Deformed natural orbitals for *ab initio* calculations

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NUMERICS

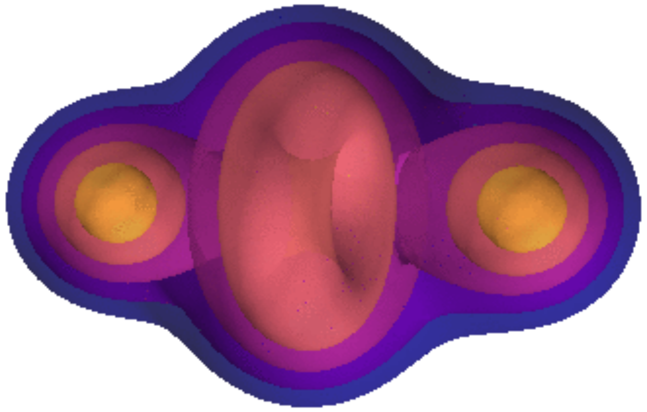
International PhD Program in Numerical Simulation at CEA

Deformed Bogoliubov MBPT

†M. Frosini et al., Eur. Phys. J. A **57**, 151 (2021)

dBMBPT

- Strength of the method:
  - Based on symmetry breaking reference states (U(1), SO(3))
  - Ideal to explore **doubly-open shell** systems
  - Low-polynomial scaling
  - **Cheap** yet accurate (for low-momentum interactions)
  - **Bulk observables** (**energies**, **radii**), axial deformation β_2



- Ongoing projects:
  - **Large scale calculations** along the nuclear chart
  - Specific applications around the $N = 20$ **island of inversion**
  - Role of correlations in semi-magic (**spherical**) vs open-shell (**deformed**) nuclei
  - Extraction of **natural orbitals** from the correlated density matrix $\rho_{\alpha\beta} = \langle \Psi | c^{\dagger}_{\alpha} c_{\beta} | \Psi \rangle$

Natural Orbitals

†J. Hoppe et al., Phys. Rev. C **103**, 014321

Basis informed by MB correlations suited to **efficiently capture correlations** in the wave-functions

- Main objective: reduce the cost of an expensive calculation
- How it can be done: via an **auxiliary cheaper calculation**

V_{ijkl} HO (e_{max})

$\tilde{e}_{max} \ll e_{max}$

Mean-field calculation

Cheap (B)MBPT

ρ_{ij}^{BMBPT}

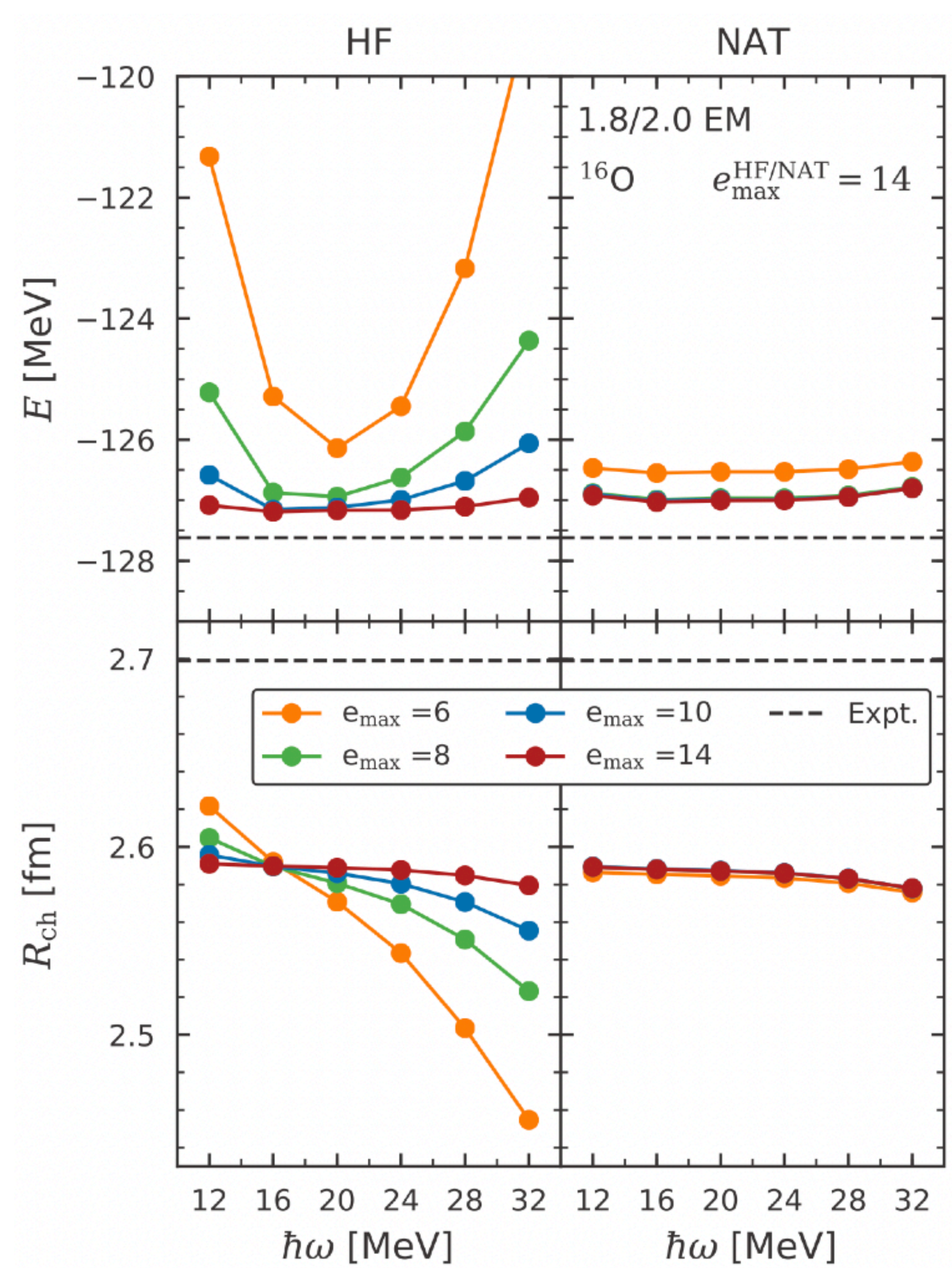
V_{ijkl} NAT (e_{max})

truncation

V_{ijkl} NAT ($\tilde{e}_{max}$)

$V_{\alpha\beta\gamma\delta}$ HF(B)

Expensive beyond mean-field calculation

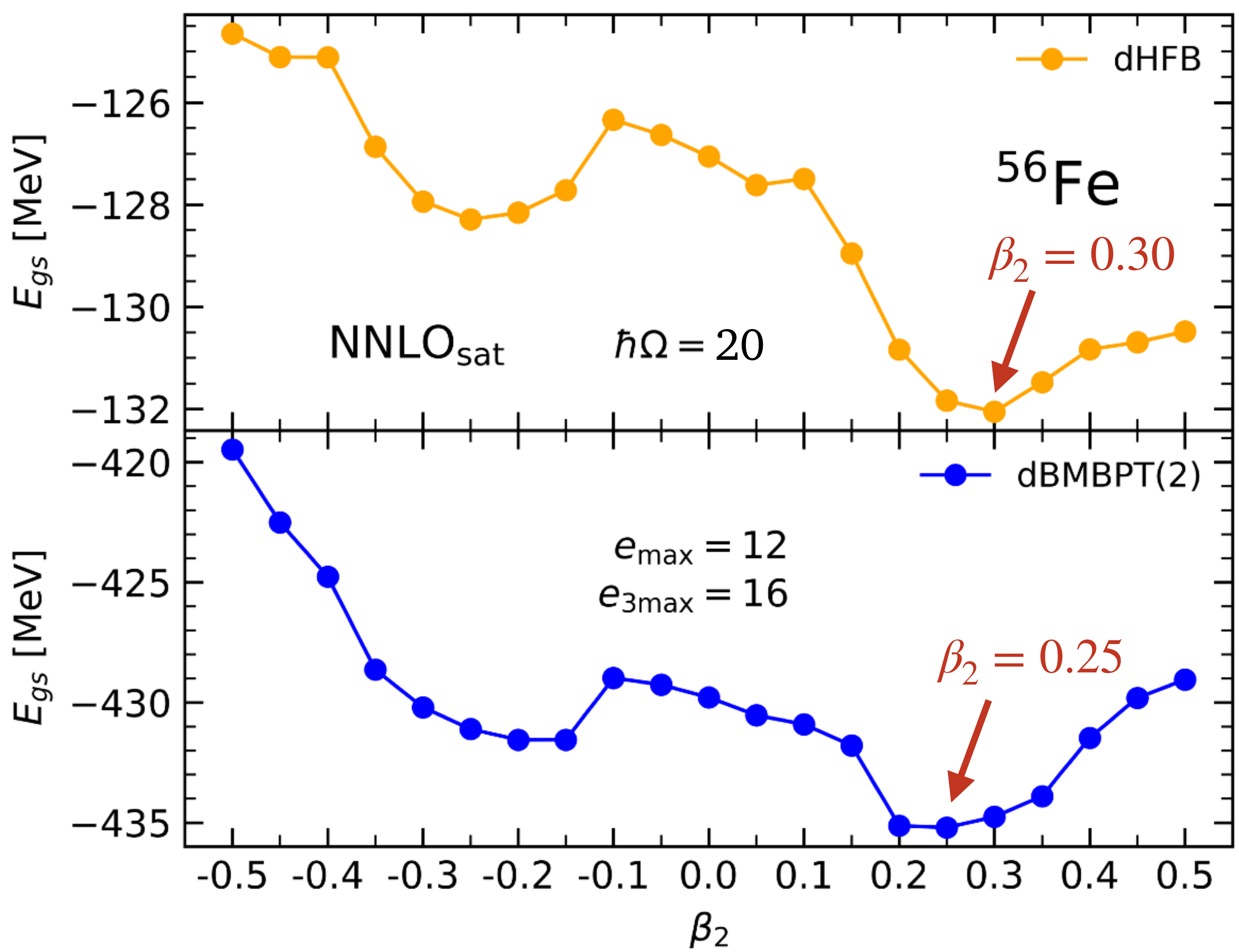


Deformed Natural Orbitals

†A. Scalesi et al., *in preparation*

- Extension to extract natural orbitals for **open-shell** nuclei
- Based on dBMBPT(2) performed on top of the **HFB minimum** w.r.t. the axial deformation β_2

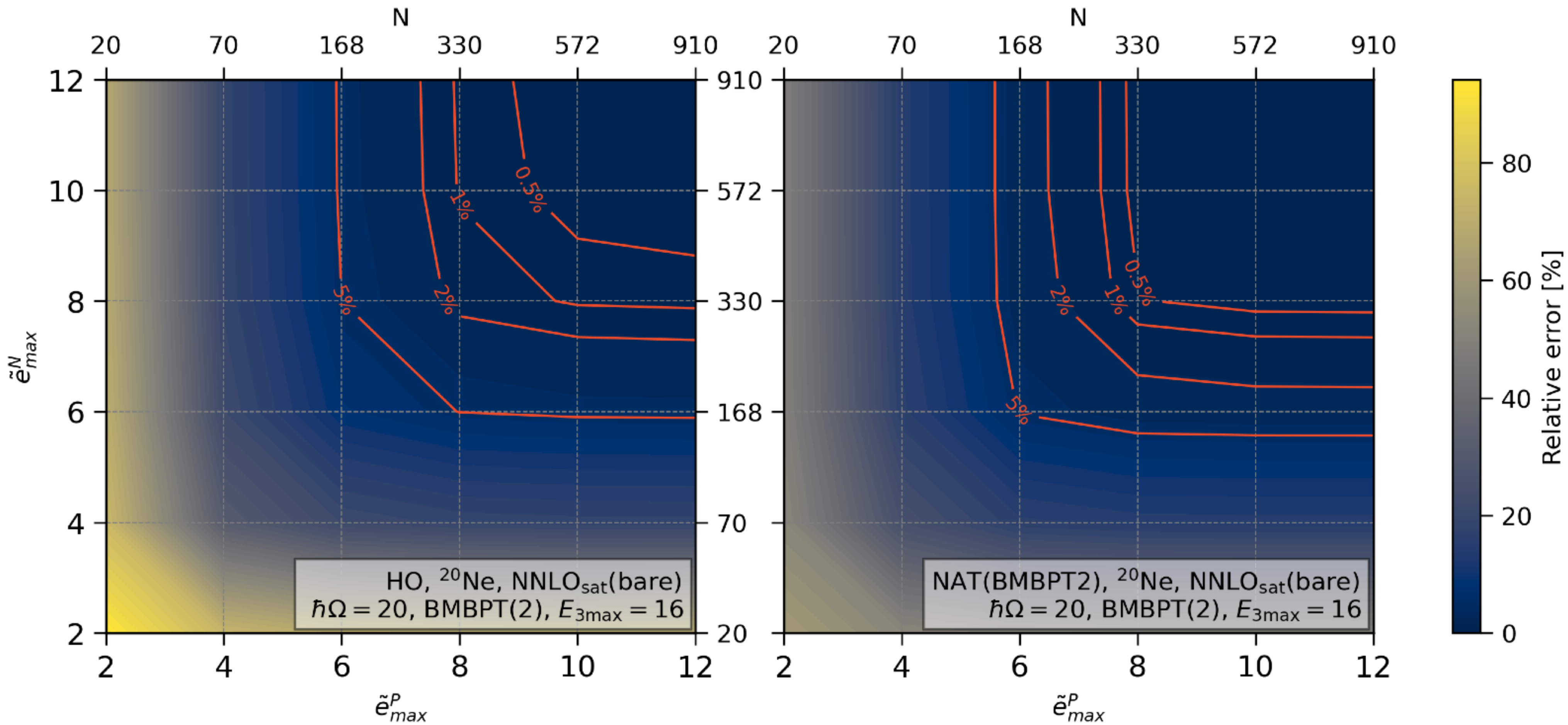
Total Energy Surface (TES)



Convergence of the ground-state energy

†A. Scalesi et al., *in preparation*

- ^{56}Fe
- NNLO$_{sat}$
- $\hbar\Omega = 20$
- BMBPT(2)
- $E_{3max} = 16$

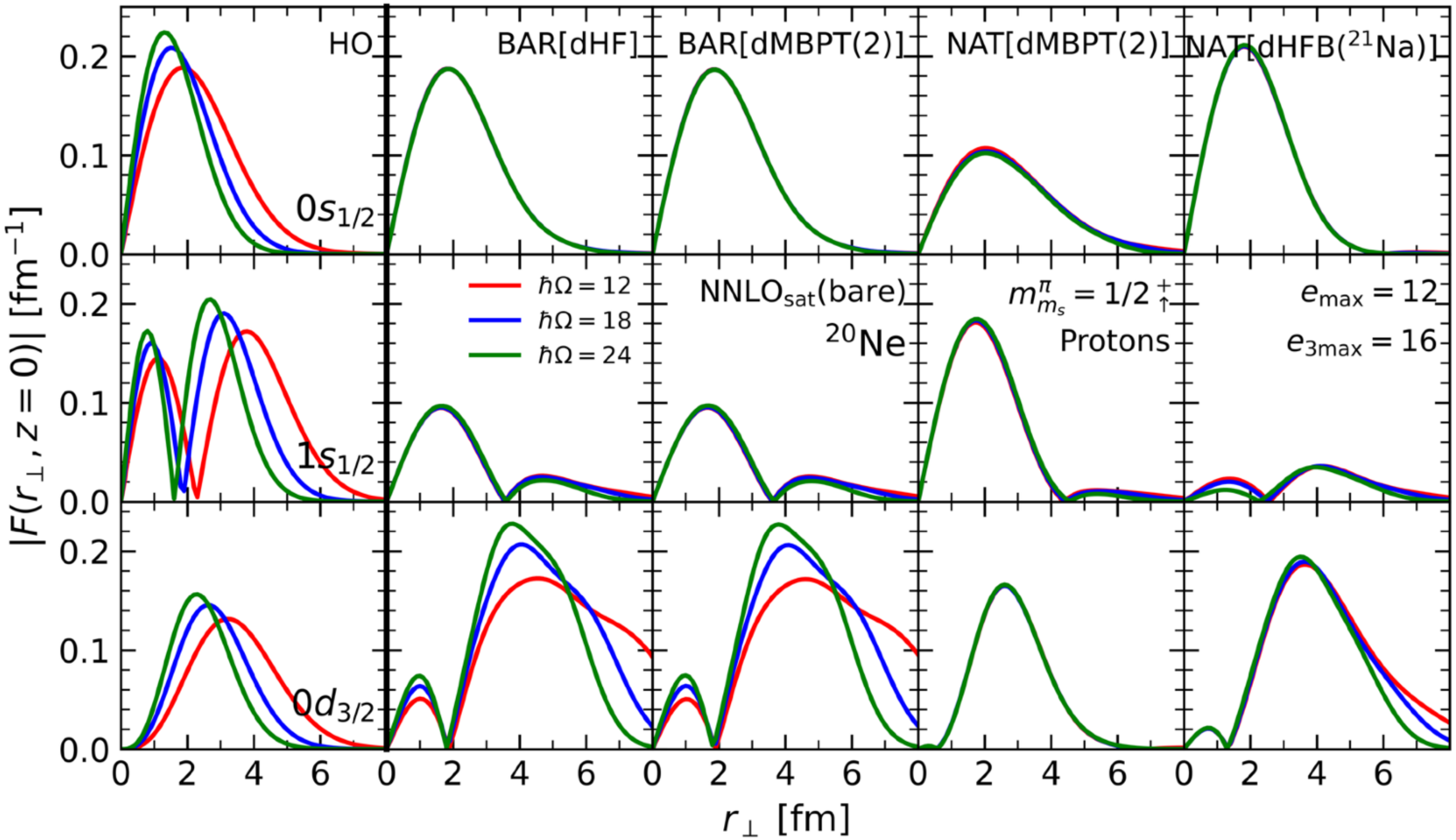


- NAT are **$\hbar\Omega$-independent**, the advantage of NAT w.r.t. HO is $\hbar\Omega$-dependent
- Here the optimal $\hbar\Omega$ is showed, which leads to the minimal gain for NAT
- Typical minimal gain of **2** e_{max} in all the studied cases for a relative precision of 0.5%
- Significant reduction in the **number of states** for N^p scaling methods in m-scheme

→ For a N^5 method $\dfrac{N^{p=5}[e_{max} = 10]}{N^{p=5}[e_{max} = 8]} = 16.6$

$\hbar\Omega$-dependency of the wave functions

MB correlations ⟷ Localization of WFs ⟷ Independence of HO $\hbar\Omega$



- Select block m, π, t
- Mix n and j
- Select **spin** component

- **Baranger basis (BAR)**

  ⟶ $\hbar\Omega$-independent in occupied states

- **NAT basis from dMBPT(2)**

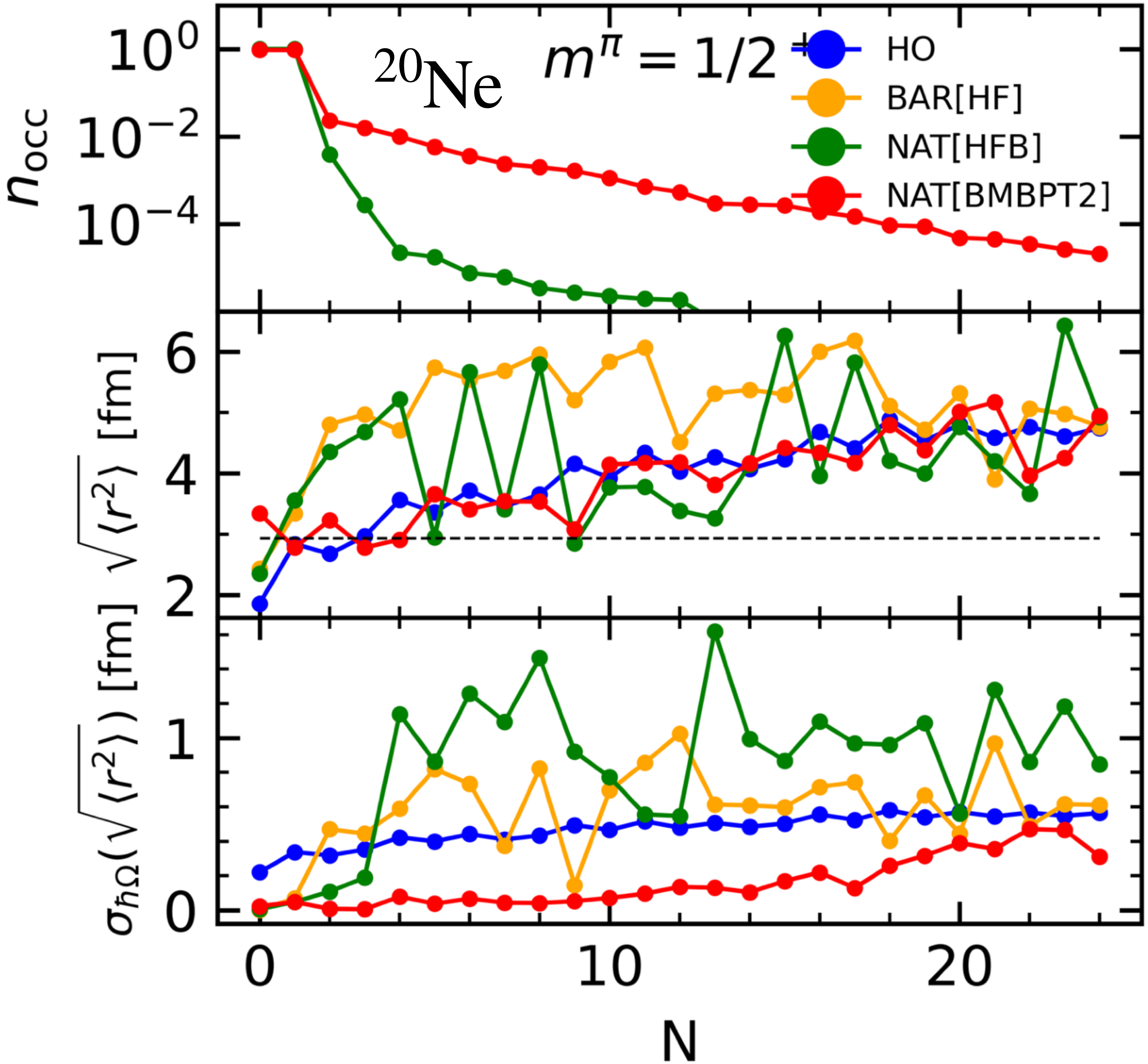
  ⟶ always $\hbar\Omega$-independent

- **NAT basis from dHFB**

  ⟶ $\hbar\Omega$-independent in occupied states

  ⟶ weak $\hbar\Omega$-dependence above the Fermi surface

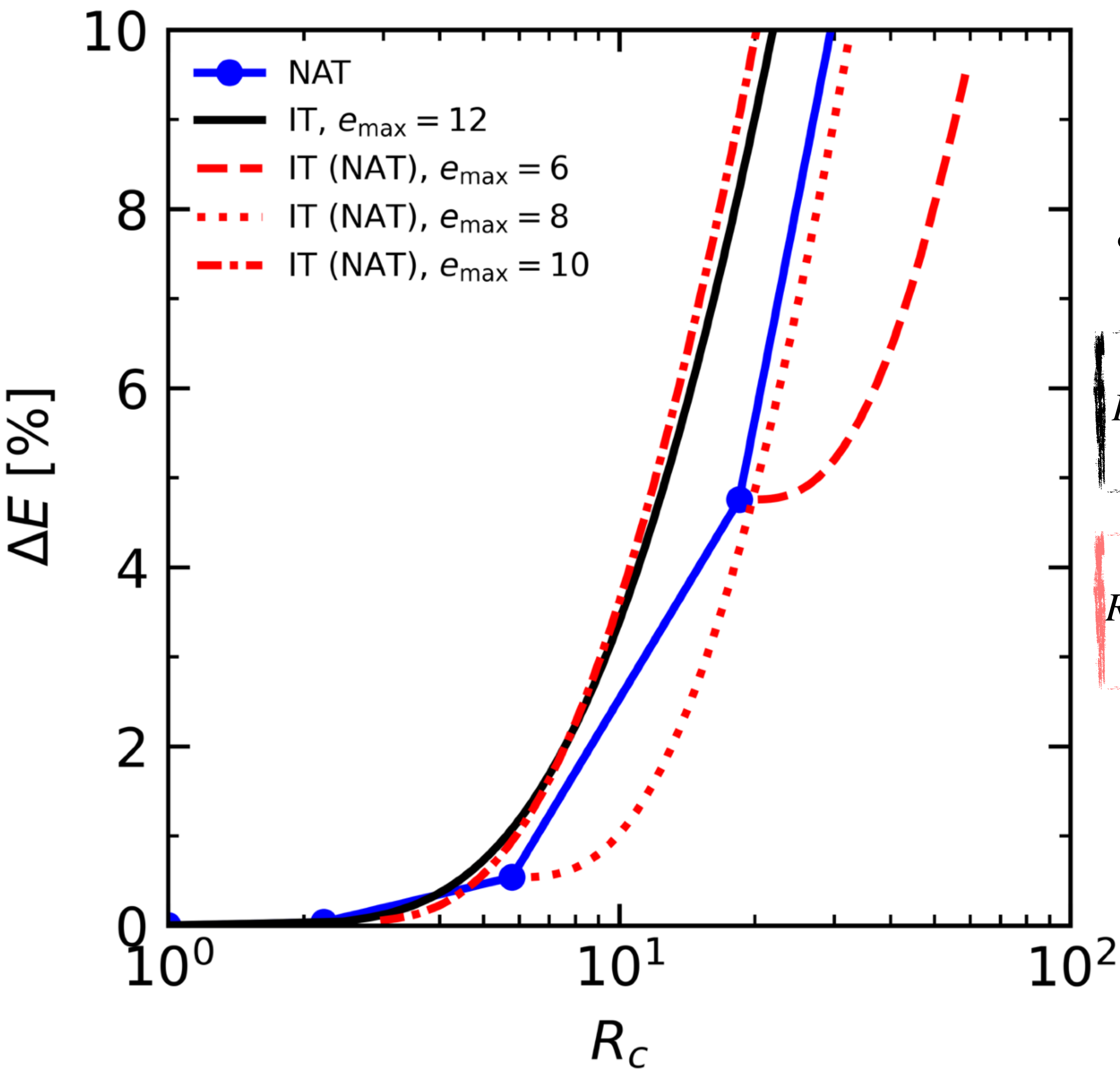
Single-particle radii



- n_{occ}: **occupation number**
- $\sqrt{\langle r^2 \rangle}$: **rms matter radius**

  - - - rms system radius
- $\sigma_{\hbar\Omega}\left(\sqrt{\langle r^2 \rangle}\right)$: **std. dev.**

Importance truncation



- **Compression factor R_c**

$$R_c^{\mathrm{IT}}(\epsilon^{\mathrm{IT}}) \equiv \frac{n_{\mathrm{conf}}^{\mathrm{MBPT(2)}}(e_{\max} = 12, \epsilon^{\mathrm{IT}} = 0)}{n_{\mathrm{conf}}^{\mathrm{MBPT(2)}}(e_{\max} = 12, \epsilon^{\mathrm{IT}})}$$

$$R_c^{\mathrm{NAT}}(\tilde{e}_{\max}) \equiv \frac{n_{\mathrm{conf}}^{\mathrm{MBPT(2)}}(e_{\max} = 12, \epsilon^{\mathrm{IT}} = 0)}{n_{\mathrm{conf}}^{\mathrm{MBPT(2)}}(\tilde{e}_{\max}, \epsilon^{\mathrm{IT}} = 0)}$$