LA-UR-19-22719

Title: Description of fission, Number of particles in fission fragments with a Monte-Carlo approach

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Intended for: Possible presentation at LLNL

Issued: 2019-03-26

Description of fission

Number of particles in fission fragments with a Monte-Carlo approach

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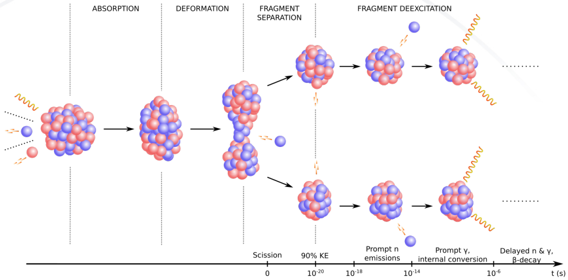
Context

1. National security
   - nuclear deterrence
   - non-proliferation
2. Energy
   - nuclear power plants
3. Fundamental Science
   - formation of elements in nucleosynthesis (r-process)
   - stability of superheavy elements

Neutron induced fission process



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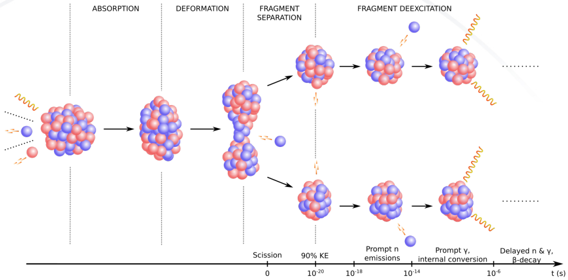

Observables

- Pre-neutron fission fragment yields
- Prompt ν & γ emission
- Total kinetic energy
- Total angular momentum
- Excitation energy
- Delayed ν & γ emission...

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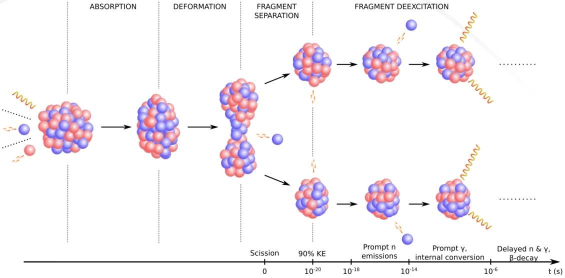

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Fission fragment yields

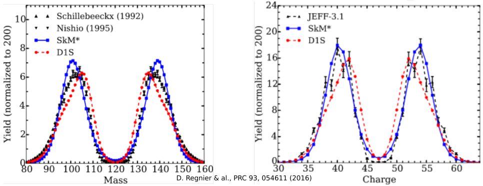


Figure: Pre-neutron mass (left)/charge (right) yields for the reaction ^{239}Pu(n,f)

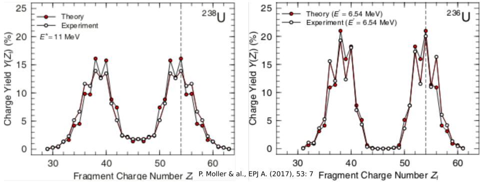
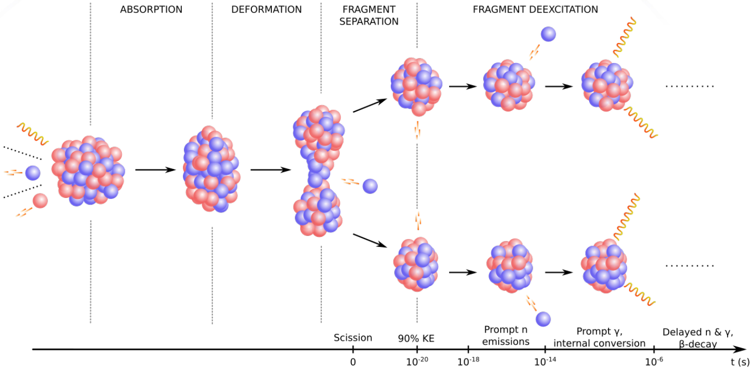


Figure: Pre-neutron charge yields for the reactions ^{237}U(n,f) (left) and ^{235}U(n,f) (right)

Neutron induced fission process



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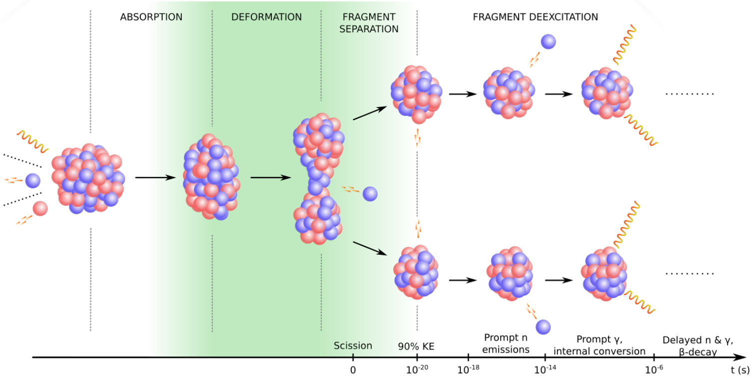

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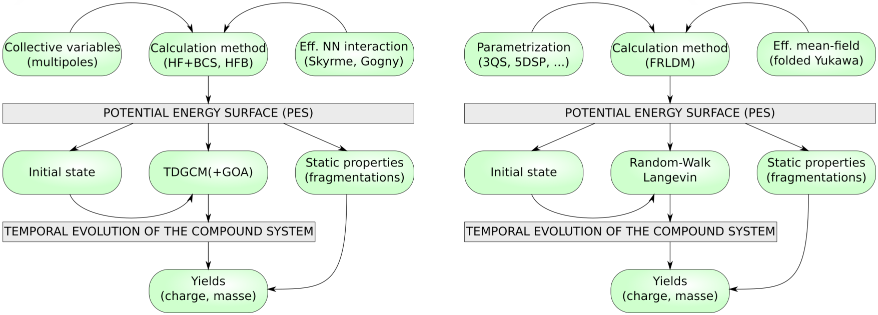

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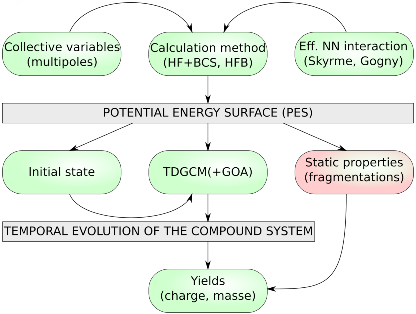

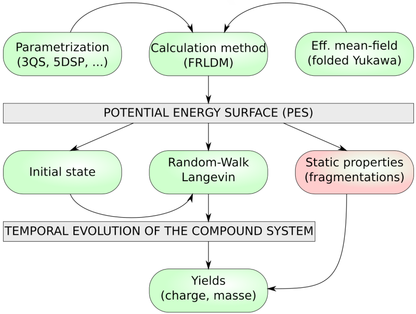

Existing methods

From the shape parametrization

- based on the geometric shapes of the nucleus (α_g) at scission,
- no dispersion in particle number,
- non-integer fragmentation.

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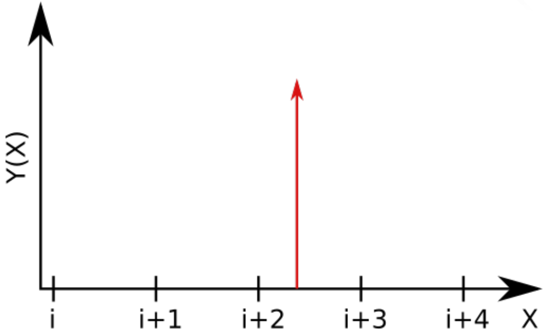
From the 1-body local density

- integration of the 1-body density on the left/right fragments for each quantum states at scission,
- no dispersion in particle number,
- non-integer fragmentation.

Existing methods



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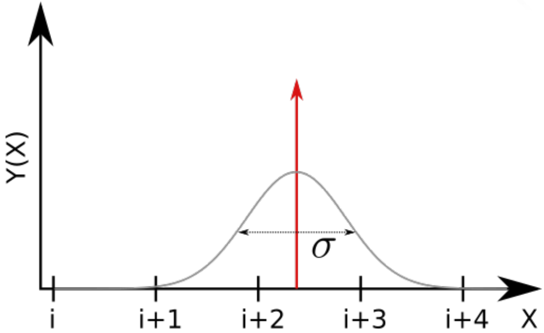

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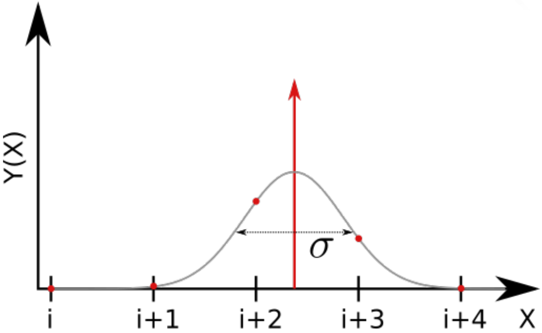

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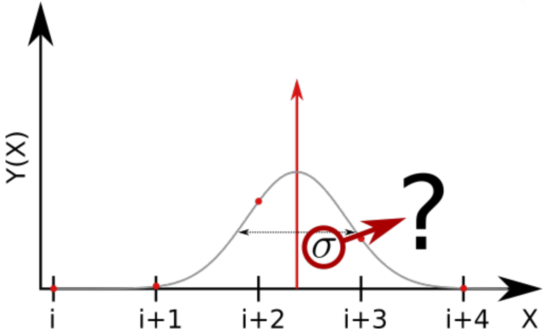

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Projection on the fragments

- projection on each possible fragment charge/mass,
- dispersion in particle number & integer fragmentations,
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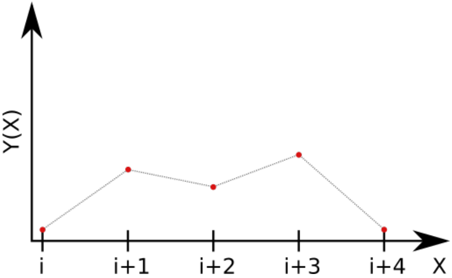

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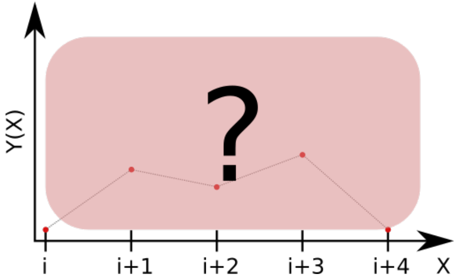

Objectives

We want to construct a method to evaluate the fragmentation probabilities with the following physical and practical considerations:

Physical considerations

- as few parameters as possible,
- integer fragmentations & dispersion,
- take into account 1- and 2-body correlations.

Practical considerations

- straitforward implementation,
- simplicity (light formalism & classical intuition),
- compatible with both macro-micro and microscopic approaches.

Outline

1. No pairing case
2. Addition of pairing correlations
3. Results
4. Conclusion

Outline

Slater determinant

$$\hat{H} = \hat{T} + \hat{V} = \sum_i \varepsilon_i \hat{a}_i^\dagger \hat{a}_i$$

$$\hat{H}|\Phi_0\rangle = E_0|\Phi_0\rangle$$

$$|\Phi_0\rangle = \hat{a}_1^\dagger \cdots \hat{a}_N^\dagger |-\rangle, E_0 = \sum_{i=1}^{N} \varepsilon_i$$

- $|-\rangle$: particle vacuum,
- $\hat{a}_i^\dagger / \hat{a}_i$: Fermion creation/annihilation operators, creates/annihilates a Fermion with energy ε_i,
- N-body state for non-interacting Fermions.

Position of the neck

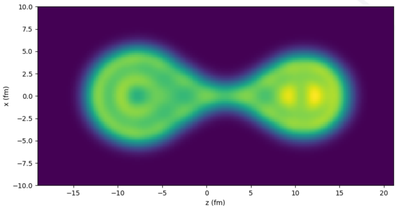

Figure: Proton local density $\langle \Phi_0 | \hat{\rho}_{\mathrm{prot.}}(x, 0, z) | \Phi_0 \rangle$ of $|\Phi_0\rangle$, ^{240}Pu near scission

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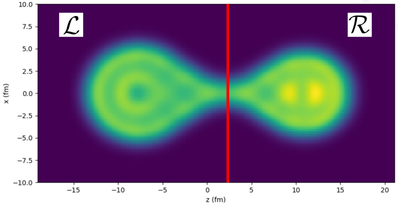

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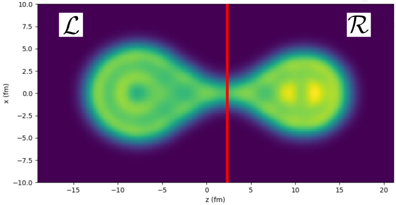

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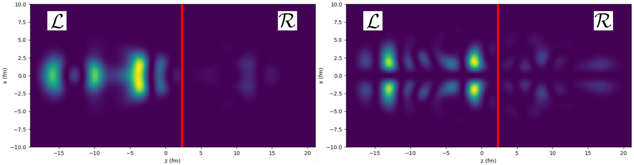
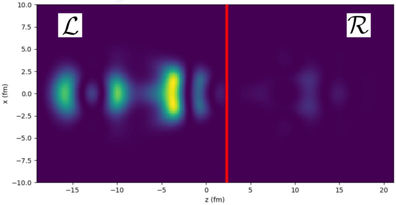
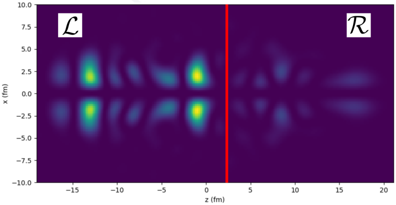


Left and right bases





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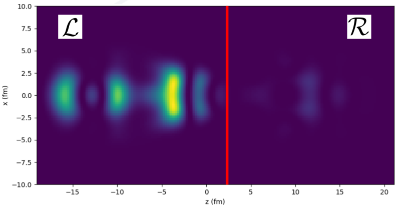

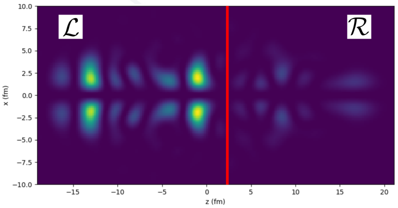

$$\alpha_i^{\mathcal{L}\,2} = \sum_\sigma \int_\mathcal{L} \mathrm{d}\vec{r} |\langle \vec{r}\sigma | \hat{a}_i^\dagger | - \rangle|^2$$

$$\alpha_i^{\mathcal{R}\,2} = \sum_\sigma \int_\mathcal{R} \mathrm{d}\vec{r} |\langle \vec{r}\sigma | \hat{a}_i^\dagger | - \rangle|^2$$

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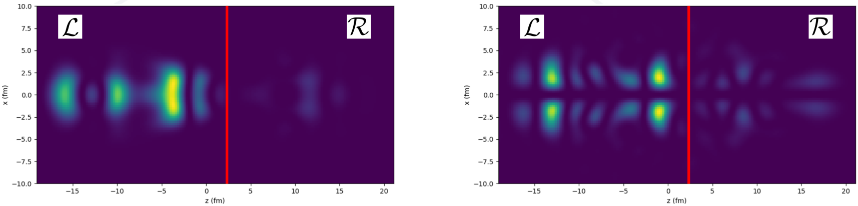

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$$\alpha_i^{\mathcal{L}\,2} + \alpha_i^{\mathcal{R}\,2} = 1$$

$$\hat{a}_i^\dagger = \alpha_i^{\mathcal{L}} \hat{a}_i^{\mathcal{L}\dagger} + \alpha_i^{\mathcal{R}} \hat{a}_i^{\mathcal{R}\dagger}$$

Decomposition of the norm

$$\langle \Phi_0 | \Phi_0 \rangle = \sum_{f} \sum_{\sigma \in \mathfrak{S}_N} \left[\prod_{i=1}^{N} \alpha_i^{f_i} \alpha_i^{f_{\sigma(i)}} \right] \det \left(\mathrm{S}|_{f, f \circ \sigma} \right)$$

where f iterate over all N-uplets of $\{\mathcal{L}, \mathcal{R}\}$.

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- This expression requires the calculation of $\approx 2^{2N}$ determinants,
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Assumption

- This expression requires the calculation of $\approx 2^{2N}$ determinants,
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- **near scission, we can expect $\mathrm{S} \approx \mathrm{I}$.**

$$\langle \Phi_0 | \Phi_0 \rangle \approx \sum_f \left[\prod_{i=1}^{N} {\alpha_i^{f_i}}^2 \right]$$

Fragmentation probabilities

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$\mathbb{P}_K^{\mathcal{L}}$: probability to have K nucleons in the left fragment

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- $\prod_{i=1}^{N} {\alpha_i^{f_i}}^2$: Probability to be in the state $\prod_{i=1}^{N} \hat{a}_i^{f_i \dagger} |-\rangle$
- **estimation of $\mathbb{P}_K^{\mathcal{L}}$ using Monte Carlo**

Outline

Quasi-particle Slater determinant

Quasi-particle Slater determinant (QPSD)

- $|\Phi\rangle = \prod_i \hat{\beta}_i |-\rangle$, where $\hat{\beta}_i$ annihilates a quasi-fermion in state i,
- $\hat{\beta}_i^\dagger$ is a weighted sum of fermion creation and annihilation operators,
- many-body state for non-interacting quasi-particles,
- good number of particle **in average.**

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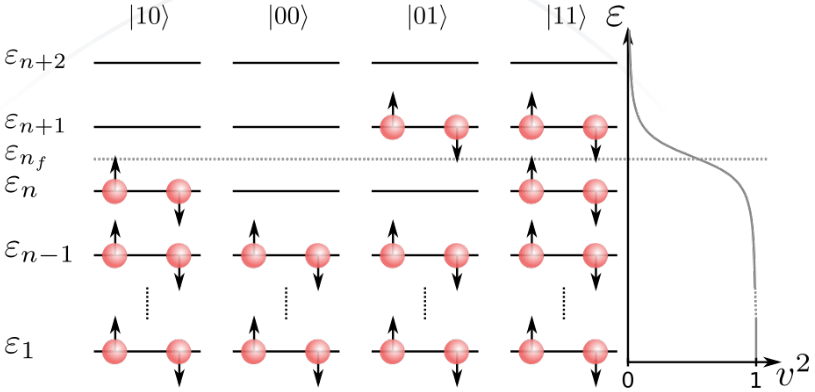
Up to a phase:

$$|\Phi\rangle = \prod_i (u_i + v_i \hat{a}_i^\dagger \hat{a}_{\bar{i}}^\dagger)|-\rangle,$$

- v_i: occupation amplitude and $u_i^2 + v_i^2 = 1$,
- $\bar{i}$: time-reversal state of i.

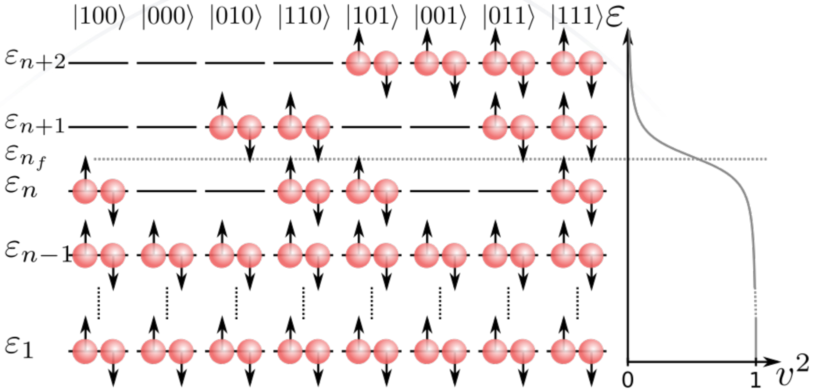
Quasi-particle Slater determinant



$$|\Phi\rangle = \hat{a}_1^\dagger \hat{a}_{\bar{1}}^\dagger \cdots \hat{a}_{n-1}^\dagger \hat{a}_{\overline{n-1}}^\dagger (u_n + v_n \hat{a}_n^\dagger \hat{a}_{\bar{n}}^\dagger)(u_{n+1} + v_{n+1} \hat{a}_{n+1}^\dagger \hat{a}_{\overline{n+1}}^\dagger)|-\rangle$$

$$|\Phi\rangle = v_n u_{n+1}|10\rangle + u_n u_{n+1}|00\rangle + u_n v_{n+1}|01\rangle + v_n v_{n+1}|11\rangle$$

Quasi-particle Slater determinant



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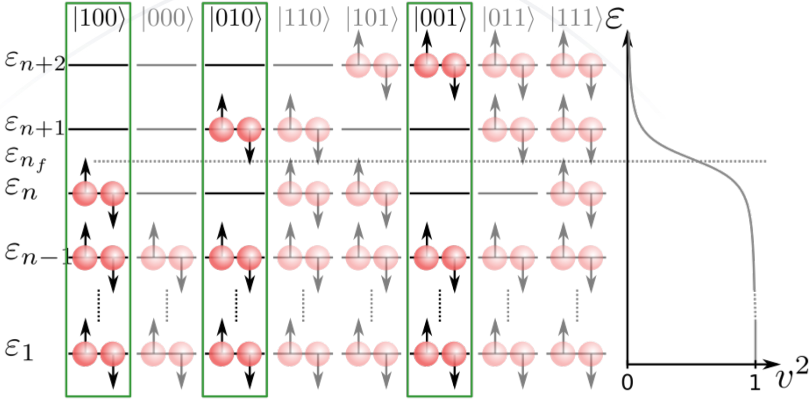

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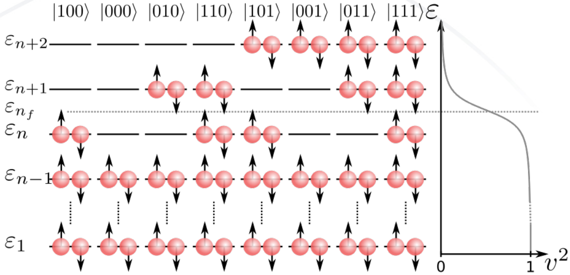
Algorithm



1. Random selection of the filled levels according to the v_i^2.
2. If the number of particle is not the good one, goto 1.
3. Calculation of the fragmentation probabilities associated with the particle Slater determinant (No pairing case).
4. Goto 1 up to convergence.

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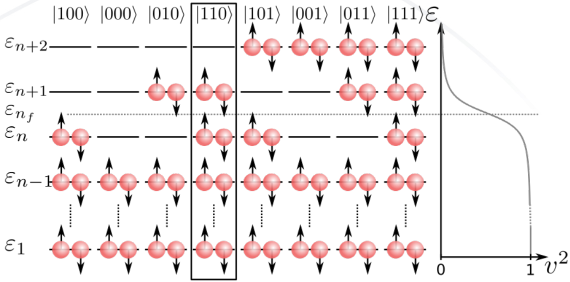

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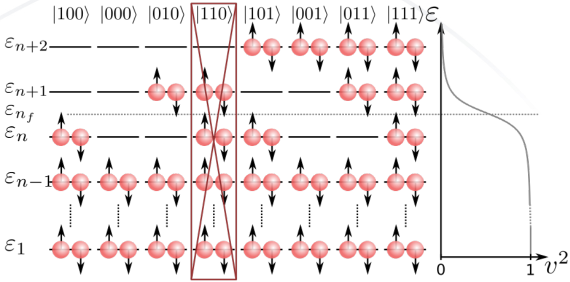

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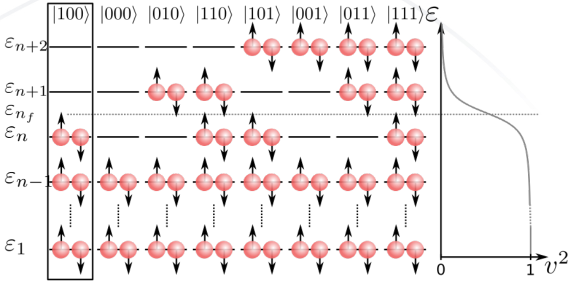

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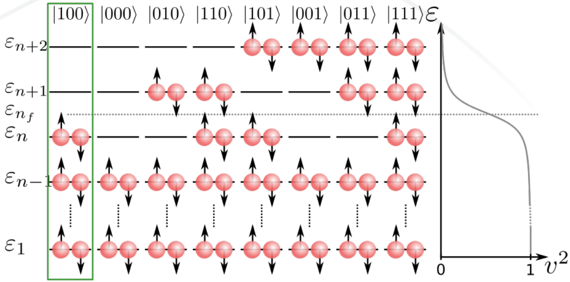

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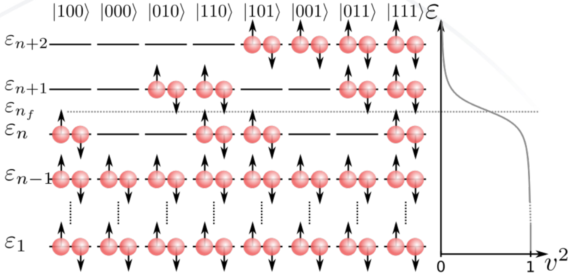

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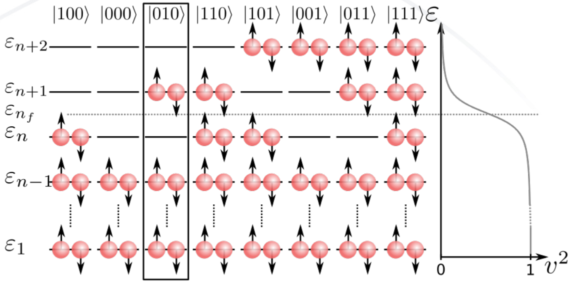

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Outline

Macro-Micro, ^{240}Pu

Shape parametrization

Tri-Quadratic Surface (3QS), 5 parameters

- α_2, α_3: mass asymmetry,
- σ_1, σ_2, σ_3: distance between the fragments, curvature of the neck & elongation of the fragments

Parametrized mean-field + pairing

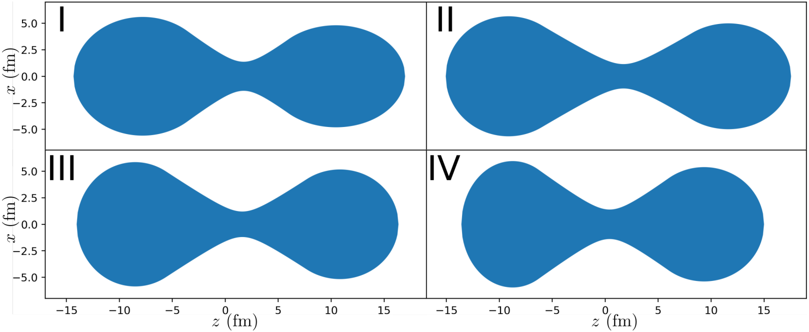
- Folded Yukawa,
- Axial HO basis with $N_{\mathrm{sh}} = 35$,
- Lipkin-Nogami with Seniority Pairing approximation

Macro-Micro, ^{240}Pu

Shape	α_2	α_3	σ_1	σ_2	σ_3	A_L	Z_L
I	0.30	0.192	3.500	-0.576	0.640	99.61	39.78
II	0.25	0.203	3.889	-0.365	0.810	101.33	40.91
III	0.25	0.250	3.500	-0.450	1.000	102.36	41.82
IV	0.20	0.605	3.182	-0.545	1.210	112.29	44.95

Macro-Micro, ^{240}Pu

Shape	α_2	α_3	σ_1	σ_2	σ_3	A_L	Z_L
I	0.30	0.192	3.500	-0.576	0.640	99.61	39.78
II	0.25	0.203	3.889	-0.365	0.810	101.33	40.91
III	0.25	0.250	3.500	-0.450	1.000	102.36	41.82
IV	0.20	0.605	3.182	-0.545	1.210	112.29	44.95



Macro-Micro, ^{240}Pu

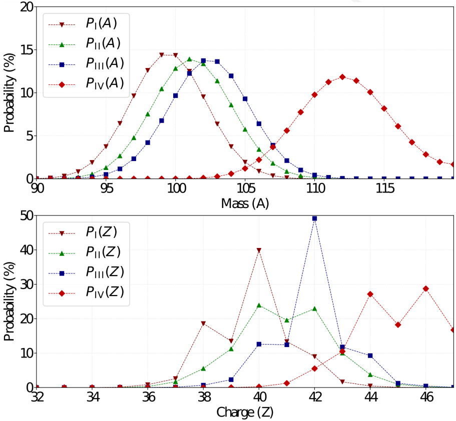


Figure: Mass (upper) and charge (lower) fragmentation probabilities associated with each shape

Macro-Micro, ^{240}Pu

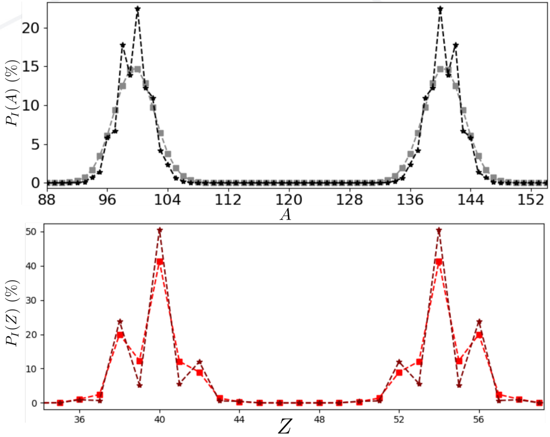


Figure: Comparison between the fragmentation probabilities obtained with the Monte Carlo method (light curves, square) and the projector method (dark curves, star) for the shape I

Microscopic, ^{240}Pu

Skyrme-HFB state calculated with HFBTHO (N. Schunck), $\langle \hat{Q}_{20} \rangle = 345$b.

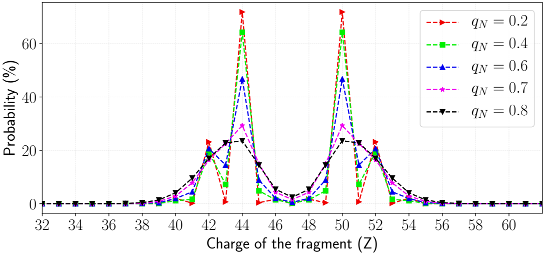


Figure: Evolution of the charge probability for the scission configuration associated with the least-energy fission path for ^{239}Pu(n,f) as a function of the expectation value of the Gaussian neck operator.

Outline

Objectives

We want to construct a method to evaluate the fragmentation probabilities with the following physical and practical considerations:

Physical considerations

- as few parameters as possible,
- integer fragmentations & dispersion,
- take into account 1- and 2-body correlations.

Practical considerations

- straitforward implementation,
- simplicity (light formalism & classical intuition),
- compatible with both macro-micro and microscopic approaches.

Objectives

We want to construct a method to evaluate the fragmentation probabilities with the following physical and practical considerations:

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Thank you!

arXiv:1811.05568 [nucl-th]