AB INITIO NUCLEAR STRUCTURE CALCULATIONS OF ATOMIC NUCLEI UP TO OXYGEN-16

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OBJECTIVES

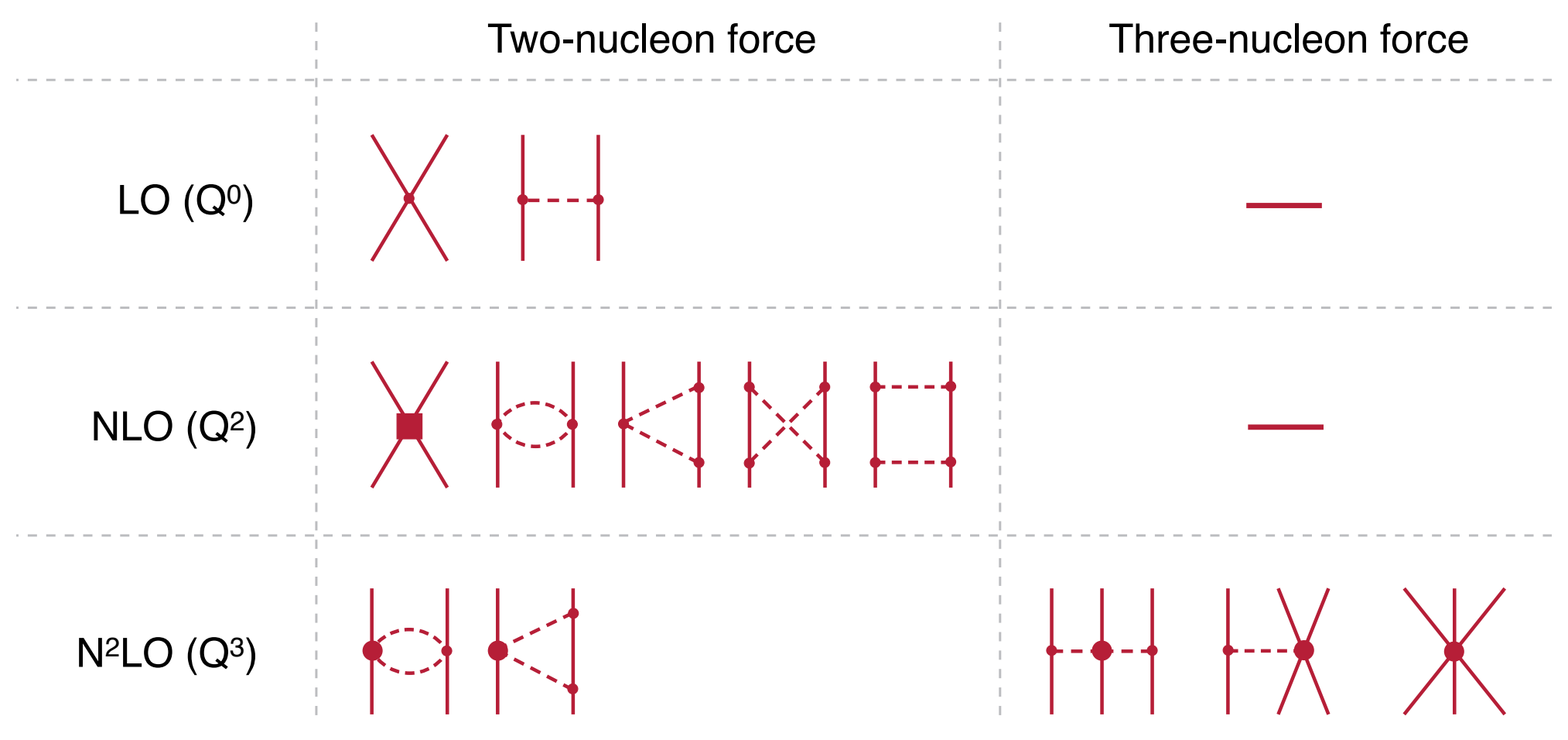
Description of the structure of nuclei as self-bound quantum many-body systems using realistic 2- and 3-body forces between protons and neutrons

$$\hat{\mathbf{H}} \;=\; \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

- Ground state (gs) and excitation energies
- Radii and electromagnetic moments

NUCLEAR INTERACTION

Chiral Effective Field Theory (χEFT) up to next-to-next-to-leading order (N^{2}LO)



- Low-energy constants (LECs) for 2-body potential fitted to NN scattering data [1]
- Two additional LECs for 3-body force fitted to $A = 3$ system [2]

Phenomenological 2-body potential: **Daejon16**

- Based on chiral EFT potential at N^{3}LO
- Off-shell behavior fitted to 10 energy levels from $A = 4$ to $A = 16$ [3]

NO-CORE CI

Solve eigenvalue problem for wave function Ψ

$$\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) \;=\; \lambda\,\Psi(r_1,\ldots,r_A)$$

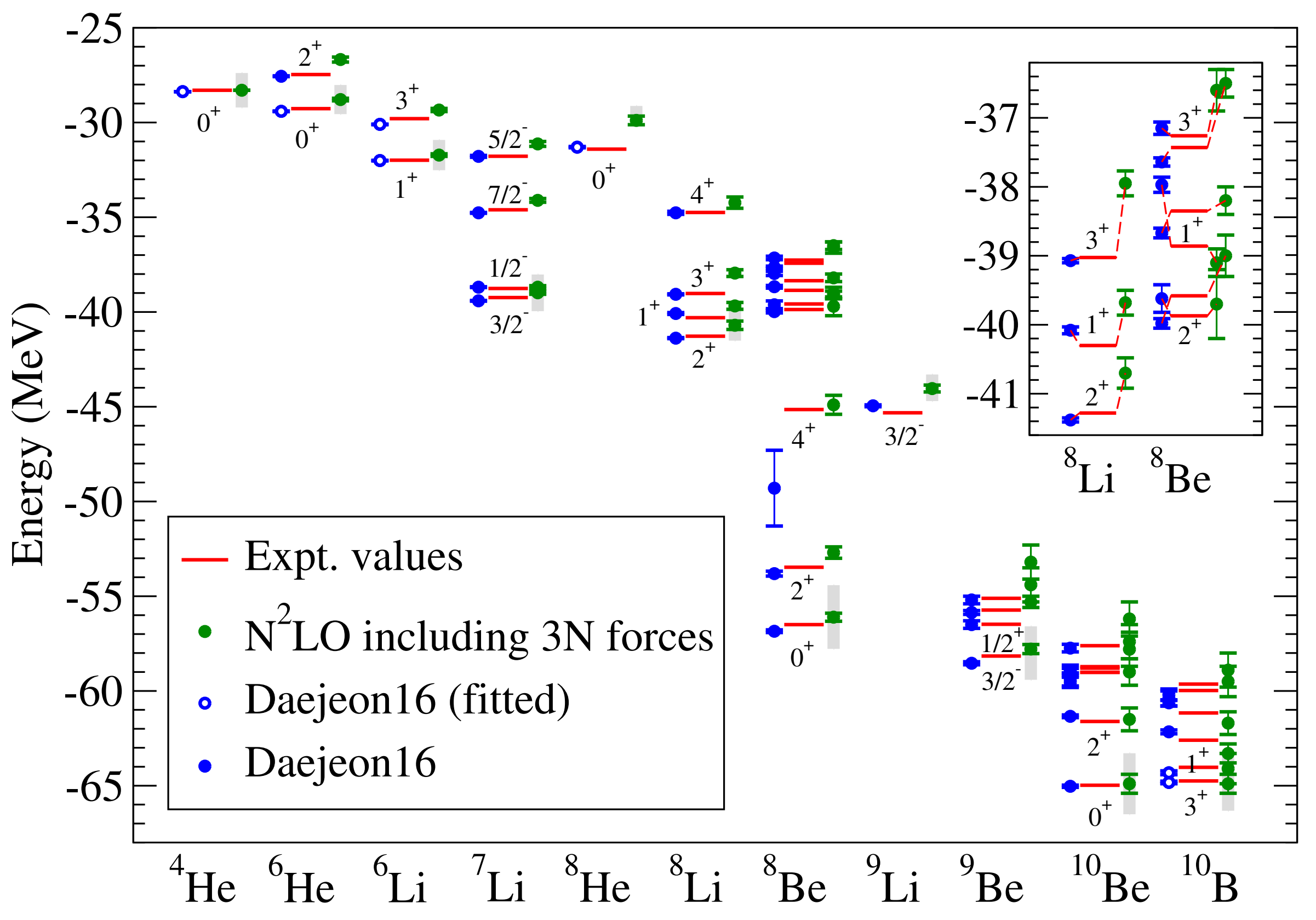
by expanding the A-body wave function Ψ in Slater Determinants of single-particle HO states ϕ

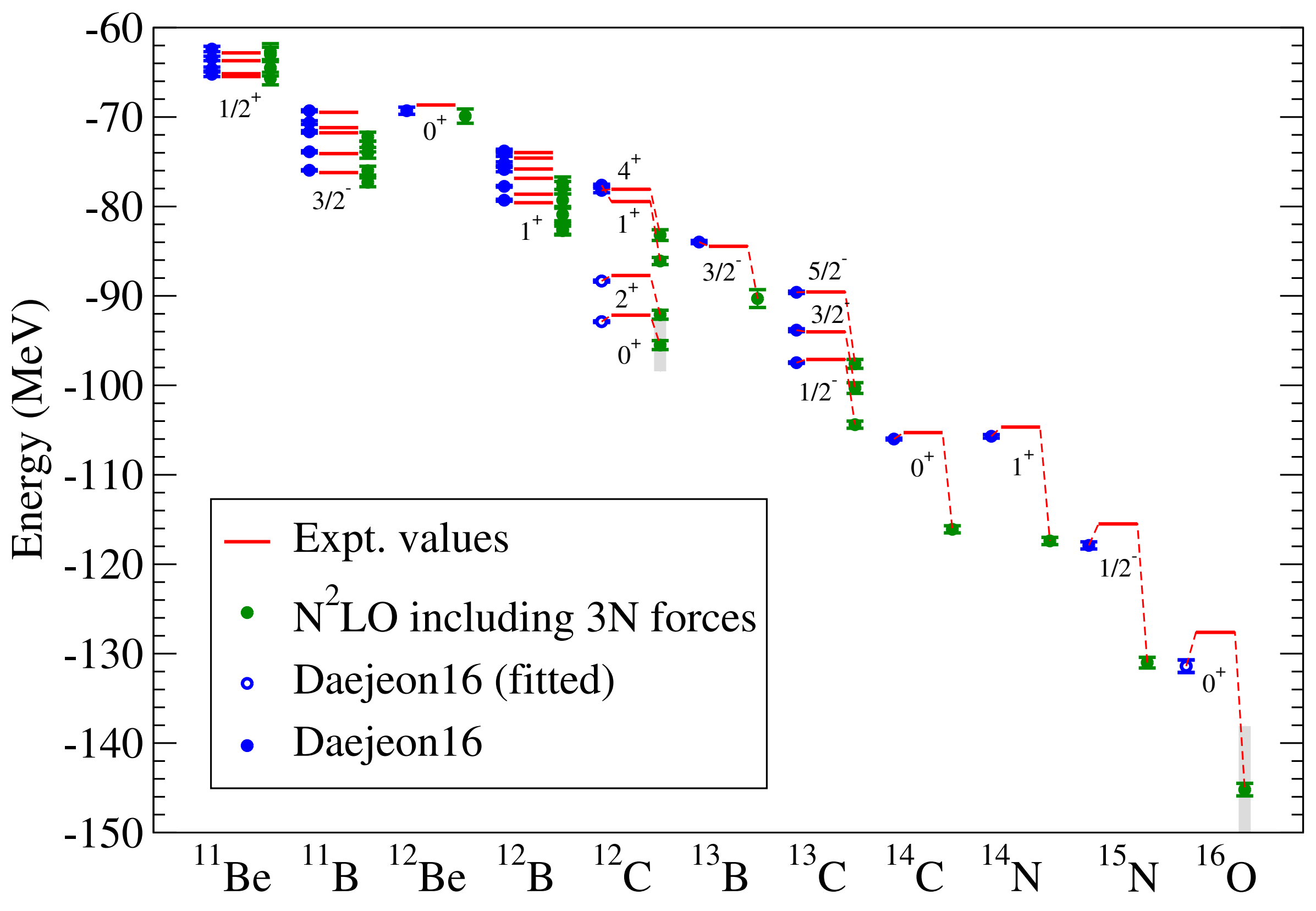
$$\Psi(r_1,\ldots,r_A) \;=\; \sum c_i \Phi_i(r_1,\ldots,r_A)$$

$$\Phi_i(r_1,\ldots,r_A) \;=\; \frac{1}{\sqrt{(A!)}} \begin{vmatrix} \phi_{i1}(r_1) & \ldots & \phi_{iA}(r_1) \\ \vdots & \ddots & \vdots \\ \phi_{i1}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

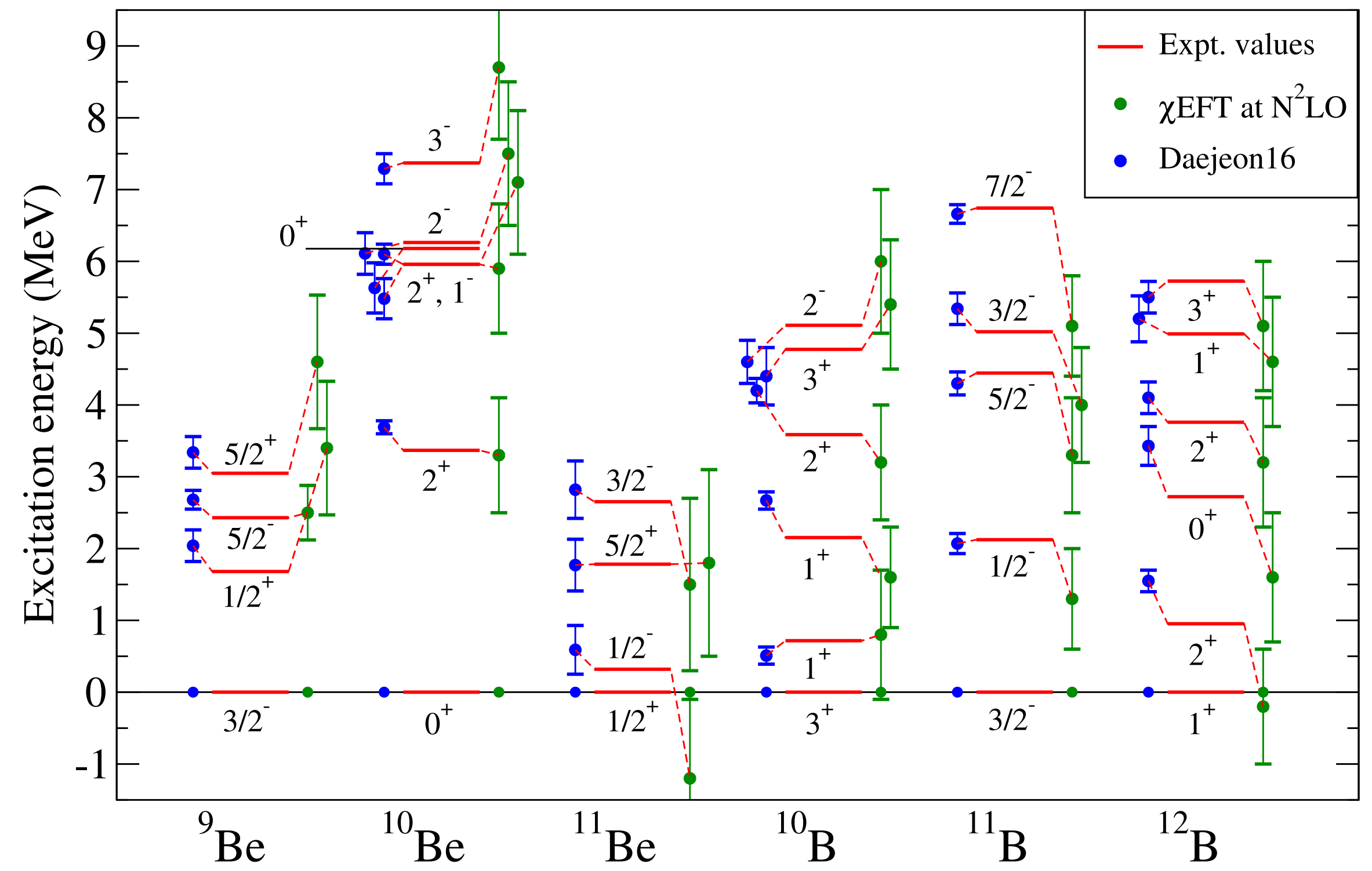
- Truncate on total number of HO excitations, such that Center-of-Mass motion factorizes
- Calculate physical observables $\langle \Psi_f | \hat{\mathcal{O}} | \Psi_i \rangle$
- Increase basis until observables converge

RESULTS FOR ENERGY LEVELS [4]



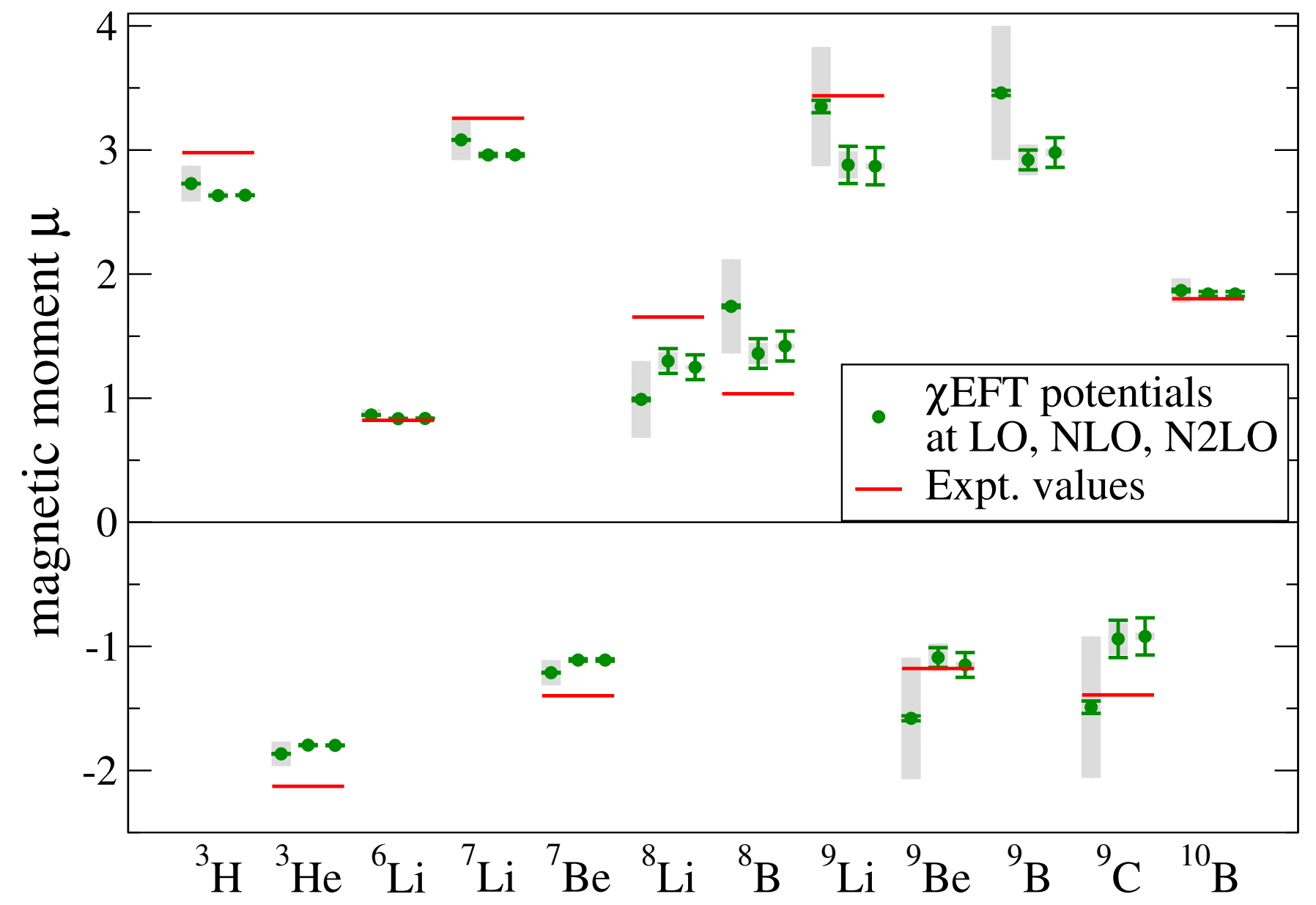


- Energies extrapolated to complete basis (see poster by J.P. Vary using ANN for extrapolation)
- χEFT: gs energies within chiral truncation error estimate (grey bands) through $A = 12$, but ^{16}O is significantly overbound [2]
- **Daejon16**: good agreement for gs energies through $A = 14$, but ^{16}O slightly overbound
- Excitation energies: difference of extrapolated energies
- Natural parity spectra in agreement with experiment up to at least $A = 12$
- Unnatural parity states too high with χEFT, but well-described by **Daejon16**



MAGNETIC MOMENTS [1]

Results with LO, NLO, and N^{2}LO potentials using LO M1 operator, with chiral truncation estimates



- Without χEFT corrections to M1 operator, nearly converged in chiral expansion
- No such corrections up to N^{2}LO for isospin T=0 states ^{6}Li and ^{10}B, which agree with data
- Discrepancy with data for T > 0 states consistent with estimates of meson-exchange contributions to M1 operator at N^{2}LO

CONCLUSIONS

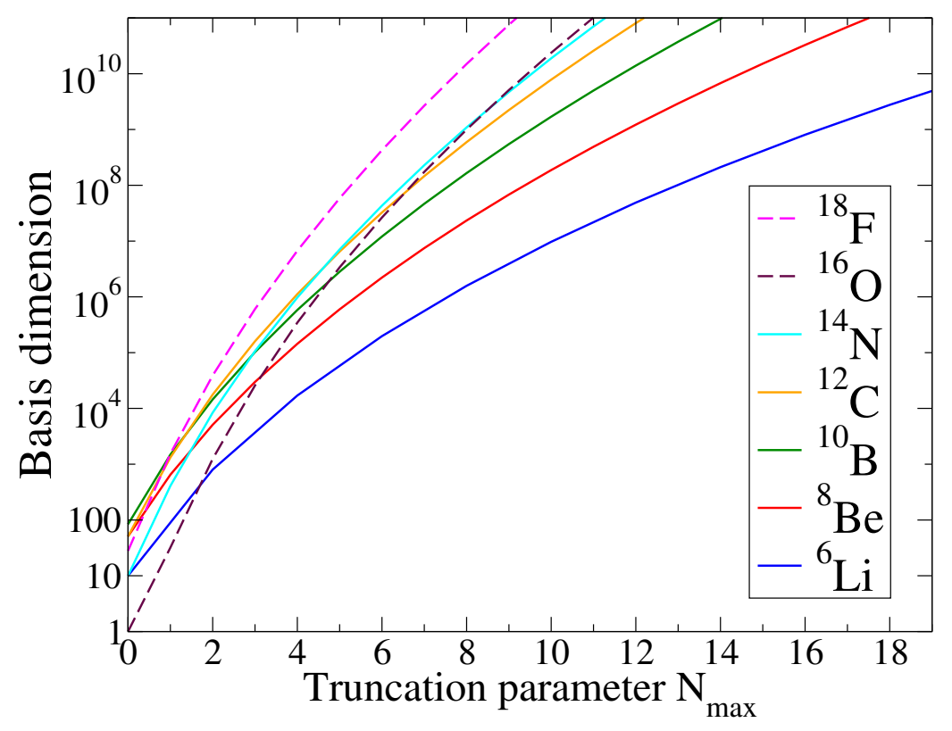
- Good description of more than 70 states, excluding isobaric analog states
- Agreement with data improves noticably when select many-body input is used in determining the nuclear interaction
- χEFT potential fitted to $A = 2$ and 3 only agreement with data decreases for $A \geq 12$
- **Daejon16** fitted to 10 energy levels in p-shell gives better agreement above $A = 12$ and for unnatural parity states

WORK IN PROGRESS

- Improved, higher-order χEFT interactions
- Consistent electroweak operators
- Electroweak transitions, including (neutrinoless) double-β decay
- Heavier nuclei using effective Shell Model interactions based on NCCI calculations for $A = 17$ and 18 nuclei

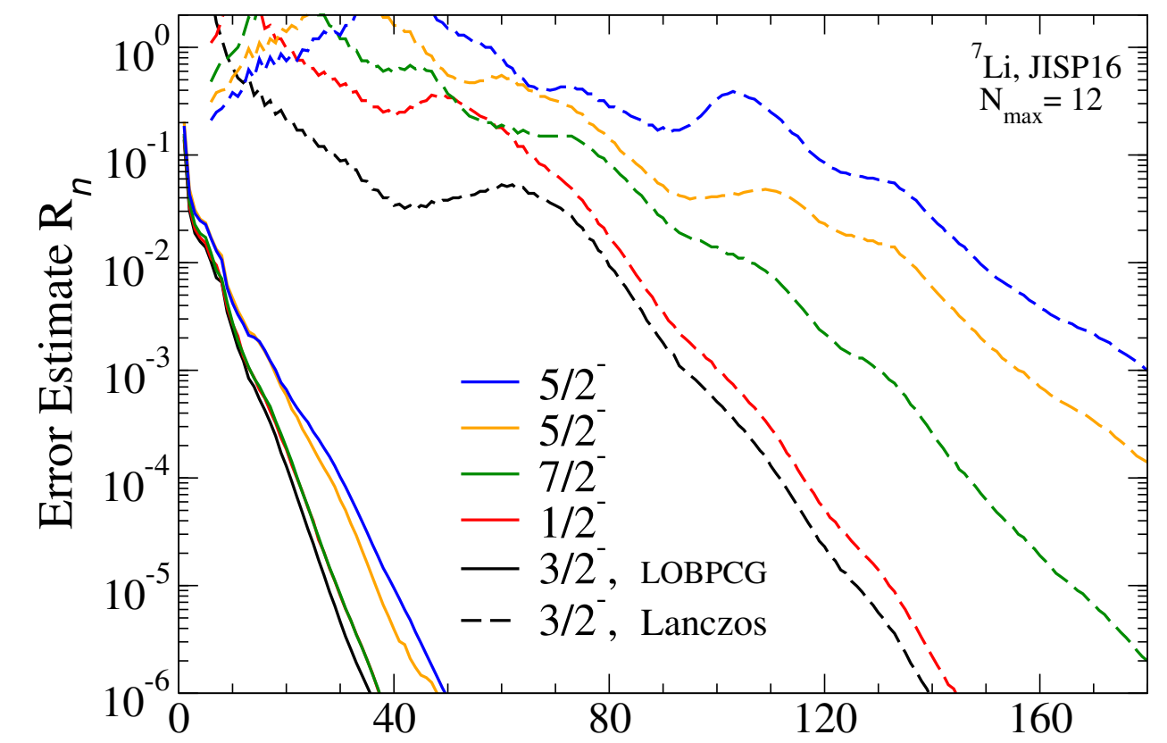
COMPUTATIONAL CHALLENGES

Eigenvalue problem for large sparse matrix. Convergence of energies, radii, moments, decays, etc, require dimensions well over 10^{10}.



ITERATIVE SOLVER [5]

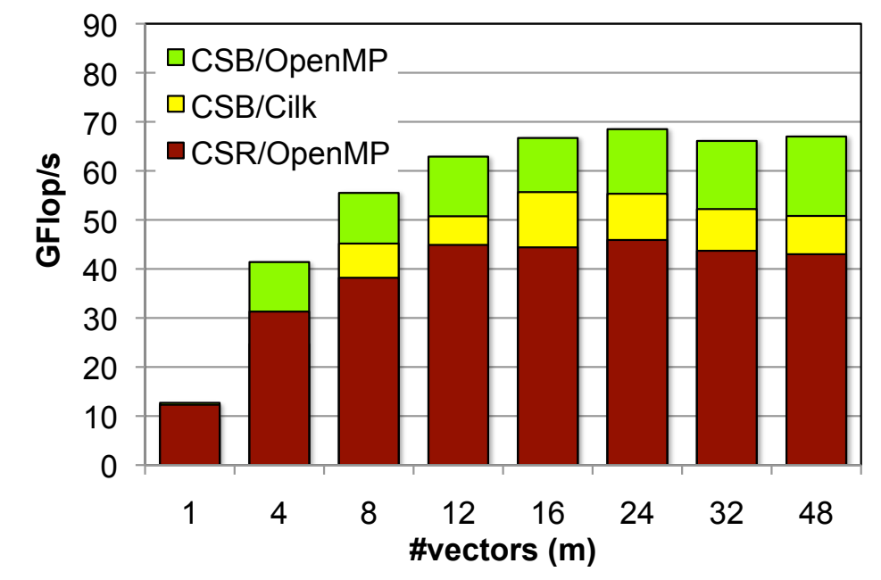
Locally Optimized Block Preconditioned Conjugate Gradient (LOBPCG): SpMV acting on block of vectors, which improves cache performance, allows for vectorization, and needs significantly less iterations compared to Lanczos algorithm

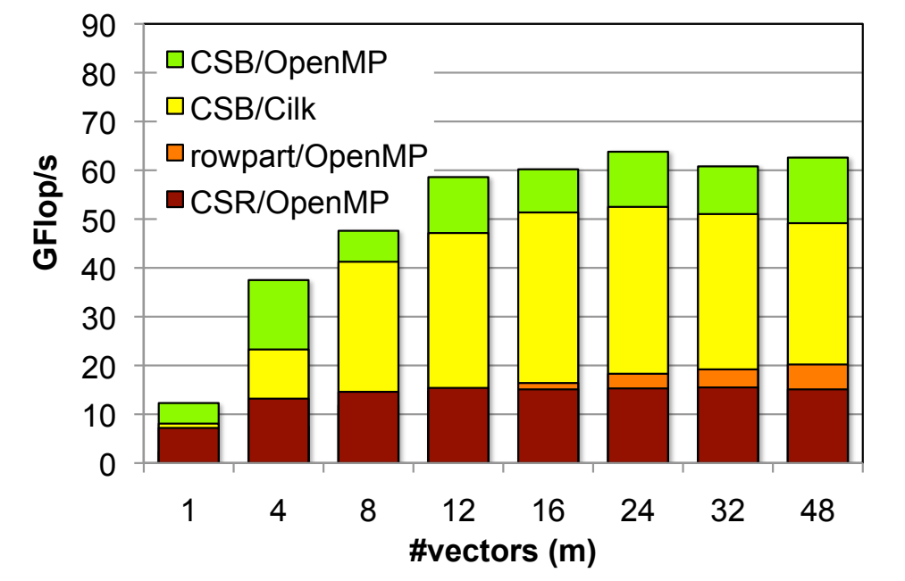


- SpMV most time-consuming kernel
- Memory bound
- Use only half of symmetric matrix for both SpMV and SpMV$^\mathrm{T}$

DISTRIBUTED SPMV/SPMM [6]

- Compressed Sparse Row works okay for SpMV (left), but inefficient for SpMV$^\mathrm{T}$ (right) in hybrid MPI/OpenMP applications
- Compressed Sparse Block improves data locality, and allows for efficient OpenMP parallelization of both SpMV and SpMV$^\mathrm{T}$





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