Level densities from mean-field approaches

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Models for level densities

- `Simple' (constant T, Fermi gas, ...)
  Very effective but low predictive power
- Shell Model (Direct level counting)
  (Limited) Studies up to Fe region
- `Mean-field' (Mostly combinatorial)
  Applicable everywhere (EDFs!)
- **S**hell **M**odel **M**onte **C**arlo
  Exact up to statistical errors, $A \sim 160$

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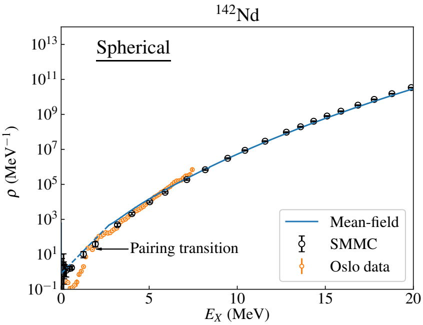

Mean-field vs. SMMC

- Same interaction, same s.p. space
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- . . . after variation

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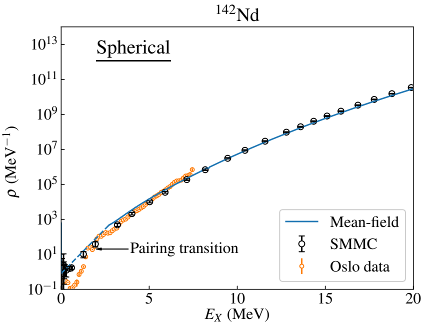

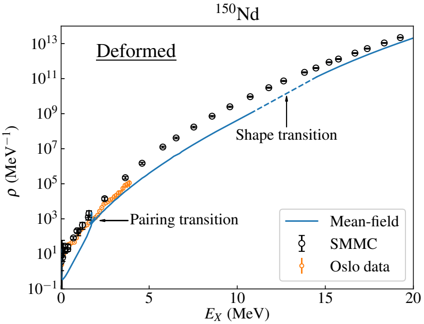

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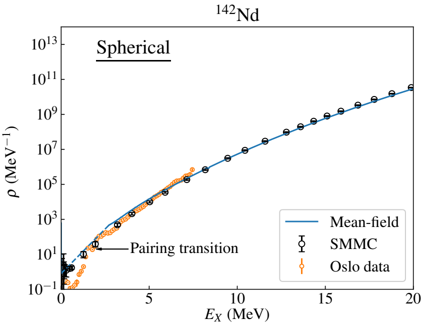
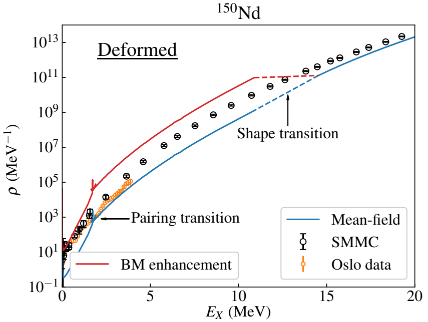
Bohr & Mottelson's collective enhancement model

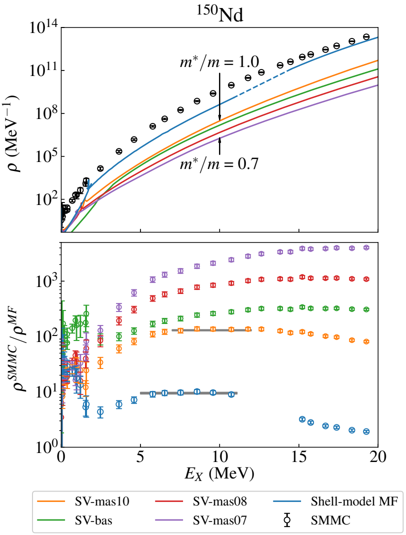
$$\rho_{\text{rot.}}(E, J) \sim \sum_{K=-J}^{J} \rho_{\text{intr.}}\left[E - E_{\text{rot.}}(K, J), K\right]$$





Level densities from Skyrme EDFs?

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



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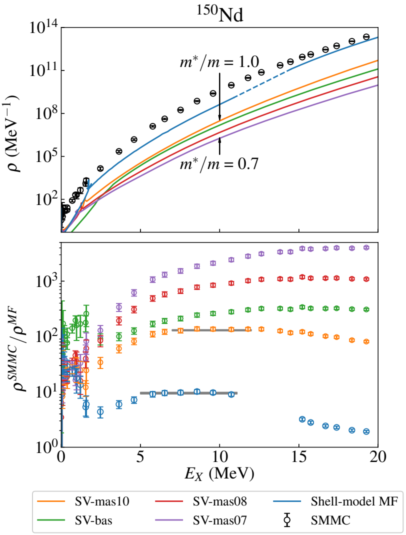

It seems m^*/m should be $\sim$ 1!

Empirical corrections for small m^* have been included for decades

M. Barranco and J. Treiner, NPA **351** (1981),
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And the authors of the largest compilation of MF level densities agree ($m^*/m \sim 1.05$!)

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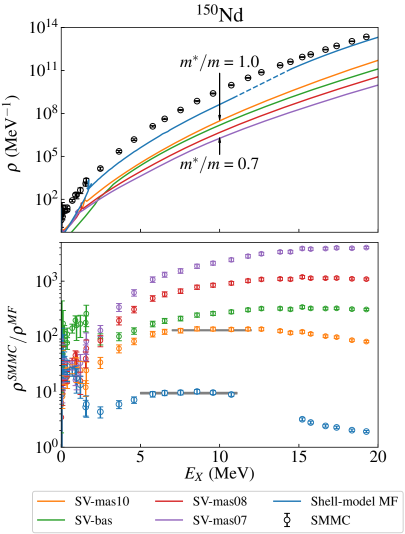

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Two issues

- Can we model collective enhancements microscopically?
- Can we expect reliable level densities from current EDFs?

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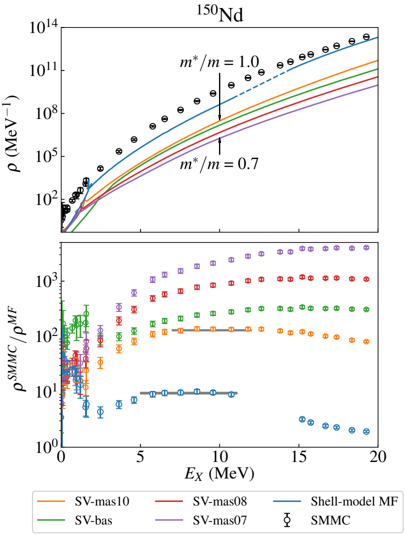

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Future work: SYSTEMATICS

- Systematics of lanthanides
- SMMC calculations for actinides
- Comparison to combinatorial models

Systematic construction of SMMC interactions!

Thanks!

Thanks for...

...all things "cool" ($T=0$) .

- Paul-Henri Heenen — ULB
- Michael Bender — IPN Lyon

...all things "hot" ($T \neq 0$)

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

...the CPU time!

- NERSC, DOE, USA.
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…your **attention**!

Questions for discussion

Collective effects

- Is there a more in-depth modelling of collective effects ?

  S. Bjørnholm, A. Bohr and B. Mottelson, Proc. Third IAEA Symp. on Physics and Chemistry of Fission, pp. 367-372 (1973).
- How about the Bohr-Mottelson enhancement for reflection asymmetric shapes? Non-axial shapes?
- What about Landau thermal averaging? Seems good for one-body observables, but what about the entropy S?

Level densities from EDFs

- Can we model beyond-mean-field effects for the effective mass?
- What about 'surface-peaked' effective mass?

Reading list

Approximate projection on particle number

- Y. Alhassid et al., PRC **93**, 044320 (2016).
- P. Fanto et al., PRC **96**, 014305 (2017) and P. Fanto, PRC **96** 051301(R) (2017).

Collective enhancements

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

State of the art mean-field level densities

- P. Demetriou and S. Goriely, NPA **695**, 95-108 (2001).
- S. Hilaire et al., PRC **86**, 064317 (2012).
- R. Capote et al., Nucl. Data Sheets **110** 3107-3214 (2009).

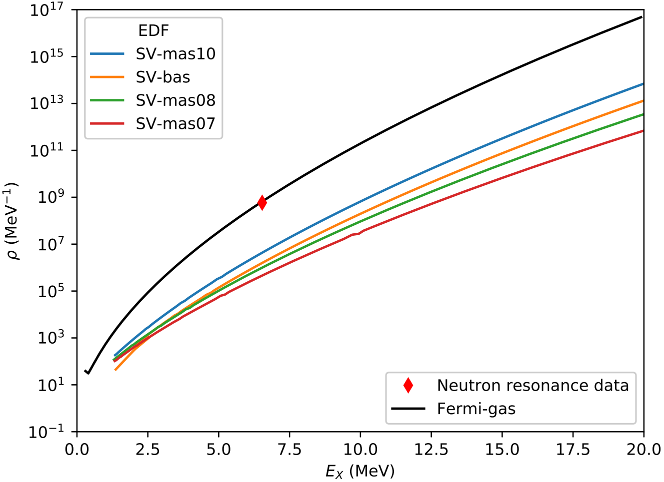
Effective mass issues with level densities

- M. Barranco and J. Treiner, NPA **351** (1981).
- M. Prakash et al., PLB **128** (1983), and many others . . .

Surface peaked effective mass for EDFs

- M. Zalewski et al., PRC **81**, 044314 (2010)
- A. F. Fantina et al., J. Phys. G: Nucl. Part. Phys. **38**, 025101 (2011).

^{240}Pu



EDF
SV-mas10
SV-bas
SV-mas08
SV-mas07
Neutron resonance data
Fermi-gas
ρ (MeV^{-1})
E_X (MeV)
10^{17}
10^{15}
10^{13}
10^{11}
10^{9}
10^{7}
10^{5}
10^{3}
10^{1}
10^{-1}
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

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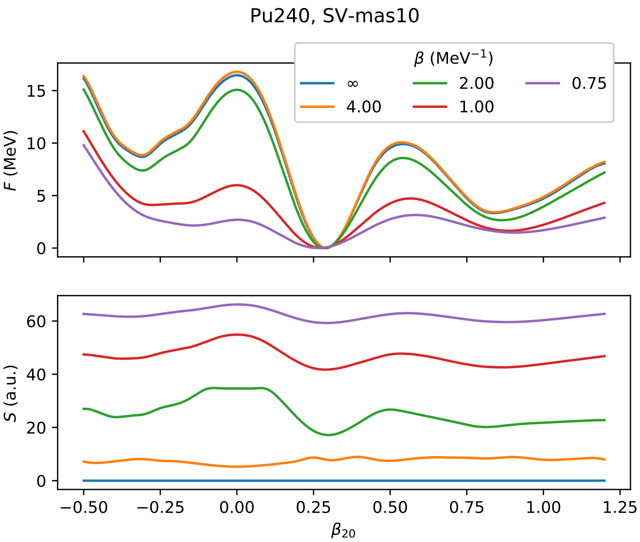

Pu240, SV-mas10
β (MeV⁻¹)
∞
4.00
2.00
1.00
0.75
F (MeV)
S (a.u.)
β20
15
10
5
0
60
40
20
0
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
1.25

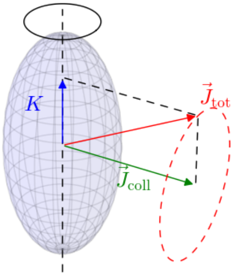
Bjørnholm-Bohr-Mottelson formula

For axially symmetric configurations

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

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

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

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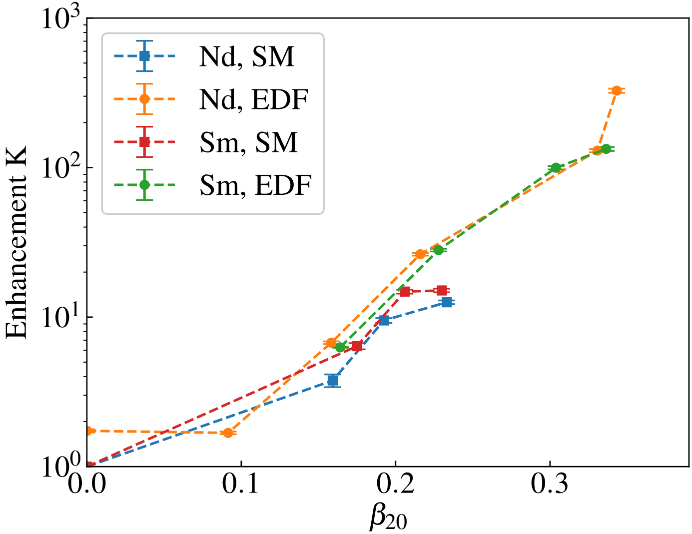
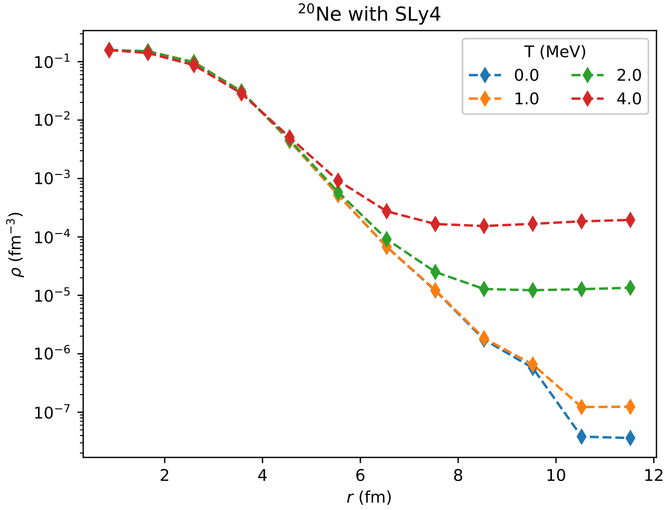
Collective enhancements

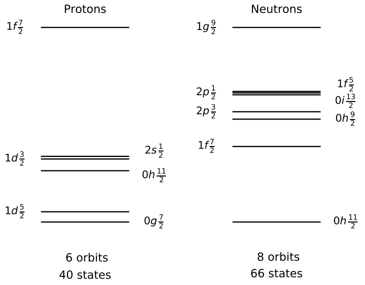


Nucleus plus gas



Model

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



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

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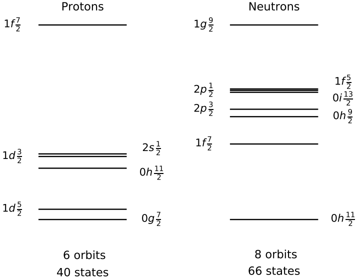

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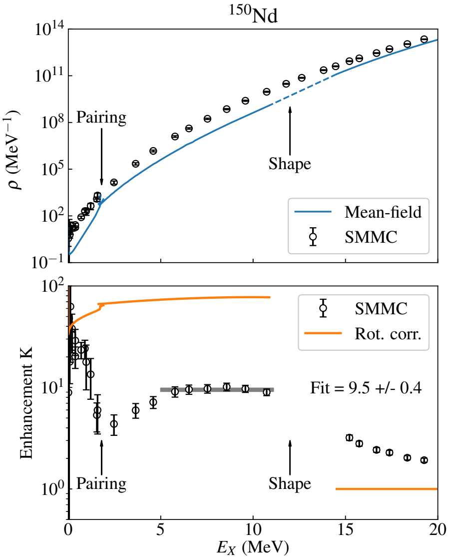

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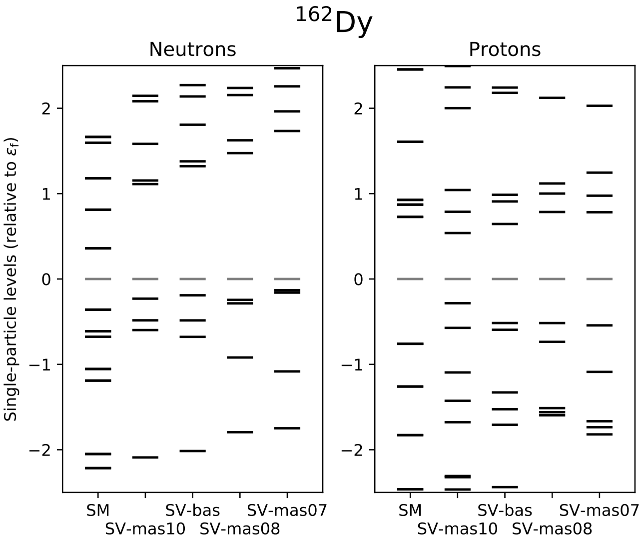
S.p. spectrum of ^{162}Dy



Ensemble reduction

Canonical ensemble

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

and

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

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<u>Grand-canonical ensemble</u>

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

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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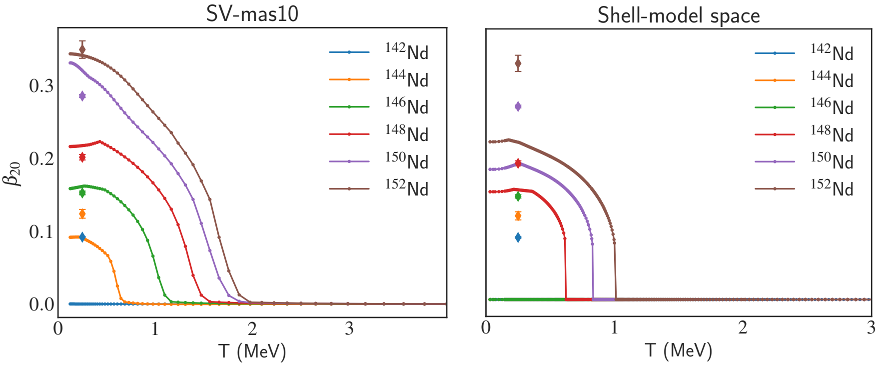
Projected grand-canonical ensemble

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

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).

Shape transitions



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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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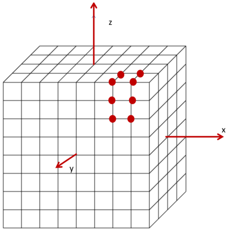

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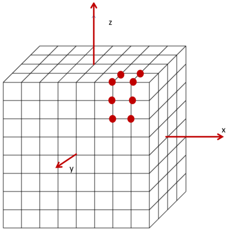

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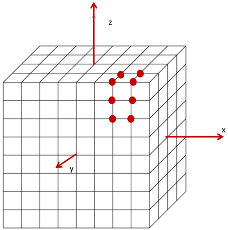

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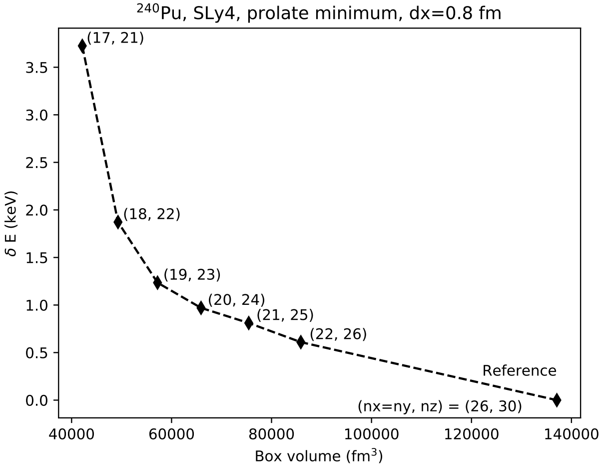
Why 3D coordinate space codes?



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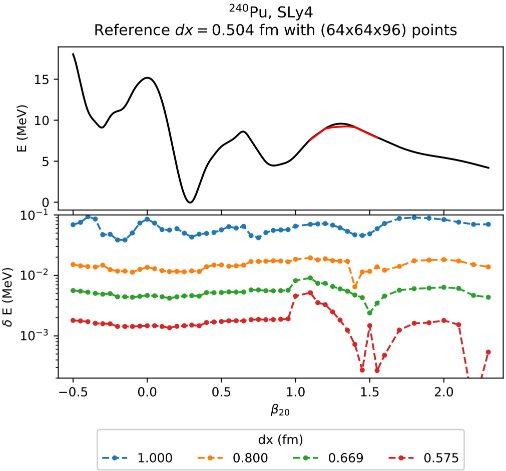

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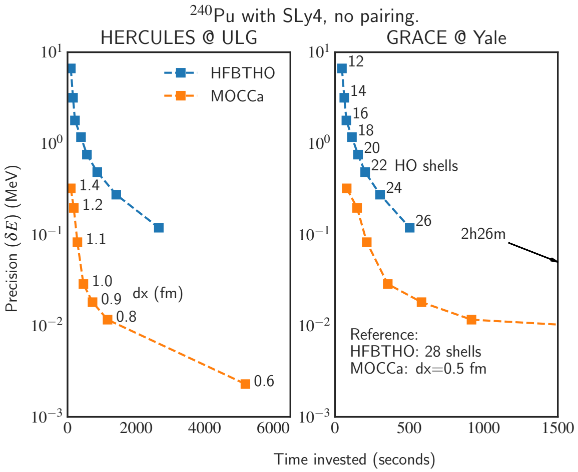

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Subproblem separation

Diagonalization subproblem:
Diagonalize $\hat{h}^{(i)}$; obtain $|\psi_l^{(i+1)}\rangle$.

↓

Pairing subproblem:
Construct auxiliary state; obtain $\rho^{(i+1)}, \kappa^{(i+1)}$.

↓

SCF iteration:
Construct new densities and potentials $\mathsf{R}^{(i+1)}, \mathsf{F}^{(i+)}$.

Optimizing quadratics

Let's minimize the quadratic form of matrix A

$$f(x) = \frac{1}{2}x^T A x$$

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$$x^{(i+1)} = x^{(i)} - \alpha \nabla f(x^{(i)})$$

Ball rolling down the hill ...

$$\alpha_{\mathrm{opt}} \sim \frac{2}{\lambda_{\mathrm{max}}} .$$

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Heavy-ball

$$x^{(i+1)} = x^{(i)} - \alpha \nabla f(x^{(i)}) + \mu \left(x^{(i)} - x^{(i-1)} \right)$$

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<u>Heavy-ball</u>

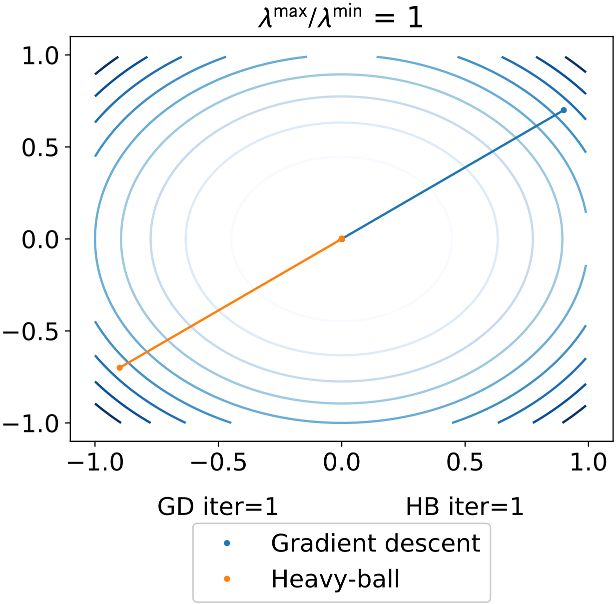
$$\begin{aligned} x^{(i+1)} = & x^{(i)} - \alpha \nabla f(x^{(i)}) \\ & + \mu \left(x^{(i)} - x^{(i-1)} \right) \end{aligned}$$

... with inertia!

$$\alpha_{\mathrm{opt}} \sim \frac{2(1 + \mu_{\mathrm{opt}})}{\lambda_{\max}} .$$

$$\mu_{\mathrm{opt}} = \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^2$$

Optimizing quadratics



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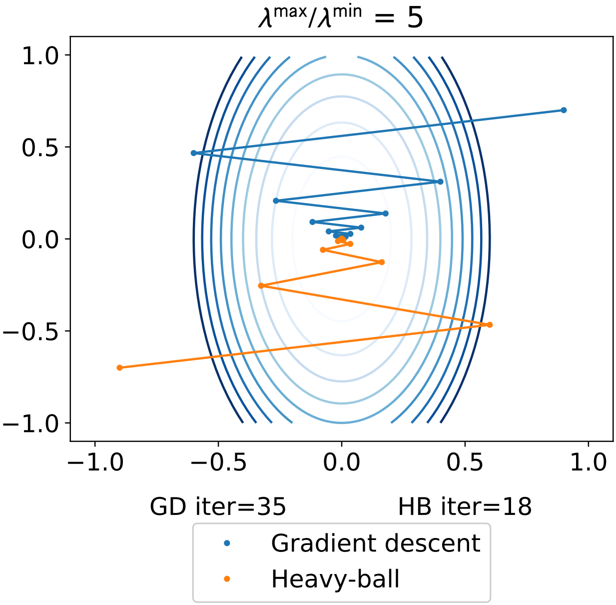

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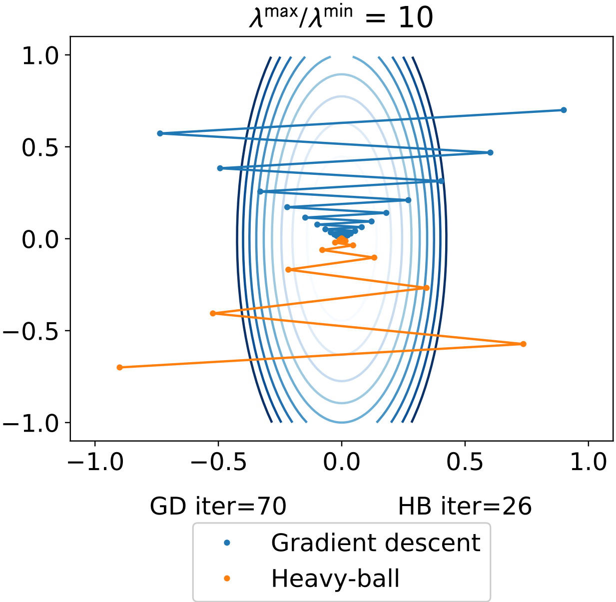

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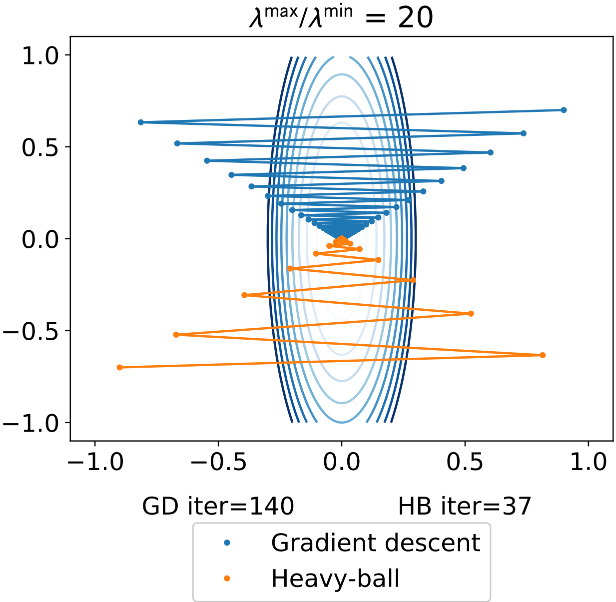

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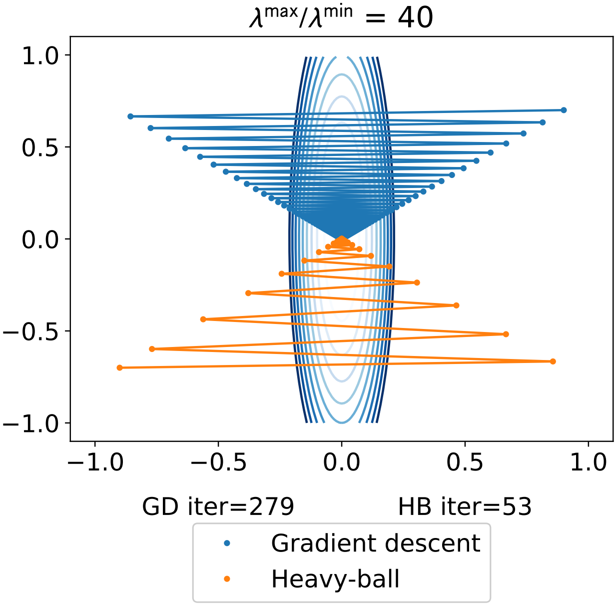
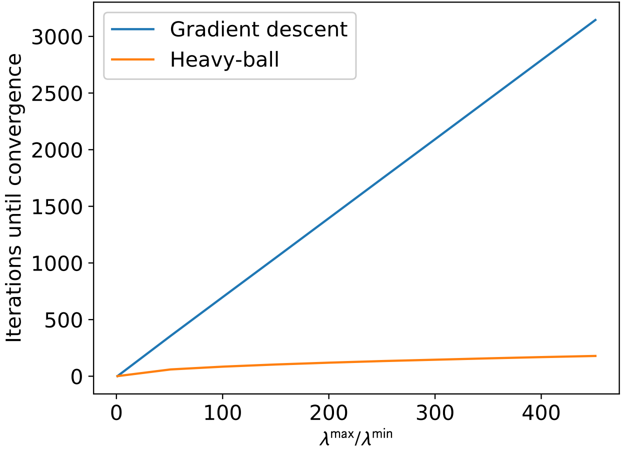


Optimizing quadratics



Constraints