Electromagnetic Strength Distributions from the Importance-Truncated No-Core Shell Model

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Motivation

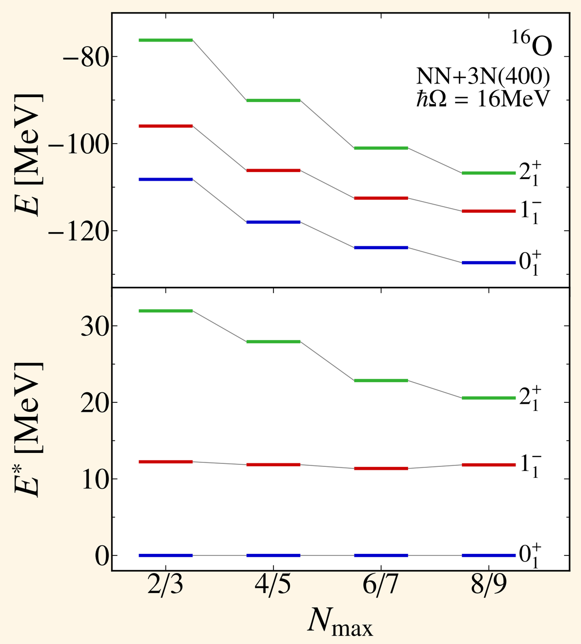
- electromagnetic transitions very sensitive to detailed form of nuclear wave function
- strength distributions can be easily related to experiments and provide excellent testing ground for theoretical models
- exact but infeasible approach: fully diagonalize the Hamilton matrix and evaluate transition strengths for all eigenstates
- Lanczos strength functions: method for ab initio calculation of strength distributions in a very simple and efficient way
- use Lanczos strength functions to validate strength distributions from approximate approaches

Importance-Truncated No-Core Shell Model

basic idea:

- introduce importance threshold $\kappa_{\min}$ as adaptive truncation criterion
- solve eigenvalue problem in IT model space tailored to Hamiltonian and target state

$\Rightarrow$ extend NCSM to larger model spaces



general concept: [1]

- start from initial approximation for the target eigenstate
- estimate relevance of basis states $\{|\Phi_\nu\rangle\}$ using the importance measure

$$\kappa_\nu = -\frac{\langle \Phi_\nu|\mathbf{H}|\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- construct IT model space from basis states with $\kappa_\nu \geq \kappa_{\min}$
- solve eigenvalue problem in IT model space
- repeat previous steps while updating reference state by most recent eigenstate
- vary $\kappa_{\min}$ and extrapolate to account for effects of excluded basis states

Simple Lanczos Method

- iterative method for computing some extreme eigenpairs of a Hermitian matrix A based on orthogonal projections onto Krylov subspaces: [2–4]

start: pivot vector $\vec{v}_1$ with $||\vec{v}_1|| = 1$
$\beta_0 = 0$, $\vec{v}_0 = \vec{0}$

iterate: for $j = 1, 2, \ldots, m$ do:

$\vec{w}_j \leftarrow A\vec{v}_j - \beta_{j-1}\vec{v}_{j-1}$

$\alpha_j \leftarrow (\vec{w}_j, \vec{v}_j)$

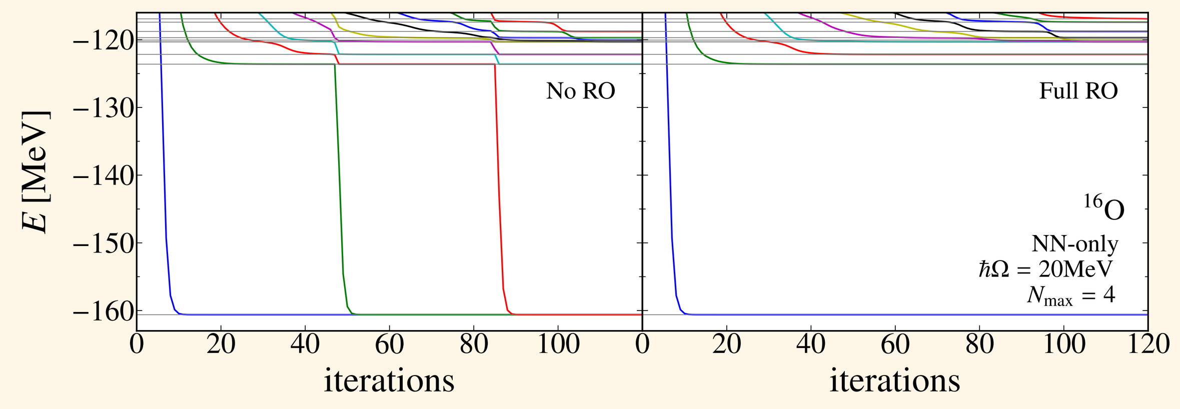
$\vec{w}_j \leftarrow \vec{w}_j - \alpha_j \vec{v}_j$

$\beta_j \leftarrow ||\vec{w}_j||$

$\vec{v}_{j+1} \leftarrow \vec{w}_j/\beta_j$

$$\Longrightarrow \quad T_m = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & & & \beta_{m-1} \\ & & & \beta_{m-1} & \alpha_m \end{pmatrix}$$

- diagonalizing T_m yields fast-converging approximations for eigenpairs of A
- loss of orthogonality due to round-off errors leads to duplicates of eigenpairs



Lanczos Strength Functions

recipe: [5]

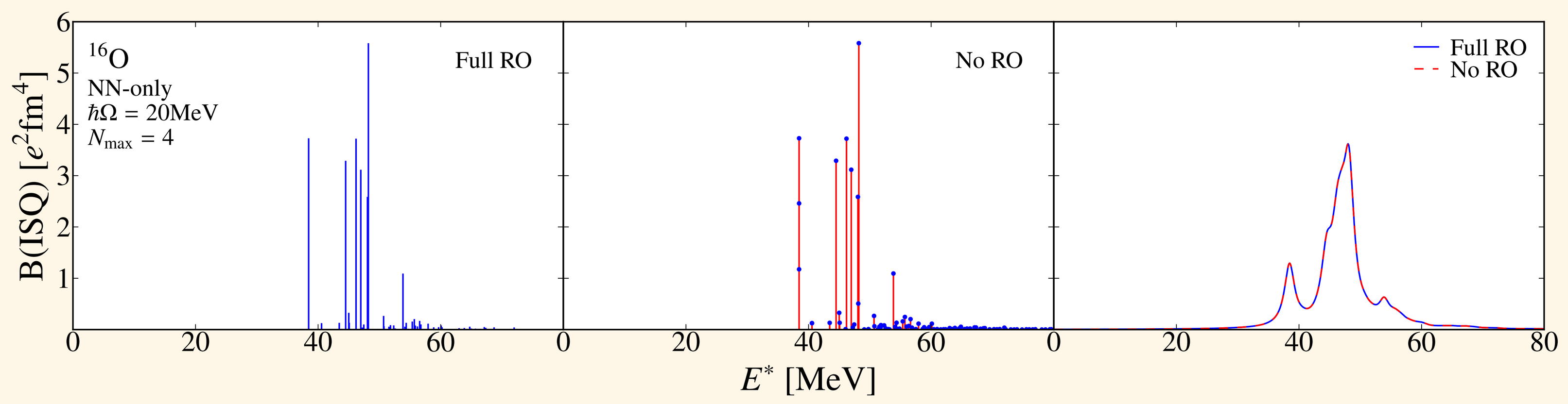
- take initial state $|\Psi^{(i)}\rangle$ from (IT-)NCSM calculation
- define pivot state:

$$|\Sigma_1\rangle = \frac{1}{\sqrt{\tilde{S}}}\mathbf{O}\,|\Psi^{(i)}\rangle\,, \quad \tilde{S} = \langle\Psi^{(i)}|\mathbf{O}^\dagger\mathbf{O}|\Psi^{(i)}\rangle$$

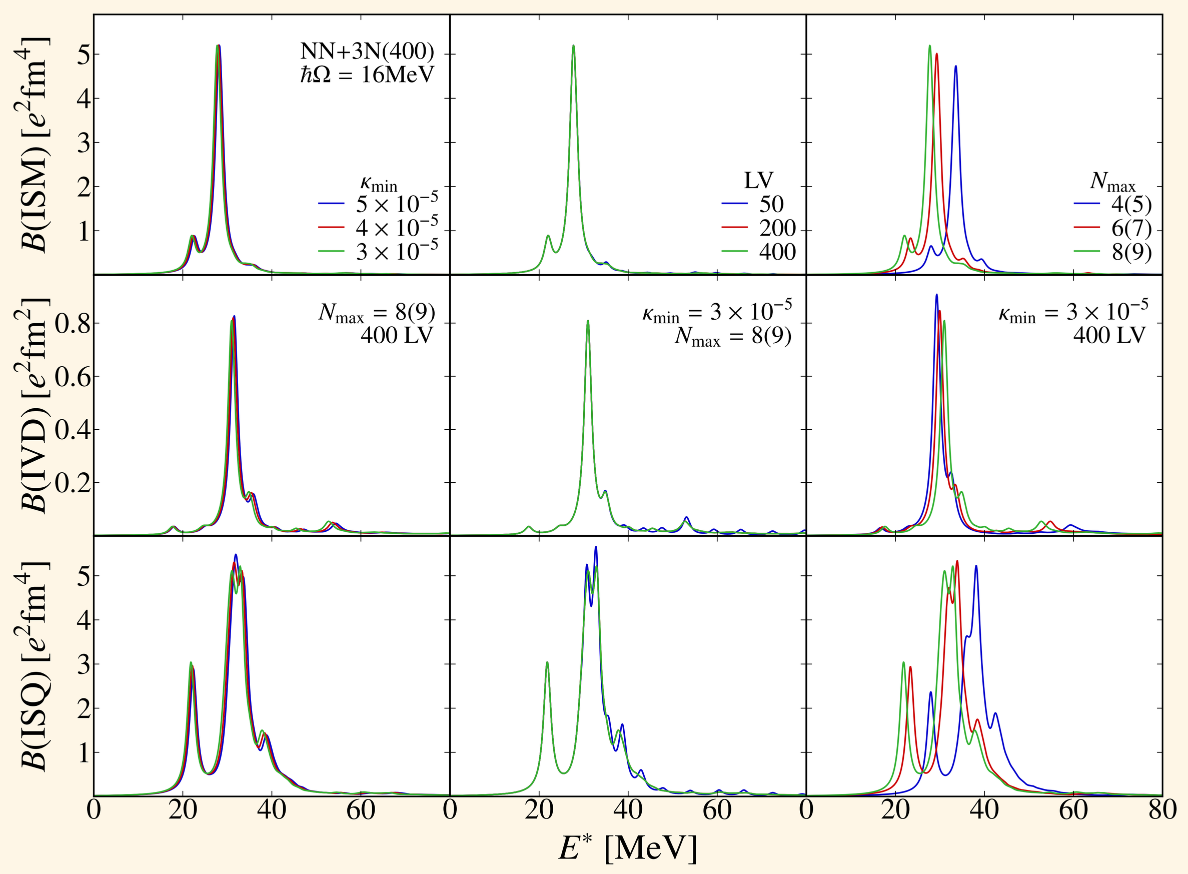
- norm $\tilde{S}$ is total strength of the operator $\mathbf{O}$ in the initial state
- obtain tridiagonal matrix T_m after m interations of the simple Lanczos algorithm applied to the nuclear Hamiltonian using $|\Sigma_1\rangle$ as initial vector
- compute eigenvalues ϵ_j and eigenvectors $\{|\Phi_j\rangle\}$ of T_m using standard diagonalization methods
- obtain strength distribution from unitary matrix that transforms T_m into eigenbasis:

$$S(E) = \sum_{j=1}^{m} \tilde{S}|\langle\Phi_j|\Sigma_1\rangle|^2\delta(E - E_j)$$
$$= \sum_{j=1}^{m} |\langle\phi_j|\mathbf{O}|\Psi^{(i)}\rangle|^2\delta(E - E_j)$$

- model continuum effects by convolving the discrete strength distribution with Lorentz curve using width 1 MeV
- empirical finding: loss of orthogonality in Lanczos basis is no issue

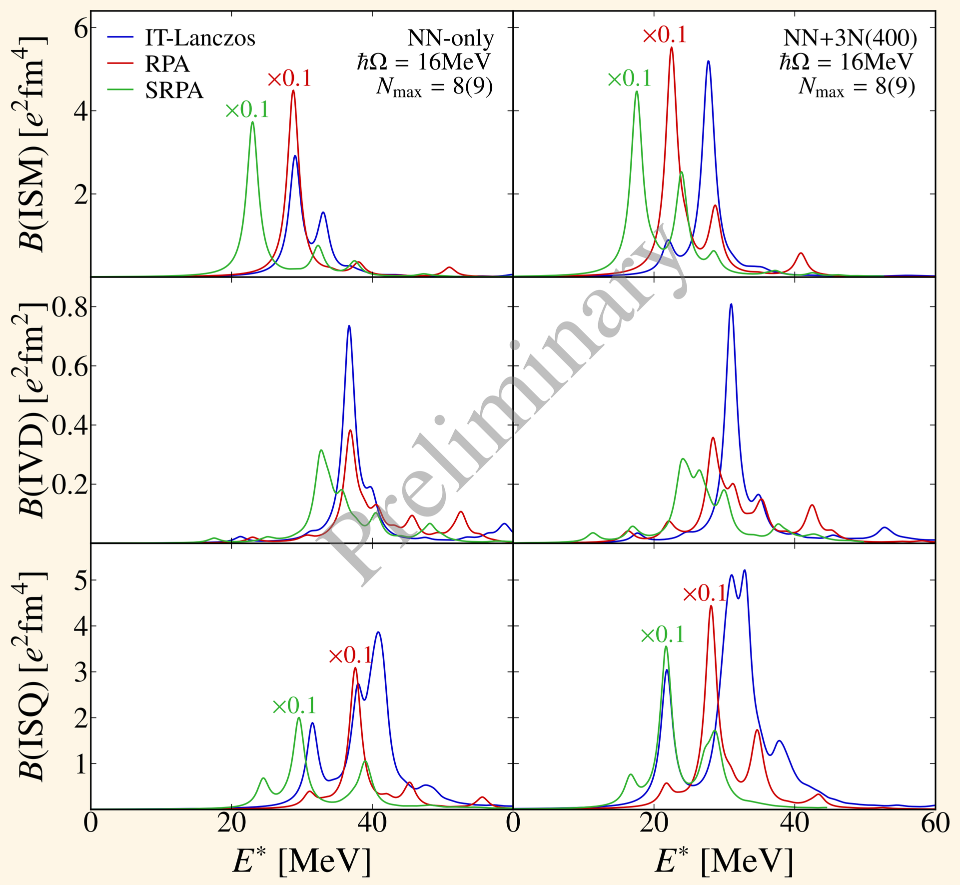


Convergence Benchmark for Lanczos Strength on ^{16}O



- no effect of importance truncation on structure of strength distributions
- only marginal dependence of peak positions in strength distributions on importance truncation
- very fast convergence behavior of strength distributions w.r.t. size of Lanczos basis
- shape of strength distribution already visible for small $N_{\max}\hbar\Omega$
- peak positions converge as the spectra
- IT model space must be tailored to eigenstate of spins involved in transition, e.g. need a 2^+ target state for $E2$ transitions

Strength Distributions for ^{16}O



- inclusion of 3N forces shifts distributions to lower energies
- qualitative agreement of Lanczos with RPA and SRPA strengths [6]
- total Lanczos strength one order of magnitude smaller than (S)RPA strength for isoscalar transitions
- need to study dependence of Lanczos strength distributions on HO frequency
- alternative: use HF single-particle basis for model-space construction

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NN-only: Idaho-500 [7]
NN+3N(400): Idaho-500+N^{2}LO 3N ($\Lambda = 400$MeV) [8]

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