Coupled-cluster effective interactions for nuclei

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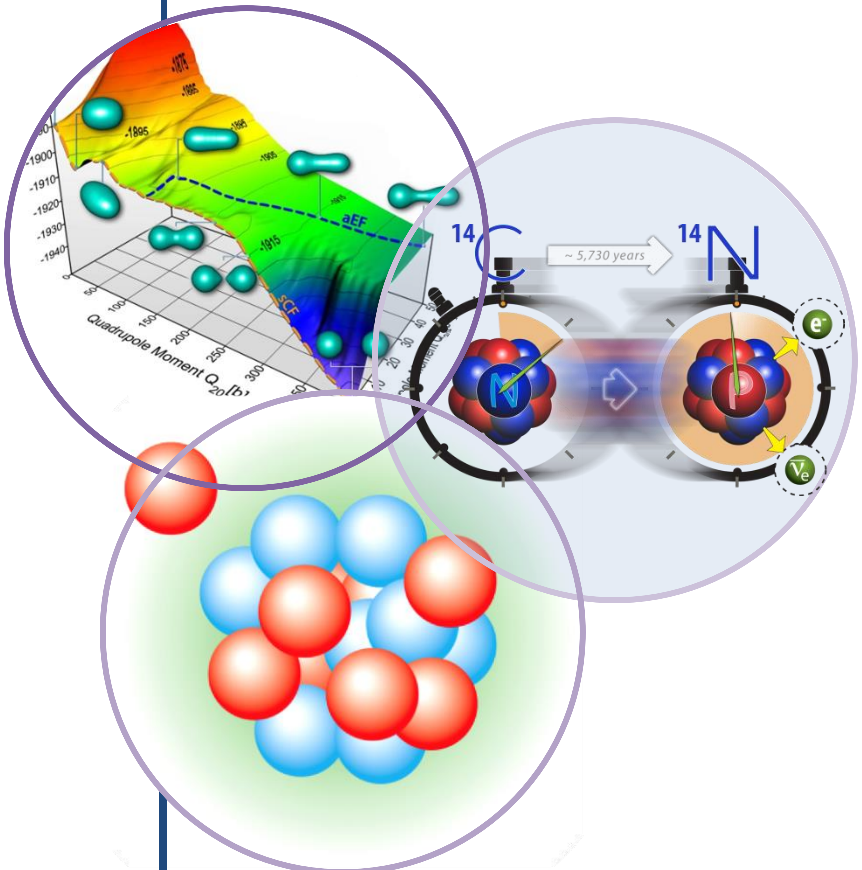


ESNT workshop, April 2, 2015

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

BSF
United States – Israel
Binational Science Foundation

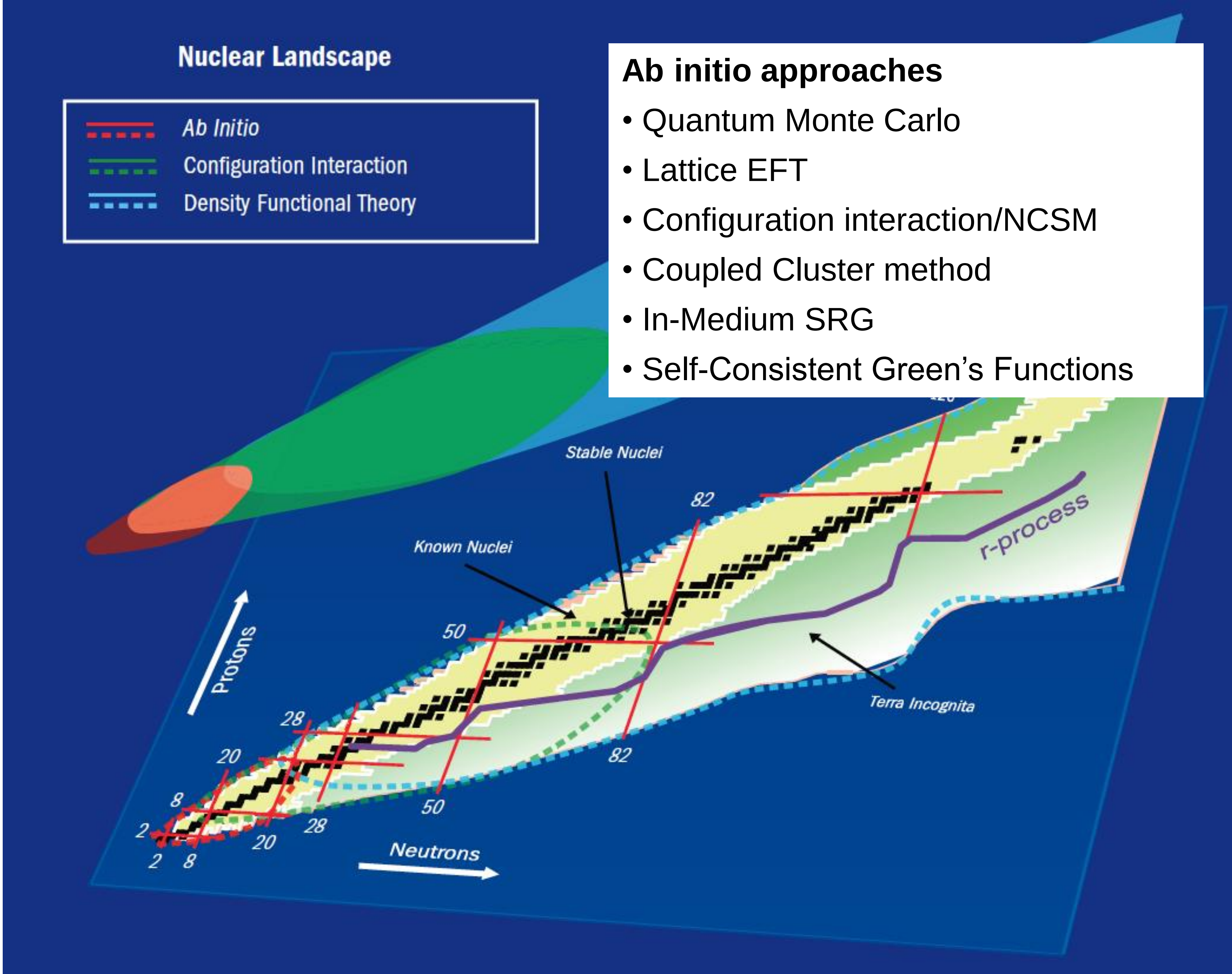
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

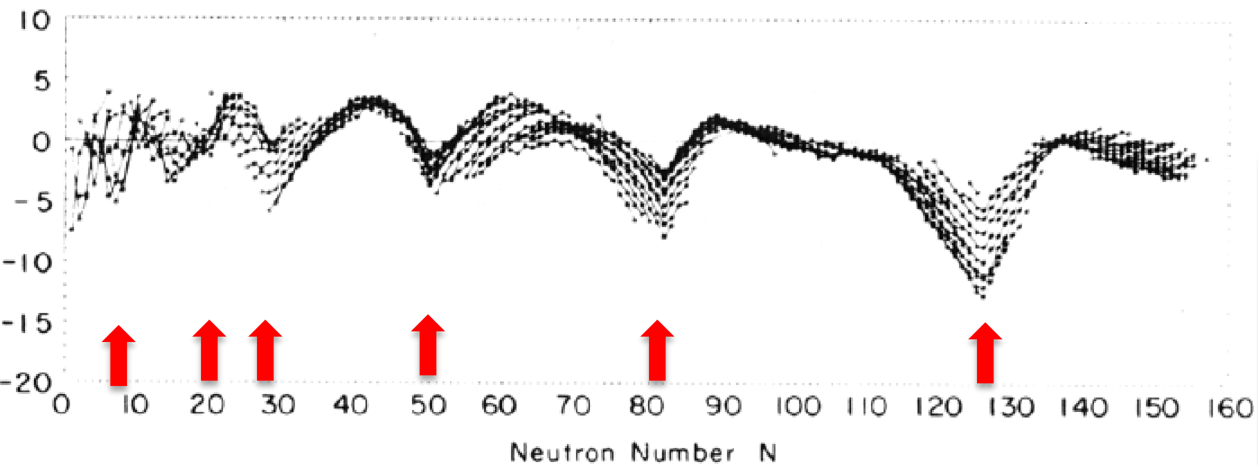
- The nuclear landscape and many-body methods
- Observation of shell structure in nuclei a paradigm for nuclear theory
- Connecting the traditional shell model (configuration interaction) with ab-initio theory.
- Coupled-cluster effective interactions (CCEI) for the shell model
- Description of neutron oxygen and carbon isotopes
- Extending CCEI to describe nuclei with protons and neutrons in the valence space.

Ab initio approaches

- Quantum Monte Carlo
- Lattice EFT
- Configuration interaction/NCSM
- Coupled Cluster method
- In-Medium SRG
- Self-Consistent Green’s Functions

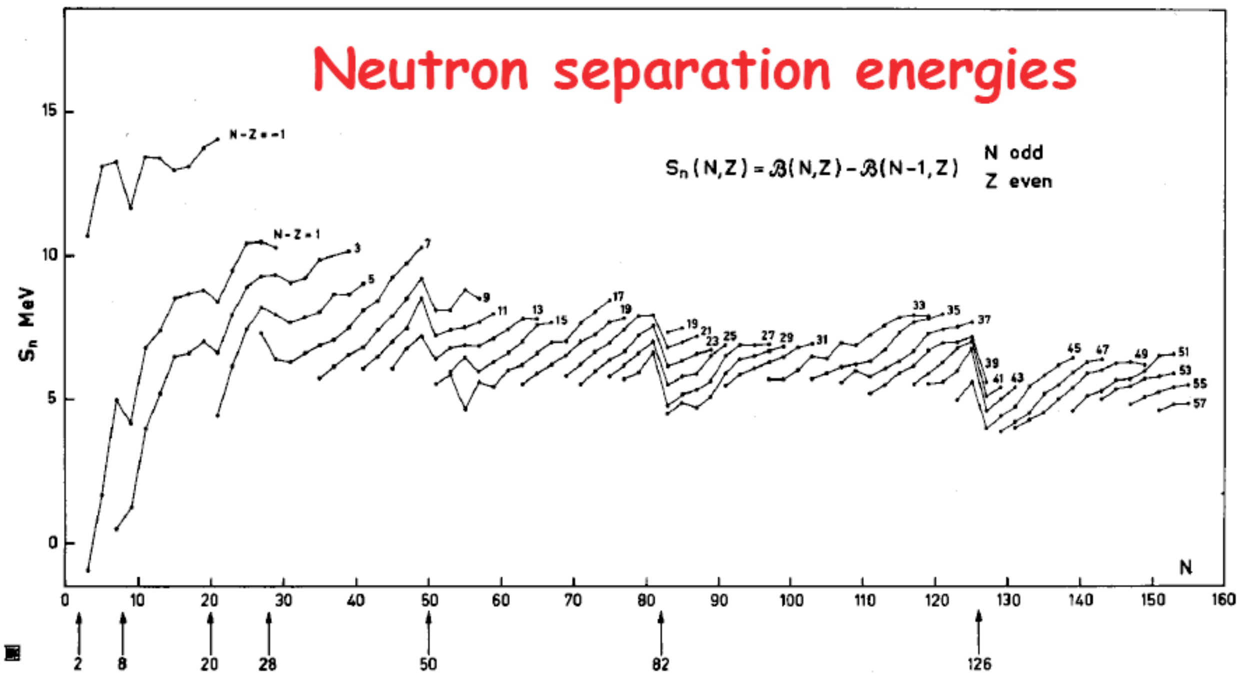


Shell structure in nuclei



From W.D. Meyers and W.J. Swiatecki, Nucl. Phys. 81, 1 (1966).

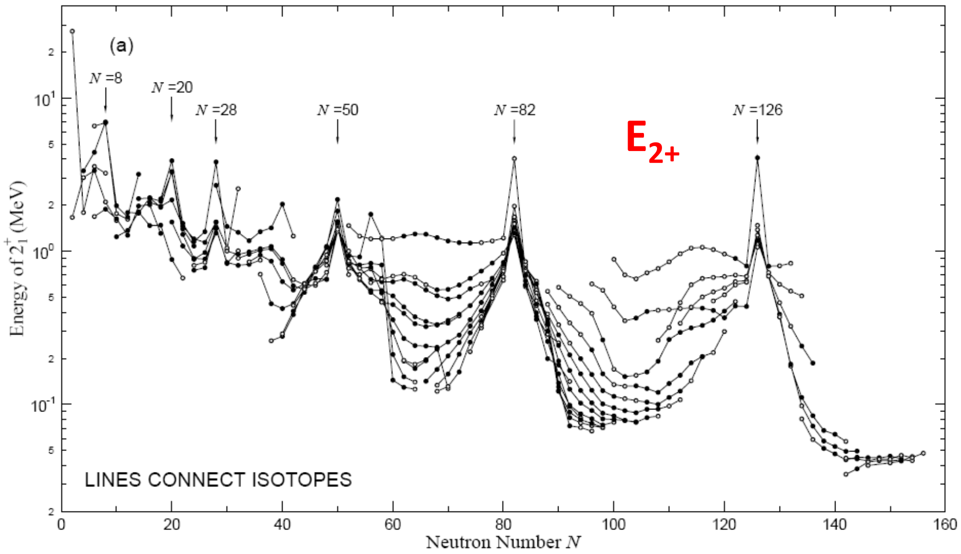
Mass differences: Liquid drop – experiment. Minima at closed shells.

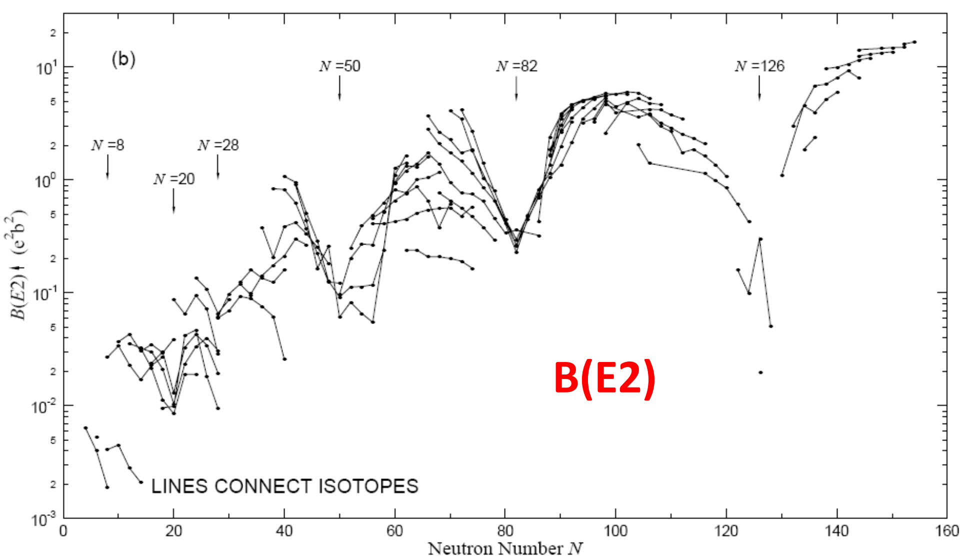


- Expensive to remove a neutron form a closed neutron shell.
- Signature of magic shell closures for N=2, 8, 20, 28, 50, 82, 128

Bohr & Mottelson, Nuclear Structure.

Shell structure in nuclei

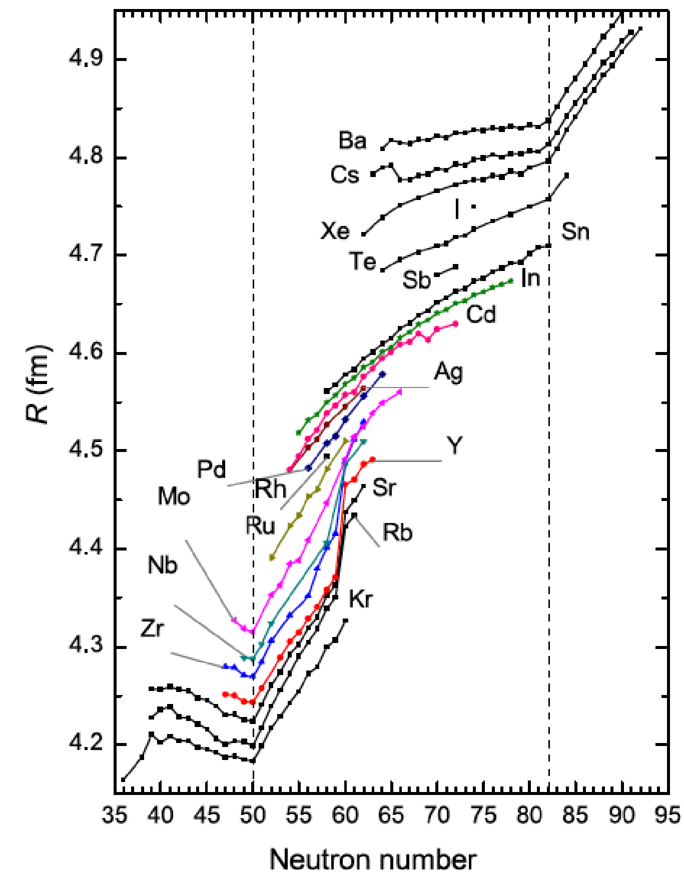




S. Raman et al, Atomic Data and Nuclear Data Tables 78 (2001) 1.

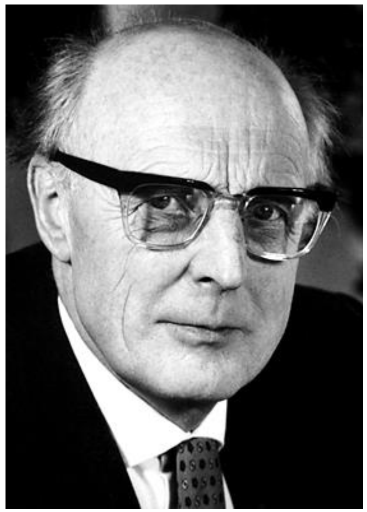
Nuclei with magic N :

- Large separation energies
- High-lying first 2^+ exited state
- Low B(E2) transition strength
- Kink/drop in charge radii



Magic numbers: 2, 8 20, 28, 50,82…

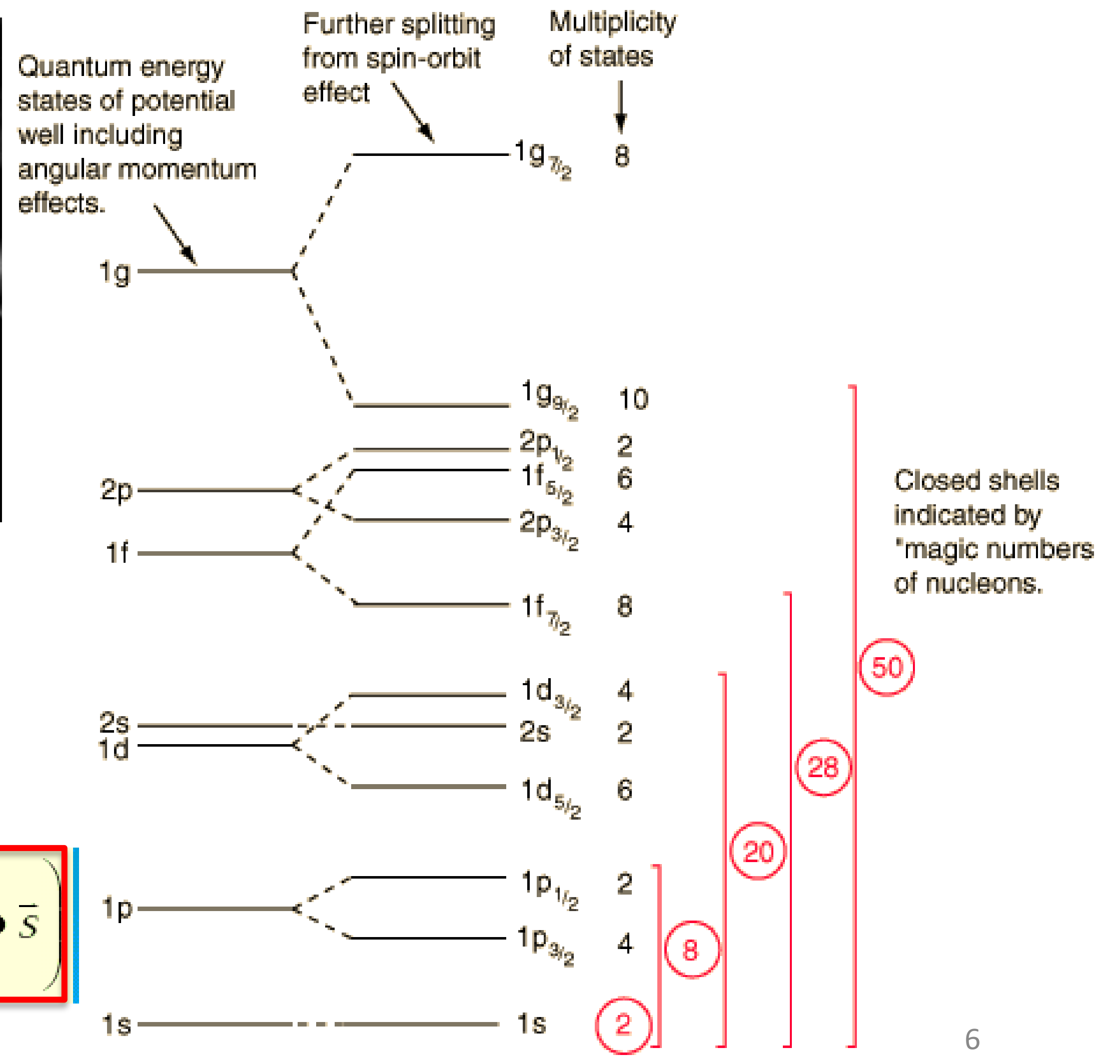
Nobel Prize 1963



Goeppert-Mayer **Jensen**

Need spin-orbit force to explain magic numbers beyond 20.

$$H_{SM} = \sum_{i=1}^{A} \left(\frac{\hbar^2}{2M} \nabla^2 + \frac{m}{2} \omega^2 r^2 + \eta_l \vec{l}^{\,2} + \xi_{ls} \vec{l} \bullet \vec{s} \right)$$



Traditional shell model

Main idea: Use shell gaps as a truncation of the model space.

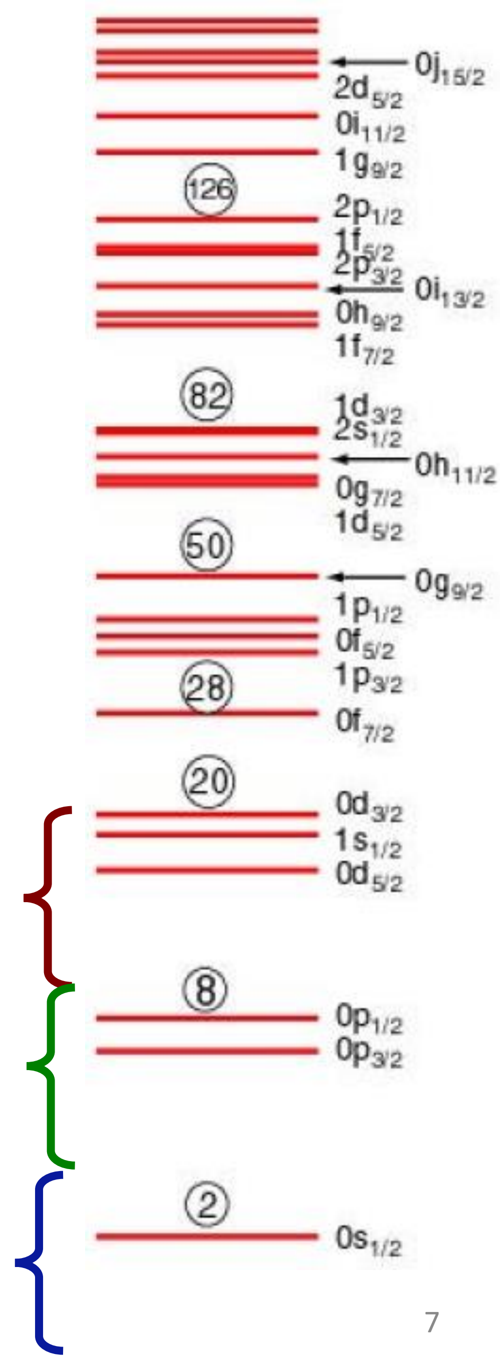
Nucleus (N,Z) = Double magic nucleus (N^*,Z^*) + valence nucleons ($N-N^*$, $Z-Z^*$)

Restrict excitation of valence nucleons to one oscillator shell.
Problematic: Intruder states and core excitations not contained in model space.

Examples:
pf-shell nuclei: ^{40}Ca is doubly magic

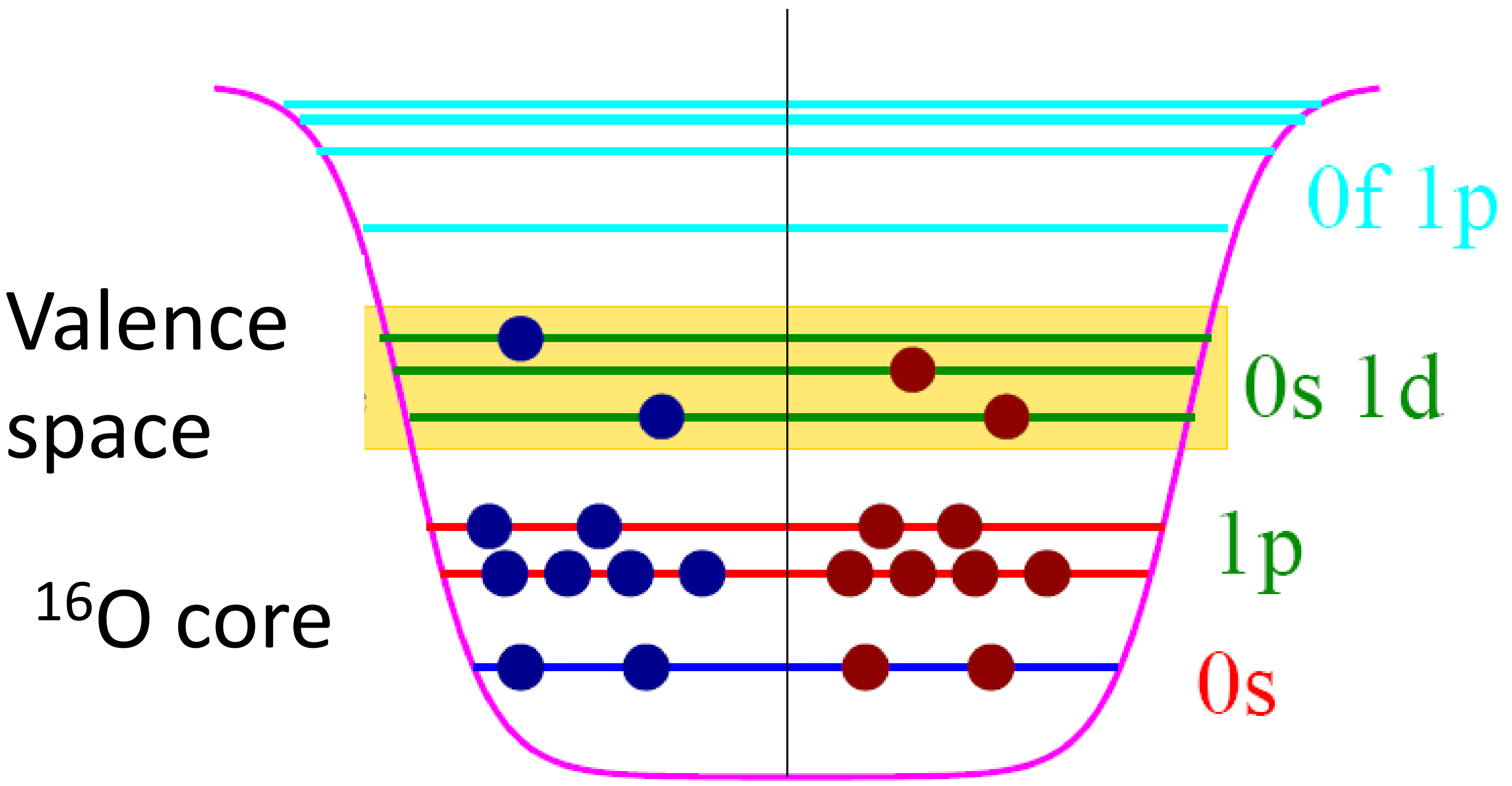
sd-shell nuclei: ^{16}O is doubly magic

p-shell nuclei: ^{4}He is doubly magic



Traditional shell model

Example: ^{20}Ne



Shell model Hamiltonian

Hamiltonian governs dynamics of valence nucleons; consists of one-body part and two-body interaction (three-body +…) :

$$\hat{H} = \sum_j \varepsilon_j \hat{a}_j^\dagger \hat{a}_j + \sum_{JTj_1j_2j_1'j_2'} \langle j_1 j_2 | \hat{V} | j_1' j_2' \rangle_{JT} \hat{A}^\dagger_{JT;j_1j_2} \hat{A}_{JT;j_1'j_2'}$$

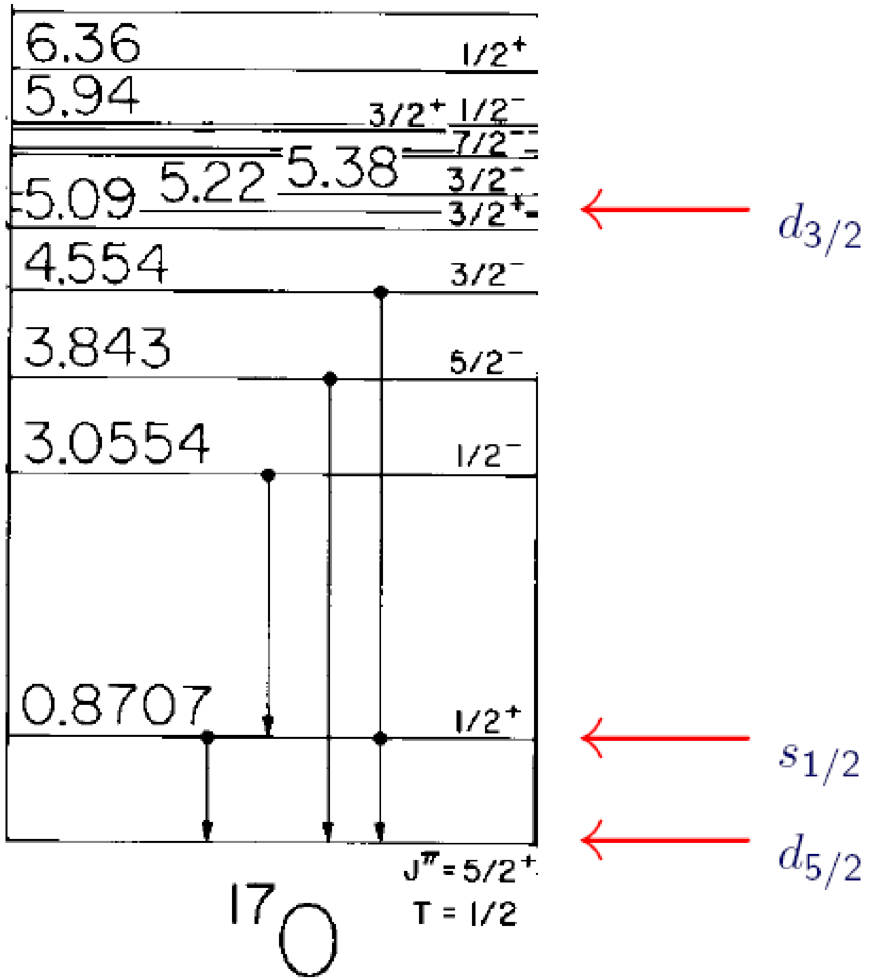
Single-particle energies (SPE)

Two-body matrix elements (TBME)
coupled to good spin and isospin

Annihilates pair of fermions

How does one determine the single-particle energies (SPE) and two-body matrix elements (TBME)?

Empirical determination of SPE and TBME



Determine SPE from neighbors of closed shell nuclei (A) having mass A +1

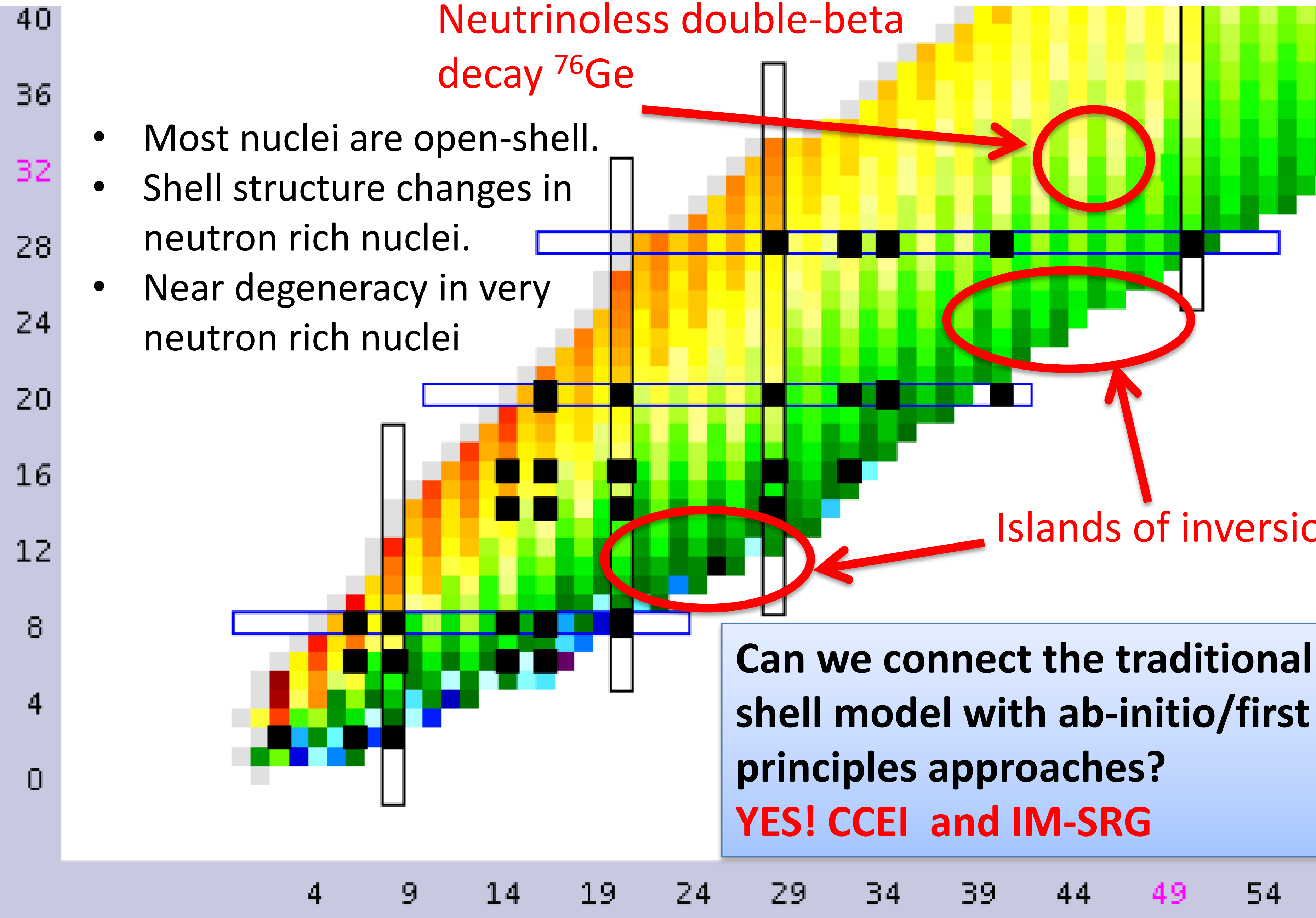
Determine TBME from fit to empirical data (e.g. excited states, transition rates)

Accurate description of nuclei in the area of the nuclear chart where they were fitted.

How to make accurate predictions for nuclei beyond the range of where the TBME were fitted?

Single reference coupled cluster theory

- Most nuclei are open-shell.
- Shell structure changes in neutron rich nuclei.
- Near degeneracy in very neutron rich nuclei



Can we connect the traditional shell model with ab-initio/first principles approaches?

YES! CCEI and IM-SRG

Valence cluster expansion: connecting ab-initio approach with the shell-model

P. Navratil et al, PRC 55, 573 (1997)
A. Lisetskiy et al. ,PRC 78, 044302 (2008), PRC 80, 023315 (2009)

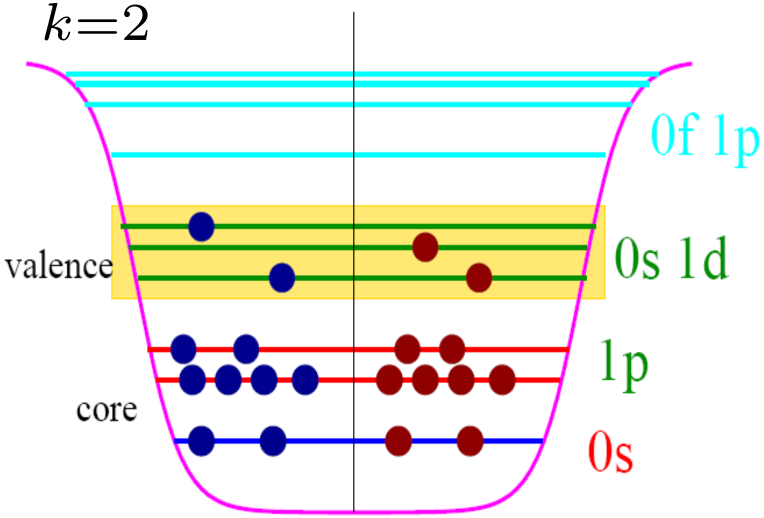
We start from the intrinsic Hamiltonian with NN and 3N forces:

$$H = \sum_{i<j} \left(\frac{(\mathbf{p}_i - \mathbf{p}_j)}{2mA} + V_{NN}^{(i,j)} \right) + \sum_{i<j<k} V_{3\mathrm{N}}^{(i,j,k)}$$

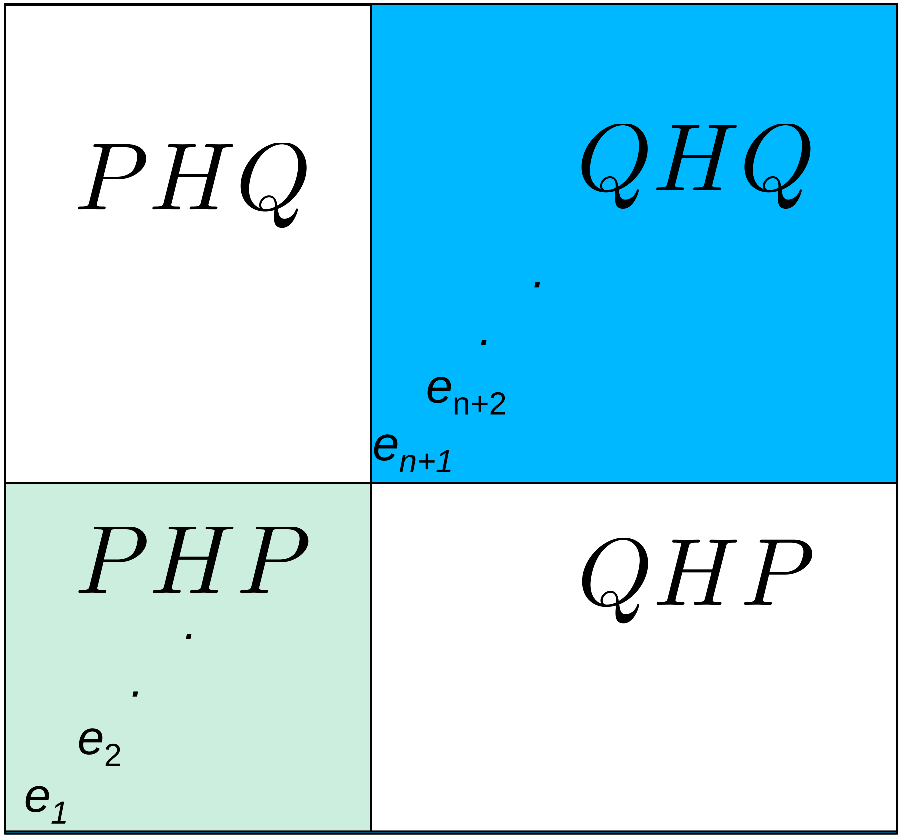
Write the intrinsic Hamiltonian as a valence cluster expansion:

$$H^A = H^{A,A_c} + H^{A,A_c+1} + \sum_{k=2}^{a_v} H^{A,A_c+k}$$

- Need to solve for the core (A_c), and the A_c+1, A_c+2,… neighboring nuclei.
- Project the A_c+1, A_c+2, … wavefunctions onto the valence space via a similarity transformation to obtain an effective Hamiltonian



Effective interactions from similarity transformations



- Define a model space *P* and complement space *Q*
- Construct a similarity transformation such that

$$Q(X^{-1}HX)P = 0$$

- This defines an effective Hamiltonian in the *P*-space which exactly reproduces *n* eigenvalues of the full Hamiltonian:

$$P\left(X^{-1}HX\right)P|\psi_k^{\text{eff}}\rangle = e_k|\psi_k^{\text{eff}}\rangle$$

Bloch-Brandow effective interaction (Lee-Suzuki similarity transformation)

Write the effective Hamiltonian in spectral representation which reproduces *d* eigenvalues of the full Hamiltonian:

$$\langle \alpha_P | H_{\text{eff}} | \alpha_{P'} \rangle = \sum_{k=1}^{d} \langle \alpha_P | \psi_k^{\text{eff}} \rangle e_k \langle \tilde{\psi}_k^{\text{eff}} | \alpha_{P'} \rangle$$

Effective eigenvectors are defined as (Bloch-Brandow):

$$|\psi_k^{\text{eff}}\rangle \equiv P|\Psi_k\rangle$$

This gives the effective Hamiltonian in the *P* space:

$$\langle \alpha_P | H_{\text{eff}} | \alpha_{P'} \rangle_{LS} = \sum_{k=1}^{d} \langle \alpha_P | \Psi_k \rangle e_k \overline{\langle \alpha_{P'} | \Psi_k \rangle}$$

Where $\overline{\langle \alpha_P | \Psi_k \rangle}$ are the matrix elements of the inverse of the matrix *U* with matrix elements: $U_{pk} = \langle \alpha_P | \Psi_k \rangle$

Coupled cluster effective interaction

Solve for the A_c+2 problems via two-particle attached equation-of-motion coupled-cluster (Talks by P. Piecuch and G. Jansen)

$$\overline{H} R_\mu^{A_c+2} |\Phi_0\rangle = \omega_\mu R_\mu^{A_c+2} |\Phi_0\rangle$$

$$\langle \Phi_0 | L_\mu^{A_c+2} \overline{H} = \omega_\mu \langle \Phi_0 | L_\mu^{A_c+2}$$

To obtain H_{eff} we can either project the left or the right solutions onto the P-space:

$$|\psi_k^{\text{eff}}\rangle \equiv P|R^{A,A_c+2}\rangle$$

Using the right eigenvector projections we obtain CCEI:

$$\langle \alpha_P | \overline{H}_{\text{eff}}^{A,A_c+2} | \alpha_{P'} \rangle = \sum_{k=1}^{d} \langle \alpha_P | R_k^{A,A_c+2} \rangle e_k \overline{\langle \alpha_{P'} | R_k^{A,A_c+2} \rangle}$$

We can hermitize H_{CCEI} by symmetric orthogonalization procedure (I. Mayer Int. J. Quantum Chem 90, 63 (2002))

$$\left[S^\dagger S \right]^{1/2} \overline{H}_{\text{CCEI}}^{A} \left[S^\dagger S \right]^{-1/2}$$

Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al.*; Entem & Machleidt; ⋯]

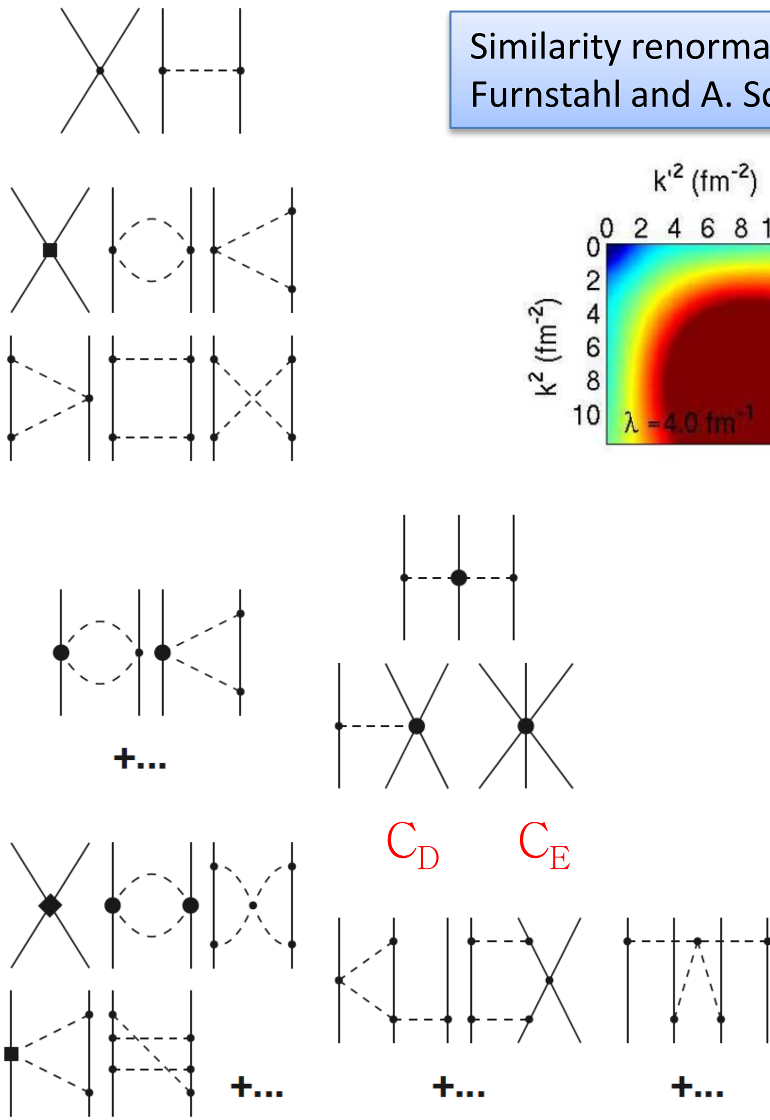
2N Force **3N Force** **4N Force**

Q^0 LO

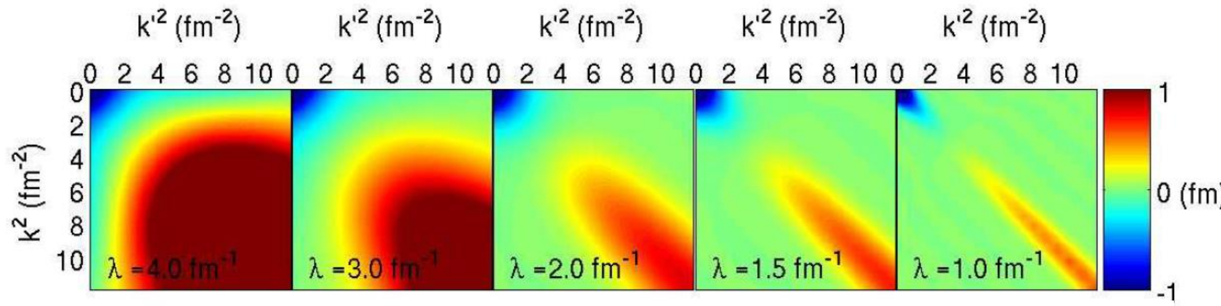
Q^2 NLO

Q^3 NNLO

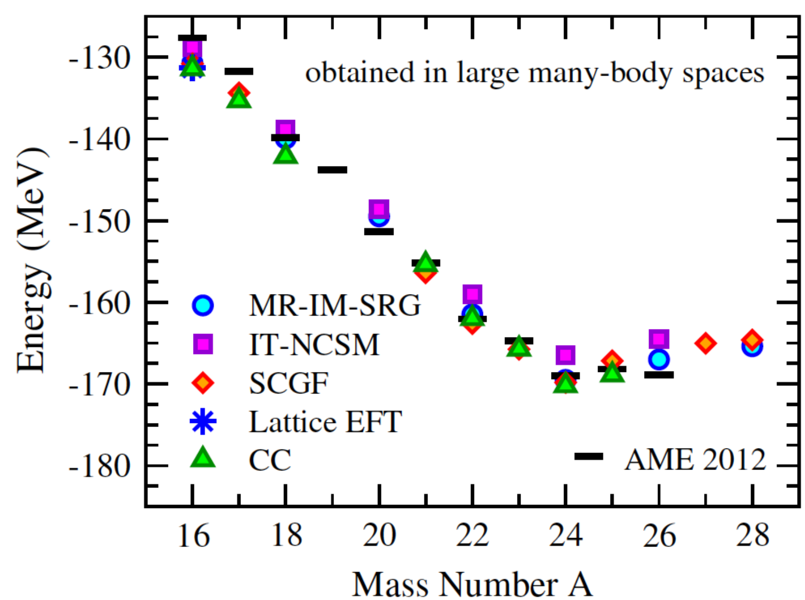
Q^4 N^3LO



Similarity renormalization group for nuclear forces: S. Bogner, R. J. Furnstahl and A. Schwenk Prog. Part. Nucl. Phys. 65, 94 (2010)

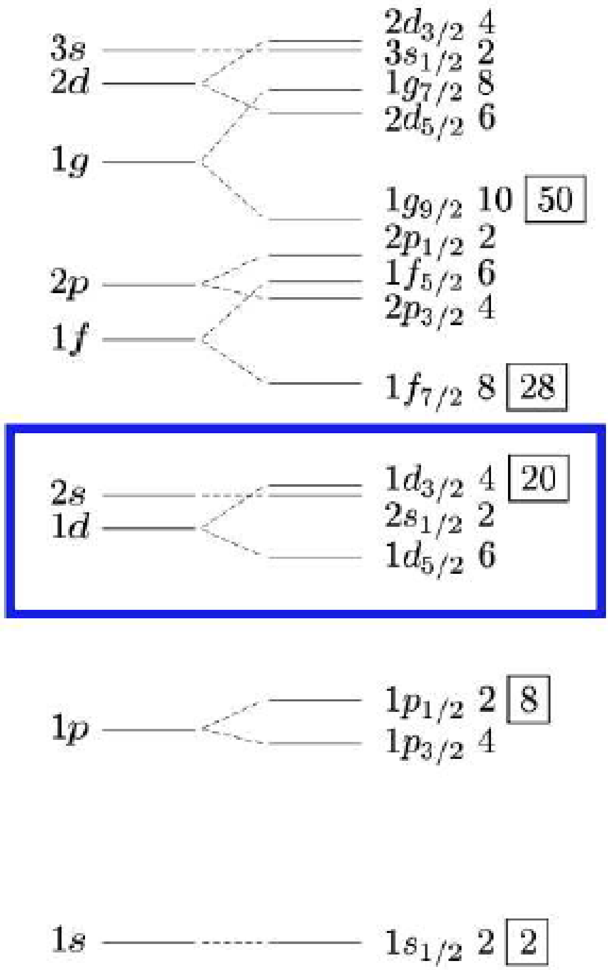


Hebeler, Holt, Menendez, Schwenk, Ann. Rev. Nucl. Part. Sci. in press (2015)



Coupled-cluster effective interaction in practice

- Obtain excited states of A_c+ 1 and A_c+ 2 from **PA-EOMCCSD(2p1h)** and **2PA-EOMCCSD(3p1h)**
- The A_c+1 Hamiltonian is diagonal and given by the A_c+1 lowest eigenvalues
- Are results sensitive to the choice of left/right eigenvector projections for *A*+2?
- How do we choose the *d* “exact” *A*+2 wavefunctions?
  - ➢ Largest overlap with model space
  - ➢ Lowest energies

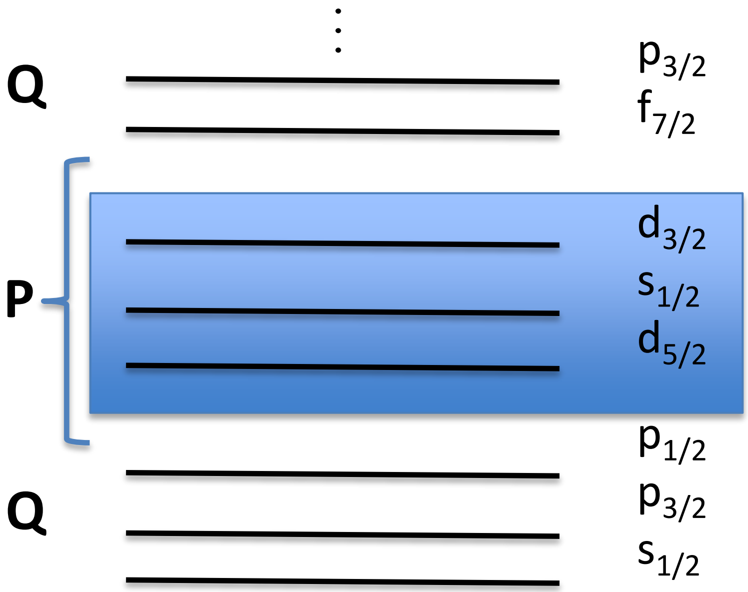


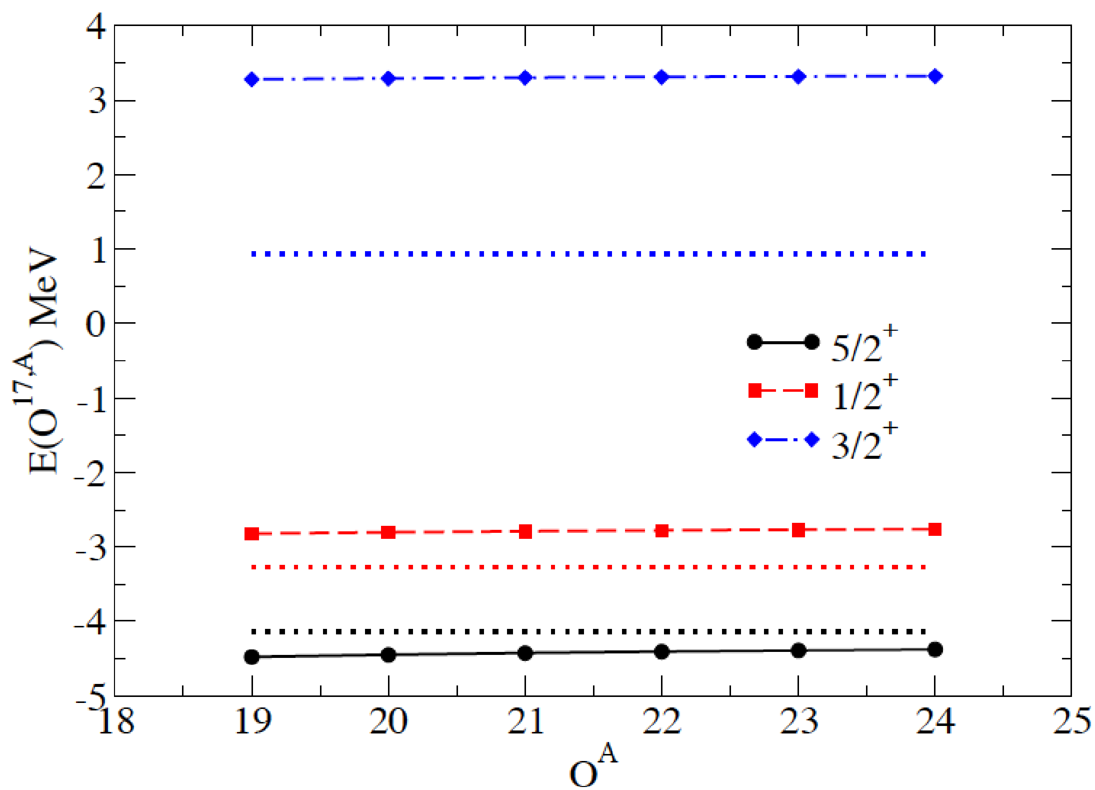
CCEI: Application to the oxygen chain

G. R. Jansen, J. Engel, G. Hagen, P. Navratil, A. Signoracci, PRL **113**, 142502 (2014).

- Start from chiral NN(N3LO$_{EM}$) + 3NF(N2LO) interactions SRG evolved to 2.0fm^{-1}
- Model space size N_{max} = E_{3max} = 12, hw = 20MeV

Low-lying states in ^{17}O as a function of *A*. These energies defines the single-particle energies of H_{eff}





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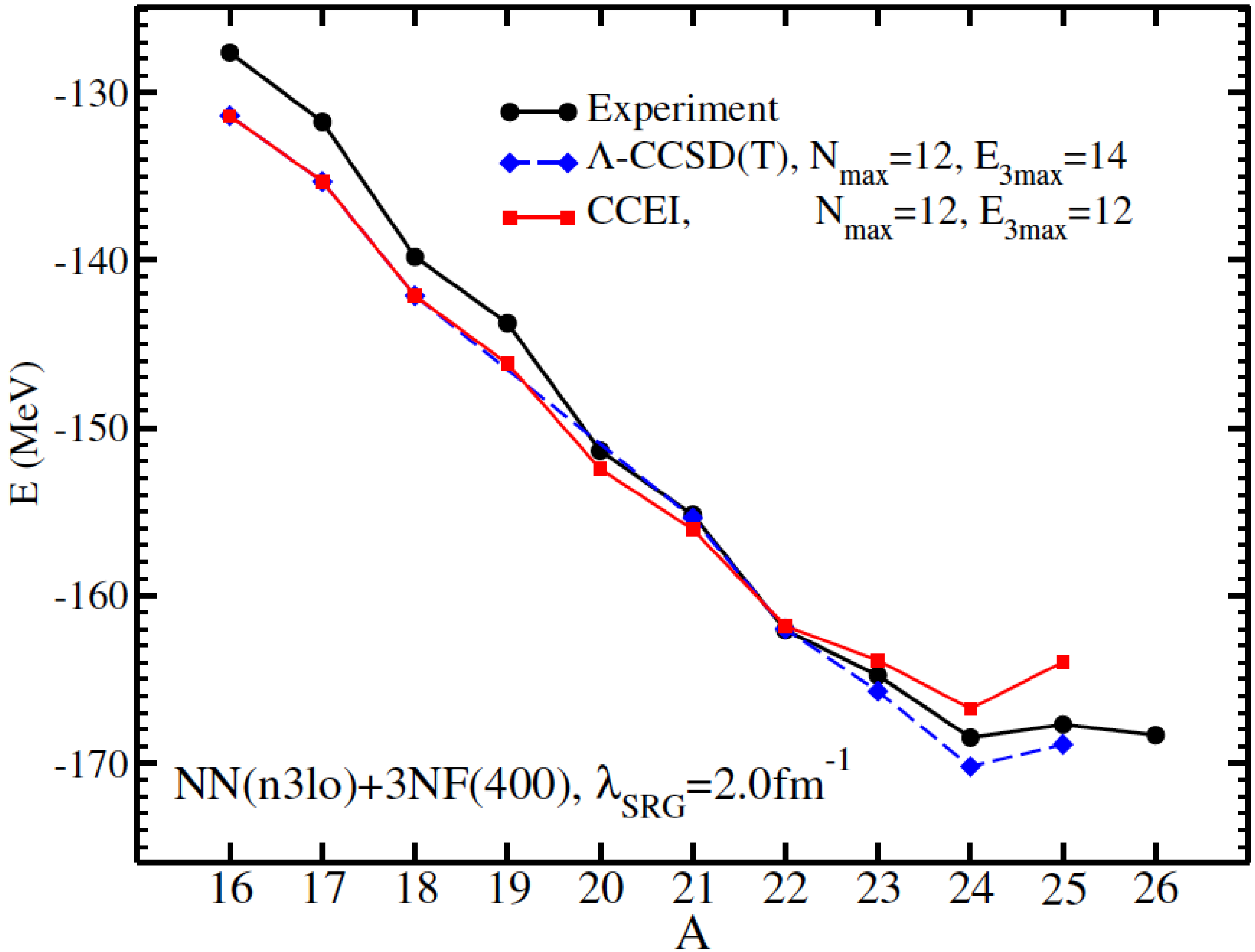
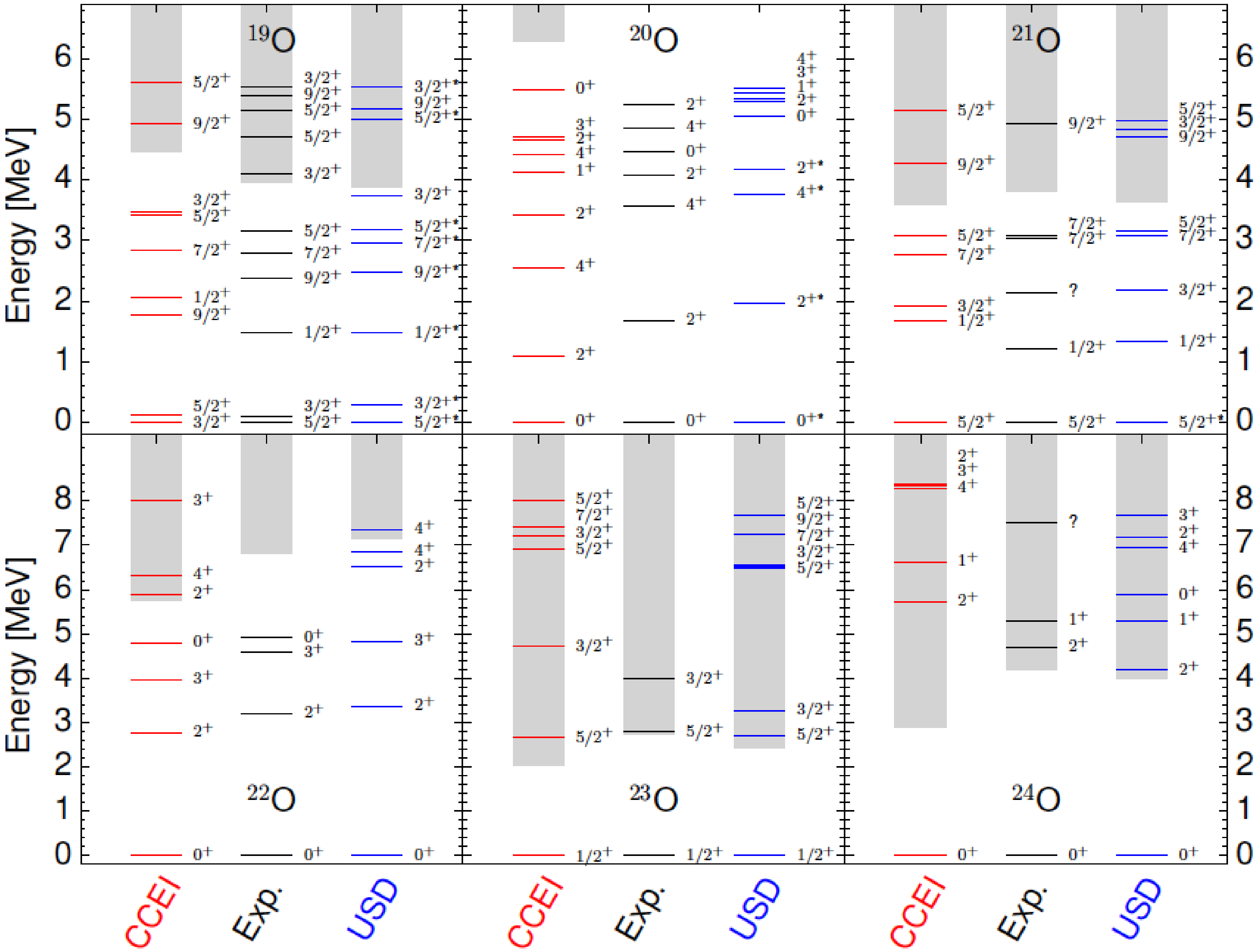
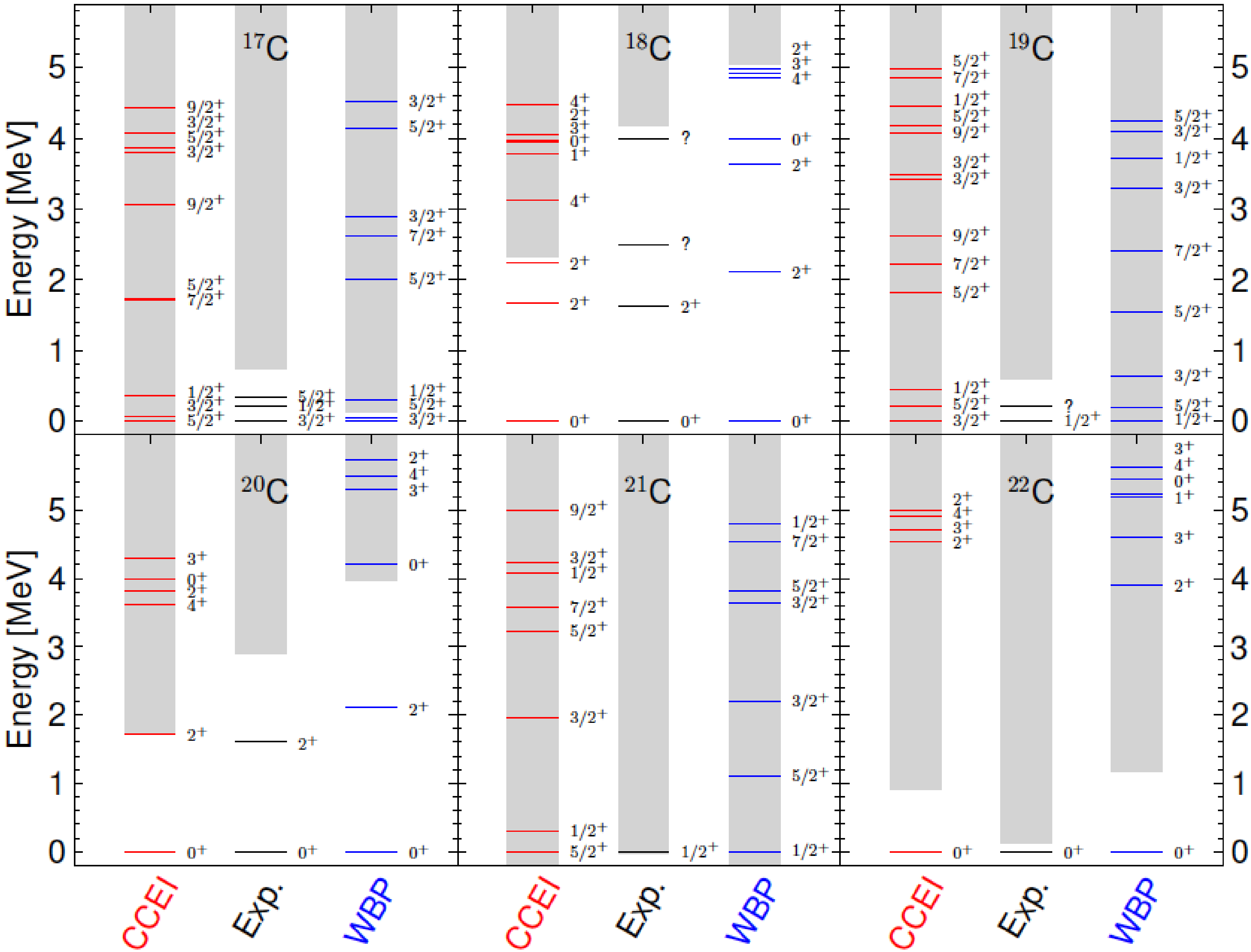


Comparison between coupled-cluster effective interaction (CCEI) and “exact” coupled-cluster calculation with inclusion of perturbative triples Λ-CCSD(T) (Talk by R. Bartlett).

Coupled-cluster effective interactions for the shell model: Oxygen isotopes



Coupled-cluster effective interactions for the shell model: Carbon isotopes



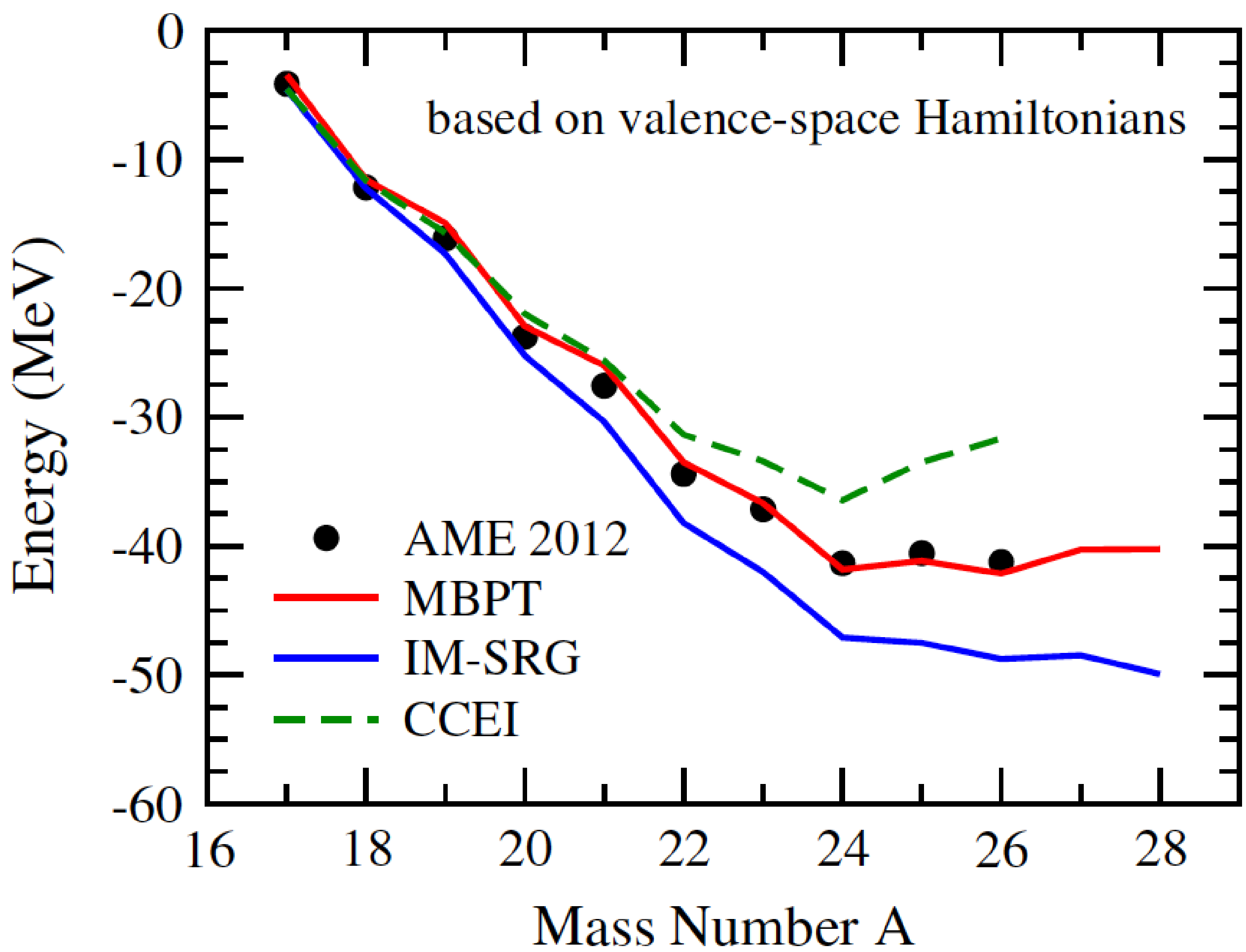
Benchmarking different methods: Binding energies oxygen isotopes

In-medium SRG

S. Bogner et al, Phys. Rev. Lett. 113, 142501 (2014)

Coupled-Cluster Effective Interactions

G. R. Jansen et al, Phys. Rev. Lett. 113, 142502 (2014)



Benchmarking different methods: Spectra in $^{22,23,24}O$

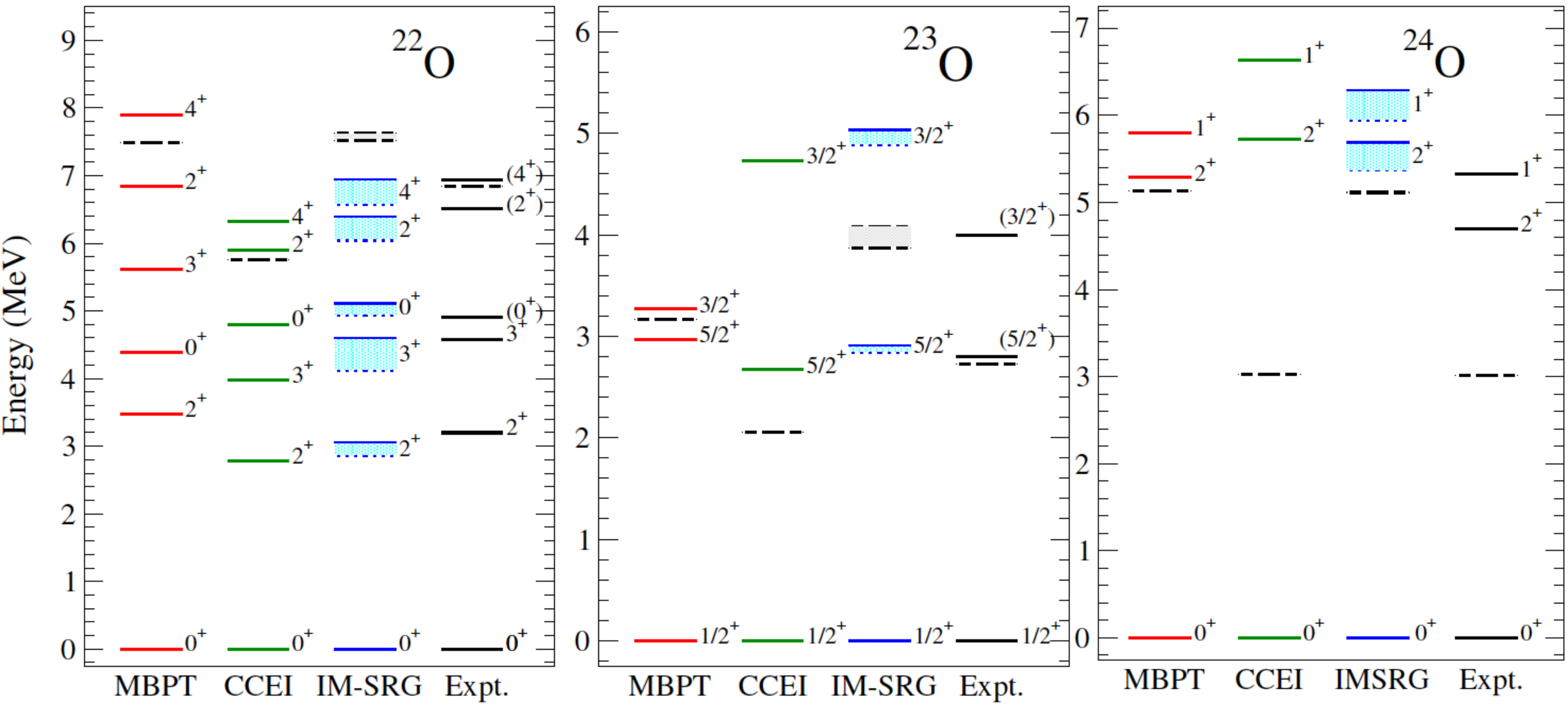
In-medium SRG

S. Bogner et al, Phys. Rev. Lett. 113, 142501 (2014)

Hebeler, Holt, Menendez, Schwenk, Ann. Rev. Nucl. Part. Sci. in press (2015)

Coupled-Cluster Effective Interactions

G. R. Jansen et al, Phys. Rev. Lett. 113, 142502 (2014)

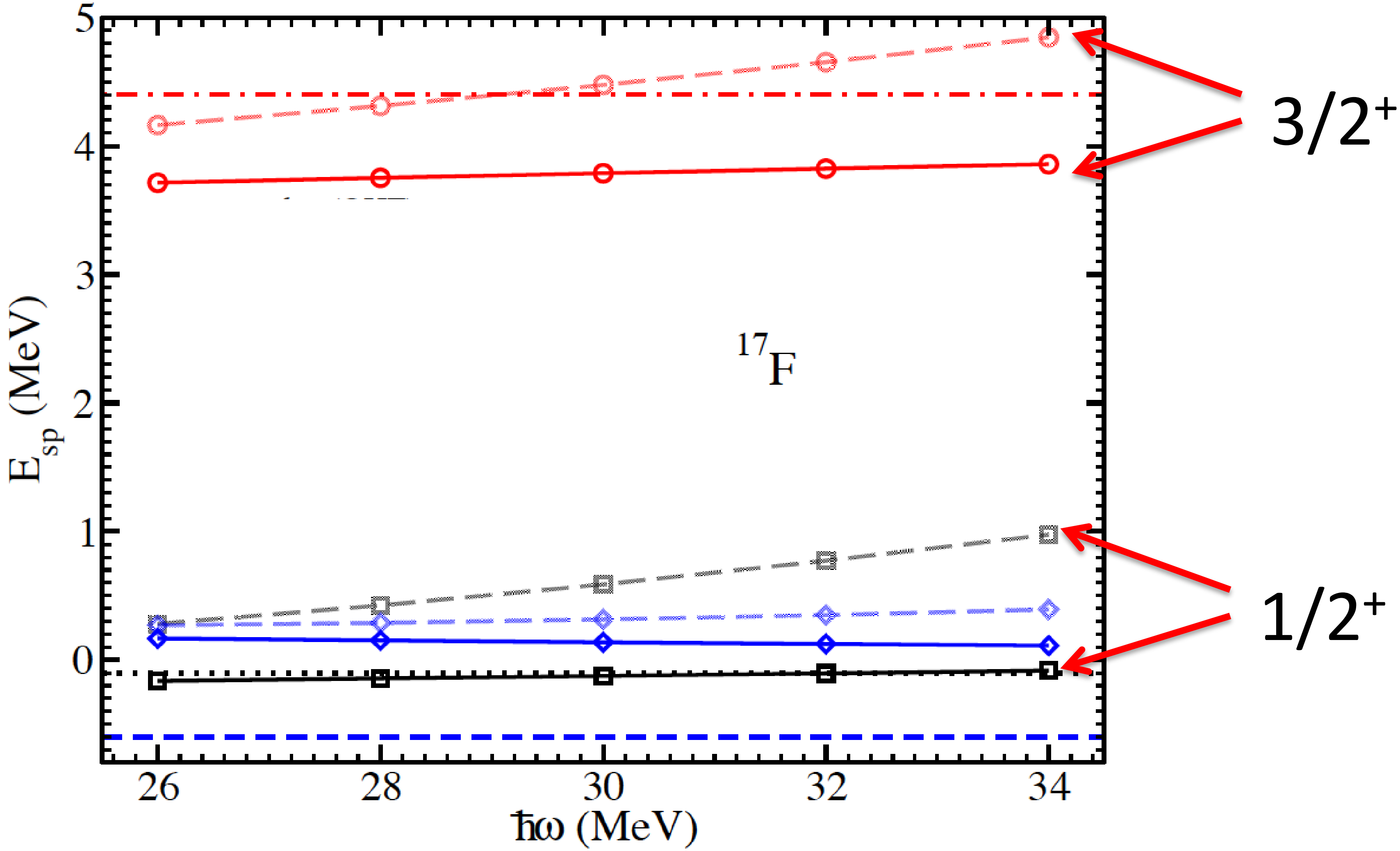


Effect of continuum on low-lying states in ^{17}F

Single-particle basis consists of bound, resonance and scattering states

- Gamow basis for $s_{1/2}$ $d_{5/2}$ and $d_{3/2}$ single-particle states
- Harmonic oscillator states for other partial waves

[G. Hagen, TP, M. Hjorth-Jensen, Phys. Rev. Lett. 104, 182501 (2010)]



Summary

- Non-perturbative shell model interactions from ab-initio coupled-cluster theory
- Spectra in oxygen and carbon isotopes in good agreement with data. Comparable in quality to phenomenological shell model interactions
- Extended CCEI to nuclei with protons and neutrons in valence space. Good agreement with data for 2+ and 4+ states in ^{20,24}Ne and ^{24}Si

- Extend CCEI to incorporate effects of continuum coupling.
- Compute observables such as radii, BE2s and beta-decay using CCEI.