Many-Body Theory and Electromagnetic Transitions

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Outline

Q: Which nuclei?

light nuclei ($A \lesssim 25$) or medium-mass ($A \lesssim 50$), depending on method

Q: Which observables?

ground-state observables, low-lying excitations,
collective excitations, electromagnetic moments & transitions

Q: Which framework?

NN, 3N, 4N interactions from chiral EFT,
ready to include two-body MEC contributions

Q: Which many-body method?

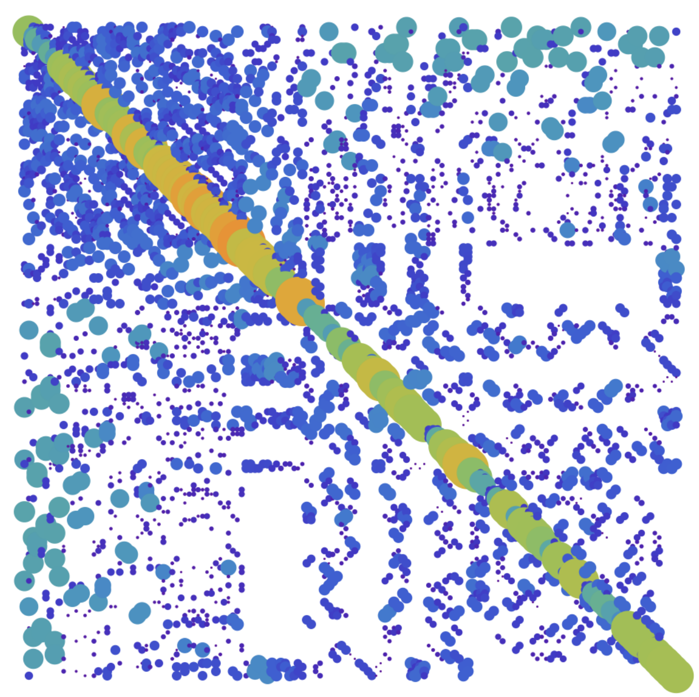
No-Core Shell Model with various add-ons

No-Core Shell Model

Barrett, Vary, Navrátil, Maris, Roth,...

no-core shell model is the
most universal and powerful ab initio approach for
light nuclei (up to A≈25)

- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$



$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

No-Core Shell Model

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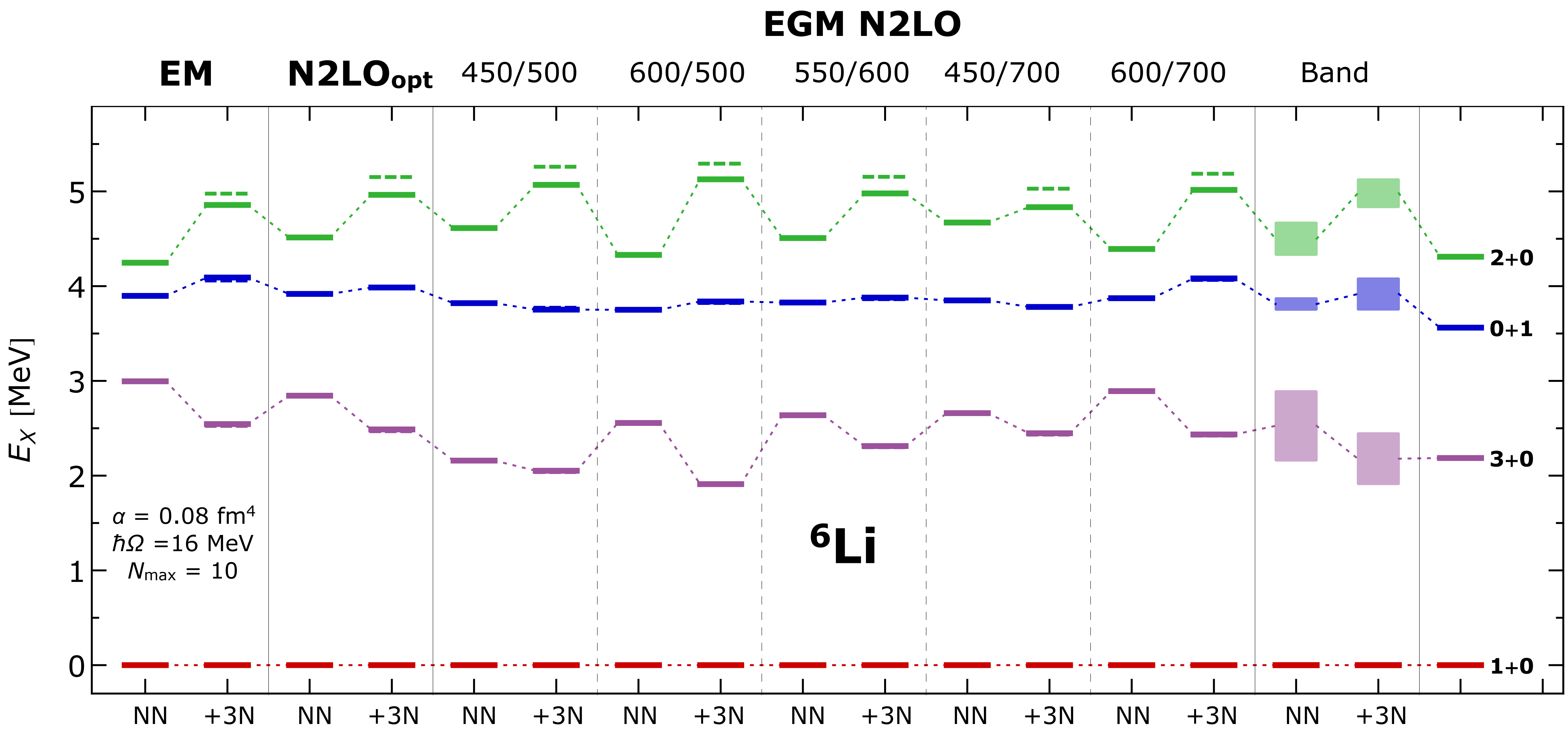
- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\mathrm{max}}\hbar\Omega$
- **advantages**: simplicity makes it powerful
  - ground and excited states obtained on the same footing
  - all observables obtained directly from the eigenvectors
  - inclusion of continuum degrees-of-freedom possible
- **limitations**: convergence of observables w.r.t. N_{max} is the only limitation and source of uncertainty
  - easy to control and quantify many-body uncertainties rigorously
  - different observables will have very different convergence rate and uncertainties

Low-Lying Excitations

Classical NCSM

p-Shell Spectroscopy: Sensitivity

Calci, Roth; PRC 94, 014322 (2016)



- of course, spectra depend on choice of initial chiral NN+3N interaction, but the dependence is not dramatic
- important contribution to the total theory uncertainty

p-Shell Spectroscopy: Sensitivity

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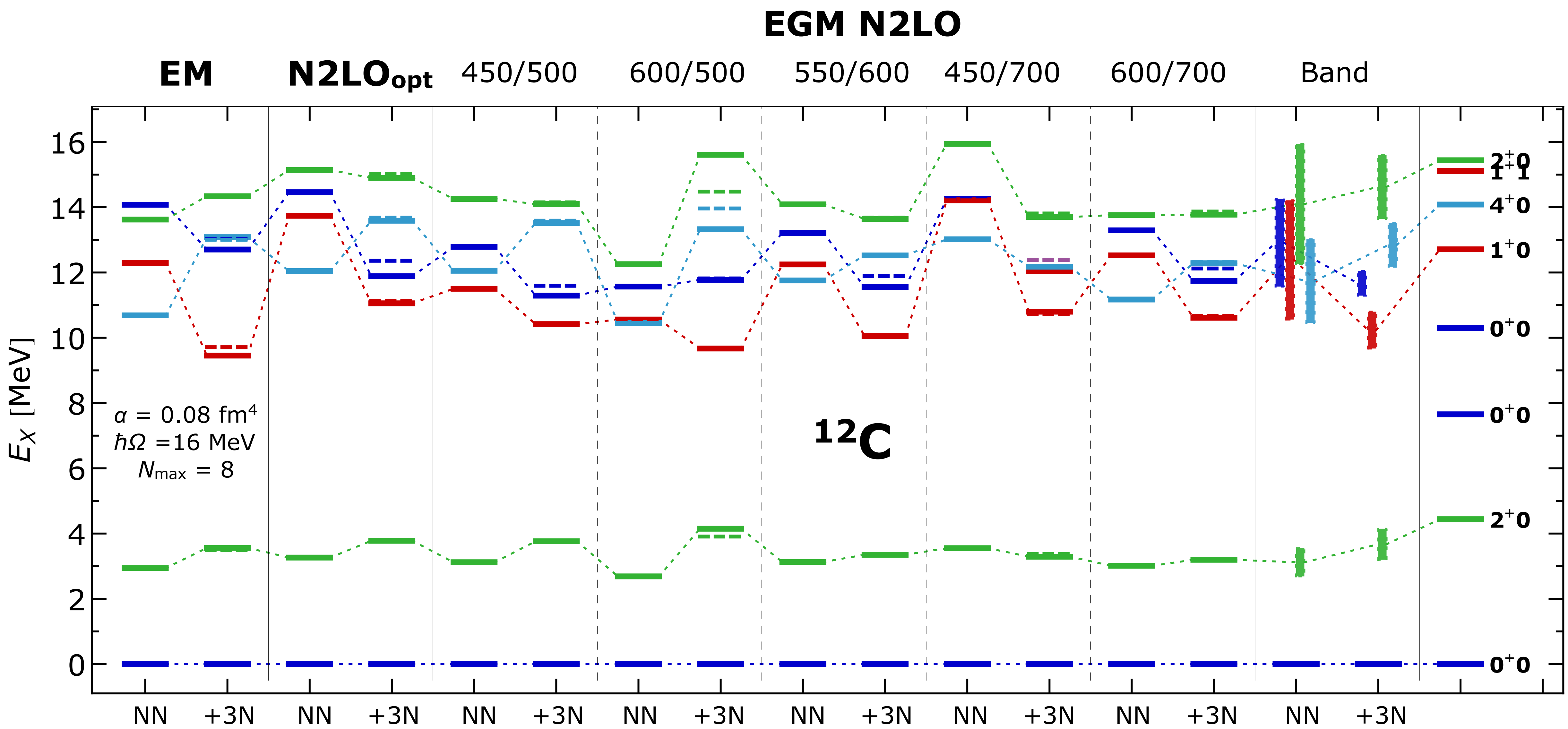
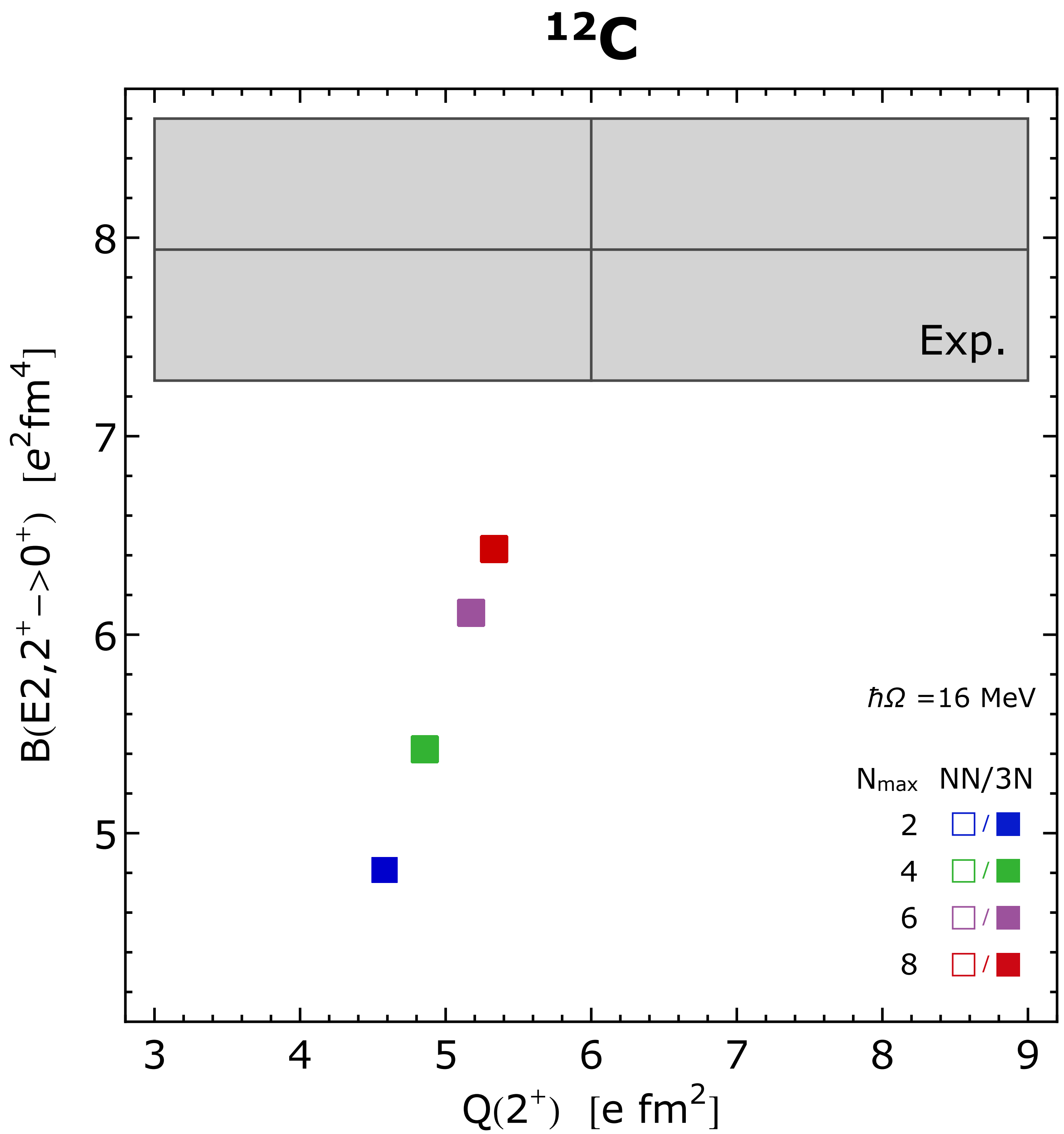


- individual states show systematic disagreement with experiment:
  - second 0^+: Hoyle state, cluster structure not captured in HO basis
  - first 1^+: systematic problem with N2LO-3N interaction ?

p-Shell Spectroscopy: Correlations

Calci, Roth; PRC 94, 014322 (2016)



- **electric quadrupole (E2)** observables involving 0^+ ground state & first excited 2^+
- model-space convergence is terrible, E2 operator sensitive to long-range wave functions

p-Shell Spectroscopy: Correlations

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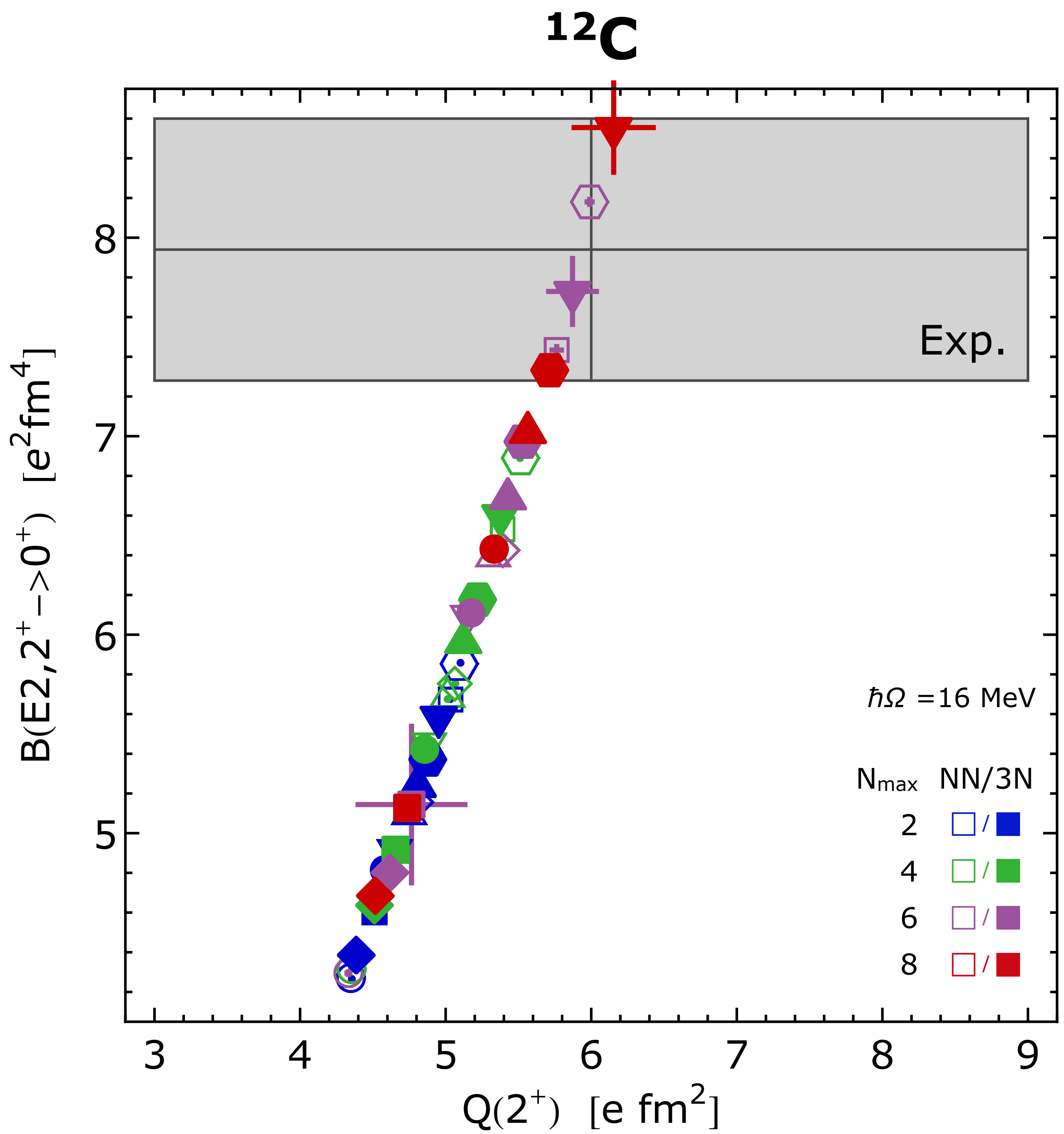

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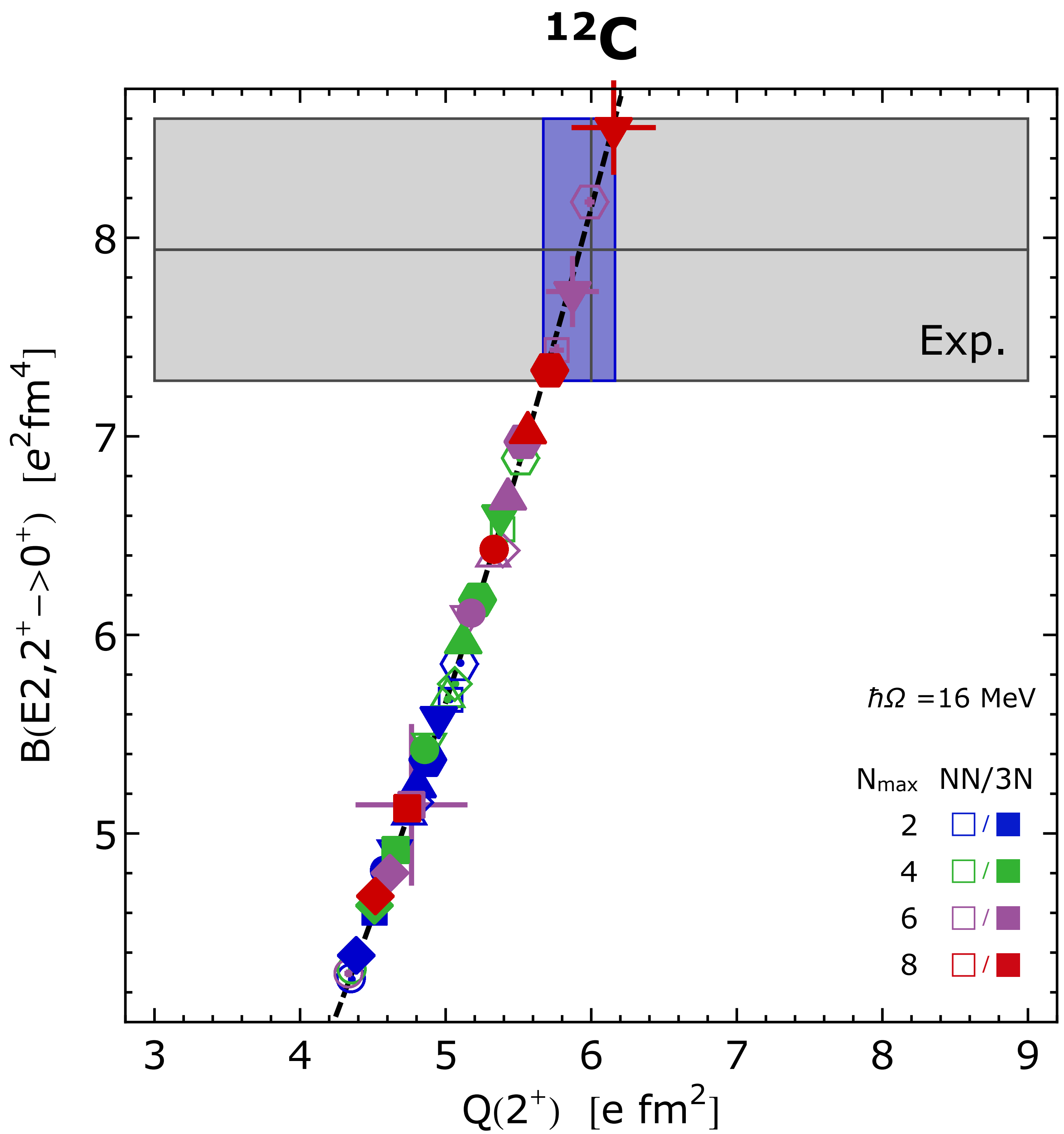

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- **extremely robust correlation** predicted by NCSM for all interactions and model spaces
- predict $Q(2^+)$ with very high accuracy based on ... al datum for ...

alternative way to exploit ab initio calculations and to bridge to effective models

p-Shell Spectroscopy: Correlations

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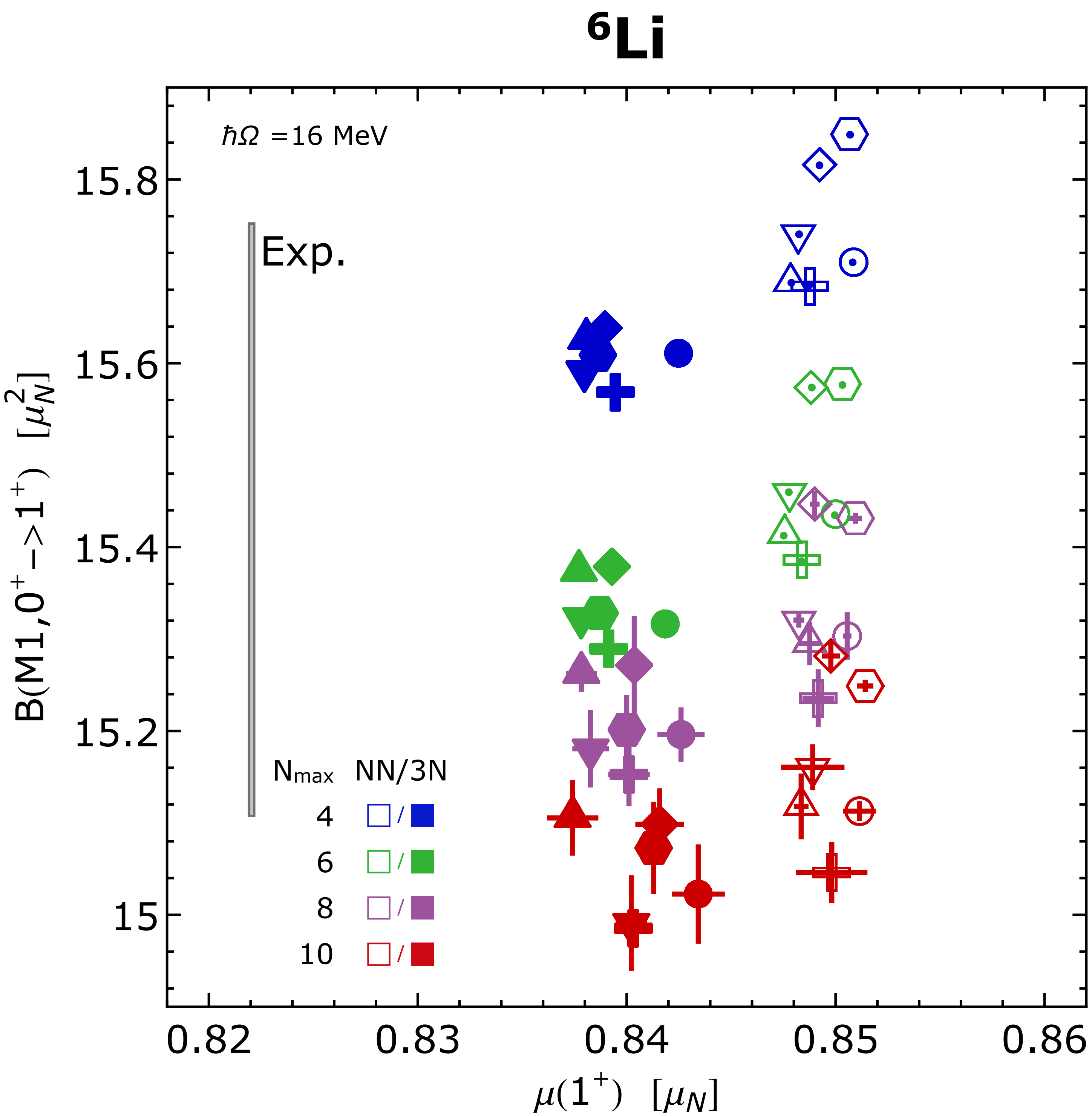


- **magnetic dipole (M1)** observables involving 1^+ ground state & 0^+ excited state
- dipole moment and B(M1) are **very robust** (few % changes)
- mild systematic model-space dependence of B(M1)
- dipole moment affected by 3N interaction and in slight disagreement with experiment

ready for precision studies, e.g., on electromagnetic two-body currents

Collective Excitations

Strength-Function NCSM

Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

NCSM
ground state

- regular NCSM calculation for ground state for a range of N_{max} truncations
- access to all open-shell nuclei

NCSM
strength distribution

- prepare pivot vector by applying transition operator to ground-state vector
- use simplistic Lanczos iterations to generate strength distribution

Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

- perform **NCSM calculation for ground state** $|E_0\rangle$
- prepare **pivot vector with transition operator**

$$|v_1\rangle = \mathcal{N}\, \mathrm{O}_\lambda\, |E_0\rangle \quad ; \quad \mathcal{N} = \langle E_0|\, \mathrm{O}_\lambda^\dagger \mathrm{O}_\lambda\, |E_0\rangle^{-1/2}$$

- perform **Lanczos algorithm** with Hamiltonian: obtain eigenvectors $|E_n\rangle$ as superposition of Lanczos vectors

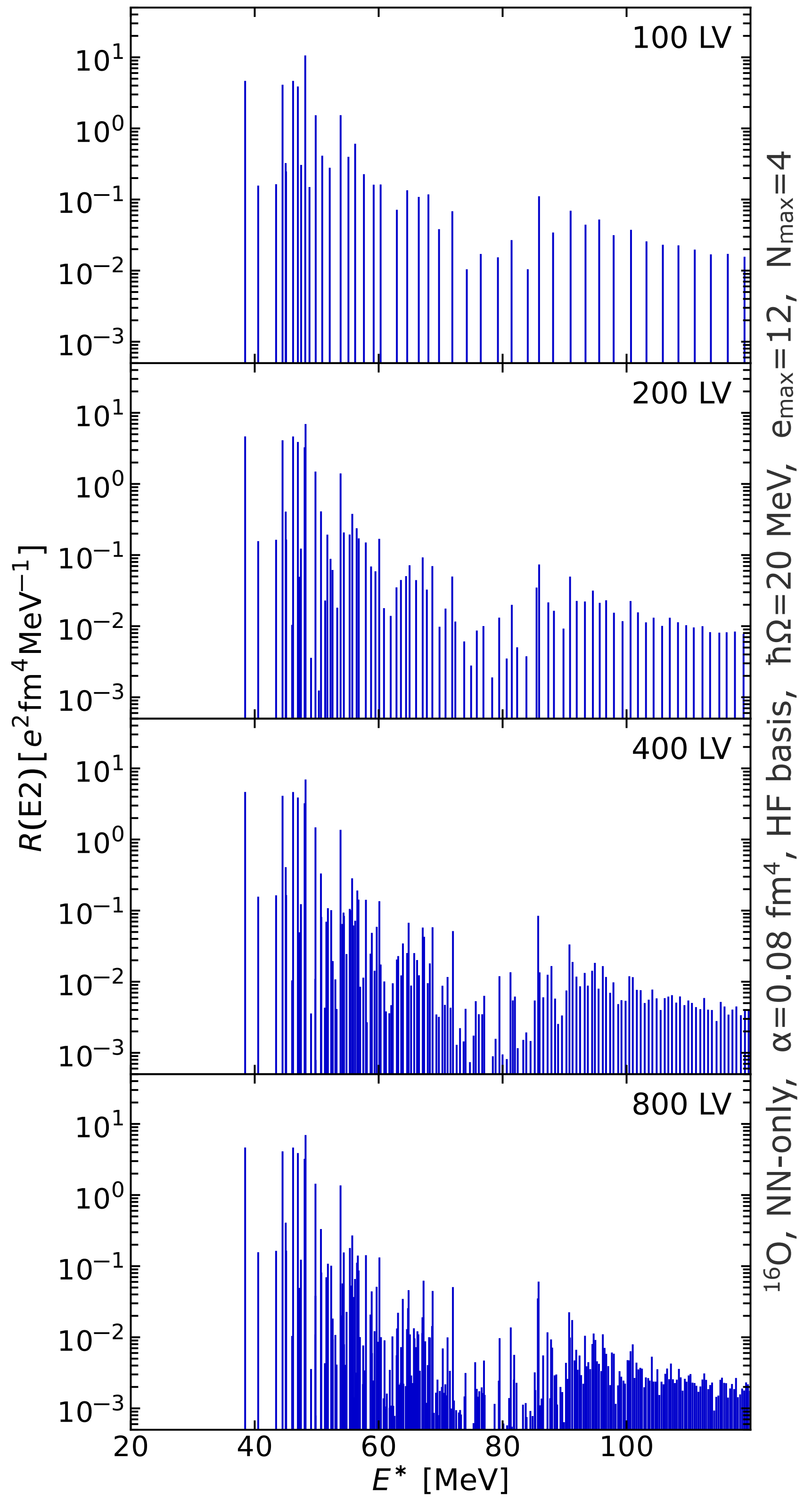
$$|E_n\rangle = \sum_{i=1}^{I} C_i^{(n)}\, |v_i\rangle$$

- first coefficient provides **transition matrix element**

$$C_1^{(n)} = \langle v_1|E_n\rangle = \mathcal{N}\, \langle E_0|\, \mathrm{O}_\lambda\, |E_n\rangle$$

- construct **discrete strength distribution**

$$R(E\lambda, E^*) = \sum_n |\langle E_0||\mathrm{O}_\lambda||E_n\rangle|^2\, \delta(E^* - (E_n - E_0))$$

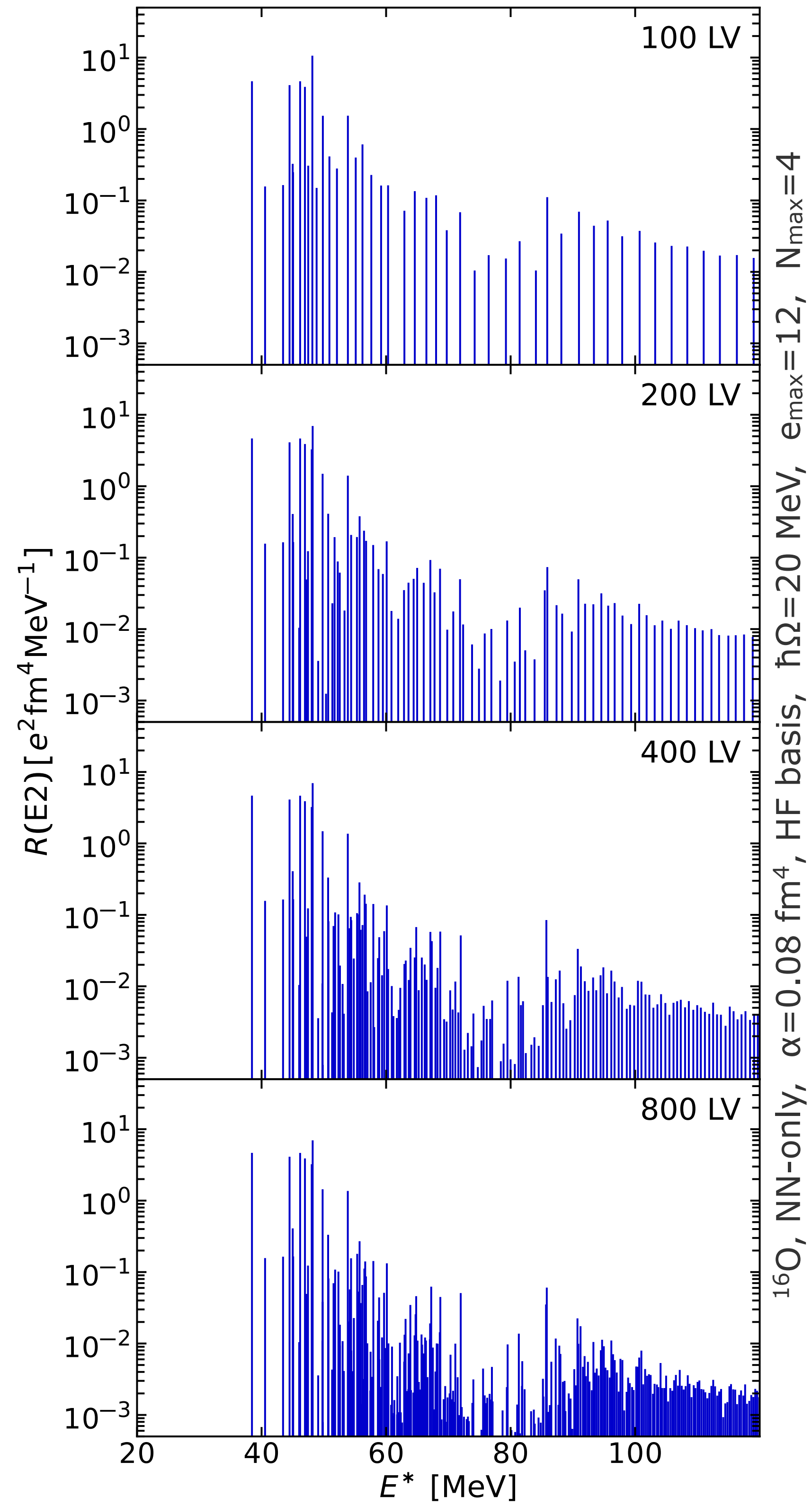


Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

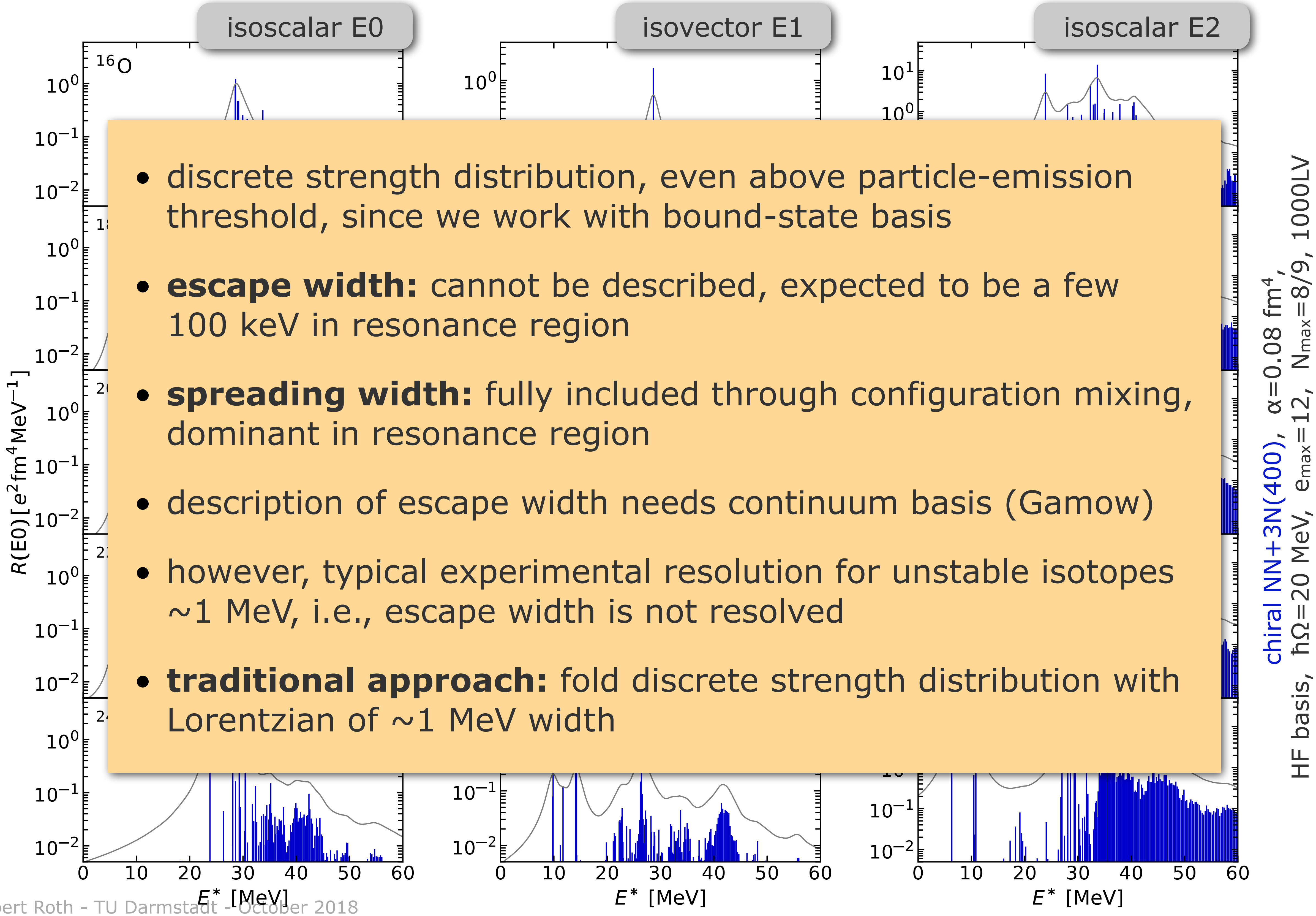
ab initio approach to strength distributions with many advantages

- works with simplest Lanczos algorithm (no reorthogonalization, Lanczos vectors discarded)
- same computational reach as regular NCSM
- no ad-hoc truncations, convergence in N_{max} and Lanczos iterations can be demonstrated explicitly
- full convergence of individual transitions in the relevant energy regime after ~800 iterations
- full access to fine structure of giant resonances
- full access to below-threshold features



Discrete Strength Distribution

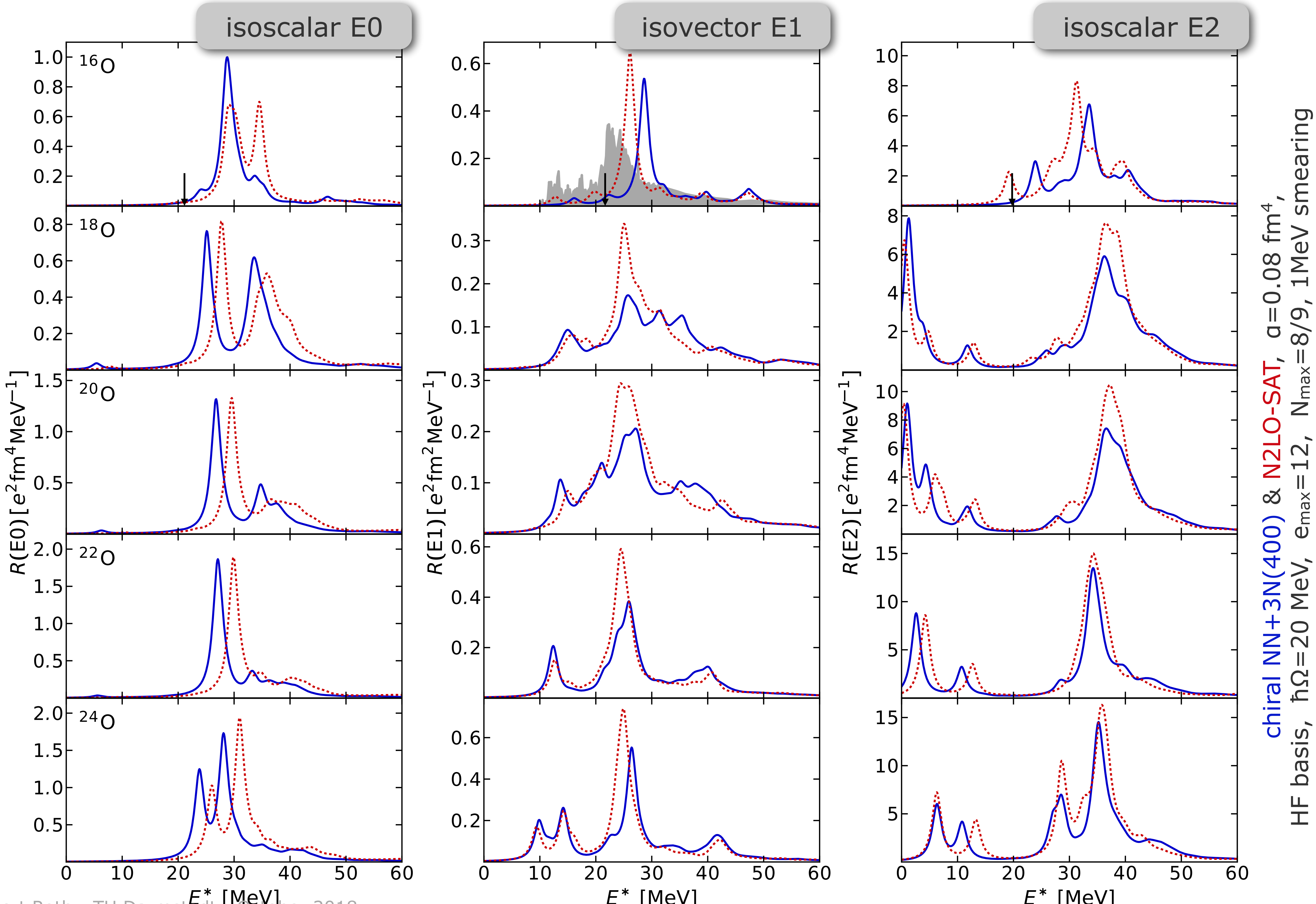
Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- discrete strength distribution, even above particle-emission threshold, since we work with bound-state basis
- **escape width:** cannot be described, expected to be a few 100 keV in resonance region
- **spreading width:** fully included through configuration mixing, dominant in resonance region
- description of escape width needs continuum basis (Gamow)
- however, typical experimental resolution for unstable isotopes ~1 MeV, i.e., escape width is not resolved
- **traditional approach:** fold discrete strength distribution with Lorentzian of ~1 MeV width

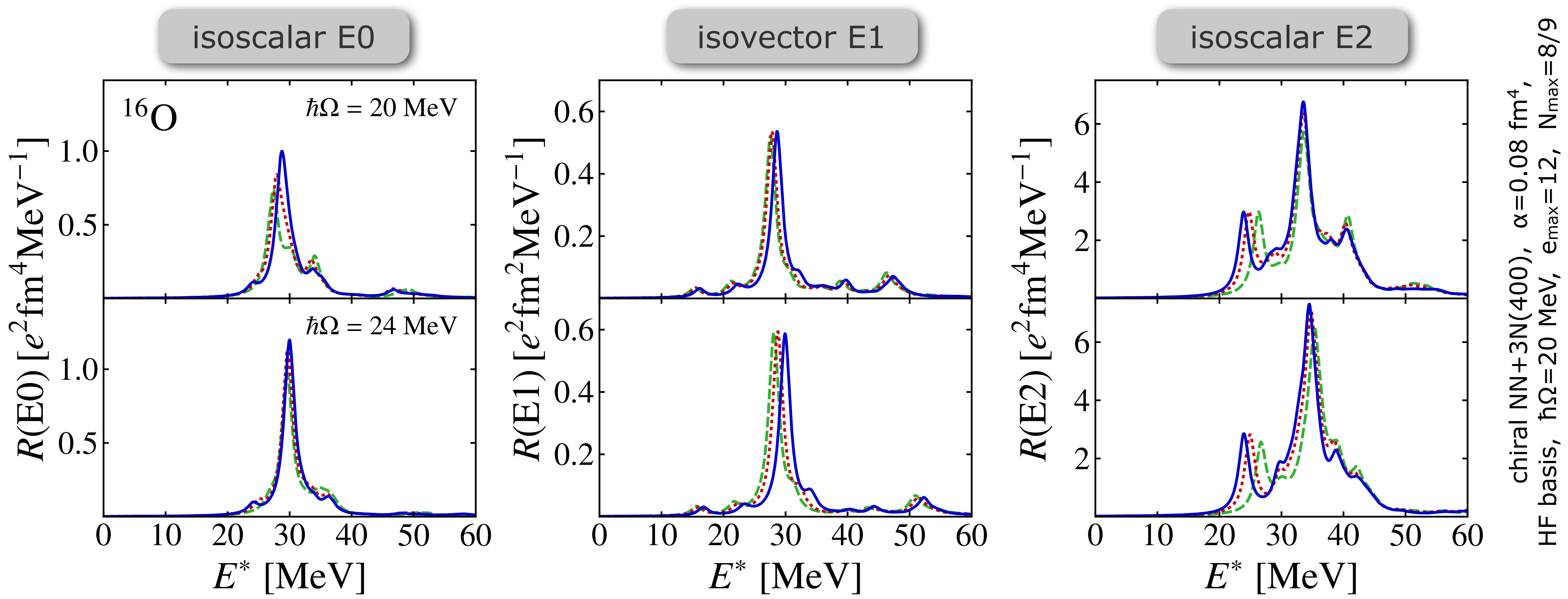
Strength Distribution

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



Model-Space Convergence

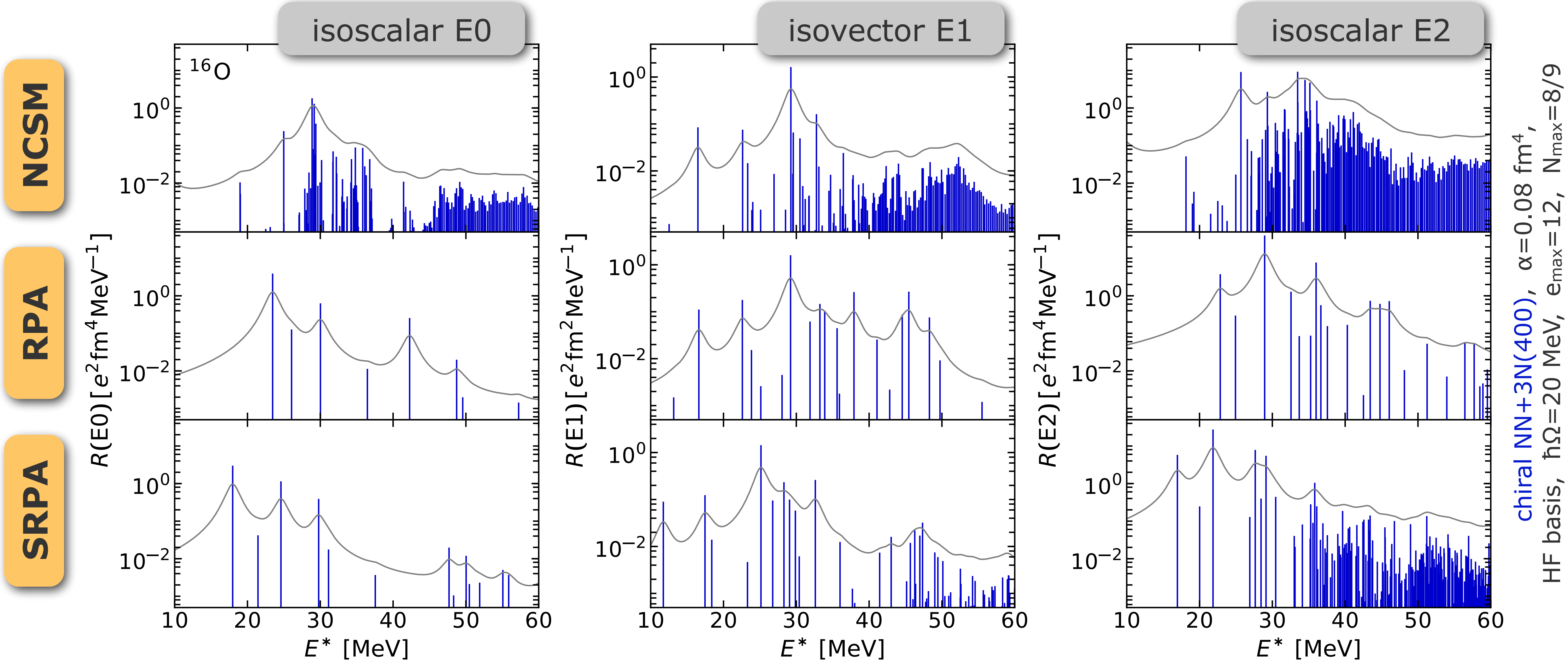
Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- N_{max} is the only relevant active truncation parameter
- very stable N_{max} convergence and independence of frequency of underlying HO basis

Comparison with RPA and SRPA

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



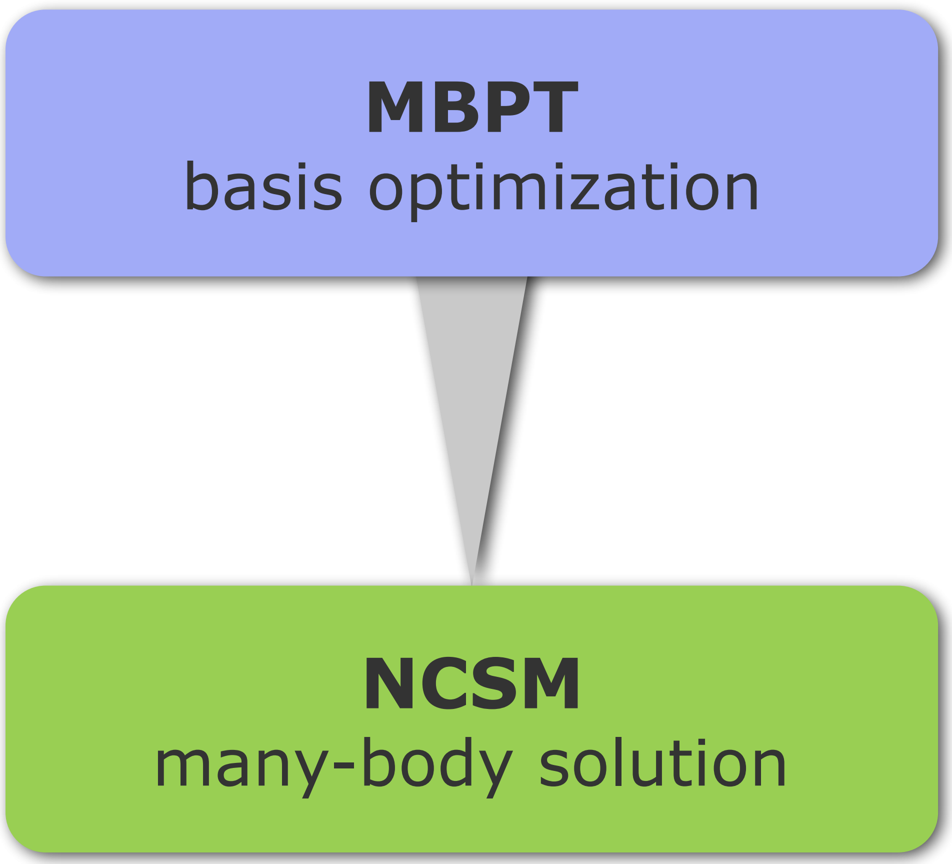
- collective excitations traditionally described in RPA or SRPA
- RPA (1p1h) cannot describe fragmentation, therefore, go to SRPA (2p2h)
- NCSM shows much more fine structure than SRPA and resolves notorious problem with pathological SRPA energy-shifts

Improving Convergence I

Natural-Orbital NCSM

Natural-Orbital NCSM

Tichai, Müller, Vobig, Roth; arXiv:1809.07571

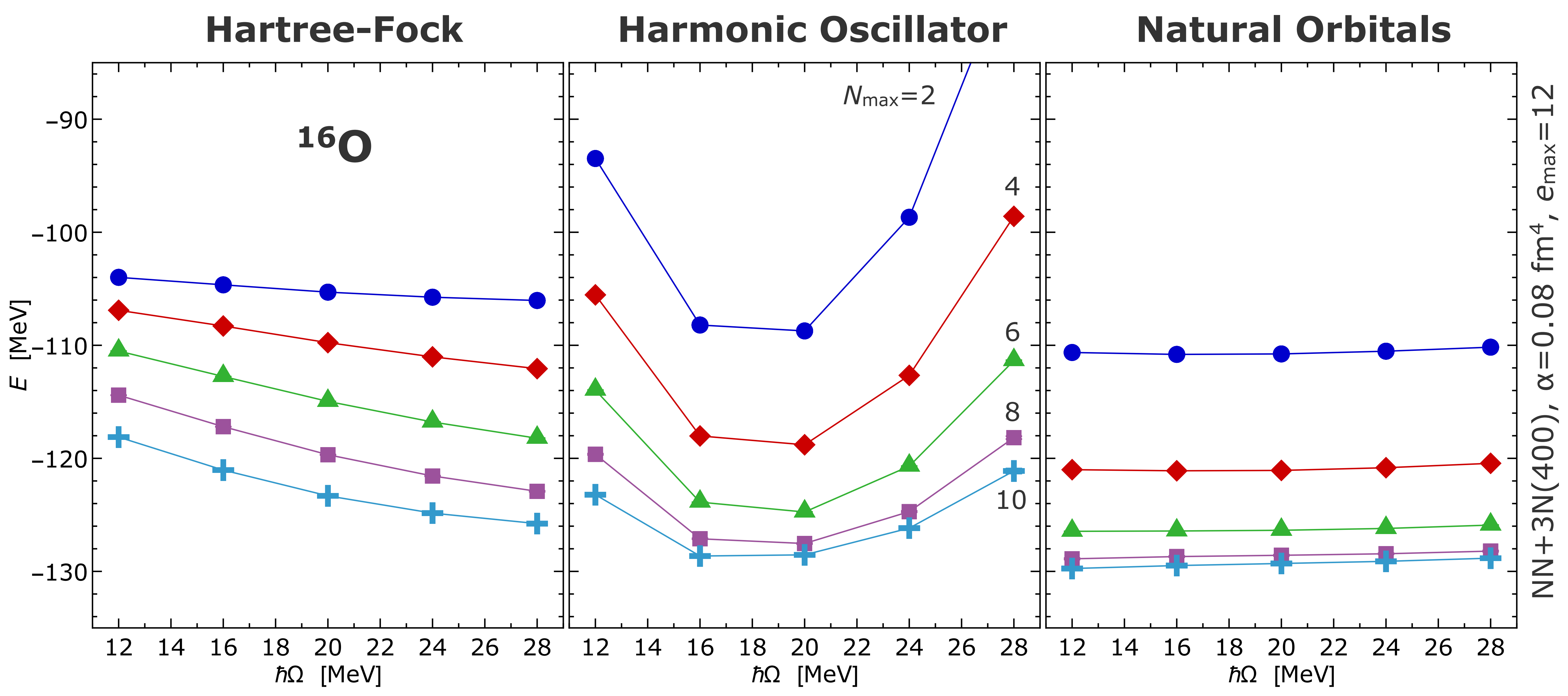


- construct HF basis in large single-particle space
- compute perturbative corrections to one-body density matrix up to second order
- determine natural orbitals from one-body density matrix and transform matrix elements

- NCSM calculation with natural-orbital basis
- use importance truncation for large spaces and heavier nuclei (optional)
- use normal-order two-body approximation to include 3N interactions (optional)

NCSM Convergence: Energies

Tichai, Müller, Vobig, Roth; arXiv:1809.07571



- MBPT natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

NCSM Convergence: Energies

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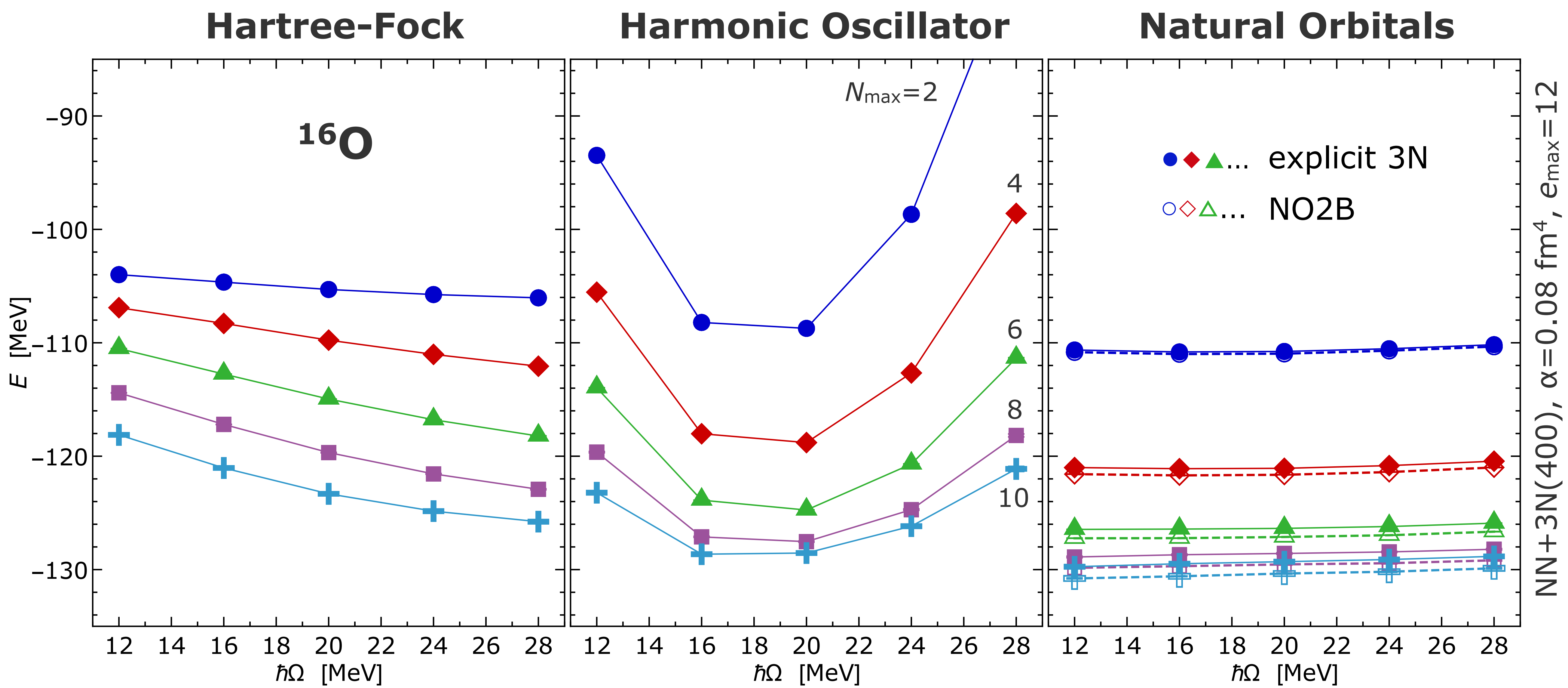

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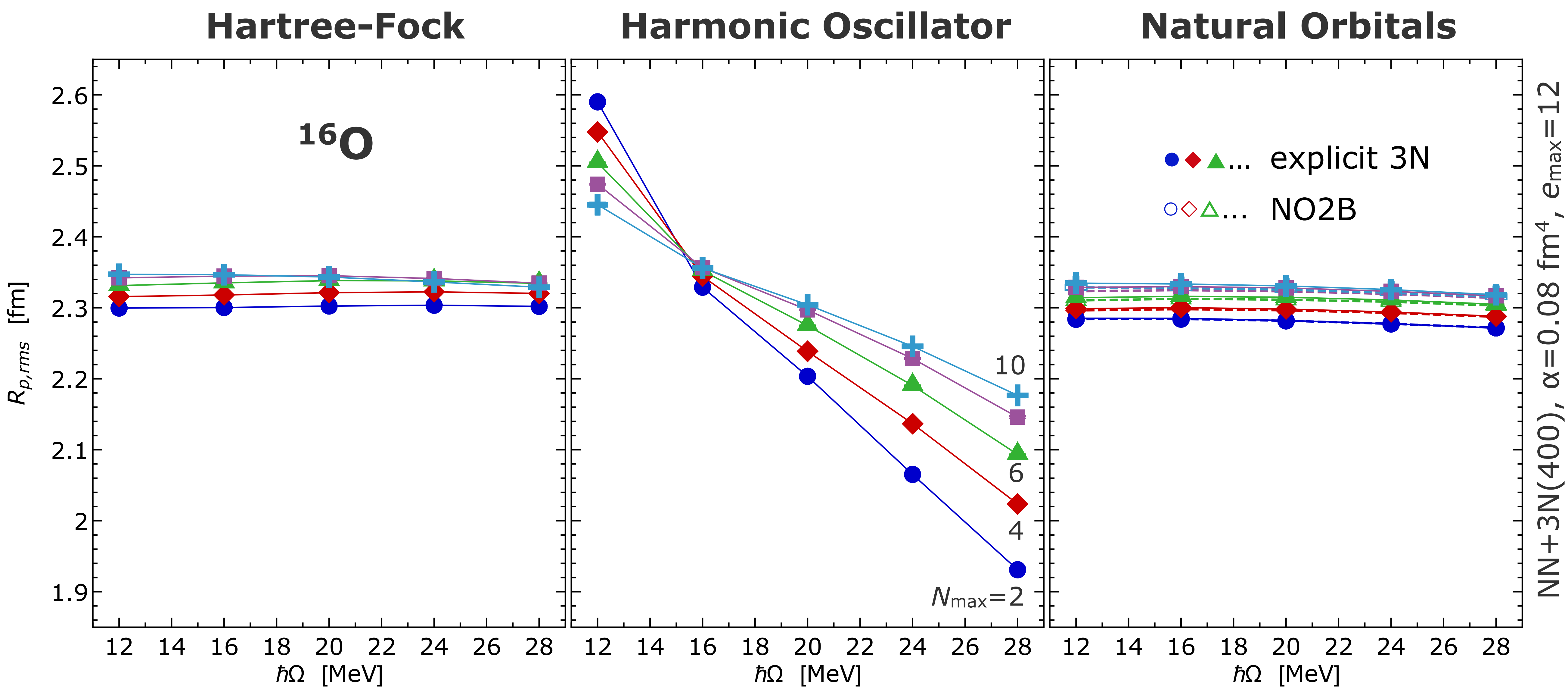
NCSM Convergence: Radii

Tichai, Müller, Vobig, Roth; arXiv:1809.07571



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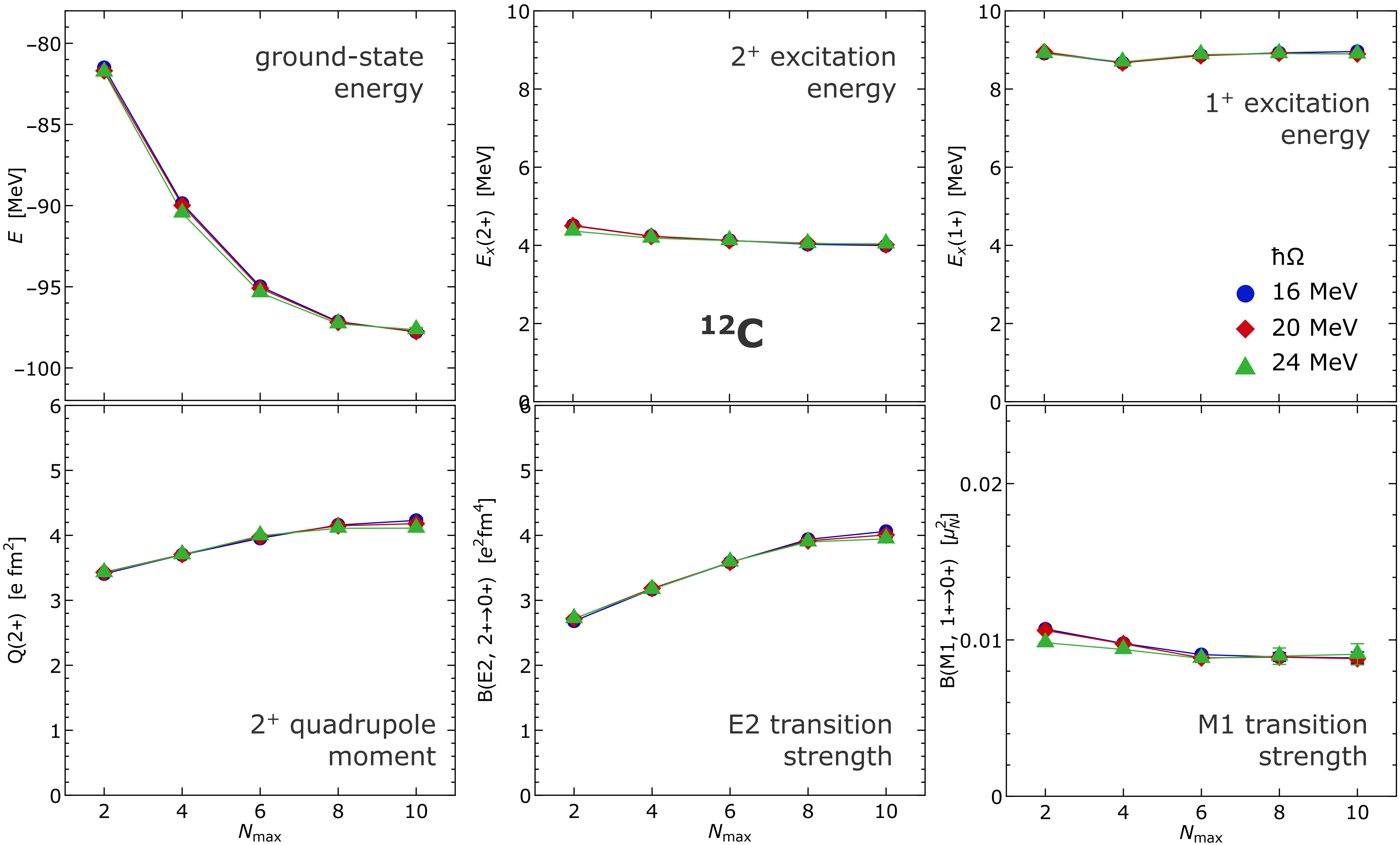
NCSM Convergence: Spectroscopy

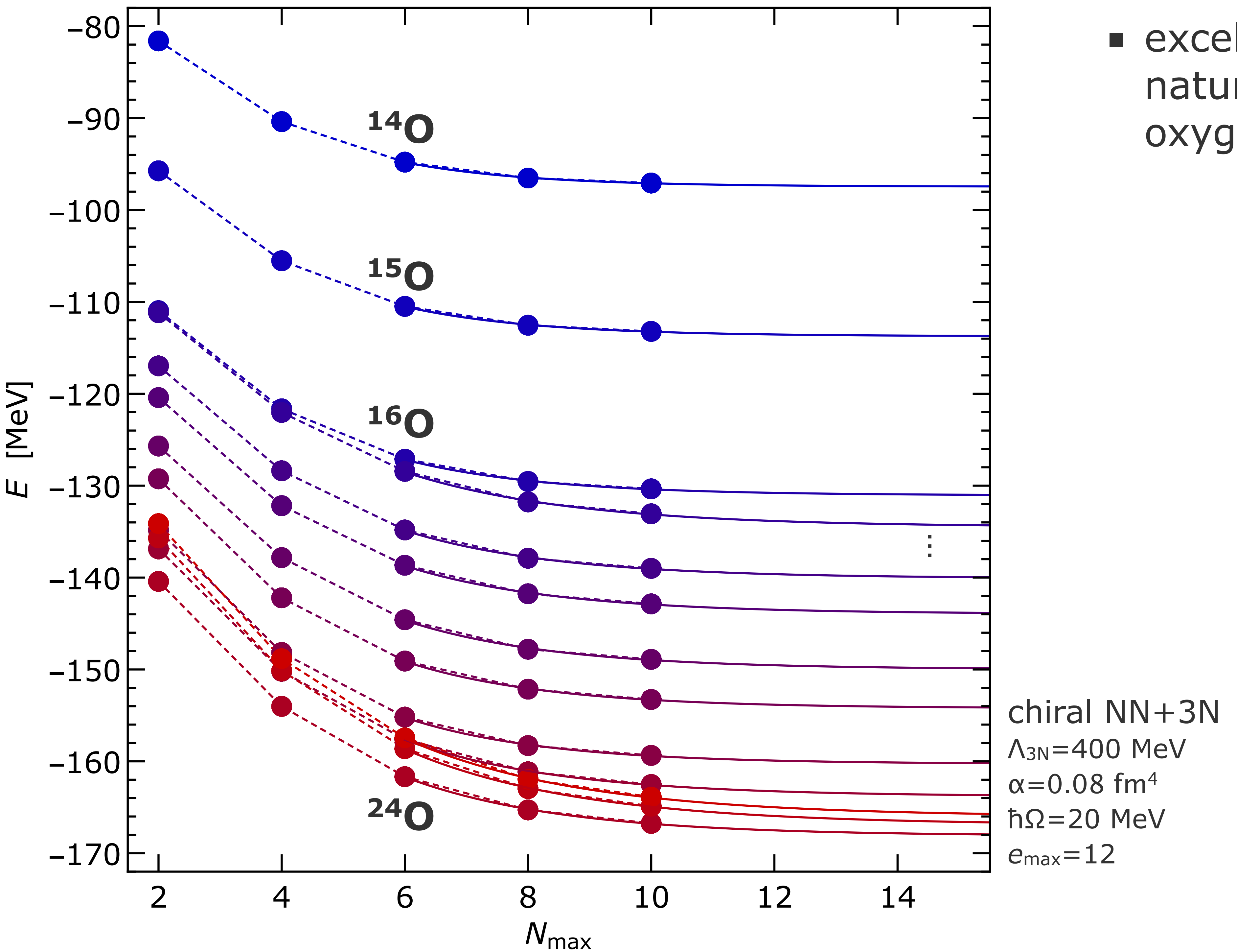
Tichai, Müller, Vobig, Roth; arXiv:1809.07571



NN+3N(500), α=0.08 fm^4, e_{max}=12

Oxygen Isotopes

Tichai, Müller, Vobig, Roth; arXiv:1809.07571



- excellent convergence with natural-orbital basis for all oxygen isotopes

Oxygen Isotopes

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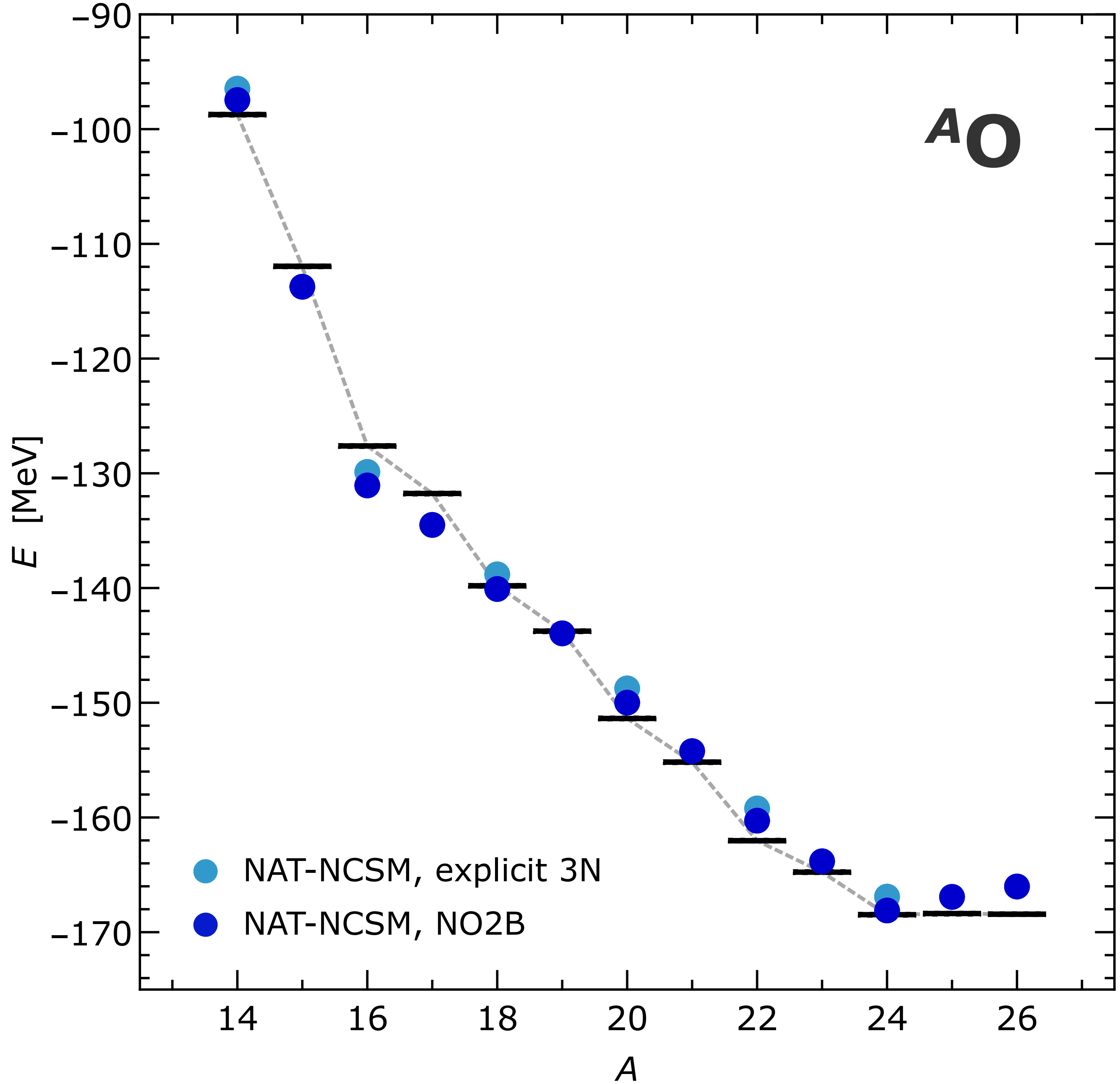

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

- excellent convergence with natural-orbital basis for all oxygen isotopes
- very good agreement with experimental systematics and dripline
- NO2B instead of explicit 3N causes ~1% overbinding

Epilogue

- **thanks to my group and my collaborators**
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