Ab Initio Description of Collective Excitations

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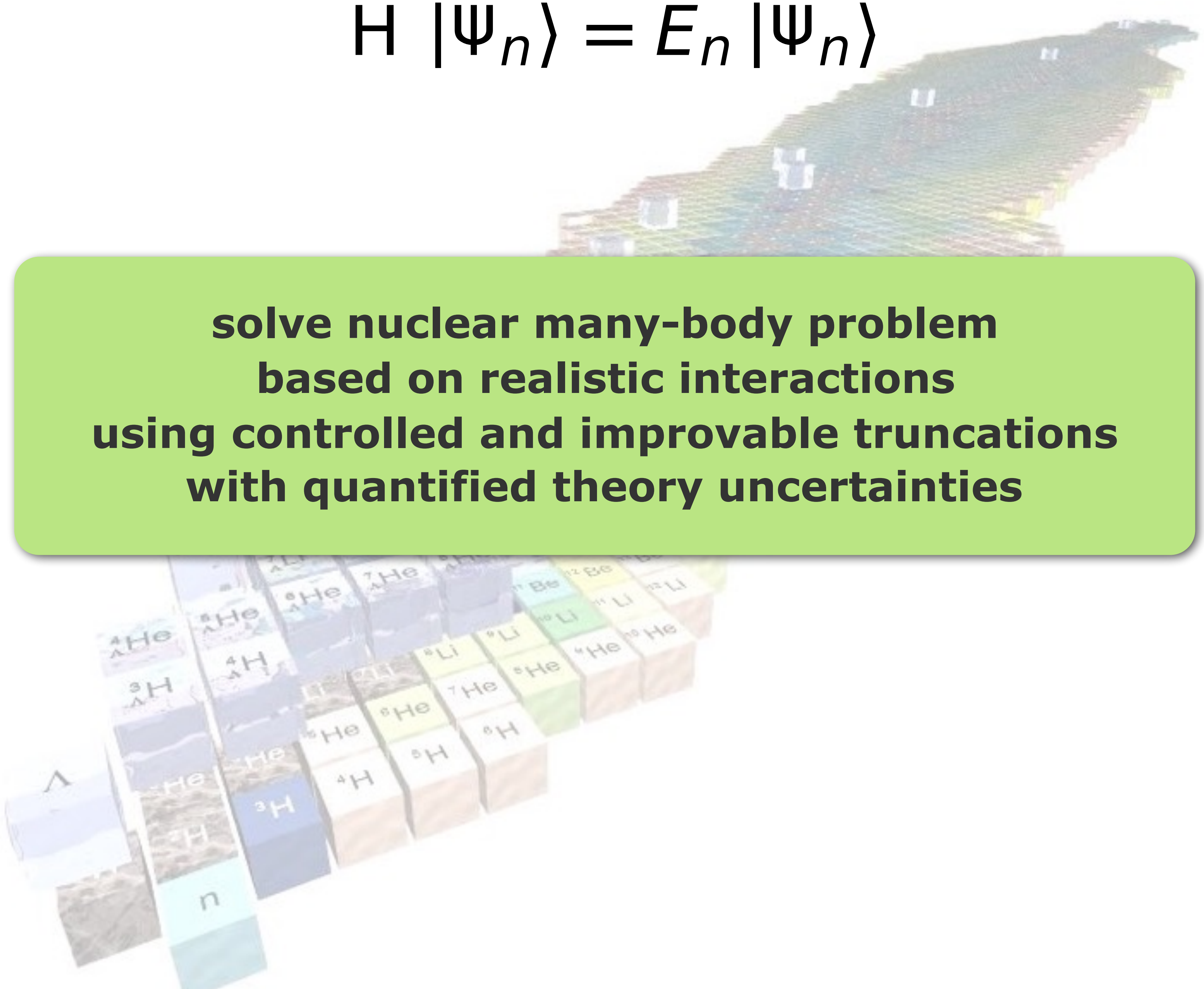
Ab Initio - Definition

$$H\ |\Psi_n\rangle = E_n\,|\Psi_n\rangle$$



solve nuclear many-body problem
based on realistic interactions
using controlled and improvable truncations
with quantified theory uncertainties

Ab Initio - Toolbox

Nuclear Structure & Reaction Observables

Many-Body Solution
No-Core Shell Model,...

Pre-Processing
Similarity Renormalization Group

Hamiltonian
Chiral Effective Field Theory

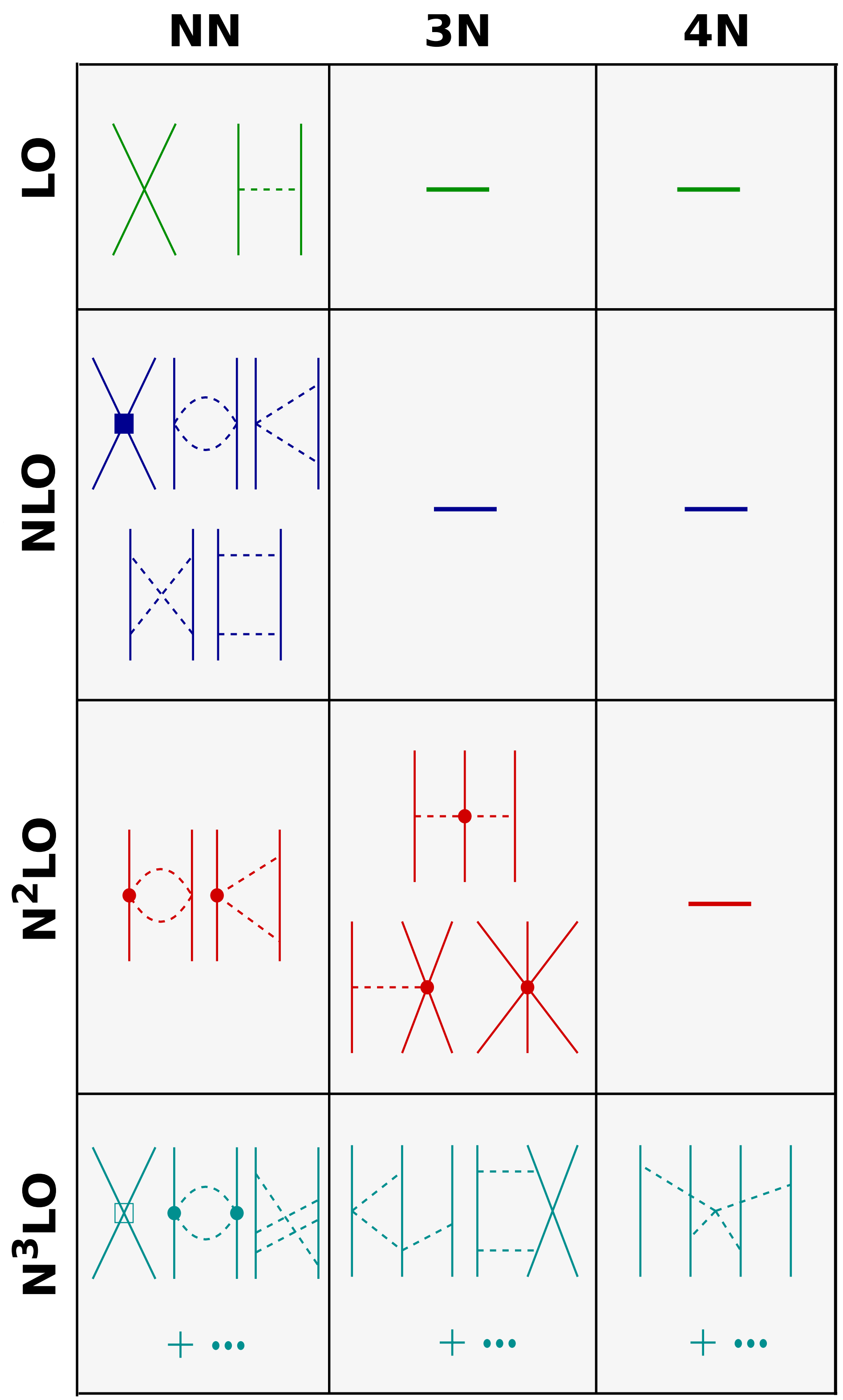
Low-Energy QCD

- systematic and improvable input for all ab initio calculations
- NN & 3N interactions give robust description of p-shell nuclei
- provides tools for theory uncertainty quantification

Nuclear Interactions from Chiral EFT

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...

- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- hierarchy of **consistent NN, 3N, 4N,...** interactions and electroweak operators
- many **recent developments**
  - improved NN up to N4LO+
  - 3N interaction up to N3LO
  - 4N interaction at N3LO
  - improved fits and error analysis
  - order-by-order uncertainty quantification



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- unitary, physics-conserving transformation of Hamiltonian
- accelerate convergence of many-body calculation, tame correlations
- induced many-nucleon interactions are sizeable, but under control

Hamiltonian
Chiral Effective Field Theory

Low-Energy QCD

Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...

continuous unitary transformation driving Hamiltonian towards diagonal form

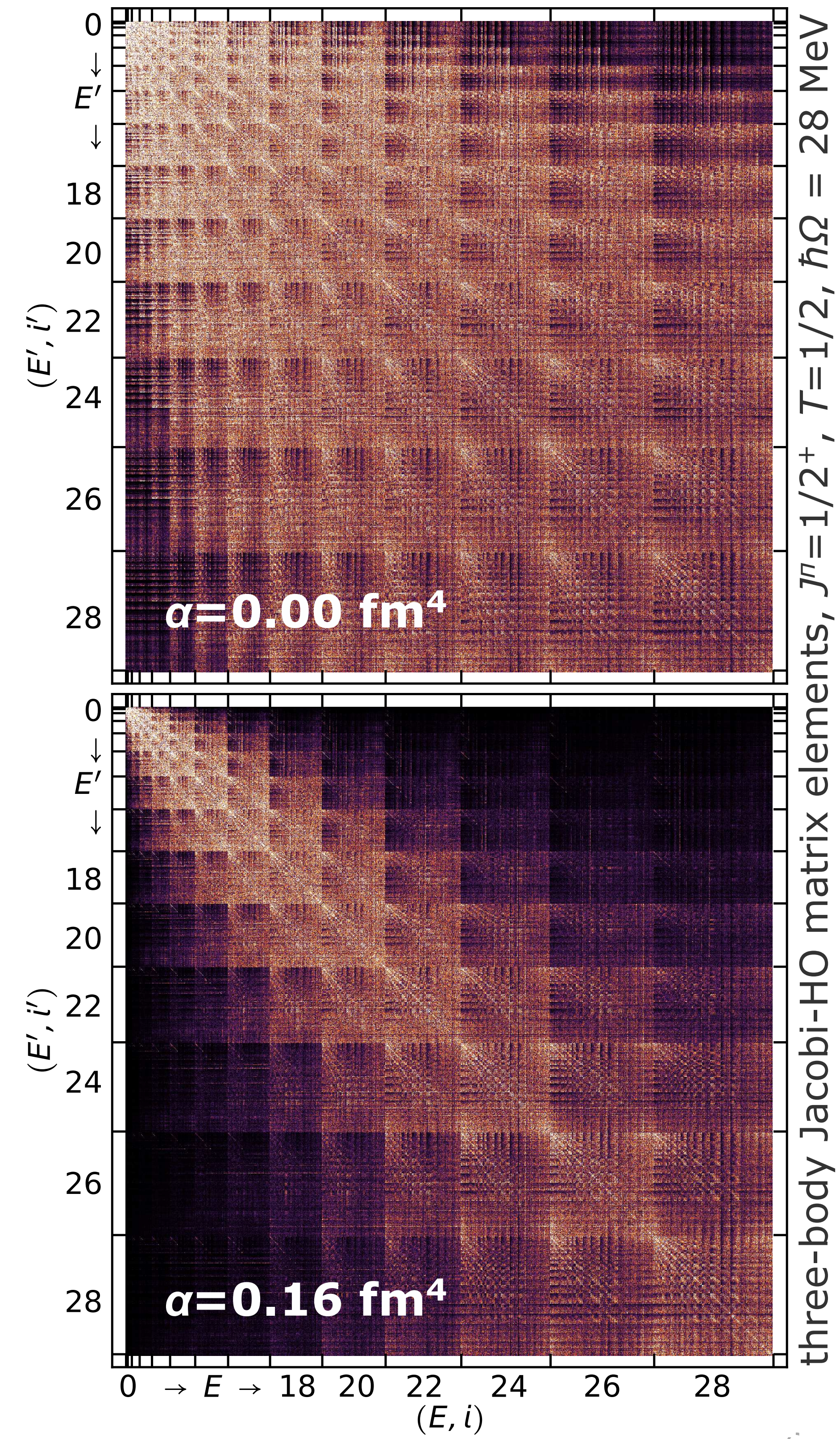
- unitary transformation via flow equation

$$\mathrm{H}_\alpha = \mathrm{U}_\alpha{}^\dagger \mathrm{H}_0\, \mathrm{U}_\alpha \quad \rightarrow \quad \frac{d}{d\alpha}\mathrm{H}_\alpha = [\eta_\alpha, \mathrm{H}_\alpha]$$

- dynamic generator determines physics of transformation

$$\eta_\alpha = (2\mu)^2\, [\mathrm{T}_{\mathrm{int}}, \mathrm{H}_\alpha]$$

- solve flow equation using matrix representation in two- and three-body space
- flow parameter α determines how far to go

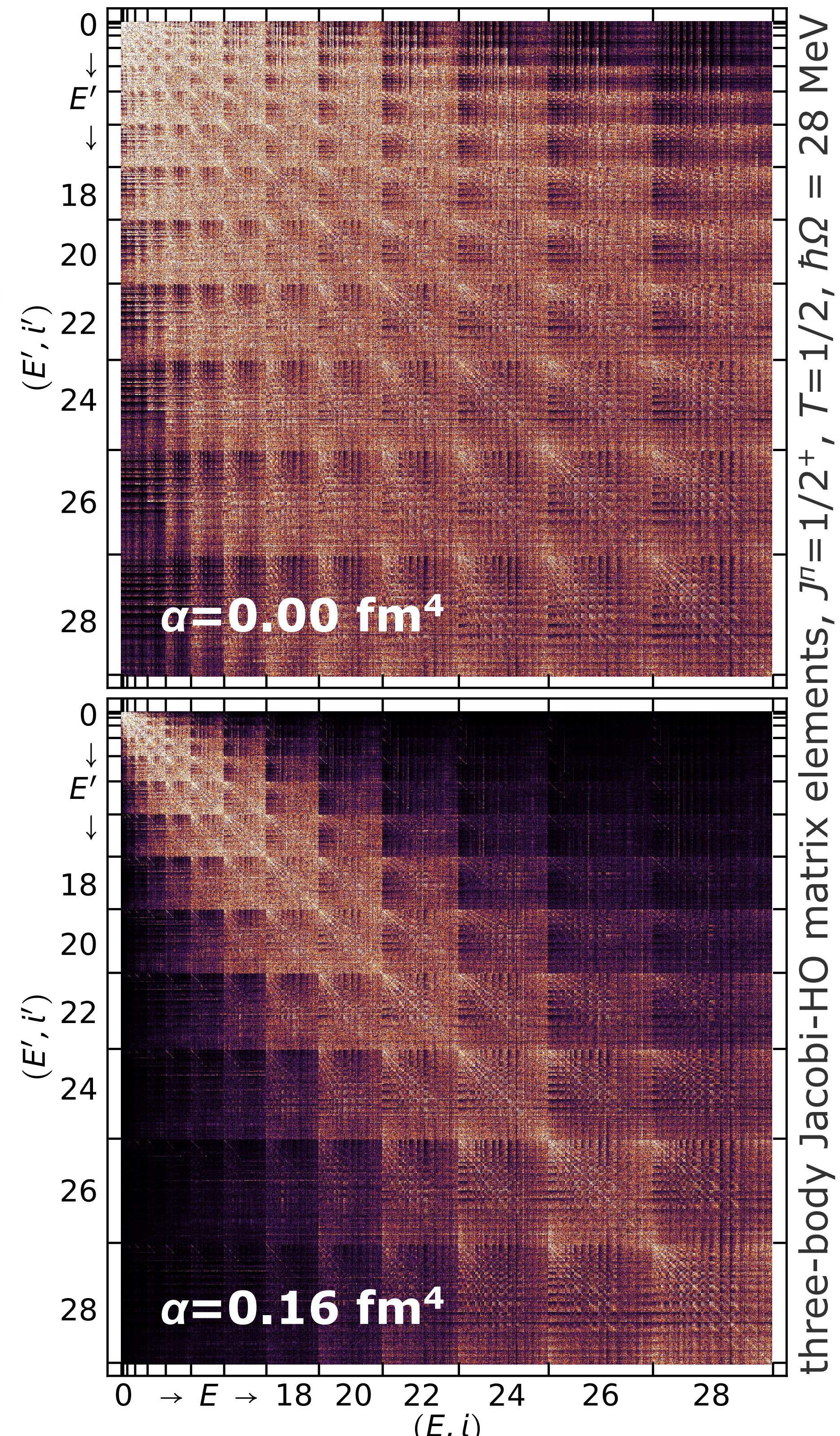


Similarity Renormalization Group

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...

pro:
improves convergence of many-body calculations

con:
induces many-body interactions



- evolved Hamiltonian and all other operators acquires many-body terms

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + \cdots$$

- need to truncate at finite particle rank

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + \cancel{H_\alpha^{[4]} + \cdots}$$

- variation of flow parameter provides diagnostic for omitted many-body terms

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Low-Energy QCD

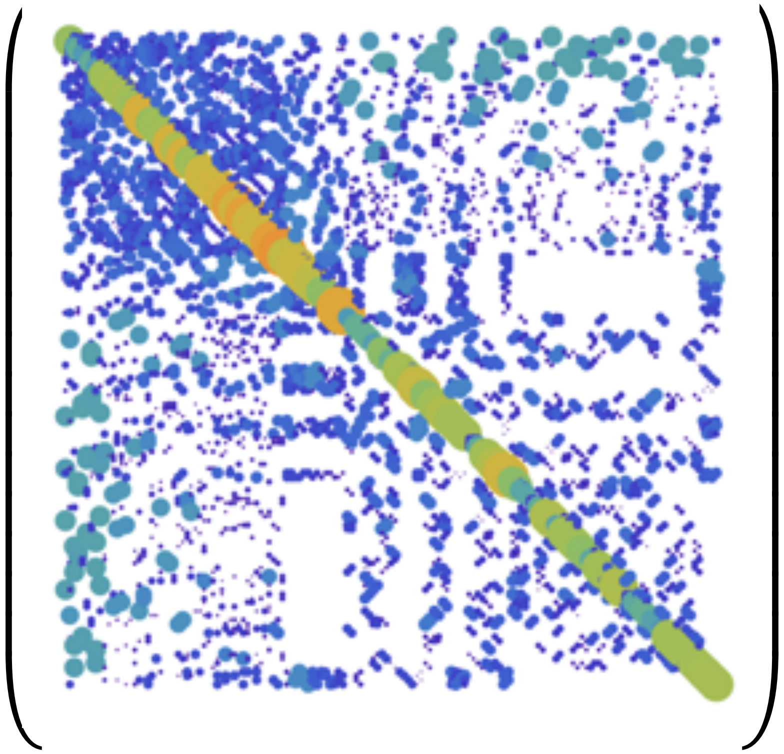
- different many-body methods for different mass regions and different observables
- light nuclei: NCSM
- medium-mass: extensions of NCSM (hybrids with MBPT or IM-SRG)

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 $N_{\max}\hbar\Omega$



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

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$$\boldsymbol{H} = \left(\; 10^{10} \times 10^{10} \; \right)$$

Lanczos Algorithm

$\vec{v}_0 := \vec{0}$
$\vec{v}_1 :=$ any norm. vector
$\beta_1 := 0$

for $i = 1, m$ **do**

$\vec{w} := \boldsymbol{H} \cdot \vec{v}_i - \beta_i \vec{v}_{i-1}$
$\alpha_i := \vec{w} \cdot \vec{v}_i$
$\vec{w} := \vec{w} - \alpha_i \vec{v}_i$
$\beta_{i+1} := ||\vec{w}||$
$\vec{v}_{i+1} := \vec{w} / \beta_{i+1}$

end for

$$\boldsymbol{T}_m = \begin{pmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_m \\ & & & \beta_m & \alpha_m \end{pmatrix}$$

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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 $N_{\max}\hbar\Omega$

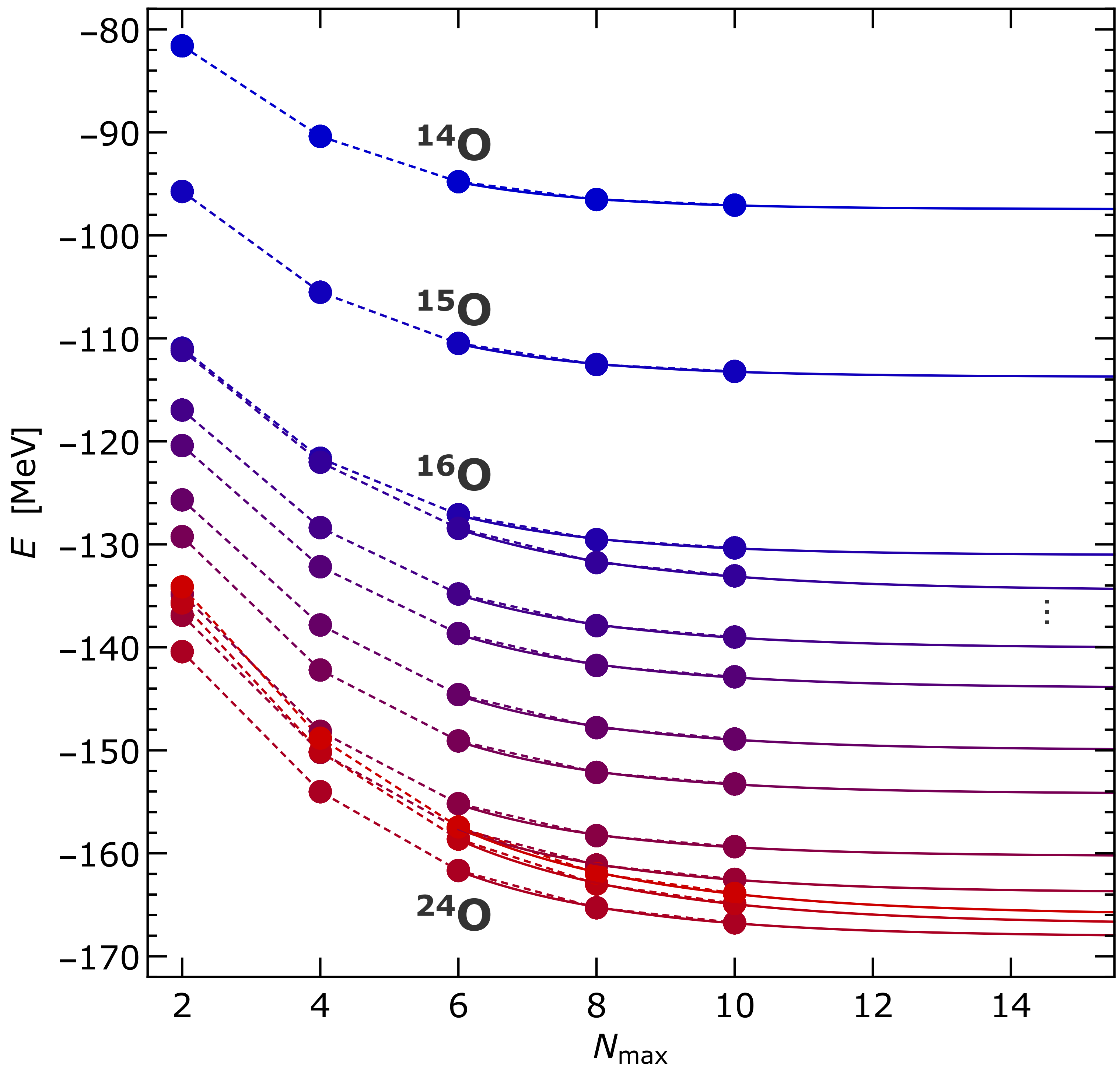
- **advantages**: simplicity makes it powerful
  - ground and excited states obtained on the same footing
  - all observables obtained directly from the eigenvectors
  - inclusion of continuum degrees-of-freedom possible

- **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 States

Ground-State Energies

Tichai, Müller, Vobig, Roth; arXiv:1809.07571

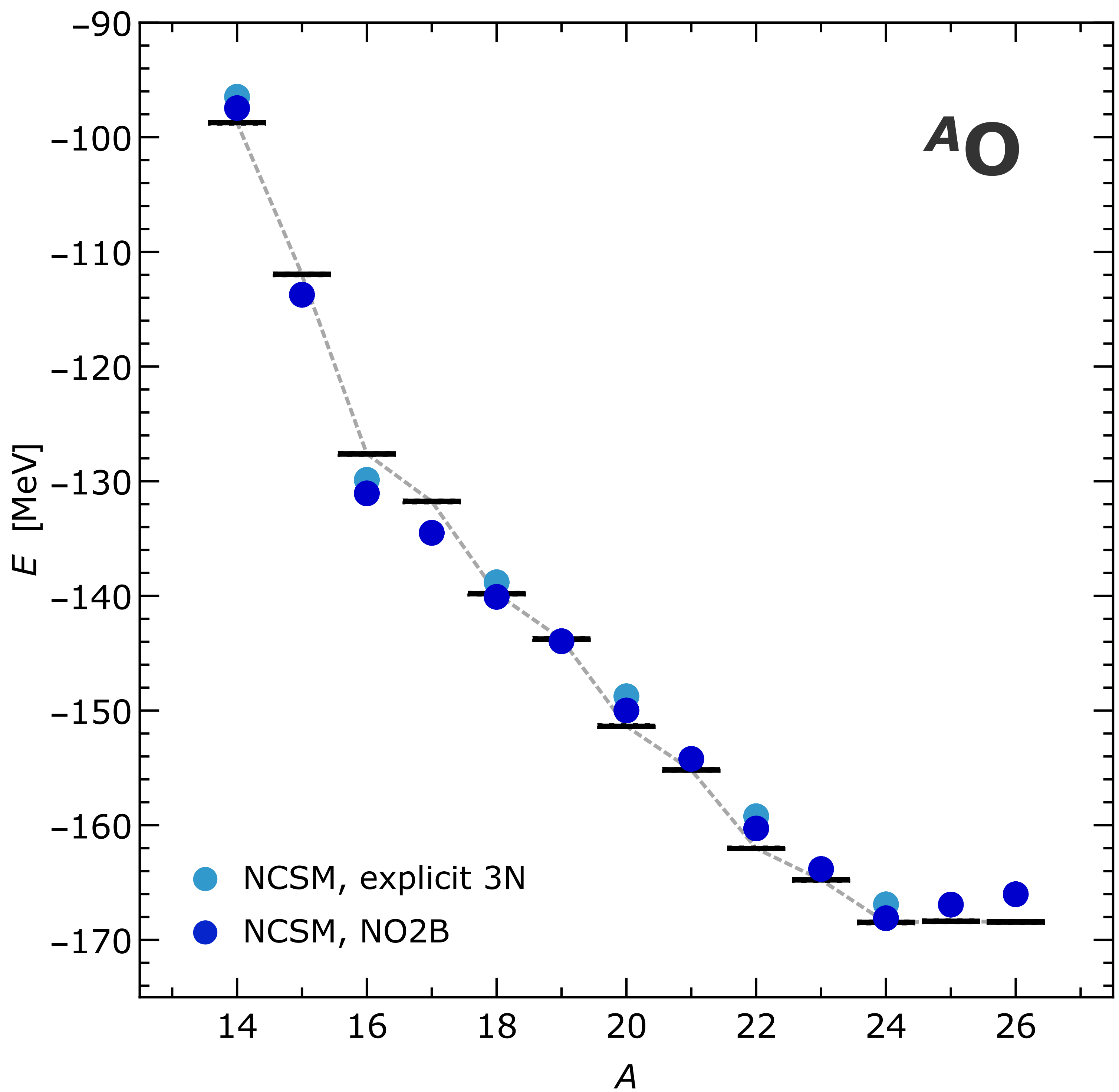


chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
ħΩ=20 MeV
e_{max}=12
NAT basis

- ground-state energies converge for N_{max} ~ 10 for all oxygen isotopes

Ground-State Energies

Tichai, Müller, Vobig, Roth; arXiv:1809.07571

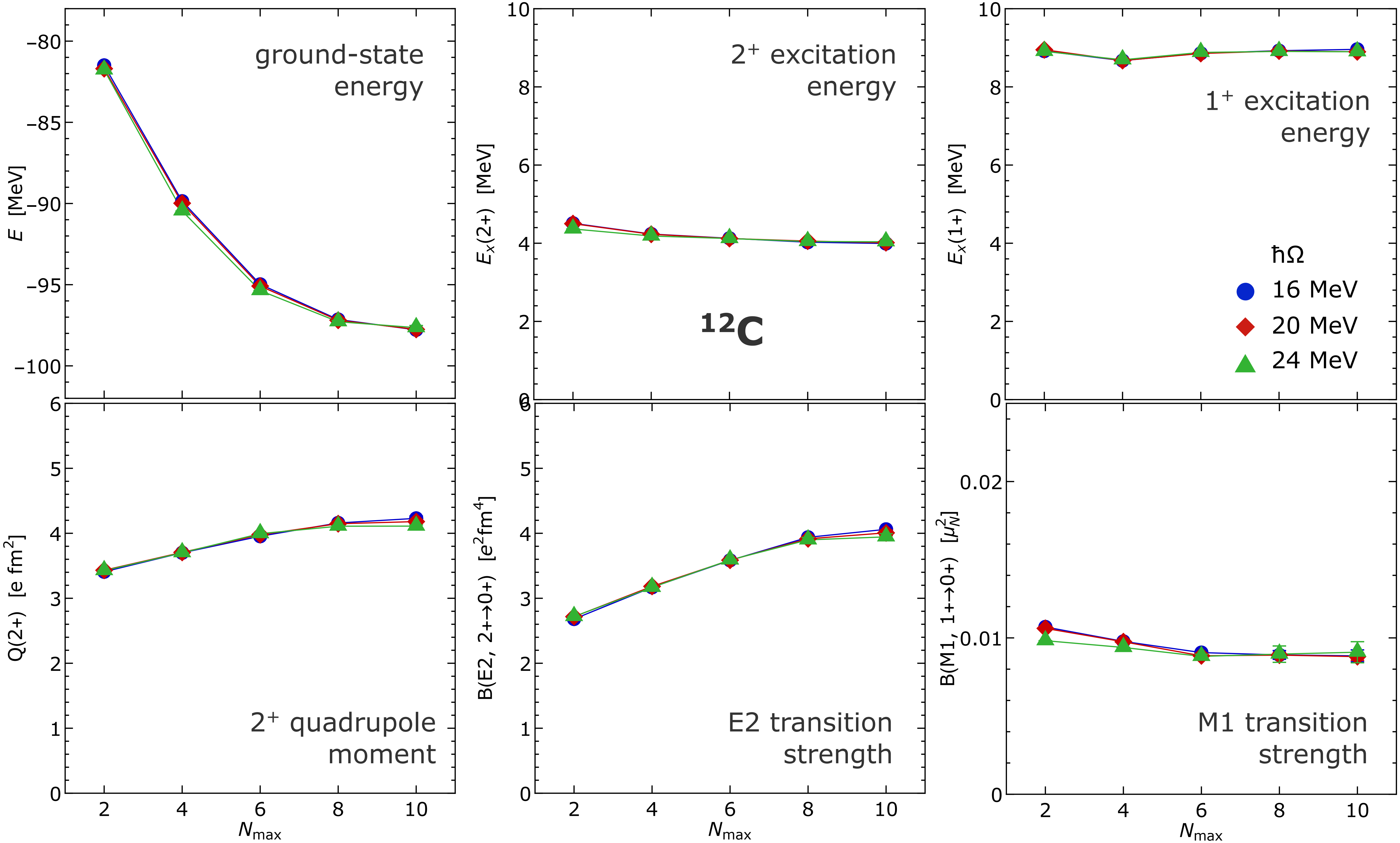


- ground-state energies converge for N_{max} ~ 10 for all oxygen isotopes
- very good agreement with experimental systematics and dripline
- NO2B instead of explicit 3N causes ~1% overbinding

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

Excited States & Spectroscopy

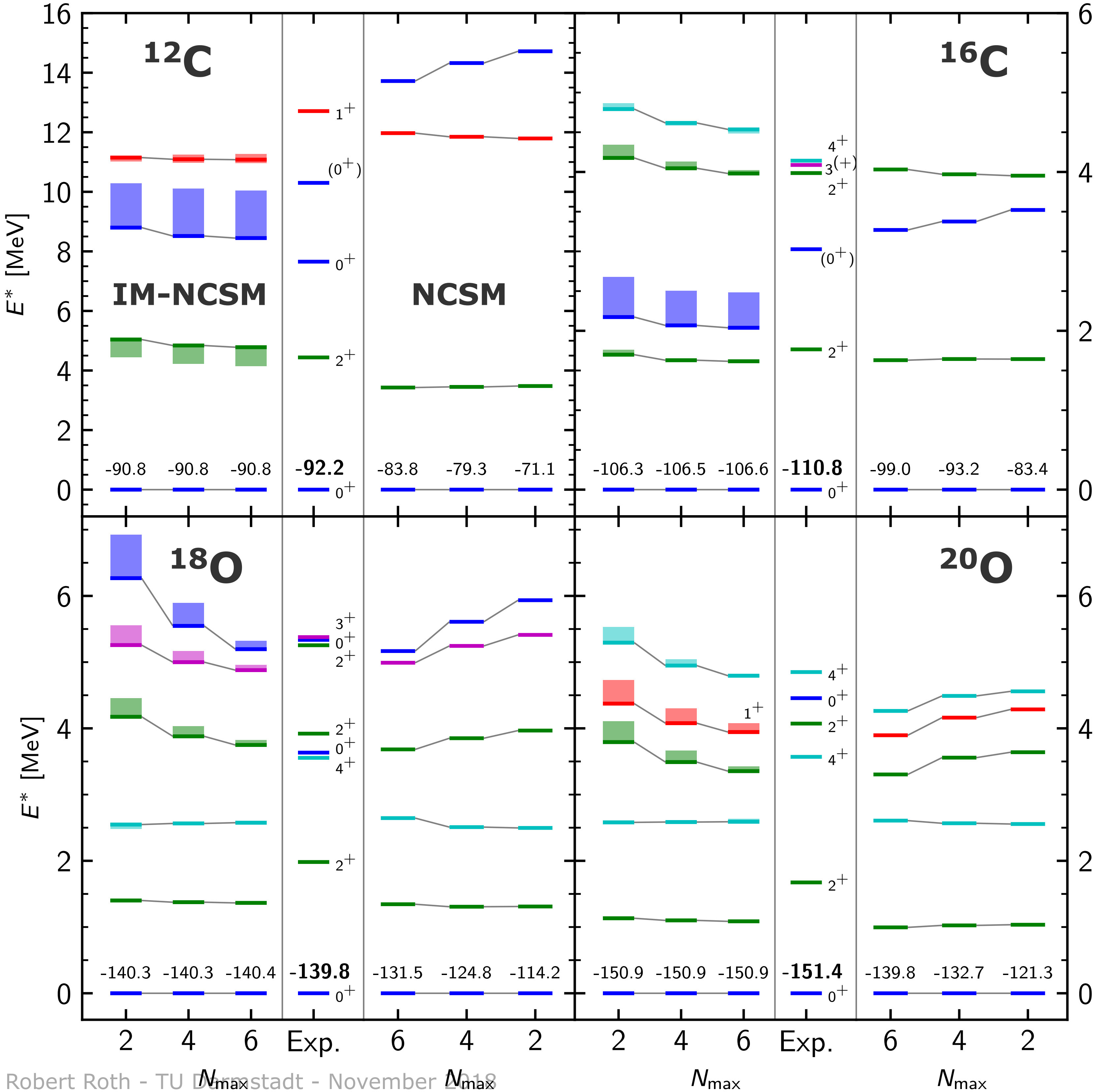
Tichai, Müller, Vobig, Roth; arXiv:1809.07571



chiral NN+3N, Λ_{3N}=500 MeV, α=0.08 fm^4, e_{max}=12, NAT basis

Excitation Spectra

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



- NCSM and IM-NCSM in excellent agreement for converged states
- consistent evolution of electromagnetic operators is available
- full access to low-lying spectroscopy

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

HF basis
N_{max}=0 reference

Collective Excitations

NCSM for Strength Distributions

- **naive idea**
  - compute the full spectrum using NCSM
  - for each eigenvector compute transition matrix element
  - computationally not feasible…

- **ingenious trick**
  - R.R. Whitehead (1980), *Moment Methods and Lanczos Methods*
  - exploit intrinsic structure of the Lanczos algorithm to extract transition strengths distribution on-the-fly
  - equivalent to naive version once converged
  - computational cost: same as for low lying-spectrum

Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

- perform **NCSM calculation for ground state** $|E_0\rangle$

- prepare **pivot vector with transition operator**

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

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

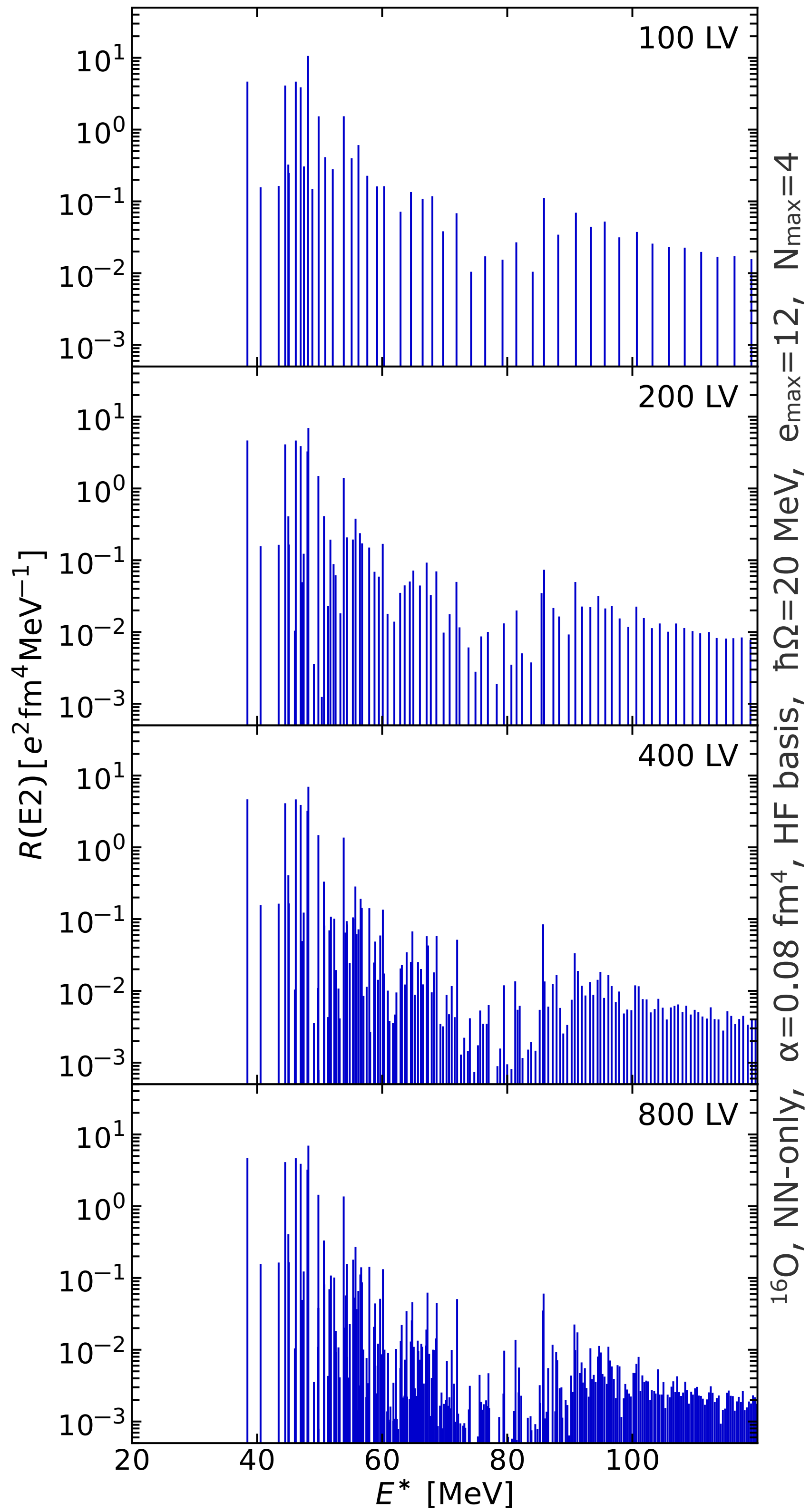
$$|E_n\rangle = \sum_{i=1}^{I} C_i^{(n)}\, |v_i\rangle$$

- 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**

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

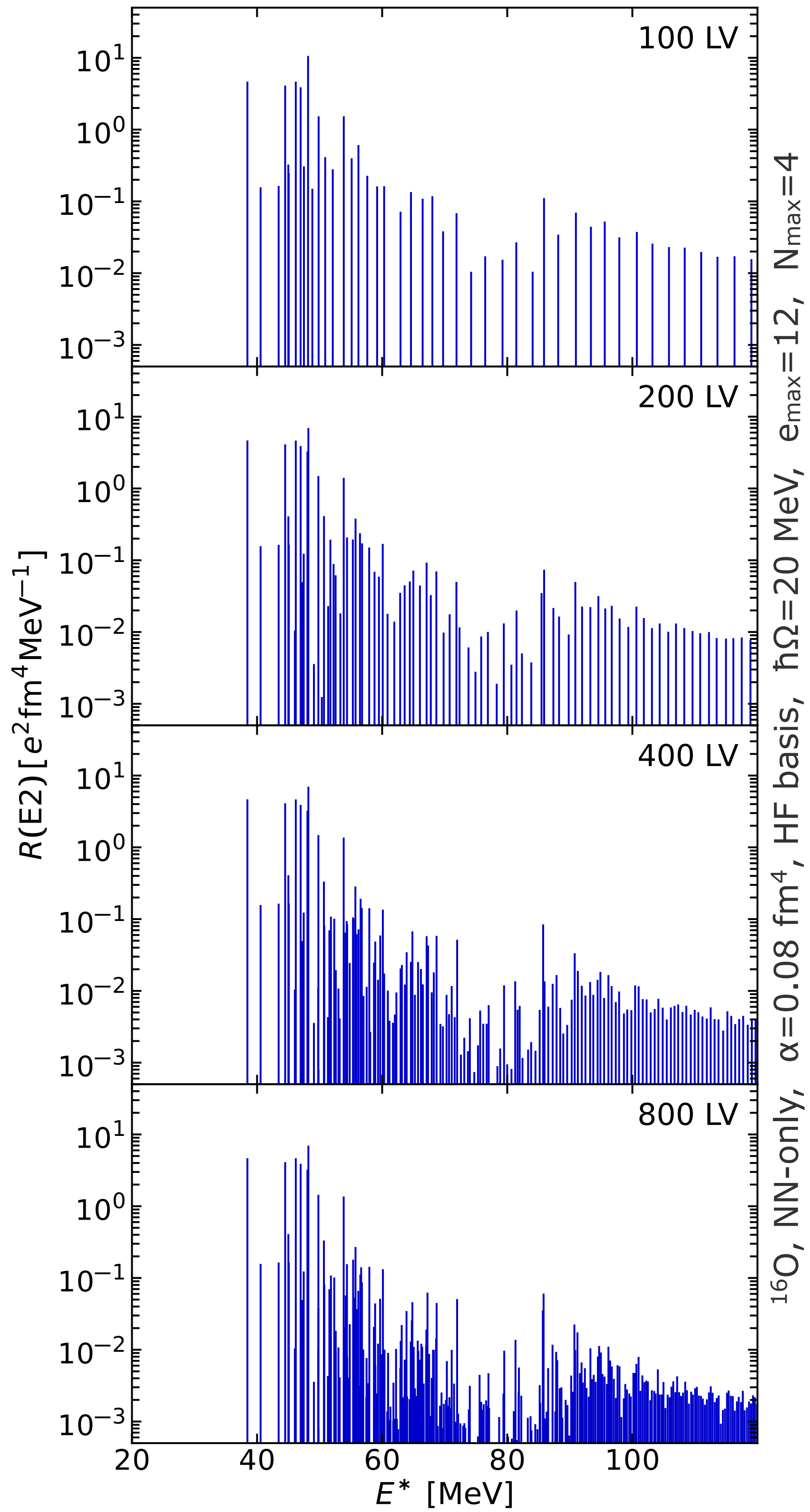


Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

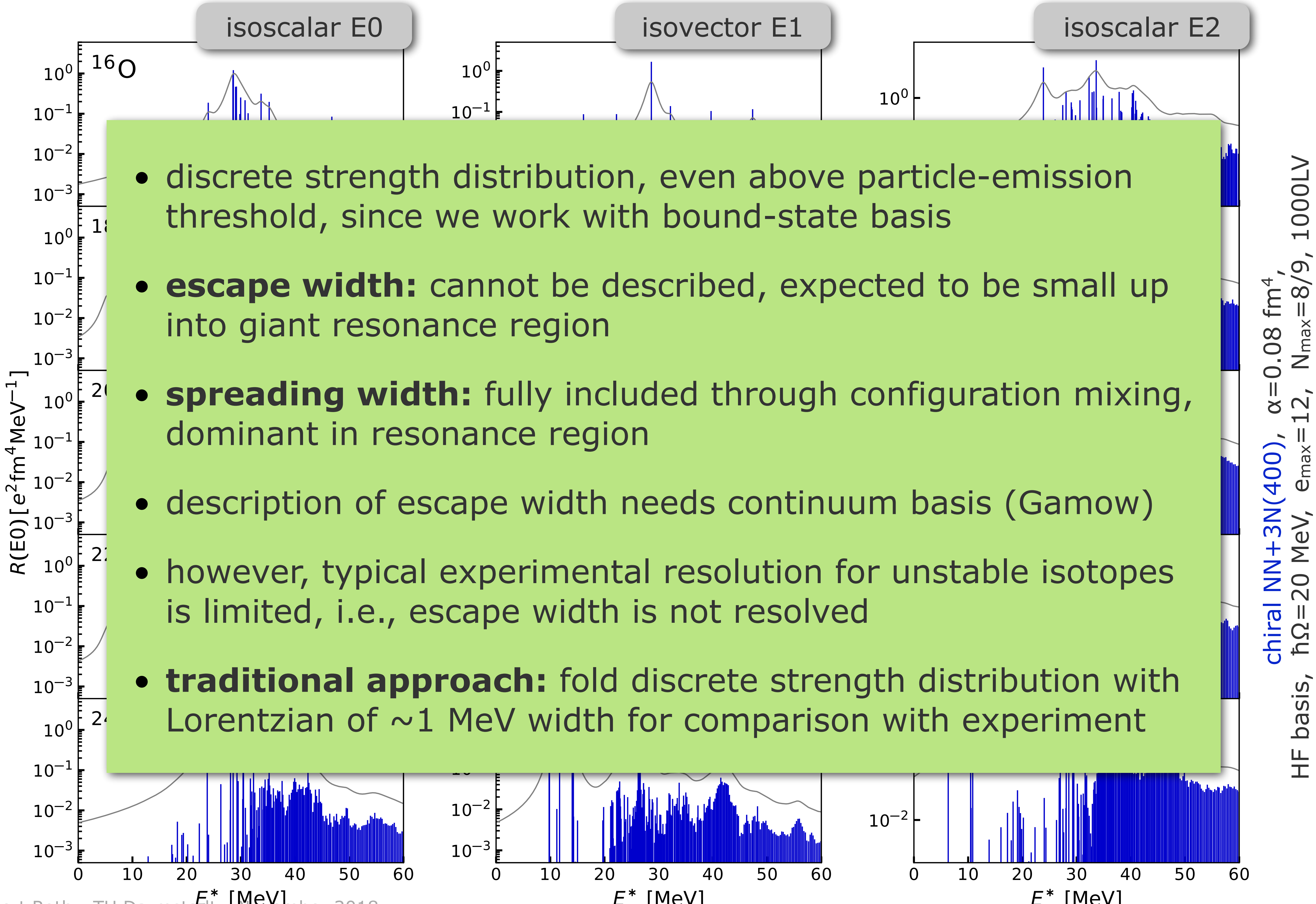
ab initio approach to strength distributions with many advantages

- 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

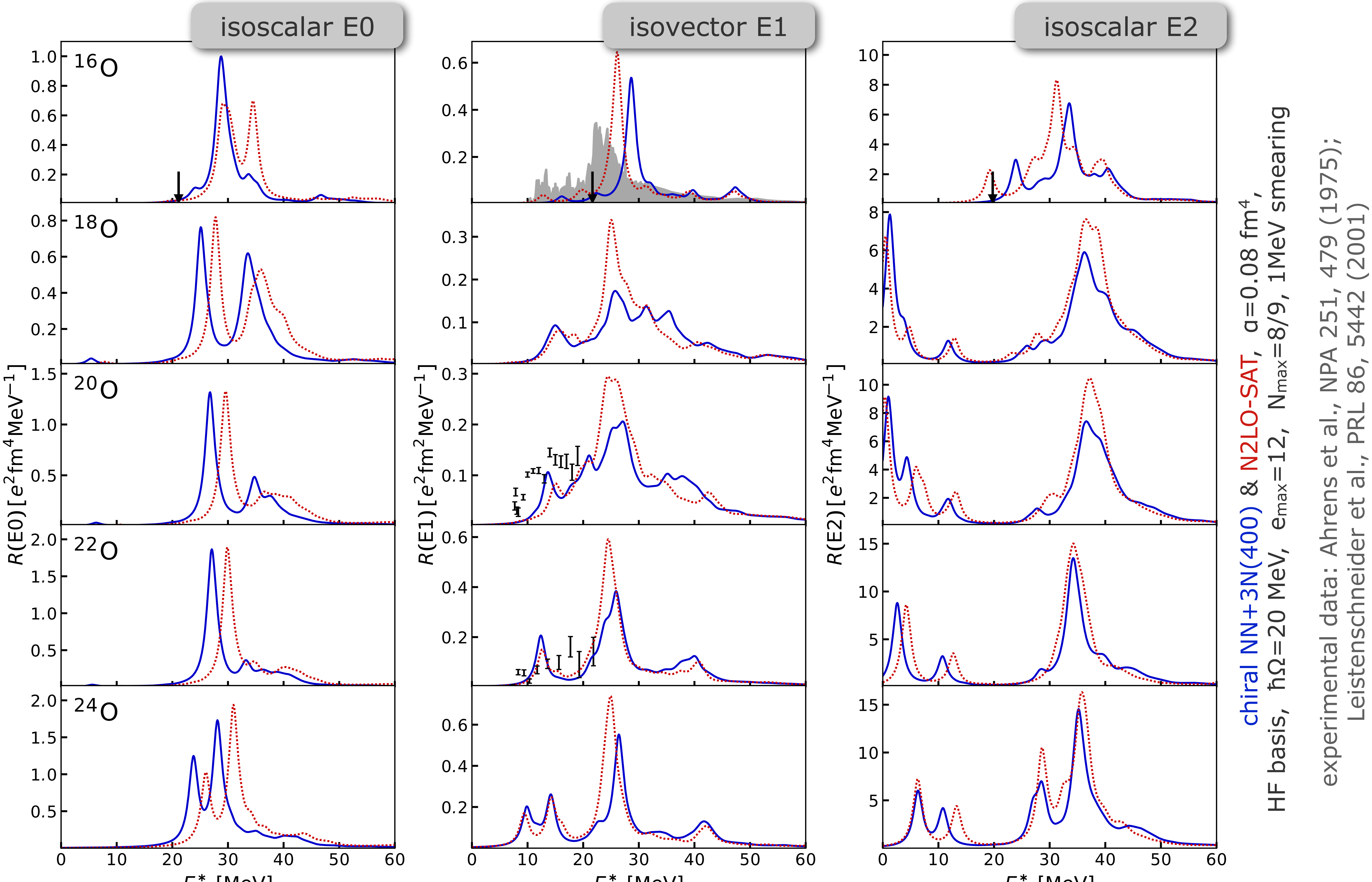
Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- discrete strength distribution, even above particle-emission threshold, since we work with bound-state basis
- **escape width:** cannot be described, expected to be small up into giant 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 is limited, i.e., escape width is not resolved
- **traditional approach:** fold discrete strength distribution with Lorentzian of ~1 MeV width for comparison with experiment

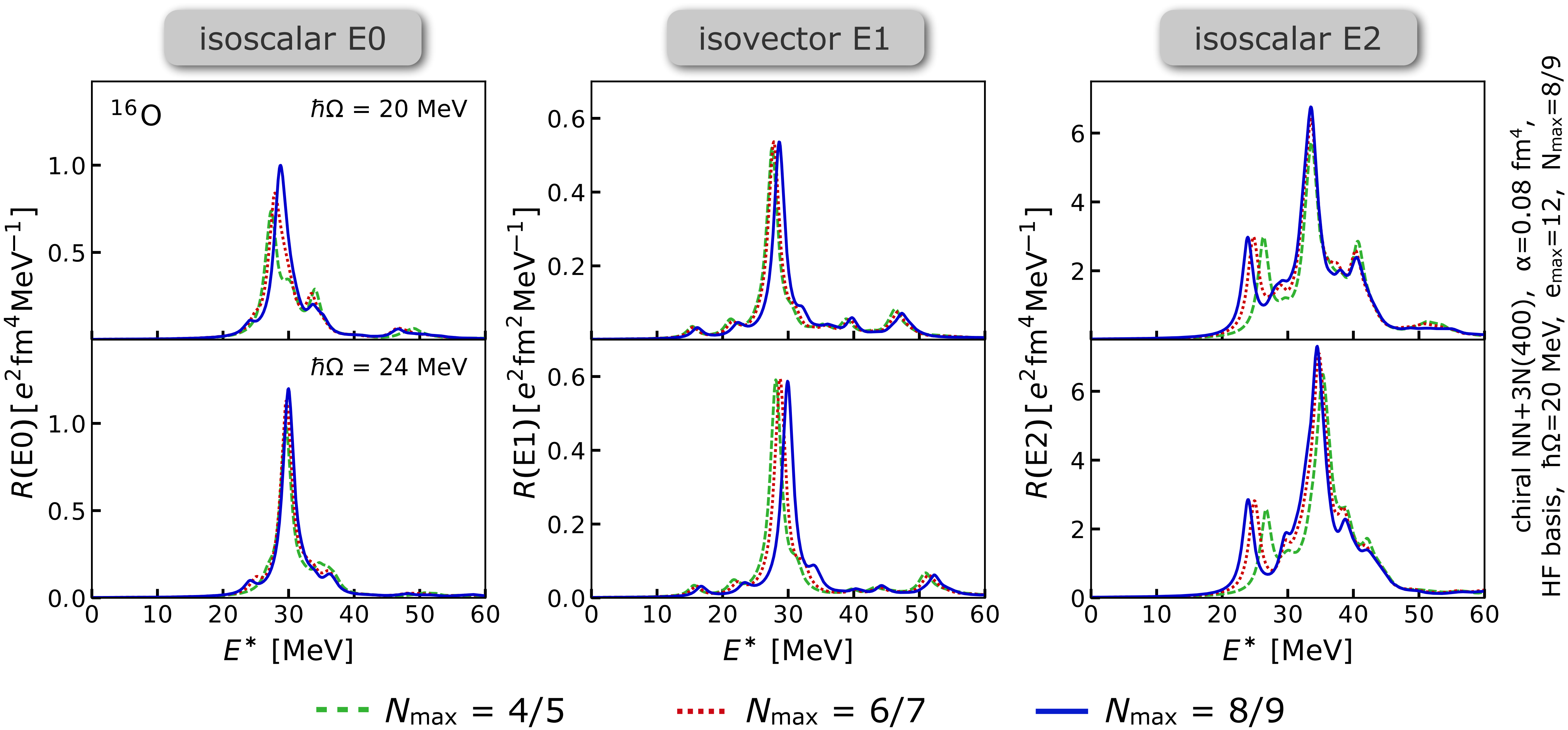
Strength Distribution

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



Model-Space Convergence

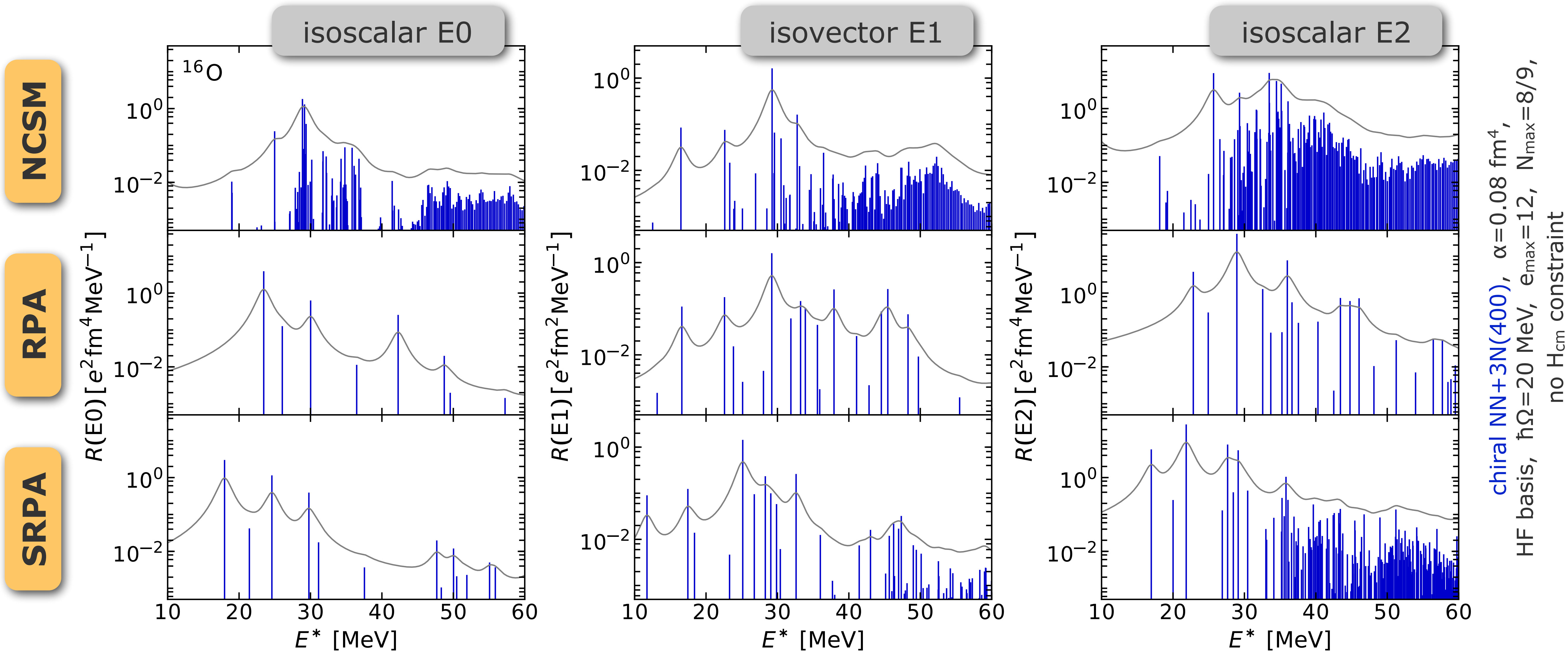
Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- N_{max} is the only model-space truncation parameter
- very stable N_{max} convergence and independence of ħΩ

Comparison with RPA and SRPA

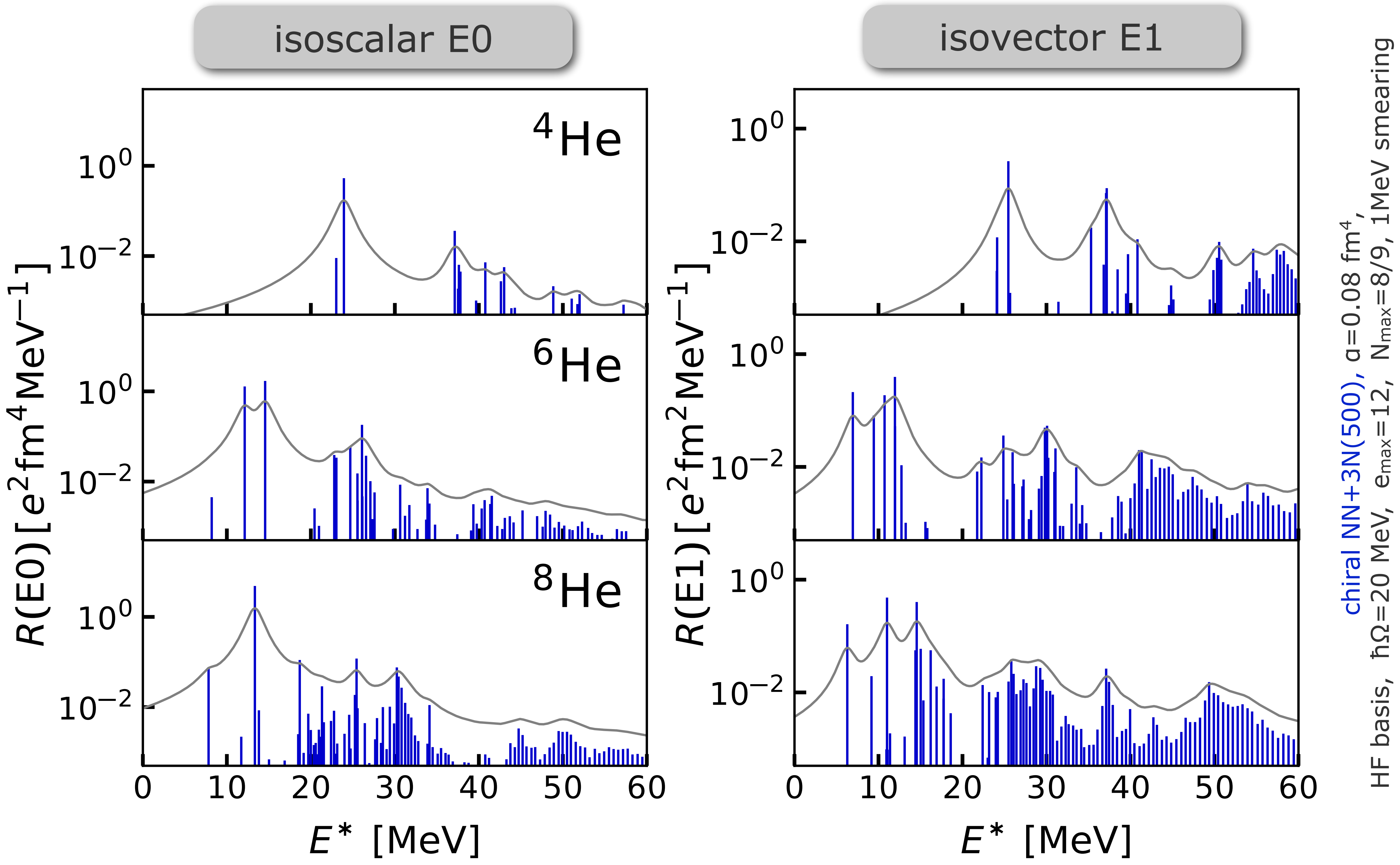
Stumpf, Wolfgruber, Roth; arXiv:1709.06840



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

Helium Isotopes

Stumpf, Mertes, Roth; in prep.



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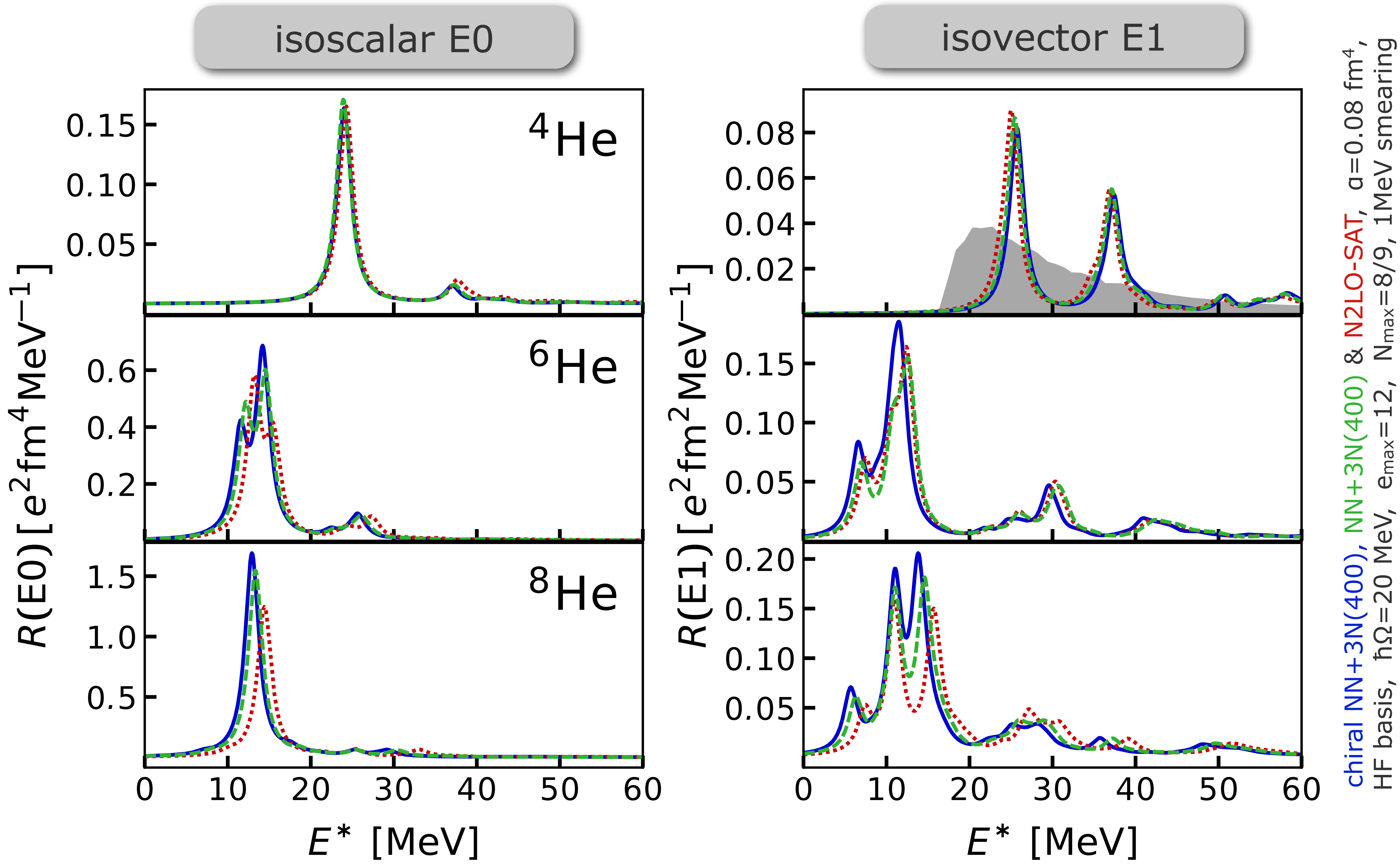
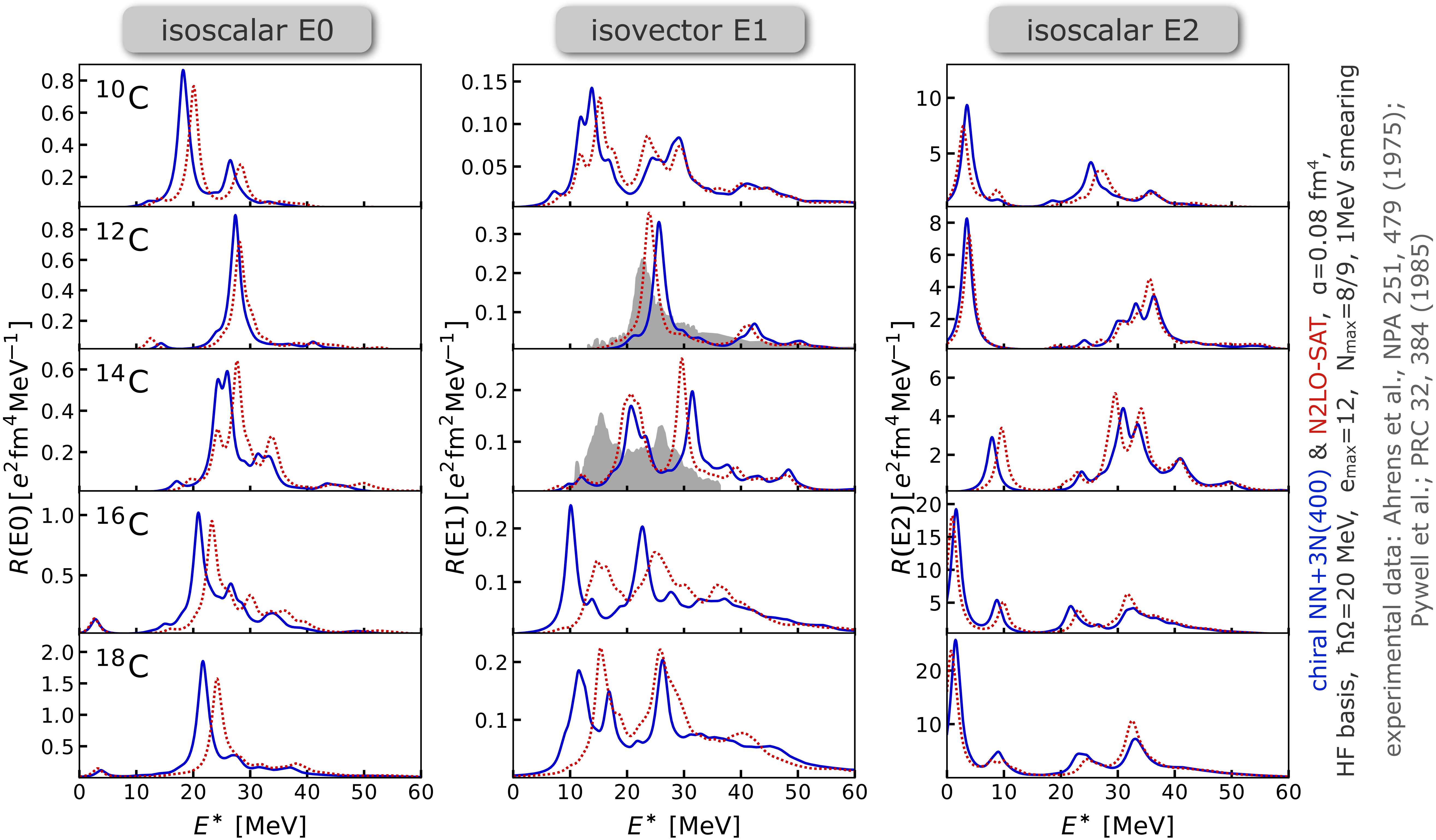


Carbon Isotopes

Stumpf, Mertes, Roth; in prep.



Summary & Outlook

- **unified ab initio framework** for ground states, low-lying excitations, and high-lying modes up to A~25

- **full access** to strength distributions, fine structure, properties of individual states (transitions densities & current densities)

- **role of interactions:** understand the impact of different chiral EFT interactions and quantify theory uncertainties

- **role of continuum:** include explicit continuum degrees of freedom via Gamow basis or Lorentz integral inversion

- **extension to A~50 regime:** transfer strength-function approach to multi-reference in-medium SRG and in-medium NCSM

Epilogue

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