A thermodynamic approach to level densities

In the framework of Skyrme energy density functionals

W. Ryssens[1] and Y. Alhassid [1].

Center for Theoretical Physics,
Sloane Physics Laboratory,
Yale University.

28th of May 2018

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A Skyrme energy density functional looks like

$$E[\Psi] = \int d^3\mathbf{r}\,\mathcal{E}_{\mathrm{Sk.}}\left[\rho(\mathbf{r}),\tau(\mathbf{r}),\ldots\right] = \int d^3\mathbf{r}\,C^{\rho\rho}\rho(\mathbf{r})^2 + C^{\rho\tau}\rho(\mathbf{r})\tau(\mathbf{r})\ldots$$

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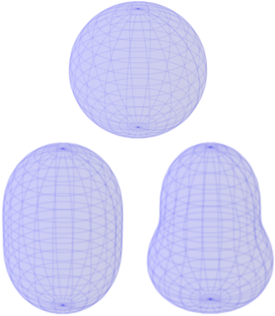
- Terms are bilinear in the densities $\rho, \tau, \dots$
- Microscopic, yet computationally cheap
- Applicable through the entire nuclear chart
- Around **10** parameters
- Fitted to masses and charge radii
- Symmetry breaking is crucial



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- Mean-field with Skyrme EDFs
  with HF, HF+BCS or HFB pairing.
- 3D coordinate mesh
  Typical basis size: 32000 $\sim$ 64000(!)

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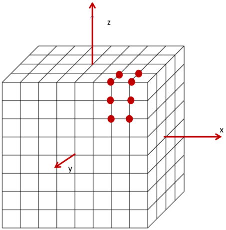

D. Baye et al. J. Phys. A 19 (1986).

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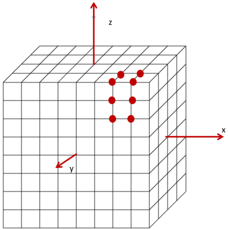
- 16 possible symmetry combinations
- Fast and easy to use
- Extremely accurate



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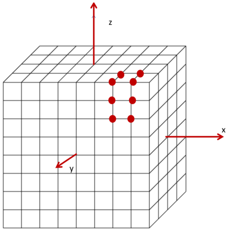
- Extended to finite temperature



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Canonical ensemble

$$Z_c = Tr[e^{-\beta \hat{H}}]$$

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Grand-canonical ensemble

$$Z_{gc} = Tr[e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}]$$

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$$\rho(E, N_n, N_p) \sim \left|\frac{\partial(E, N_n, N_p)}{\partial(\beta, \alpha_p, \alpha_n)}\right|^{-1/2} e^{S_{gc}(\beta)}$$

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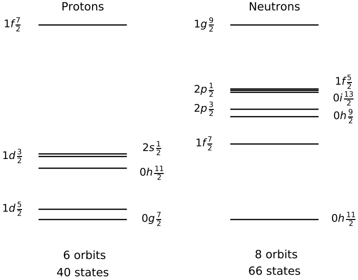
Projected grand-canonical ensemble

$$Z_{\mathrm{c}} = Tr[\hat{P}_N e^{-\beta\left(\hat{H}_{\mathrm{HFB}} - \mu \hat{N}\right)}] \,, \qquad \hat{P}_N = \frac{1}{N_s} \sum_{n=1}^{N_s} e^{-i \frac{2\pi n}{N_s} (\hat{N} - N)} \,.$$

Y. Alhassid, G.F. Bertsch, C. N. Gilbreth and H. Nakada, PRC **93**, 044320 (2016).
P. Fanto, Y. Alhassid and G.F. Bertsch, PRC **96**, 014305 (2017).

^{150}Nd as example

^{120}Sn core plus **Wood-Saxon** levels



$$\hat{H} = -\sum_{q=p,n} g_q \hat{P}_q^\dagger \hat{P}_q - \sum_{\lambda} \chi_\lambda : \hat{Q}_\lambda \cdot \hat{Q}_\lambda :$$

C. Özen, Y. Alhassid and H. Nakada, PRL **110**, 042502 (2013).

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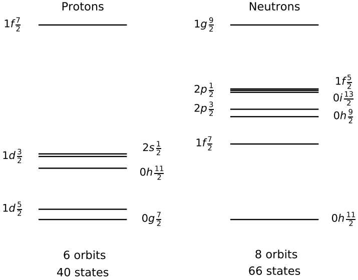

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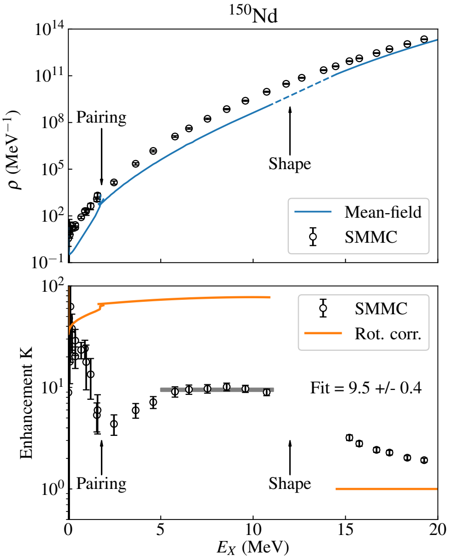

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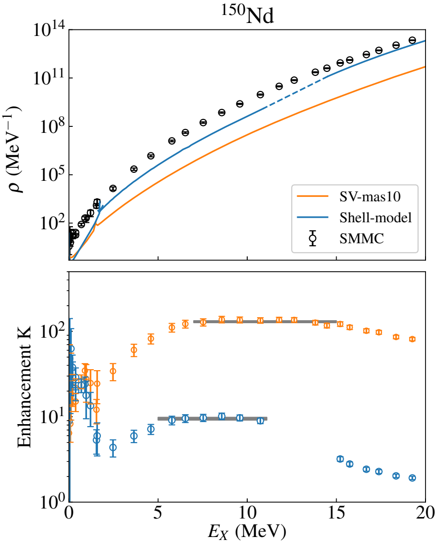
Skyrme functional

EDF of choice: **SV-mas10**

P. Klüpfel *et al.*, PRC **79**, 034310 (2009).



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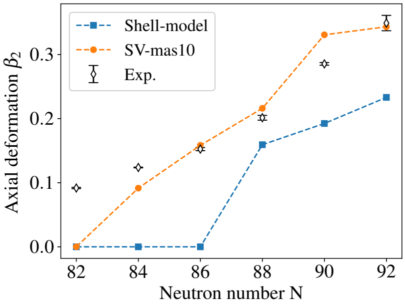

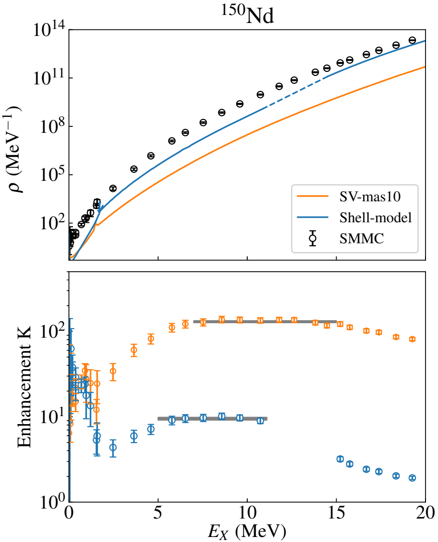

EDF	m^*/m
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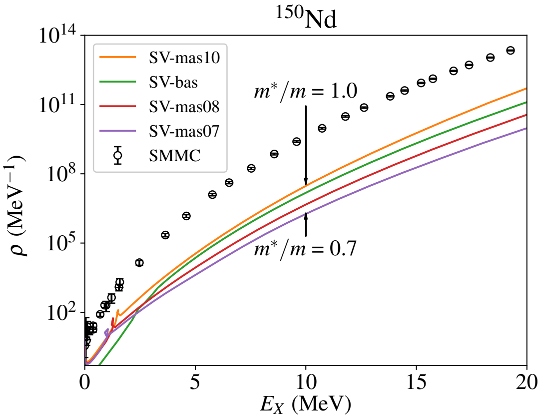

- Effective mass m^*/m controls single-particle level density

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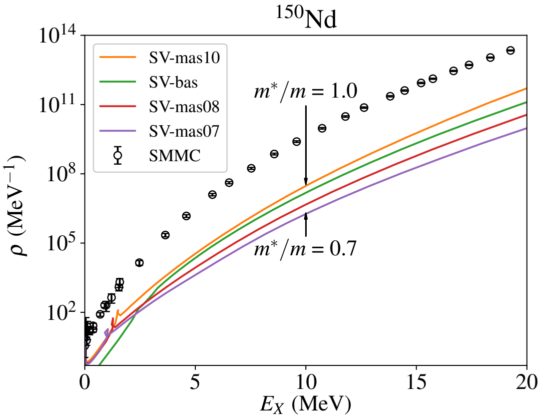

- Effective mass m^*/m controls single-particle level density
- Semiclassical methods with effective interactions often compensate for "bad" effective mass

V. Kolomietz *et al.*, PRC **97**, 064302 (2018), W.E. Ormand *et al.*, PRC **40**, 1510-1512(1989), M. Barranco *et al.*, NPA **351**, 269-284 (1981), S. Shlomo, NPA **539**, 17-36 (1992), and others . . . .

Enhancements for EDFs

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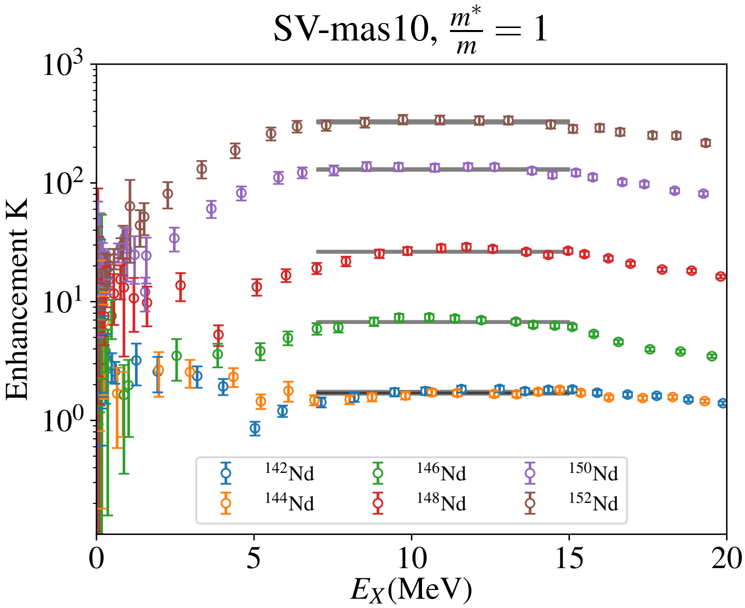
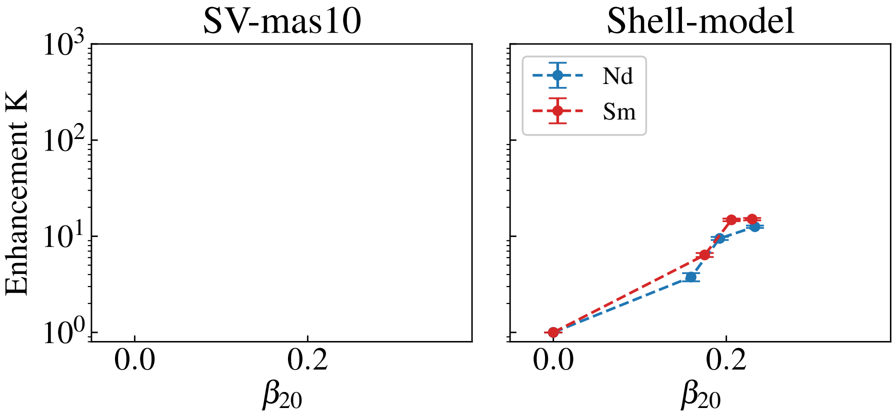
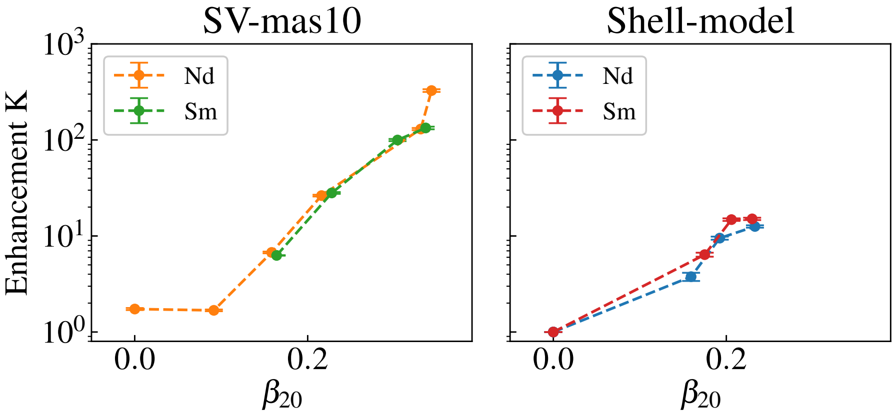
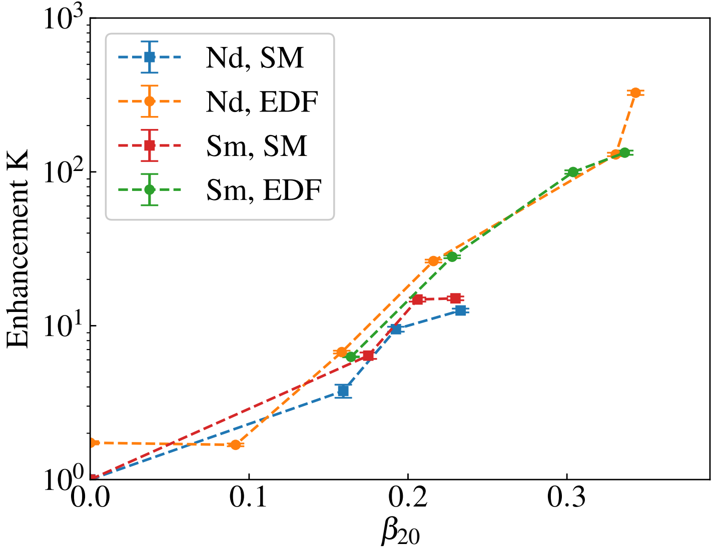


Correlating enhancements




SV-mas10
Shell-model
Enhancement K
10^3
10^2
10^1
10^0
Nd
Sm
0.0
0.2
β_{20}



Nd, SM
Nd, EDF
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We developed a model that ...

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Conclusions & Perspectives

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Open questions are . . .

- An analytical model for rotational enhancements?
- Systematic improvement of the shell-model interactions?
- Level density calculations for fission?

Thanks!

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Thanks for. . .

. . . the **help**:

- Paul-Henri Heenen ULB
- Michael Bender IPN Lyon
- Paul Fanto Yale
- Sohan Vartak Yale
- Yoram Alhassid Yale

. . . the **CPU time**!

- NERSC, DOE, USA.
- GRACE, YALE, USA.
- CÉCI network, Belgium.

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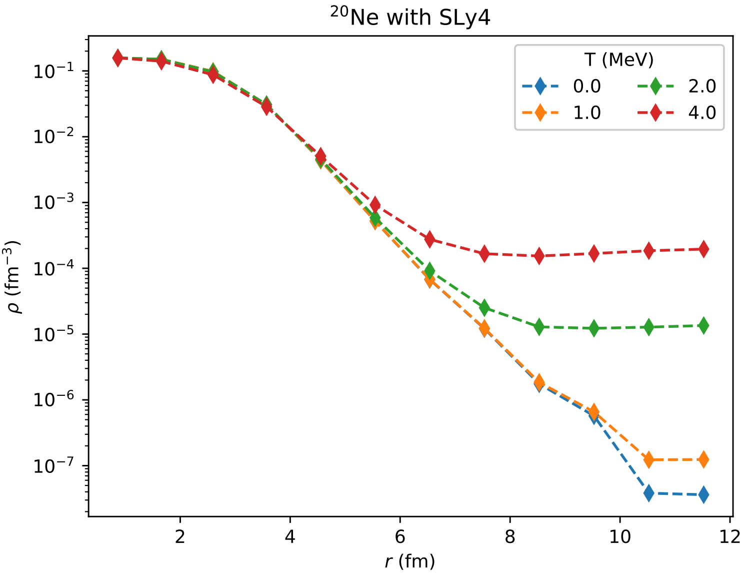
...your **attention**!


^{20}Ne with SLy4
T (MeV)
0.0
1.0
2.0
4.0
ρ (fm^{-3})
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
2
4
6
8
10
12
r (fm)

Why 3D coordinate space codes?

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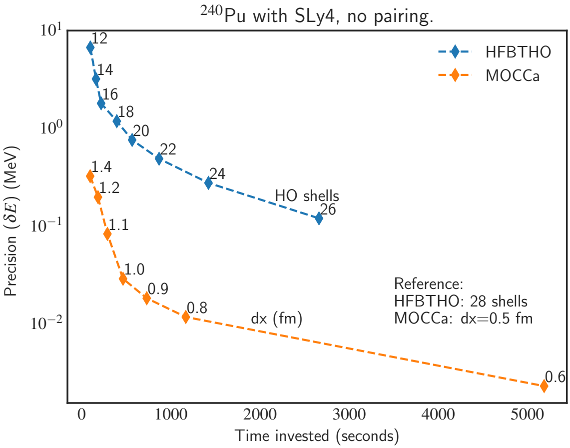
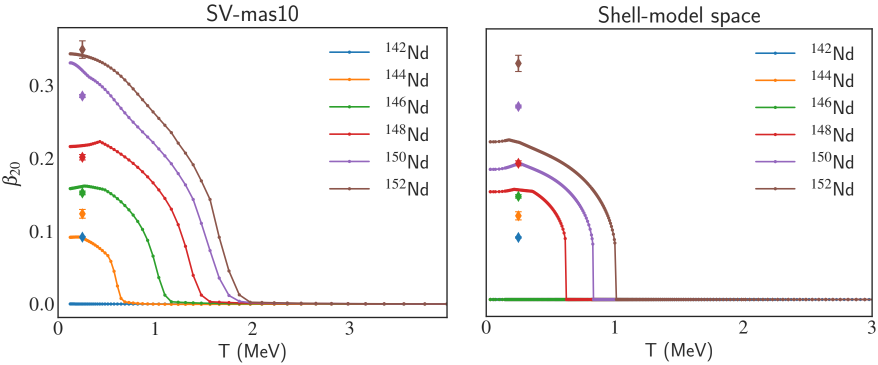


EV8: W. Ryssens *et al.*, CPC **187**, 175 - 194 (2015).
Precision: W. Ryssens *et al.*, PRC **92**, 064318 (2015).
Speed: W. Ryssens *et al.*, arXiv:1812.08262, accepted in EPJA.


SV-mas10
Shell-model space
β_{20}
0.0
0.1
0.2
0.3
0
1
2
3
T (MeV)
^{142}Nd
^{144}Nd
^{146}Nd
^{148}Nd
^{150}Nd
^{152}Nd

Analysis of enhancement

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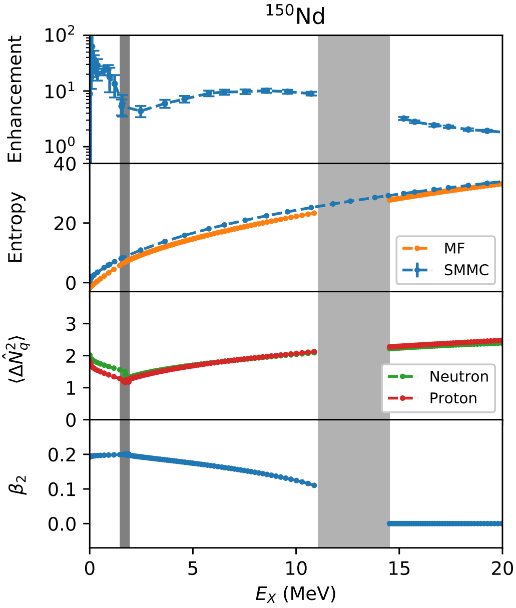

Single-particle levels "feel" a hamiltonian

$$\hat{h} \sim -\nabla \cdot \left[\frac{\hbar^2}{2m^*} \right] \nabla + U(\vec{r})$$

The effective mass m^*

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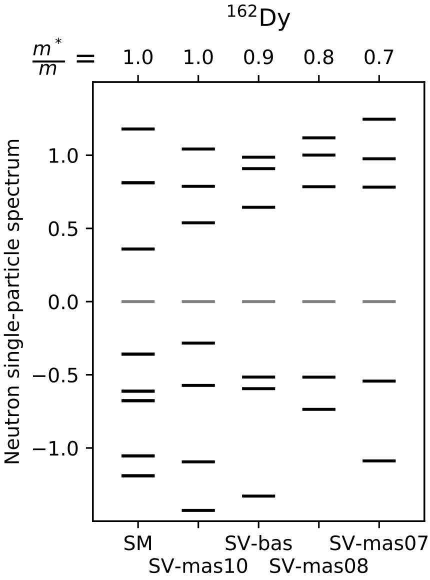

Octupole deformed Thoriums

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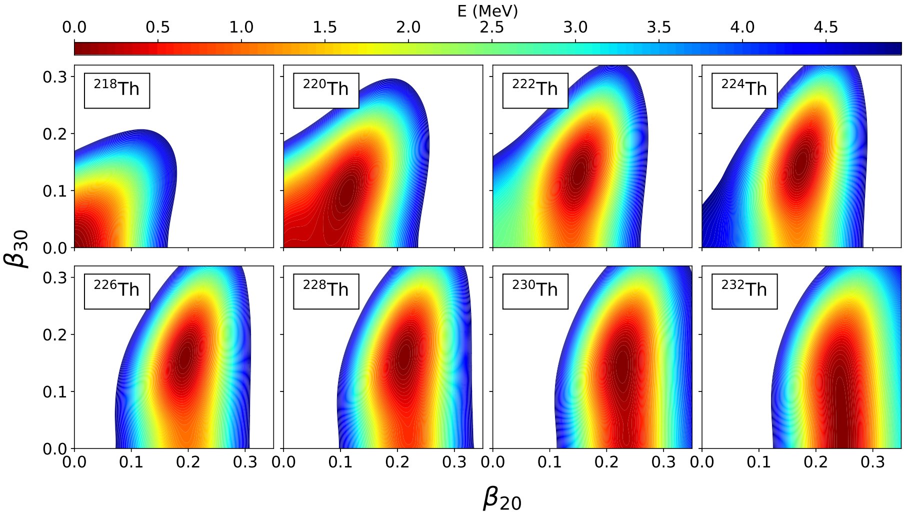
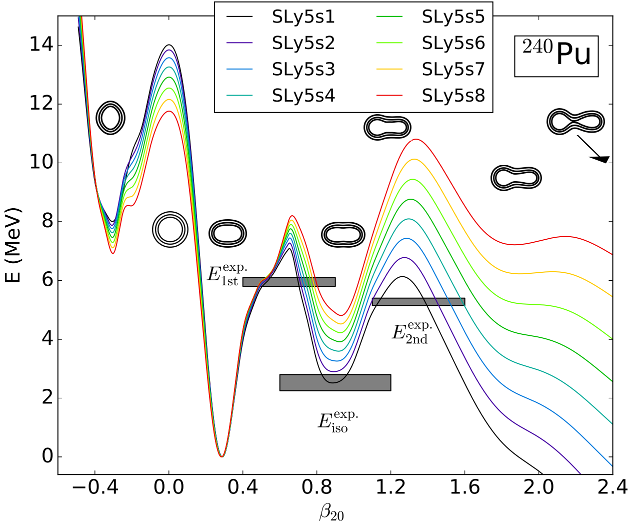


W. Ryssens, M. Bender and P.-H. Heenen, in preparation.

Fission Barriers

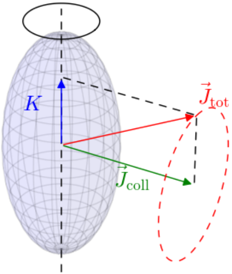


W. Ryssens et al., PRC **99**, 044315 (2019).

Bjørnholm-Bohr-Mottelson formula

For axially symmetric configurations

$$\rho_{\mathrm{intr.}}(E) = \sum_{K=\infty}^{+\infty} \rho_{\mathrm{intr.}}(E, K)\,. \qquad \frac{\rho_{\mathrm{intr.}}(E,K)}{\rho_{\mathrm{intr.}}(E)} \sim \exp\left[-\frac{K^2}{2\langle \hat{J}_z^2 \rangle}\right]\,.$$



Modelling a rotational band

$$\rho_{\mathrm{rot.}}(E, J) \sim \sum_{K=-I}^{I} \rho_{\mathrm{intr.}}\left[E - E_{\mathrm{rot.}}(K, J), K\right]$$

And the final total state density

$$\rho_{\mathrm{rot.}}(E) = \sum_{J=0}^{\infty} (2J+1)\rho_{\mathrm{rot.}}(E, J)\,.$$

S. Bjørnholm, A. Bohr and B. Mottelson,
Proc. Third IAEA Symp. on Physics and Chemistry of Fission, pp. 367-372 (1973).