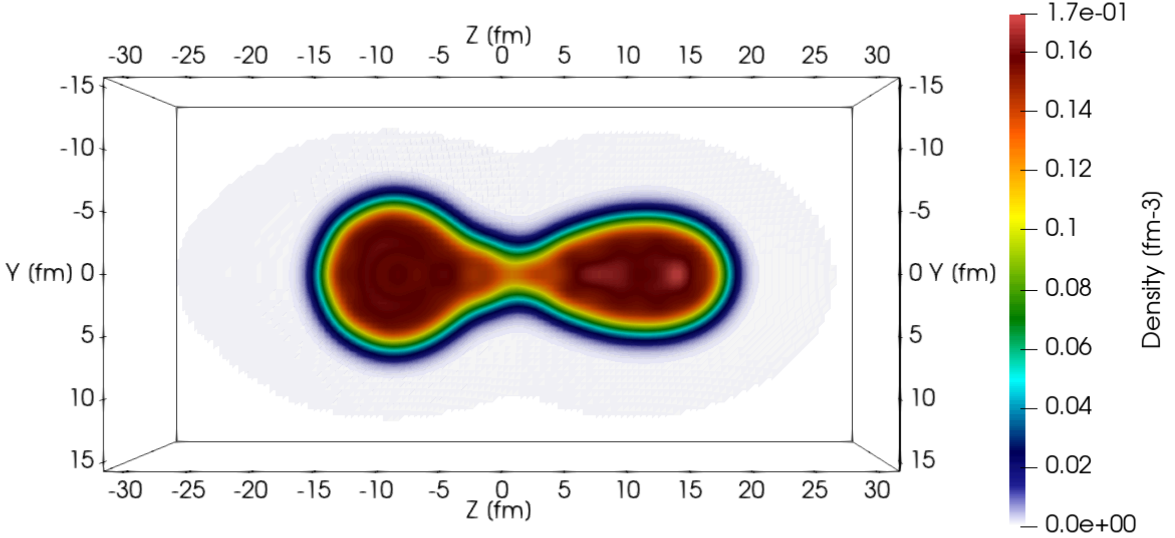
Asymmetric fission of ^{252}Cf

Potential energy surface



One point = one *constrained* HFB solution.
(Only points with $\langle \hat{Q}_{neck} \rangle > 5$ are plotted)

Selected point

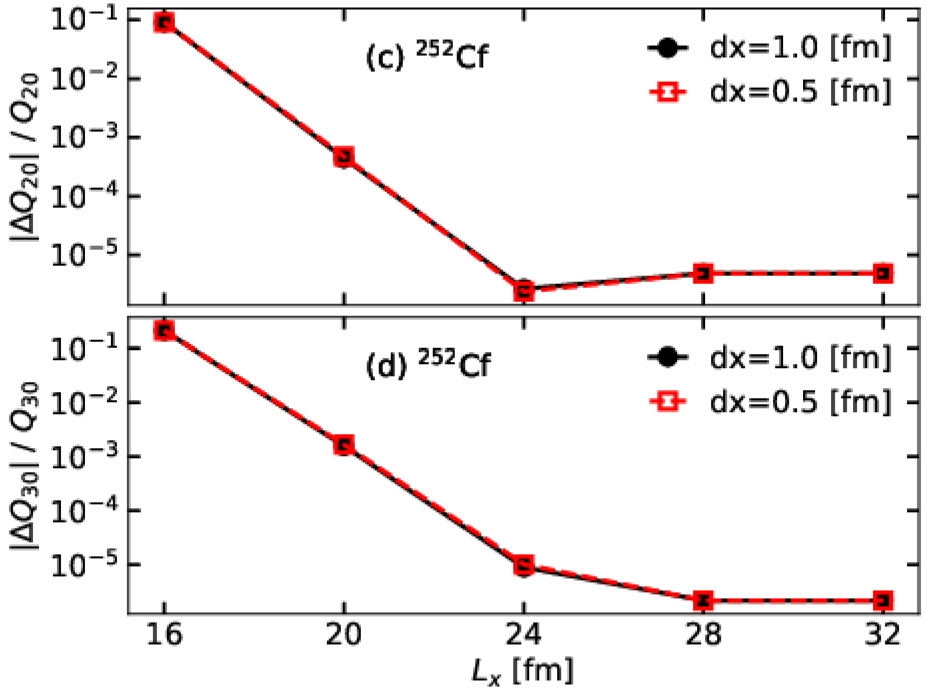


$$\langle \hat{\beta}_{20} \rangle = 4.1, \quad \langle \hat{\beta}_{30} \rangle = 1.98$$
$$\langle \hat{A}_{Left} \rangle = 143.7, \quad \langle \hat{A}_{Right} \rangle = 108.3$$
$$\langle \hat{Q}_{neck} \rangle = 3.1$$

Numerics and validation

Discretization of the wavefunction

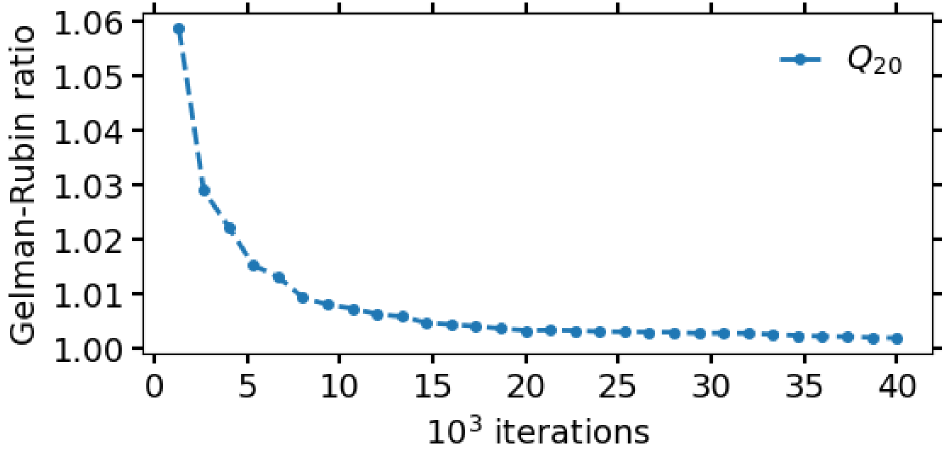
- Box: $L_x \times L_x \times 2L_x$ fm^3
- Cells: dx^3 fm^3



Monte Carlo estimation versus
deterministic values computed in an harmonic oscillator basis

Metropolis algorithm

- Independent chains: 256
- Jump: 3000 iterations
- Burn-in: $2 \cdot 10^6$ iterations



- Acceptance rate $\simeq$ 0.5
- In-chain autocorrelation $\lesssim$ 0.2
- Numerical cost $\simeq$ **6400 h.cpu**

Multipole moments distribution

Expression from the positions only

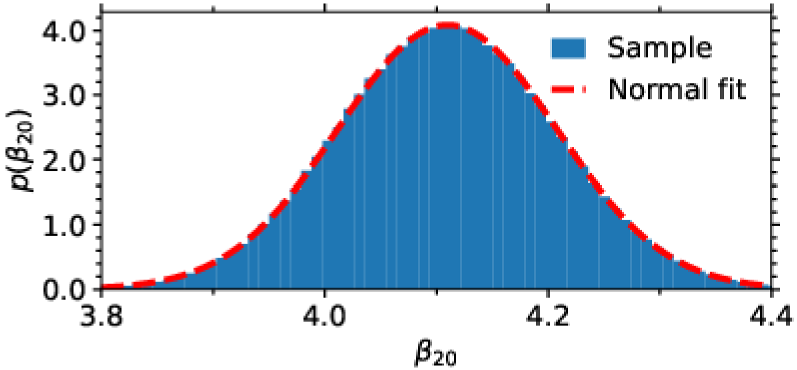
$$\beta_{20}(r_1, \cdots, r_A) \propto \sum_k^A (2z_k^2 - x_k^2 - y_k^2)$$

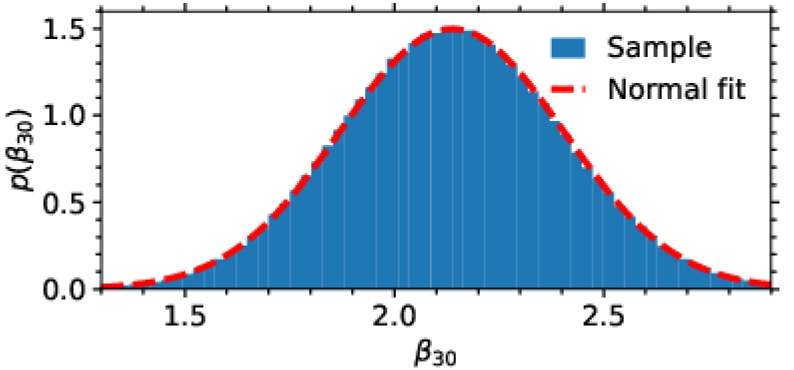
Expectation values from the sample

$$\langle \hat{\beta}_{20} \rangle = 4.10, \quad \langle \hat{\beta}_{30} \rangle = 1.98$$

Standard deviations from the sample

- Standard deviation of 2.3% for β_{20}
- Standard deviation of **12.5% for β_{30}**



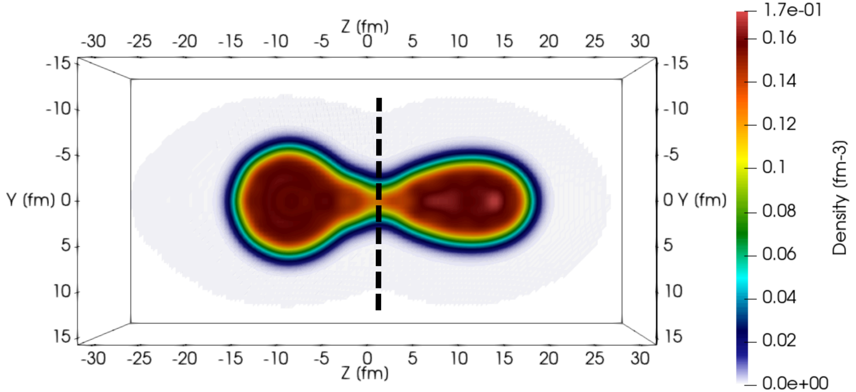


Probability distribution of the quadrupole (top) and octupole (bottom) moments

$\simeq$ Normal distributions

Particles in the pre-fragments

Number of particles in half a space:



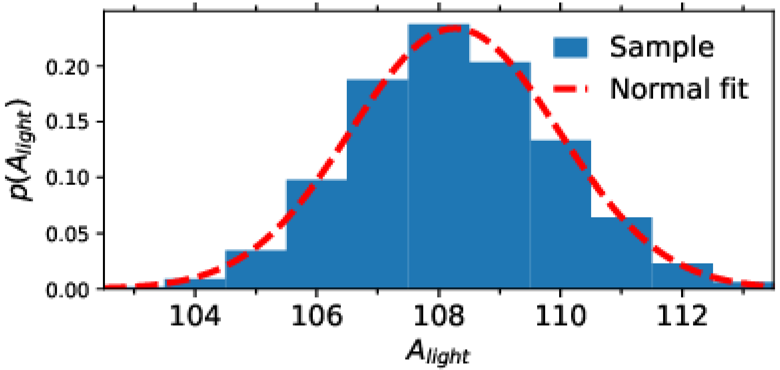
$$\hat{A}_{right} = \sum_r \Theta_{z>z_{neck}}\, c_r^\dagger c_r$$

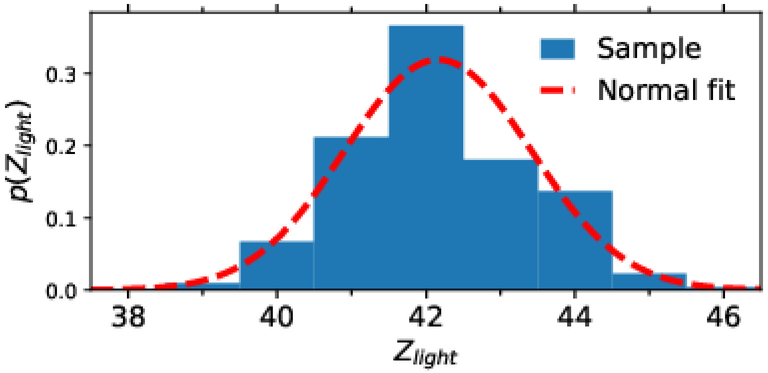
C. Simenel, Phys. Rev. Lett. **105** (2010)

- Few masses/charges width (in one Bogoliubov vacuum)

  G. Scamps *et al.*, Phys. Rev. C **92** (2015)

  M. Verriere *et al.*, Phys. Rev. C **103** (2021)

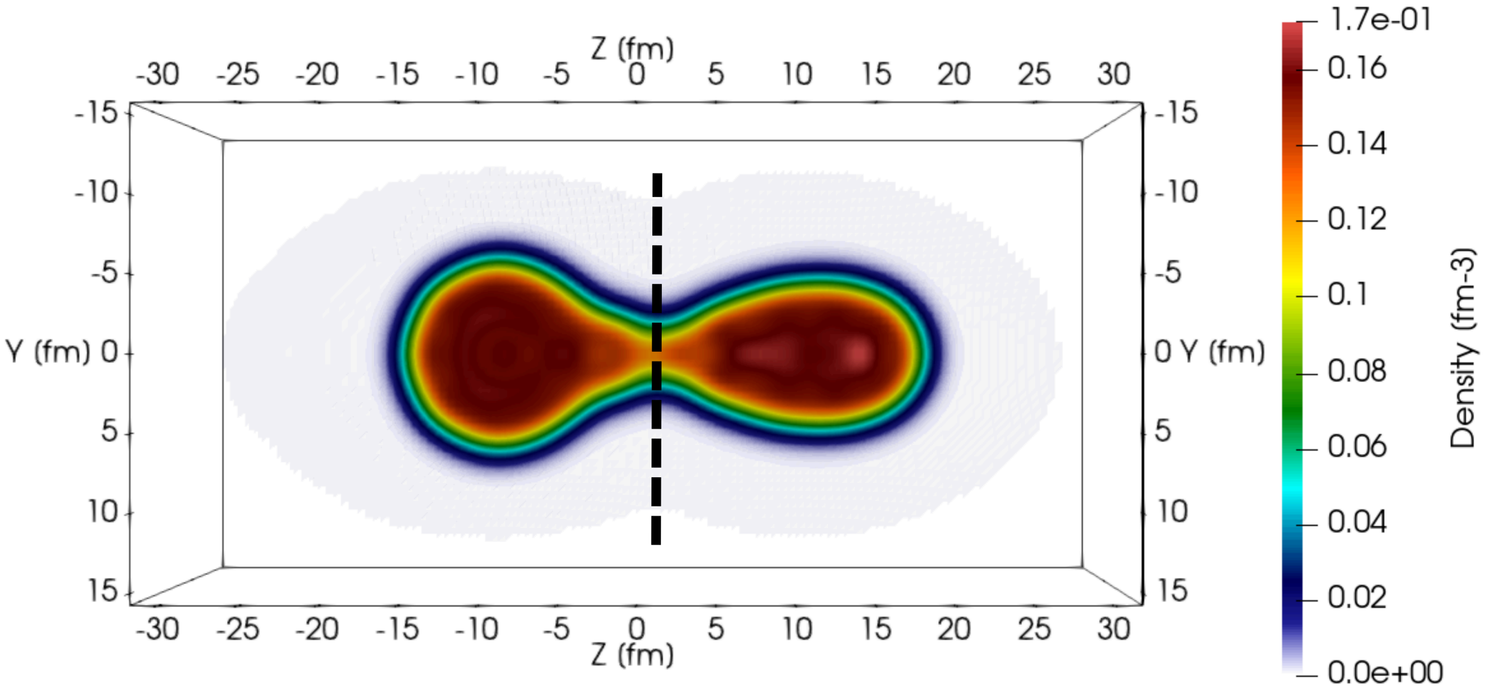




Mass and charge distribution in the light fragment

$$\sigma(\hat{A}_L) = 1.7$$
$$\sigma(\hat{Z}_L) = 1.2$$

Elongation of the pre-fragments



$$\langle \beta_{20}^{Left} \rangle = 0.26 \qquad \langle \beta_{20}^{Right} \rangle = 0.78$$

$$\sigma(\beta_{20}^{Left}) = 0.06 \qquad \sigma(\beta_{20}^{Right}) = 0.09$$

Coulomb repulsion between pre-fragments

Right/left Coulomb repulsion

$$\hat{V}^{Coul.}(r_1, \cdots, r_A) \propto \sum_{z_j < z_{neck}} \sum_{z_i > z_{neck}} \frac{1}{|r_i - r'_j|}$$

Calculation

- $\langle \hat{V}^{Coul.} \rangle = 193.8 \text{ MeV}$
- $\sigma(\hat{V}^{Coul.}) = 5.1 \text{ MeV}$

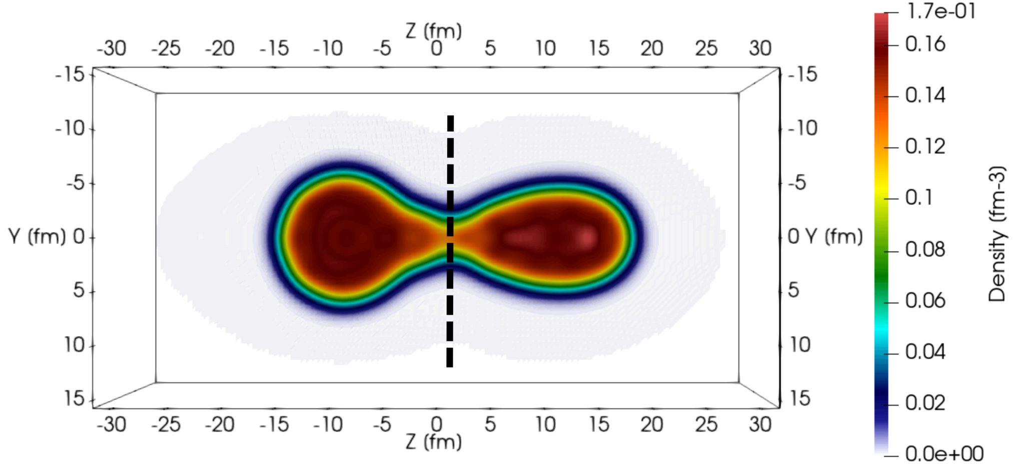
Experiment

For the same fragmentation

- $\langle TKE \rangle =$ 184.7 MeV
- $\sigma(TKE) = 8.8 \text{ MeV}$

Göök *et al.*, Phys. Rev. C **90** (2014)

✅ Estimation of the total kinetic energy within 10 MeV,
✅ **First estimation of its fluctuation**



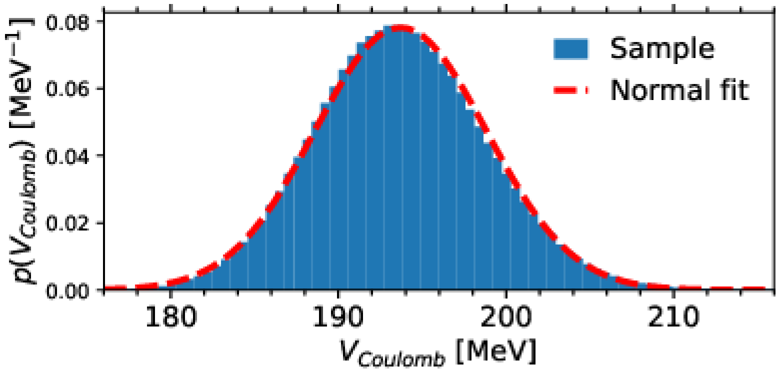


Table of contents

Final thoughts

Main conclusions

- Sampling positions for **heavy nuclei is doable**
- It gives access to the distribution of some observables
- Currently, **it is costly** ($\simeq$ 6000 h.cpu)

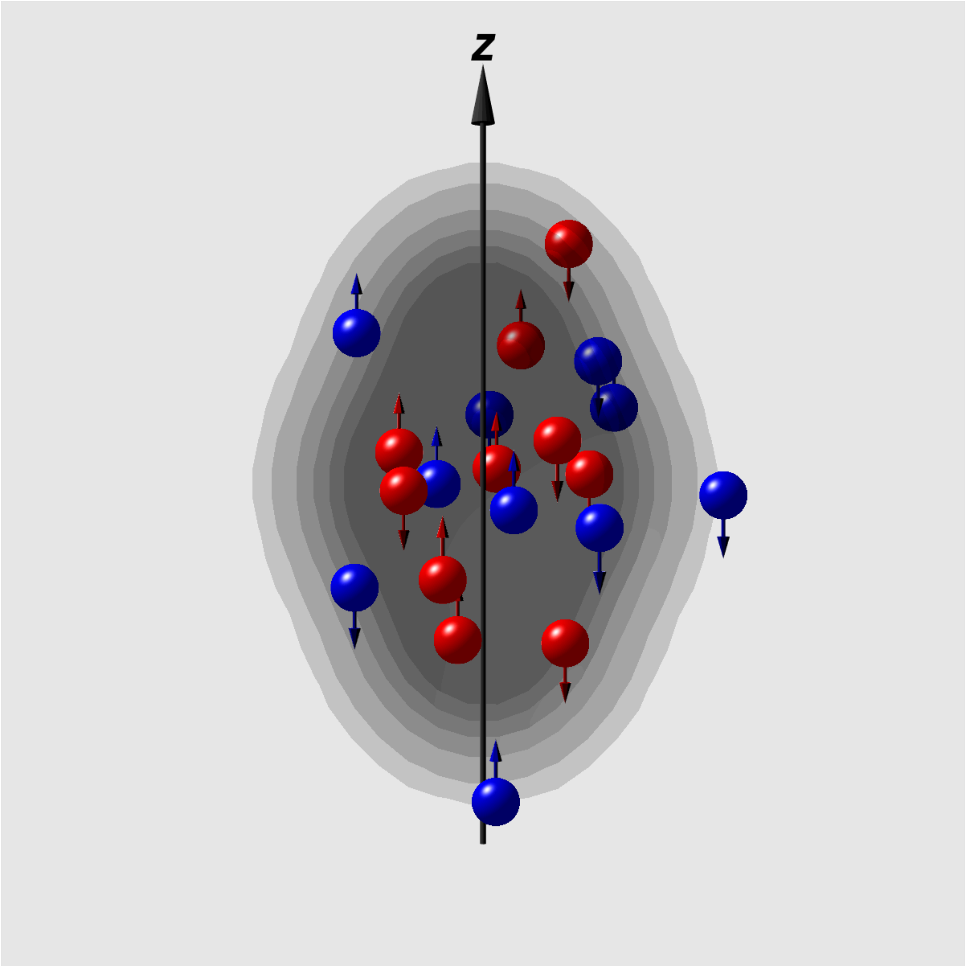
Perspectives

- Look at other observables
- Deal with non-diagonal observables
- Deal with more complex wavefunctions

Open questions

- Would you like the code to be published ?

Thank you for your attention !



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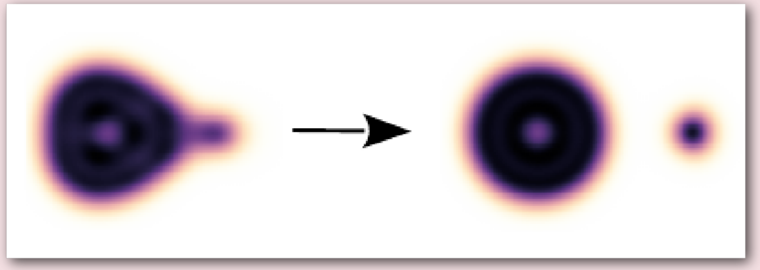
Poster session

Alice Bernard

Generative machine learning improves microscopic description of dissociation reactions

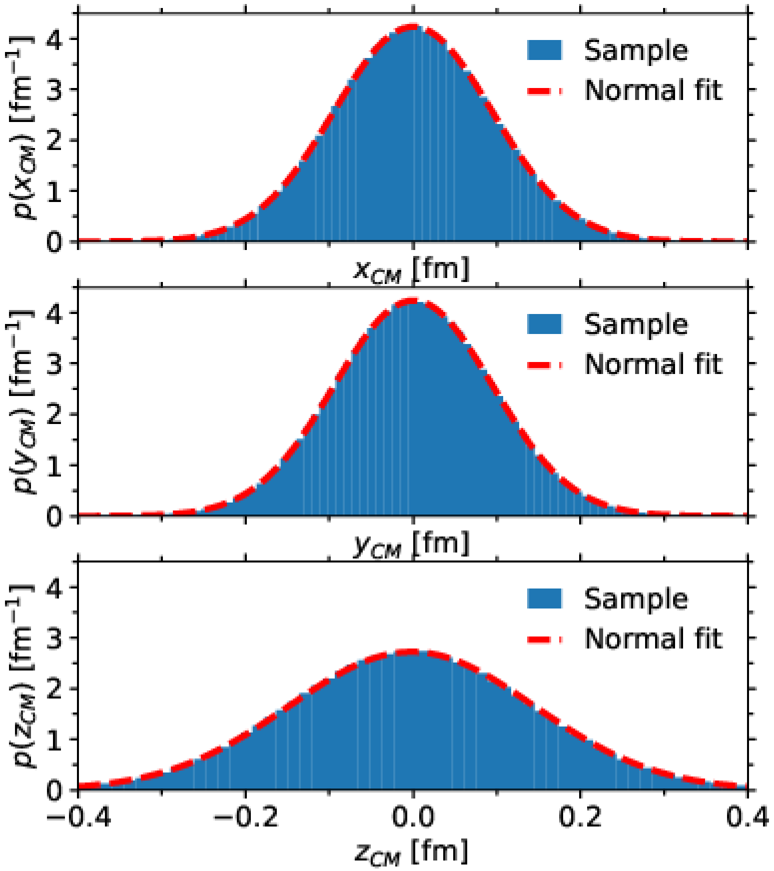


Center of mass distribution

From the generated sample:

$$\langle \hat{X}_{CM} \rangle \simeq \frac{1}{K} \sum_{k}^{K} \left(\frac{1}{A} \sum_{i}^{A} x_{ik} \right)$$

- Expectation value at the origin
- Normal distributions
- $\sigma(z_{CM}) = 0.26$ **fm**



Probability distribution for the position of the center of mass

Projecting the center of mass position

Projection = filtering

We can project the center of mass position at the origin...
by keeping only events with

$$x_{CM}, y_{CM}, z_{CM} \in [-0.05\ \mathrm{fm}, 0.05\ \mathrm{fm}]^3$$

- The projection leaves unchanged Q_{20}
- The projection **reduces by 40% the fluctuation on Q_{30}**