Thermodynamically consistent calculations of nuclear level densities

based on mean field models

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

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

15th of June 2019

Yale

What are nuclear level densities?

The nuclear level density (NLD) $\rho(\mathbf{E_X})$ counts the **number of states** at excitation energy E_X **per unit energy**.

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Why should you care?

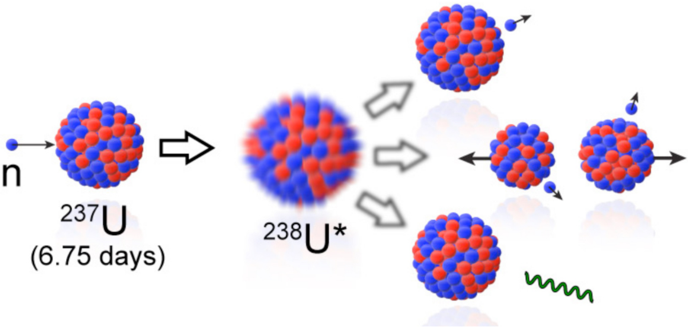

Figure adapted from J.E. Escher *et al.*, Rev. Mod. Phys. **84** 353-397 (2012).

The nuclear level density (NLD) $\rho(\mathbf{E_X})$ counts the **number of states** at excitation energy E_X **per unit energy**.

No seriously, why?

Credit: Nasa/Swift/Dana Berry

The thermodynamic approach to NLDs

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NLDs can be determined from the **partition function Z**

$$\rho[E_X(T)] \sim [C(T)]^{-\frac{1}{2}} e^{S(T)} \begin{cases} S(T) & \text{is the entropy} \\ C(T) & \text{is the heat capacity} \end{cases}$$

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$$Z = \mathrm{Tr}\left[e^{-\frac{1}{T}\hat{H}}\right]$$

Shell-model-Monte-Carlo (**SMMC**)

+ Advanced many-body technique
+ Incorporates all correlations
- Interactions and model spaces for mass regions

Mean-field (**MF**)

- Simple many-body technique
- Misses important correlations
+ Can be applied across the nuclear chart

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Goal

What can we learn from the SMMC to improve MF calculations?

Canonical partition

$$Z_C = \mathrm{Tr}_{\mathrm{N}}[\mathrm{e}^{-\frac{1}{\mathrm{T}}\hat{\mathrm{H}}}]$$

$$\uparrow$$

Trace over states with **correct N**

A note about ensembles

Canonical partition

$$Z_c = \mathrm{Tr_N}[\mathrm{e}^{-\frac{1}{\mathrm{T}}\hat{\mathrm{H}}}]$$

$$\uparrow$$

Trace over states with **correct N**

Grand-canonical partition

$$Z_{gc} = \mathrm{Tr}[\mathrm{e}^{-\frac{1}{\mathrm{T}}\left(\hat{\mathrm{H}}-\mu\hat{\mathrm{N}}\right)}]$$

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Trace over **all** states

A note about ensembles

Yale

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Grand-canonical partition

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↑

Trace over **all** states

Particle-number projected partition

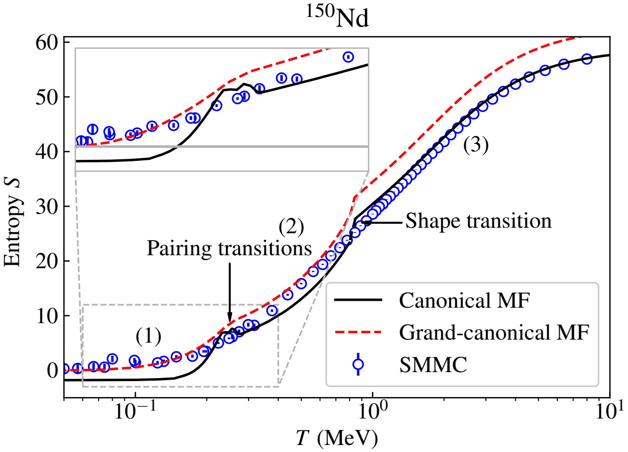
$$Z_{\mathrm{c}} = \mathrm{Tr}[\hat{\mathrm{P}}_{\mathrm{N}}\mathrm{e}^{-\frac{1}{\mathrm{T}}\left(\hat{\mathrm{H}}_{\mathrm{MF}}-\mu\hat{\mathrm{N}}\right)}] \, ,$$

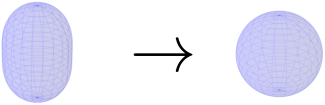
↑

$\hat{P}_N$ picks out the part with correct particle number

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





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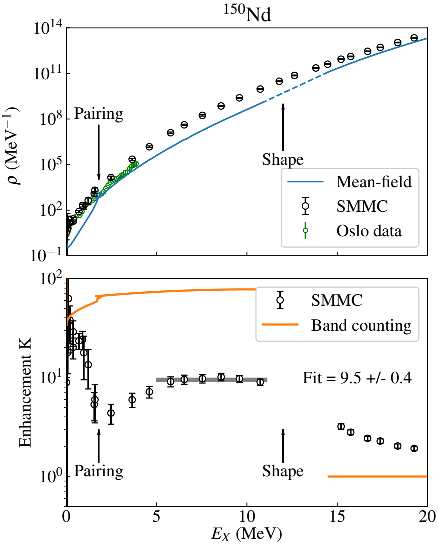

Collective enhancement factor

$$K = \frac{\rho^{\mathrm{SMMC}}}{\rho^{\mathrm{MF}}}$$

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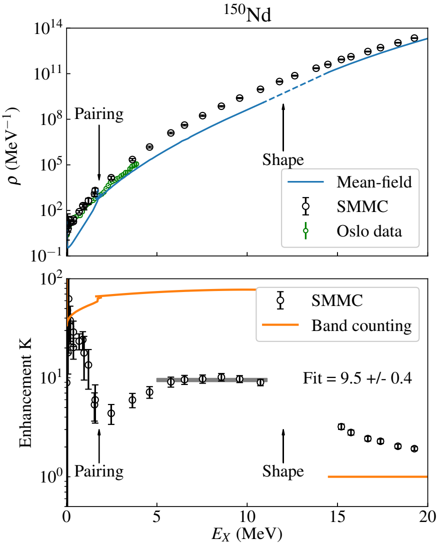
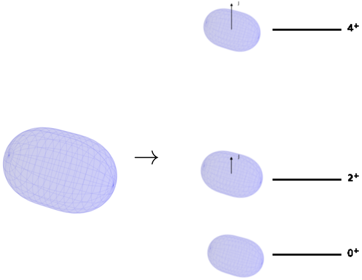


Collective enhancement factor

$$K = \frac{\rho^{\mathrm{SMMC}}}{\rho^{\mathrm{MF}}}$$

- Quantifies missing correlations
- ...mostly rotational bands

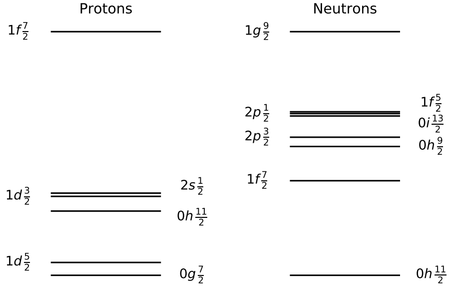


Single-particle model spaces

Shell-model space

Locally adjusted (3 parameters)

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



6 orbits
40 states

8 orbits
66 states

+ ^{120}Sn core

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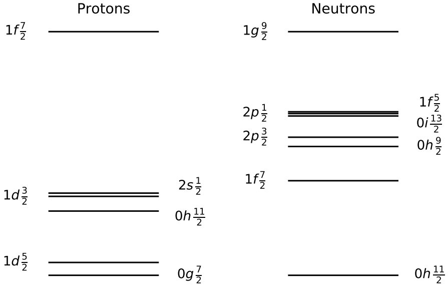

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40 states

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66 states

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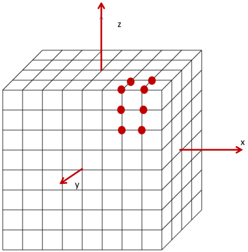
Skyrme EDFs

Globally adjusted ($\sim$ 10 parameters)

$$E[\Psi] = \int d^3\mathbf{r}\, C^{\rho\rho} \rho(\mathbf{r})^2 + C^{\rho\tau} \rho(\mathbf{r}) \tau(\mathbf{r}) \ldots$$



32000 - 64000 states

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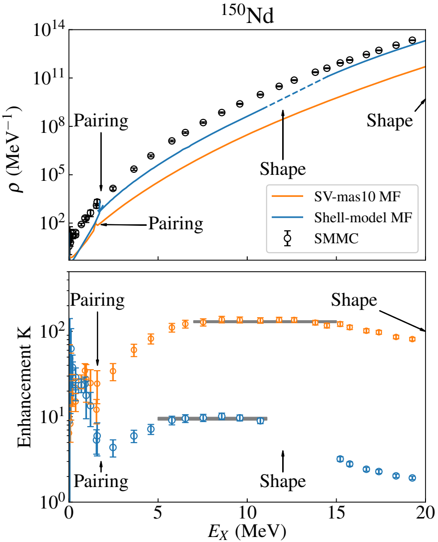
EDF of choice: **SV-mas10**

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



Back to ^{150}Nd

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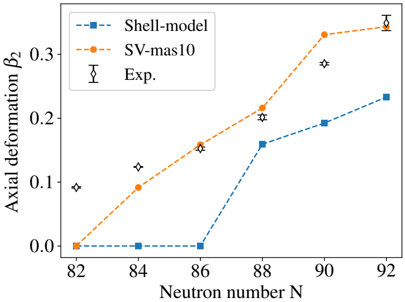
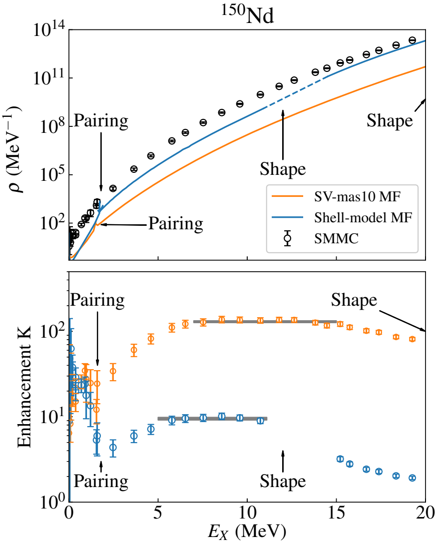
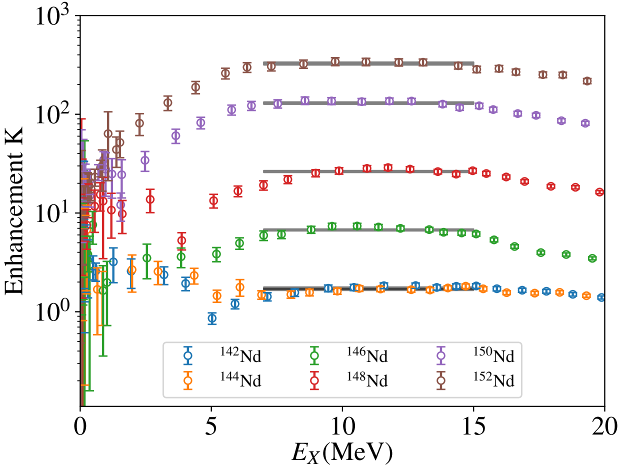
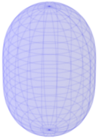
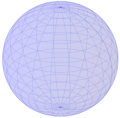






Enhancement K
10^0
10^1
10^2
10^3
0
5
10
15
20
E_X(MeV)
^{142}Nd
^{144}Nd
^{146}Nd
^{148}Nd
^{150}Nd
^{152}Nd





Correlating *K* and deformation

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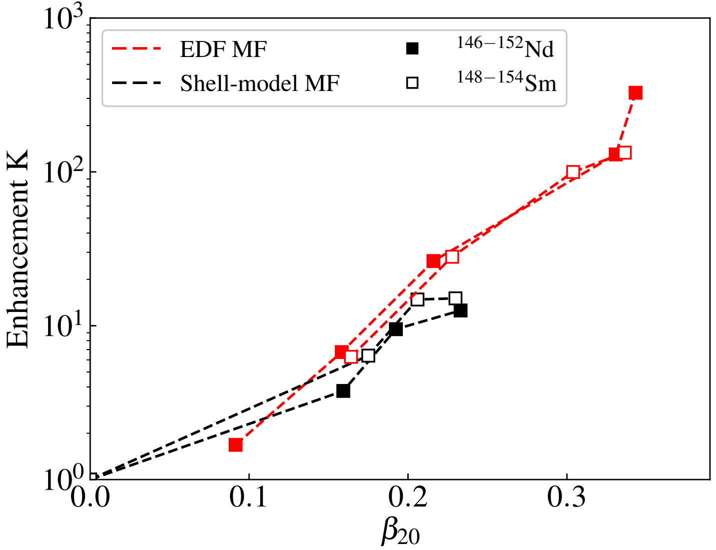

We developed a model that . . .

- is based on a **Skyrme EDF**
    - microscopic yet applicable across the nuclear chart

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- is **thermodynamically consistent**
  - derived from a mean field partition function.
  - Number projection after variation

Conclusions & Perspectives

We developed a model that . . .

- is based on a **Skyrme EDF**
  - microscopic yet applicable across the nuclear chart
- is **thermodynamically consistent**
  - derived from a mean field partition function.
  - Number projection after variation
- we are using to study **rotational enhancements**
  - which seem to correlate very well with deformation.

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  - Number projection after variation
- we are using to study **rotational enhancements**
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Open problems are . . .

- A simple model for rotational enhancements
- Systematic construction of shell-model interactions

Thanks for...

...the **help**:

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

...the **CPU time**!

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

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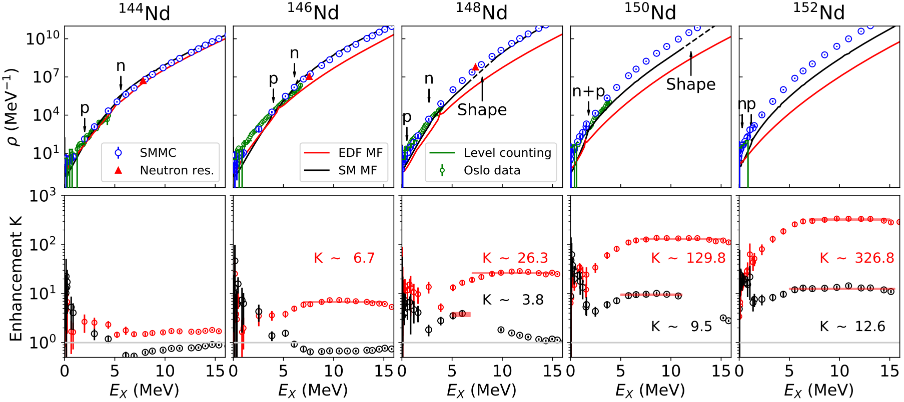
- CÉCI network, Belgium.

...your **attention**!

Yale

Bonus!

Nd isotopes

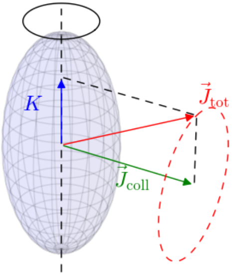


^{144}Nd
^{146}Nd
^{148}Nd
^{150}Nd
^{152}Nd
ρ (MeV^{-1})
10^{10}
10^{7}
10^{4}
10^{1}
p
n
n+p
np
Shape
SMMC
Neutron res.
EDF MF
SM MF
Level counting
Oslo data
Enhancement K
10^{3}
10^{2}
10^{1}
10^{0}
K ~ 6.7
K ~ 26.3
K ~ 3.8
K ~ 129.8
K ~ 9.5
K ~ 326.8
K ~ 12.6
0
5
10
15
E_X (MeV)

Bjørnholm-Bohr-Mottelson formula

For axially symmetric configurations

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



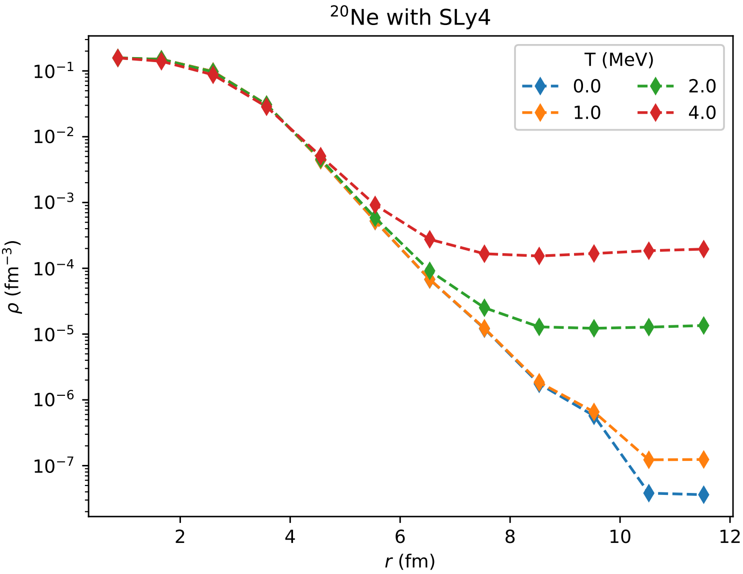
Modelling a rotational band

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

And the final total state density

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

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


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

Why 3D coordinate space codes?

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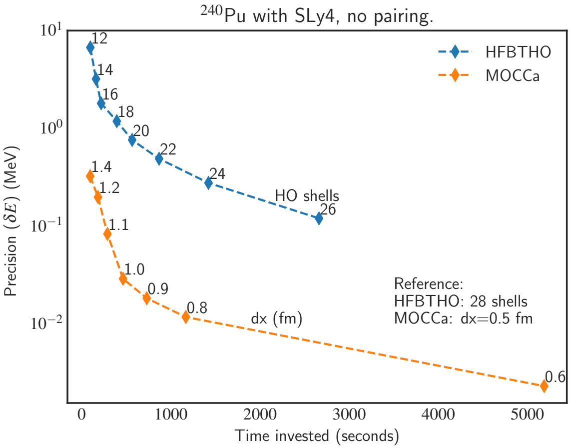

EV8: W. Ryssens *et al.*, CPC **187**, 175 - 194 (2015).
Precision: W. Ryssens *et al.*, PRC **92**, 064318 (2015).
Speed: W. Ryssens *et al.*, arXiv:1812.08262, accepted in EPJA.

Shape transitions

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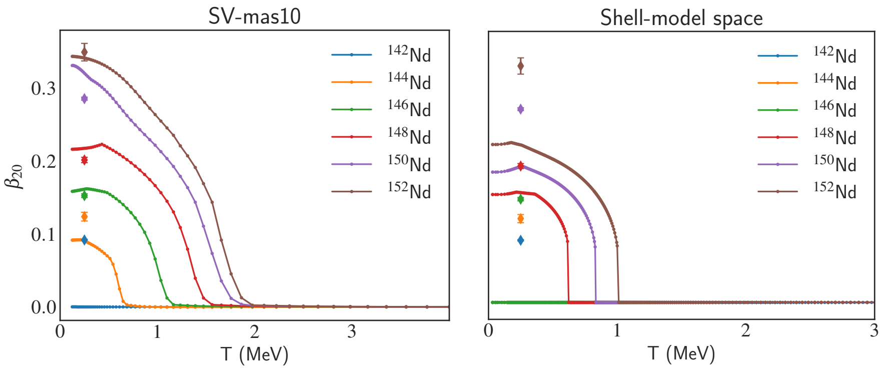
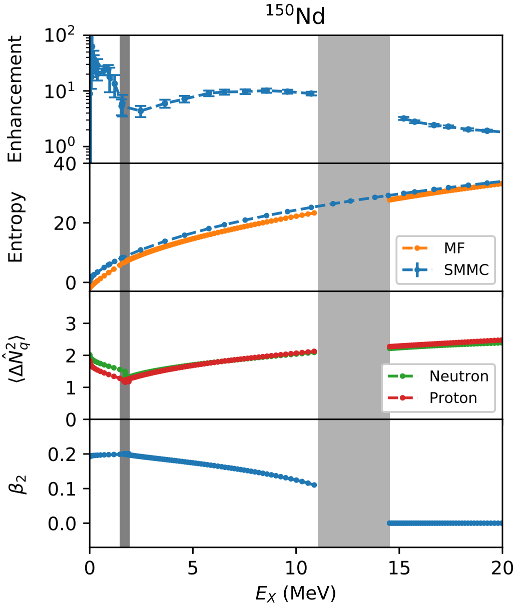


Analysis of enhancement



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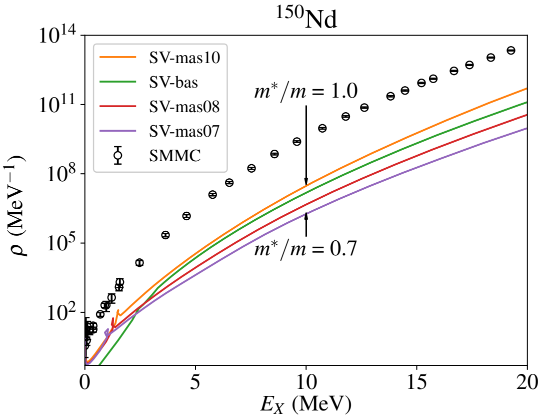
EDF	m^*/m
SV-mas10	1.0
SV-bas	0.9
SV-mas08	0.8
SV-mas07	0.7
SLy4	0.7



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

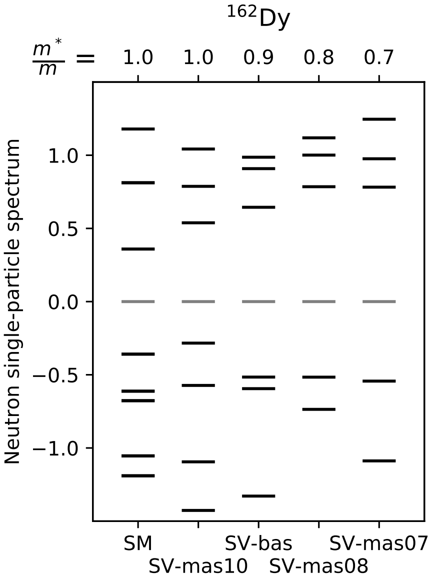
V. Kolomietz *et al.*, PRC **97**, 064302 (2018), W.E. Ormand *et al.*, PRC **40**, 1510-1512(1989), M. Barranco *et al.*, NPA **351**, 269-284 (1981), S. Shlomo, NPA **539**, 17-36 (1992), and others . . . .

Single-particle levels "feel" a hamiltonian

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

EDF	m^*/m
SV-mas10	1.0
SV-bas	0.9
SV-mas08	0.8
SV-mas07	0.7
SLy4	0.7

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



Octupole deformed Thoriums

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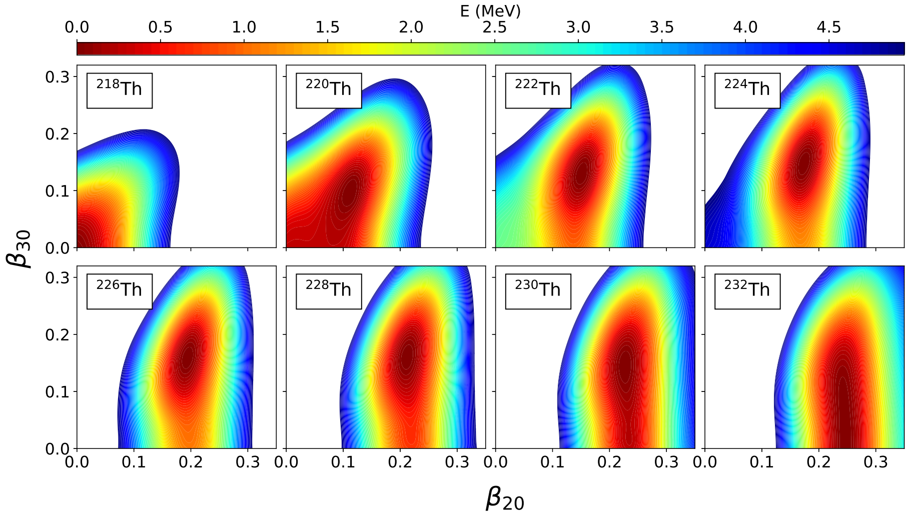
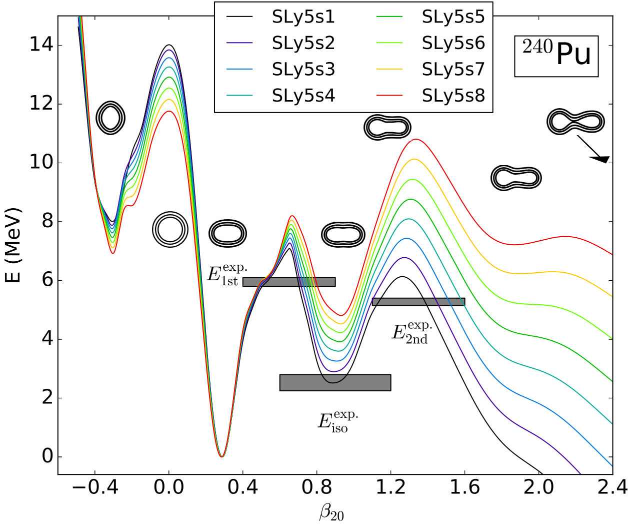


W. Ryssens, M. Bender and P.-H. Heenen, in preparation.

Fission Barriers



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

Mean-field calculations with Skyrme EDFs

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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 $\rho, \tau, \ldots$

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- Microscopic, yet computationally cheap
- Applicable through the entire nuclear chart

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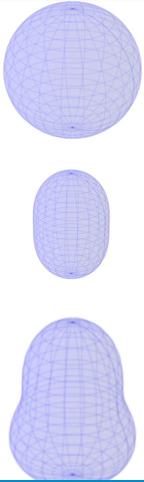

- Densities calculated from an underlying product wavefunction Ψ
- Terms are bilinear in the densities $\rho, \tau, \ldots$
- Microscopic, yet computationally cheap
- Applicable through the entire nuclear chart
- Around **10** parameters
- Fitted to masses and charge radii
- Symmetry breaking is crucial

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      `.___.'
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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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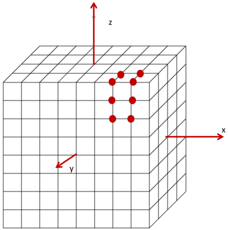

D. Baye et al. J. Phys. A 19 (1986).

MOCCa

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    '.___.'
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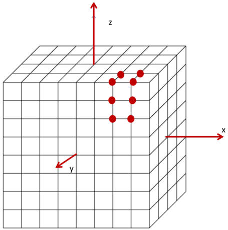
- Fast and easy to use
- Extremely accurate



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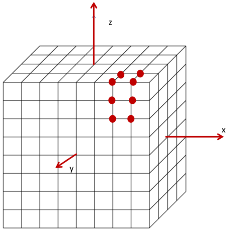
- Extremely accurate
- Extended to finite temperature



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