Level densities in heavy nuclei

Shell model Monte Carlo versus mean-field

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12th of November 2019

Nuclear level densities

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

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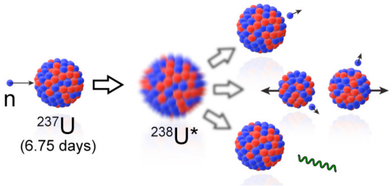

Figure adapted from J.E. Escher *et al.*, Rev. Mod. Phys. **84** 353-397 (2012).

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

Credit: Nasa/Swift/Dana Berry

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Shopping list

We want $\rho(E)$

- all nuclei
- all spins and parities, $\rho(E, J^\pi)$
- from a CONSISTENT microscopic model

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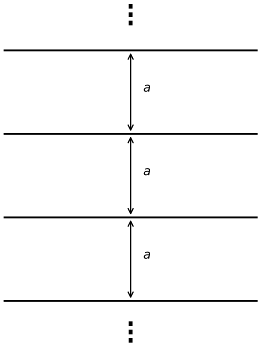
- Analytical models

  Ex: Backshifted Fermi gas, constant-T, . . .
  Low predictive power
  Used in many reaction codes



$$\rho \sim a^{-1/4} E_X^{-5/4} \exp\left[2\sqrt{a(E_X - \Delta)}\right]$$

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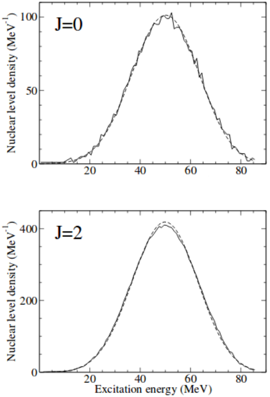
- Shell Model

  Direct level counting in a modelspace
  Studies up to $A \sim 60$



From R. Sen'kov and V. Zelevinsky, PRC 93, 064304 (2016).

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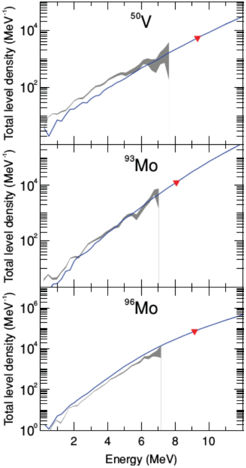
- <u>Combinatorial models</u>

  Combinations of single-particle excitations
  Using EDFs, mic-mac or analytic potentials
  Studies across the nuclear chart
  Empirical modelling of collective effects



S. Goriely, S. Hilaire and A. Koning, PRC **78**, 064307 (2008).

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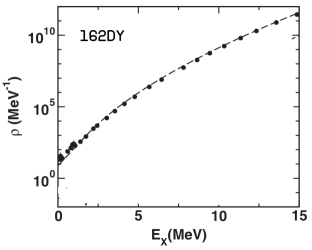
- **S**hell **M**odel **M**onte **C**arlo

  Basis dimension $> 10^{30}$!
  Involves statistical errors
  (Almost) no information on individual levels
  Up to $A \sim 160$ (for now)



Y. Alhassid et al., PRL **101**,082501 (2008).

Hubbard - Stratonovich transformation

$$\langle \hat{O} \rangle_\beta = \frac{\mathrm{Tr}\left[\hat{O}e^{-\beta\hat{H}}\right]}{\mathrm{Tr}\, e^{-\beta\hat{H}}} = \frac{\int \mathcal{D}[\sigma]\, G_\sigma \langle \hat{O} \rangle_\sigma \,\mathrm{Tr}\,(U_\sigma)}{\int \mathcal{D}[\sigma]\, G_\sigma \mathrm{Tr}\,(U_\sigma)} \begin{cases} \sigma = \text{auxiliary fields} \\ G_\sigma = \text{Gaussian weight} \\ U_\sigma = \text{one-body propagator} \end{cases}$$

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Shell **M**odel

- Single-particle modelspace
- Interaction $\hat{H}$

Monte **C**arlo

- MC evaluation of integrals
- Statistical error bars

Shell Model Monte Carlo

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Level densities from thermodynamical relations

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

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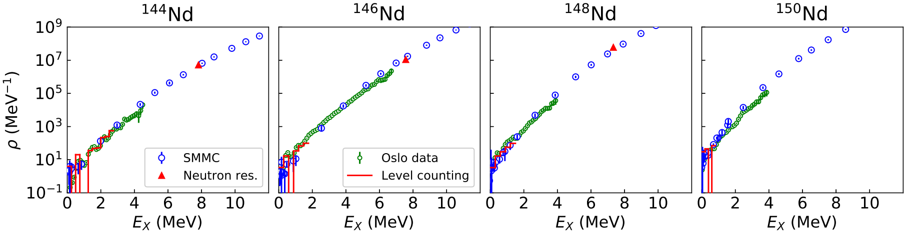
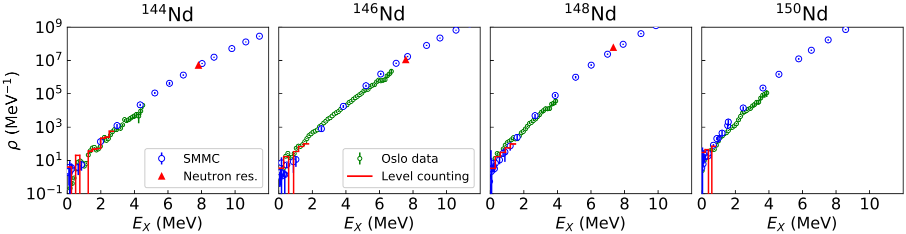


^{120}Sn core plus **Wood-Saxon** levels and **PQ** interaction

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

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

Nd isotopes as example



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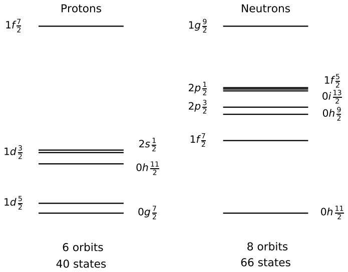

C. Özen, Y. Alhassid and H. Nakada, PRL **110**, 042502 (2013).

SMMC

- ✓ Includes all correlations
- ✓ Obtain $\rho(E, J, \pi)$ with $\hat{P}_J$, $\hat{P}_\pi$
- ✗ Computationally expensive
- ✗ Availability of model spaces
- ✗ Availability of interactions

SMMC versus mean-field

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

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Method

T-depent mean-field calculations with same model space and interaction!

Ensemble reduction

Canonical partition

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

and

$$\rho(E) \sim \left|\frac{\partial E}{\partial \beta}\right|^{-1/2} e^{S_c(T)}$$

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Grand-canonical partition

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

and

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

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Particle-number projected partition

Mean-field Hamiltonian

↓

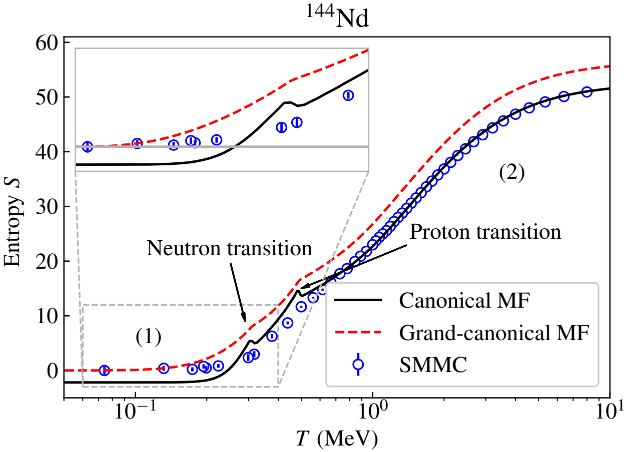
$$Z_c = \mathrm{Tr}[\hat{\mathrm{P}}_\mathrm{N} \mathrm{e}^{-\beta\left(\hat{\mathrm{H}}_\mathrm{MF} - \mu \hat{\mathrm{N}}\right)}],$$

↑

$\hat{P}_N$ 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).

Spherical: ^{144}Nd



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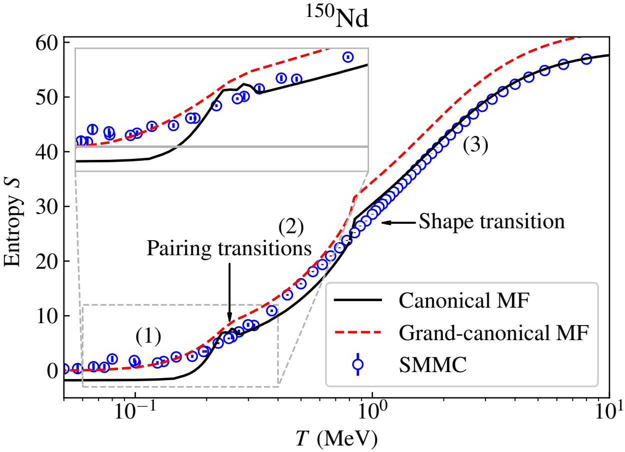
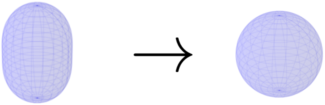
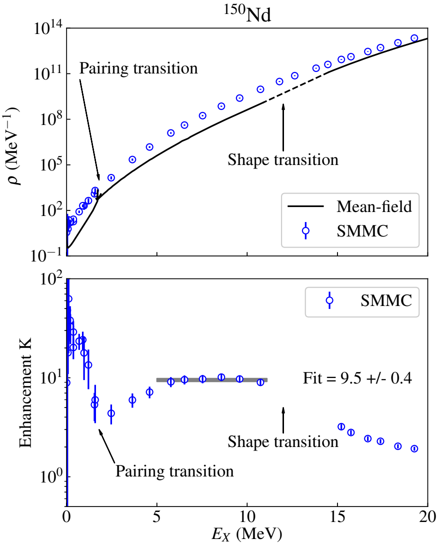


150Nd
Entropy S
T (MeV)
60
50
40
30
20
10
0
10−1
10^0
10^1
Pairing transitions
Shape transition
(1)
(2)
(3)
Canonical MF
Grand-canonical MF
SMMC



Collective enhancement

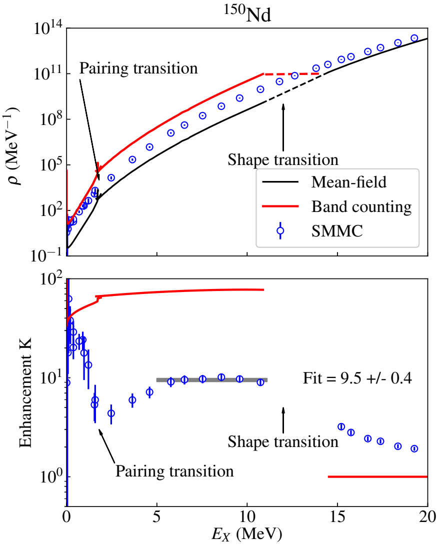


Collective factor K

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

Collective enhancement

Yale



Collective factor K

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

Simple rotational model

$$\rho_{\mathrm{intr.}}(E, K) \sim \exp[-K^2]\rho(E)$$

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

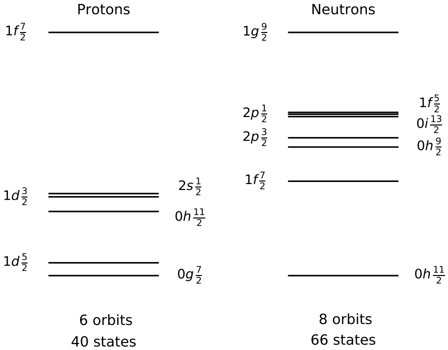
$$E_{\mathrm{rot}} = \frac{J(J+1) - K^2}{2\mathcal{I}_\perp}.$$

Single-particle model spaces

Shell-model space

Locally adjusted (3 parameters)

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



+ ^{120}Sn core

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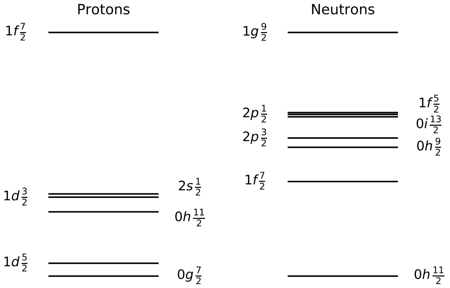


6 orbits
40 states

8 orbits
66 states

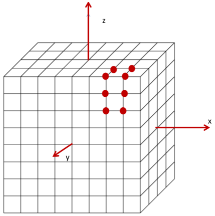
+ ^{120}Sn core

Skyrme EDFs

Globally adjusted (∼ 10 parameters)

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

Solved with **MOCCa** in coordinate space



32000 - 64000 basis dimension

EDF of choice: **SV-mas10**
P. Klüpfel *et al.*, PRC **79**, 034310 (2009).

What can we achieve with EDFs?

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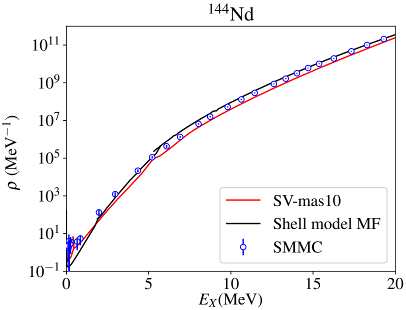

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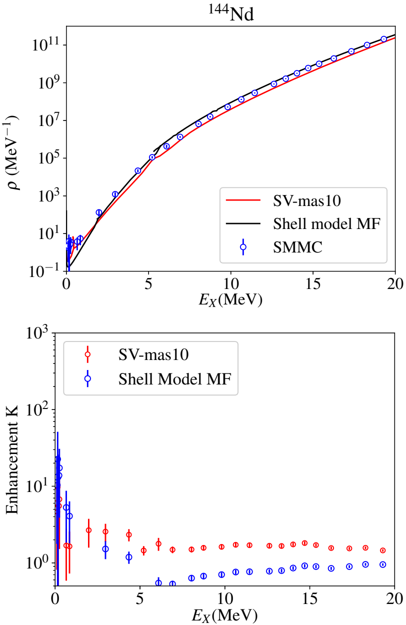

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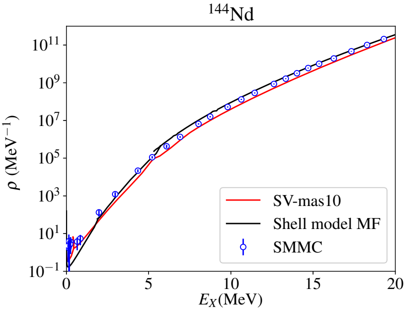

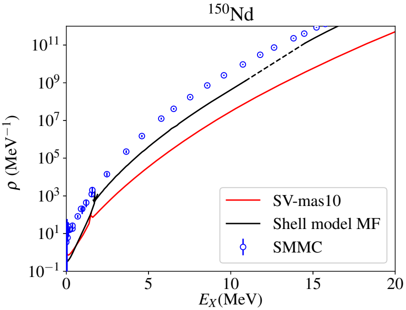

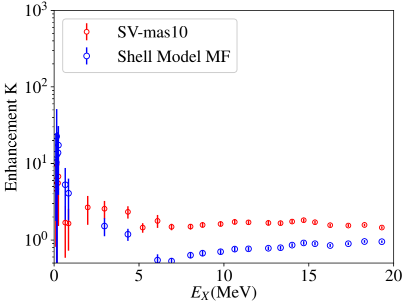

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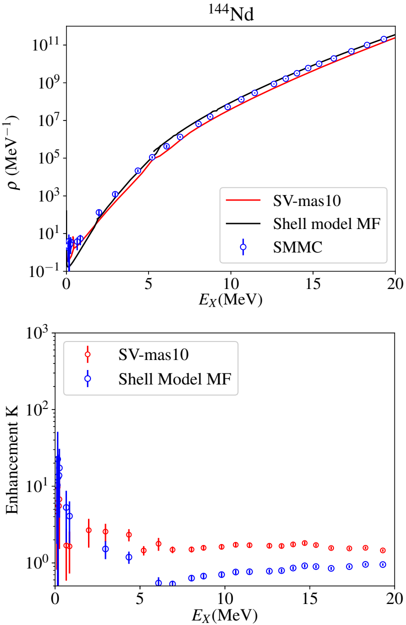
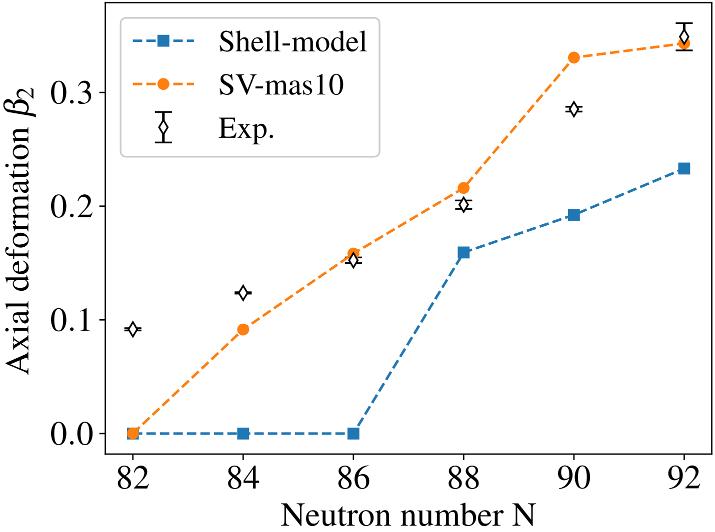


^{144}Nd
^{150}Nd
ρ (MeV^{-1})
E_X(MeV)
SV-mas10
Shell model MF
SMMC
Enhancement K
Shell Model MF

Deformations of the Nd chain



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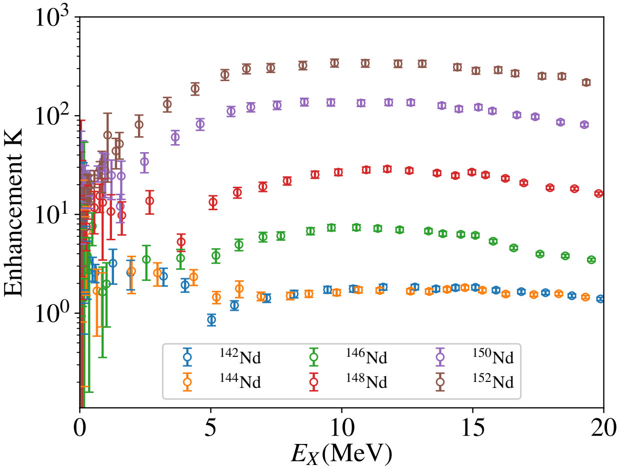
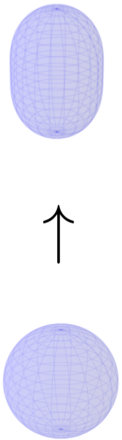

Enhancement K
10^3
10^2
10^1
10^0
0
5
10
15
20
E_X(MeV)
^{142}Nd
^{144}Nd
^{146}Nd
^{148}Nd
^{150}Nd
^{152}Nd



The effective mass m^*

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

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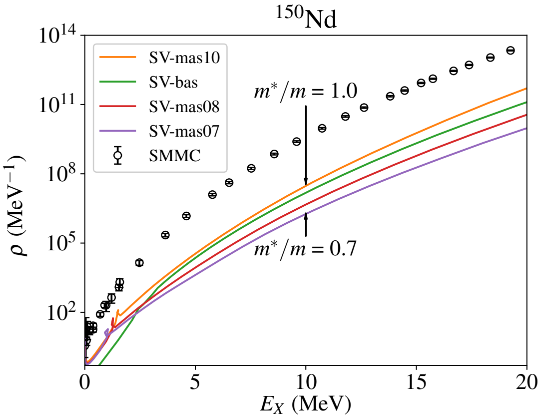

- Effective mass m^*/m controls single-particle level density

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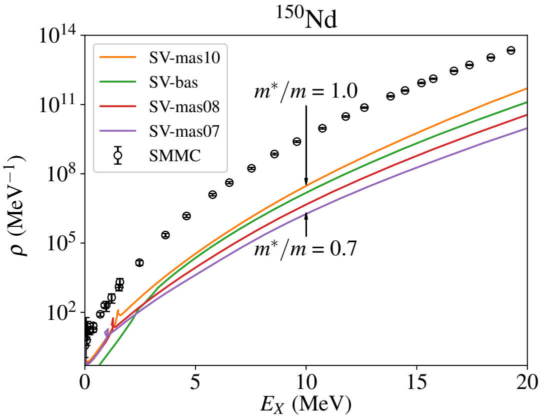

- Effective mass m^*/m controls single-particle level density
- Semiclassical methods with effective interactions often compensate for "bad" effective mass

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 . . . .

Conclusions

Thermodynamical mean-field calculations . . .

- . . . with ensemble reduction through projection.

The (bright) future

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- ...and specifically the enhancement factors!

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- How can MF(+RPA) inform the construction of SMMC interactions?
- Systematics for the lanthanides
- ... and specifically the enhancement factors!
- Make the jump to the actinides with the SMMC!

Thanks!

Yale

Thanks for. . .

. . . the **help**:

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

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- Paul Fanto — Yale
- Sohan Vartak — Yale
- Scott Jensen — Yale
- Yoram Alhassid — Yale

...the **CPU time**!

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

Thanks for. . .

. . . the **help**:

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

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. . . your **attention**!

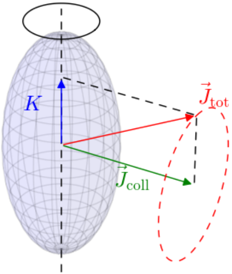
Bonus!

$$
\begin{aligned}
Z_{\mathrm{c}} &= \mathrm{Tr}[\hat{\mathrm{P}}_{\mathrm{N}} \mathrm{e}^{-\beta\left(\hat{\mathrm{H}}_{\mathrm{MF}} - \mu \hat{\mathrm{N}}\right)}] \,, \\
E_{\mathrm{c}} &= -\frac{\partial \ln Z_g c}{\partial \beta} \\
S_c &= \ln Z_{\mathrm{c}} + \beta E_{\mathrm{c}} \\
\rho(E) &\approx \left(2\pi \left| \frac{\partial E}{\partial \beta} \right| \right)^{-1/2} e^{S_{\mathrm{c}}}
\end{aligned}
$$

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

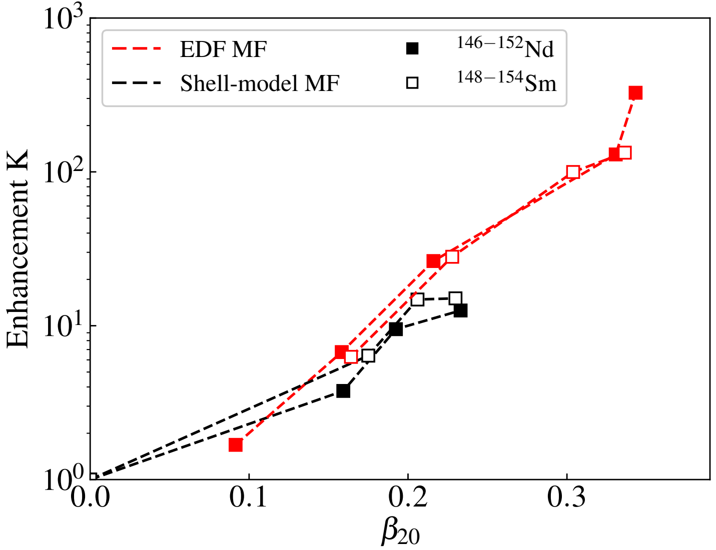
$$\rho_{\text{rot.}}(E,J) \sim \sum_{K=-I}^{I} \rho_{\text{intr.}} \left[E - E_{\text{rot.}}(K,J), K\right]$$

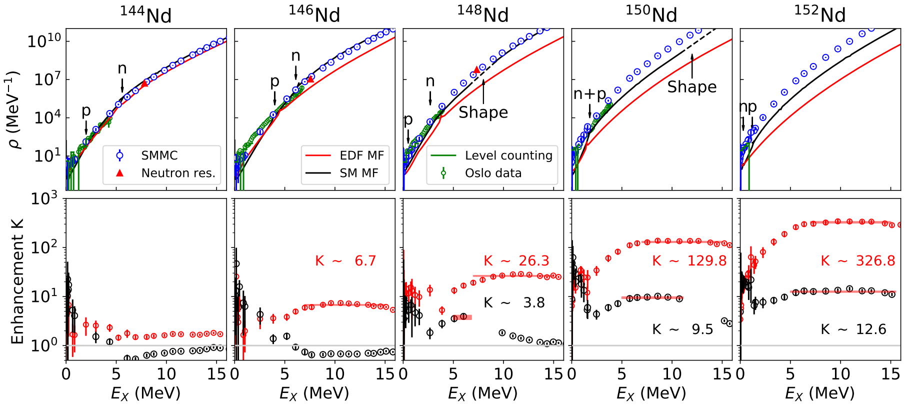
And the final total state density

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

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

Correlating *K* and deformation

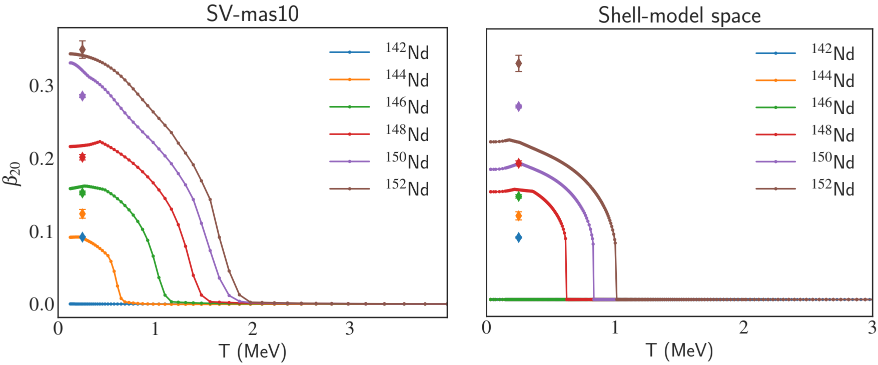




144Nd
146Nd
148Nd
150Nd
152Nd
ρ (MeV−1)
Enhancement K
p
n
n+p
np
Shape
SMMC
Neutron res.
EDF MF
SM MF
Level counting
Oslo data
K ~ 6.7
K ~ 26.3
K ~ 3.8
K ~ 129.8
K ~ 9.5
K ~ 326.8
K ~ 12.6
EX (MeV)

Shape transitions

Yale



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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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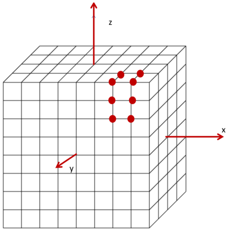

D. Baye et al. J. Phys. A 19 (1986).

Yale

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        `.___.'
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- Mean-field with Skyrme EDFs
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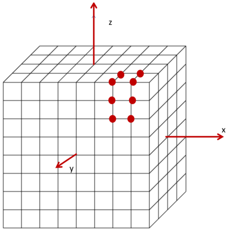
- 3D coordinate mesh
  Typical basis size: 32000 $\sim$ 64000(!)
- 16 possible symmetry combinations
- Fast and easy to use
- Extremely accurate



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- Mean-field with Skyrme EDFs
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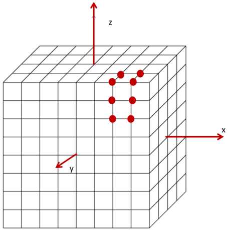
- 3D coordinate mesh
  Typical basis size: 32000 $\sim$ 64000(!)
- 16 possible symmetry combinations
- Fast and easy to use
- Extremely accurate
- Extended to finite temperature



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

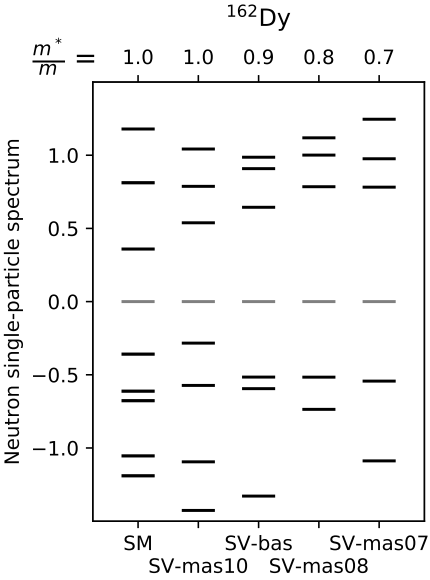
Yale

Single-particle levels “feel” a hamiltonian

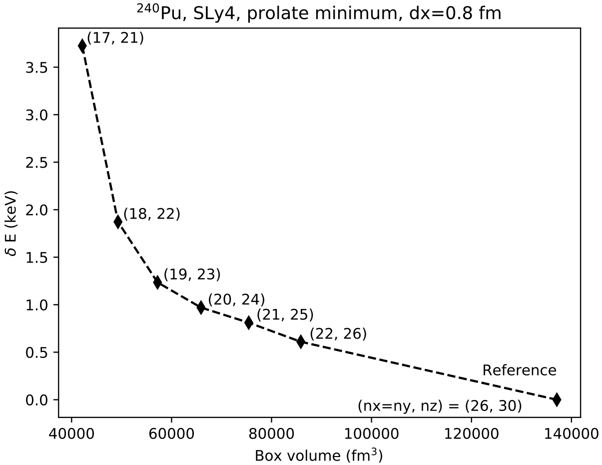
$$\hat{h} \sim -\nabla \cdot \left[\frac{\hbar^2}{2m^*}\right] \nabla + U(\vec{r})$$

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).



Why 3D coordinate space codes?



EV8:	WR, V. Hellemans, M. Bender and P.-H. Heenen, CPC **187**, 175 - 194 (2015).
Precision:	WR, M. Bender and P.-H. Heenen, PRC **92**, 064318 (2015).
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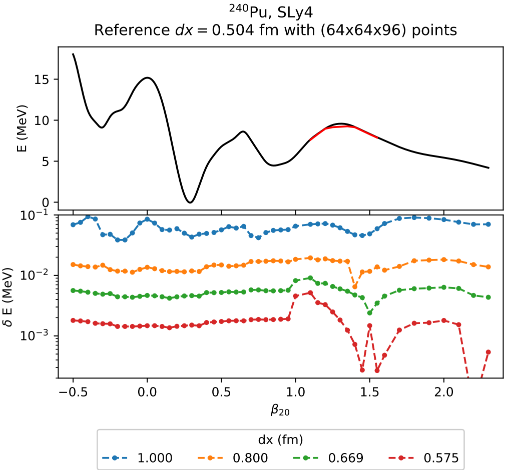

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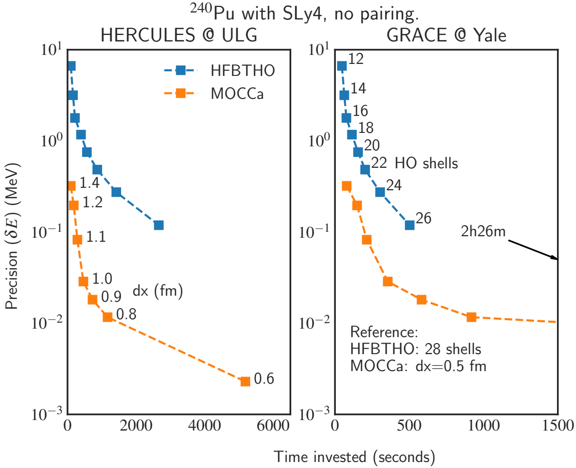

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