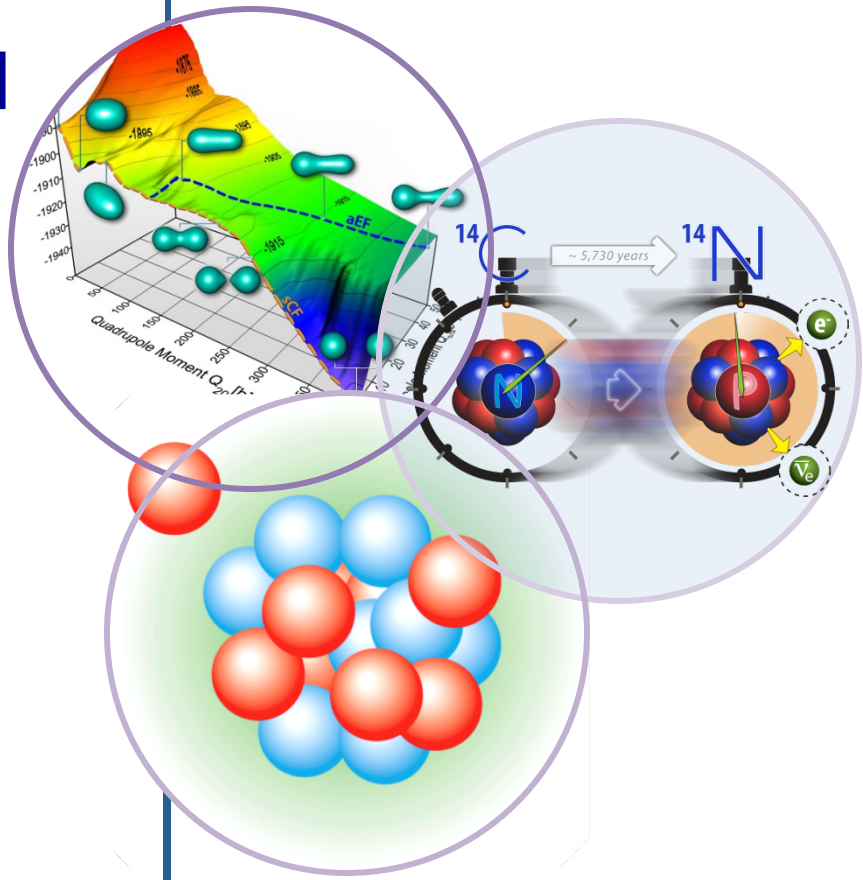
Coupled-cluster approach to open-shell nuclei

Effective interactions and the nuclear shell-model

Gaute Hagen (ORNL)

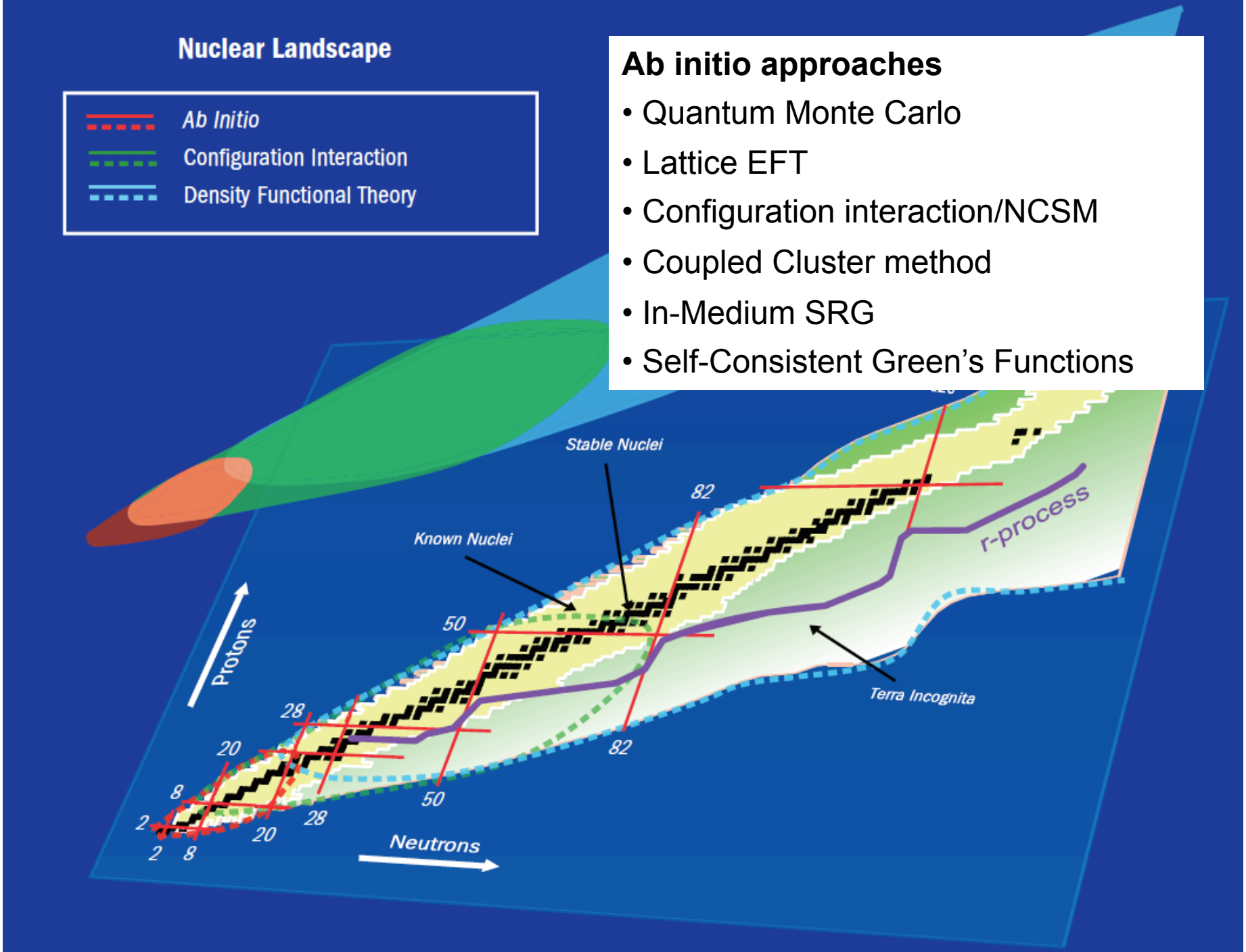


Lecture 4, TALENT school

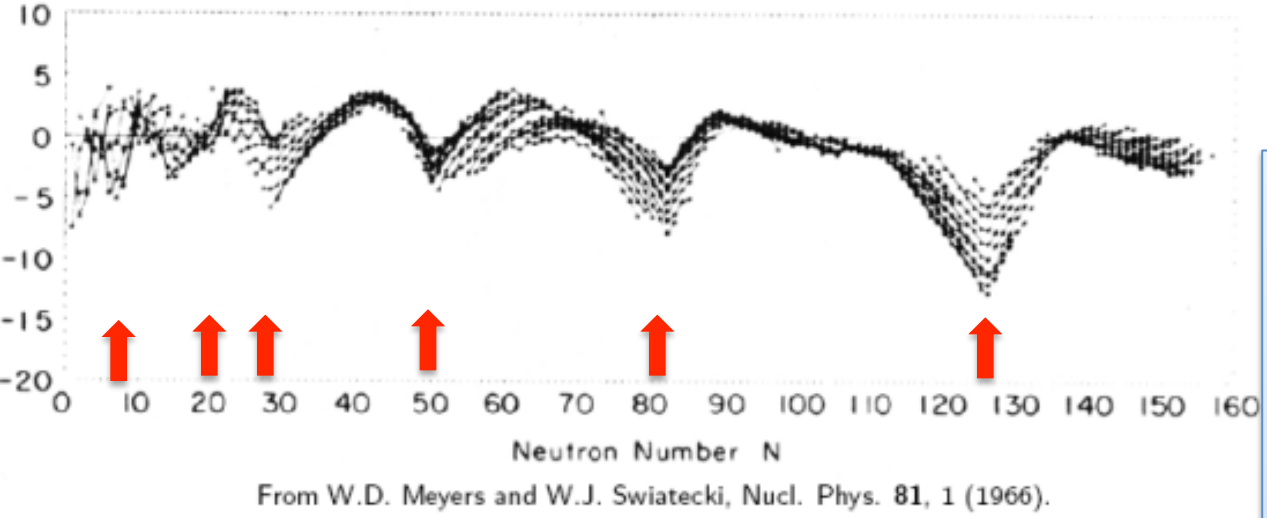
U.S. DEPARTMENT OF ENERGY
NUCLEI Nuclear Computational Low-Energy Initiative
BSF United States – Israel Binational Science Foundation
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

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

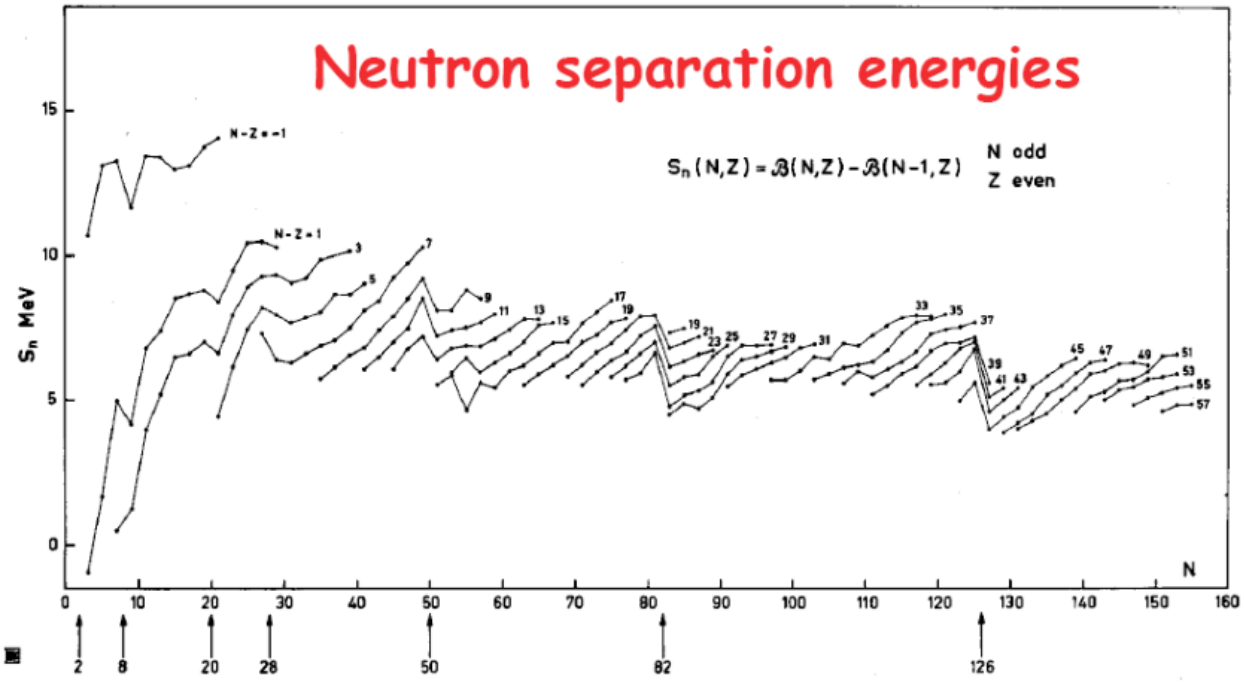

Nuclear Landscape
Ab Initio
Configuration Interaction
Density Functional Theory
Ab initio approaches
• Quantum Monte Carlo
• Lattice EFT
• Configuration interaction/NCSM
• Coupled Cluster method
• In-Medium SRG
• Self-Consistent Green's Functions
Stable Nuclei
Known Nuclei
r-process
Terra Incognita
Protons
Neutrons
2
8
20
28
50
82

Shell structure in nuclei



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

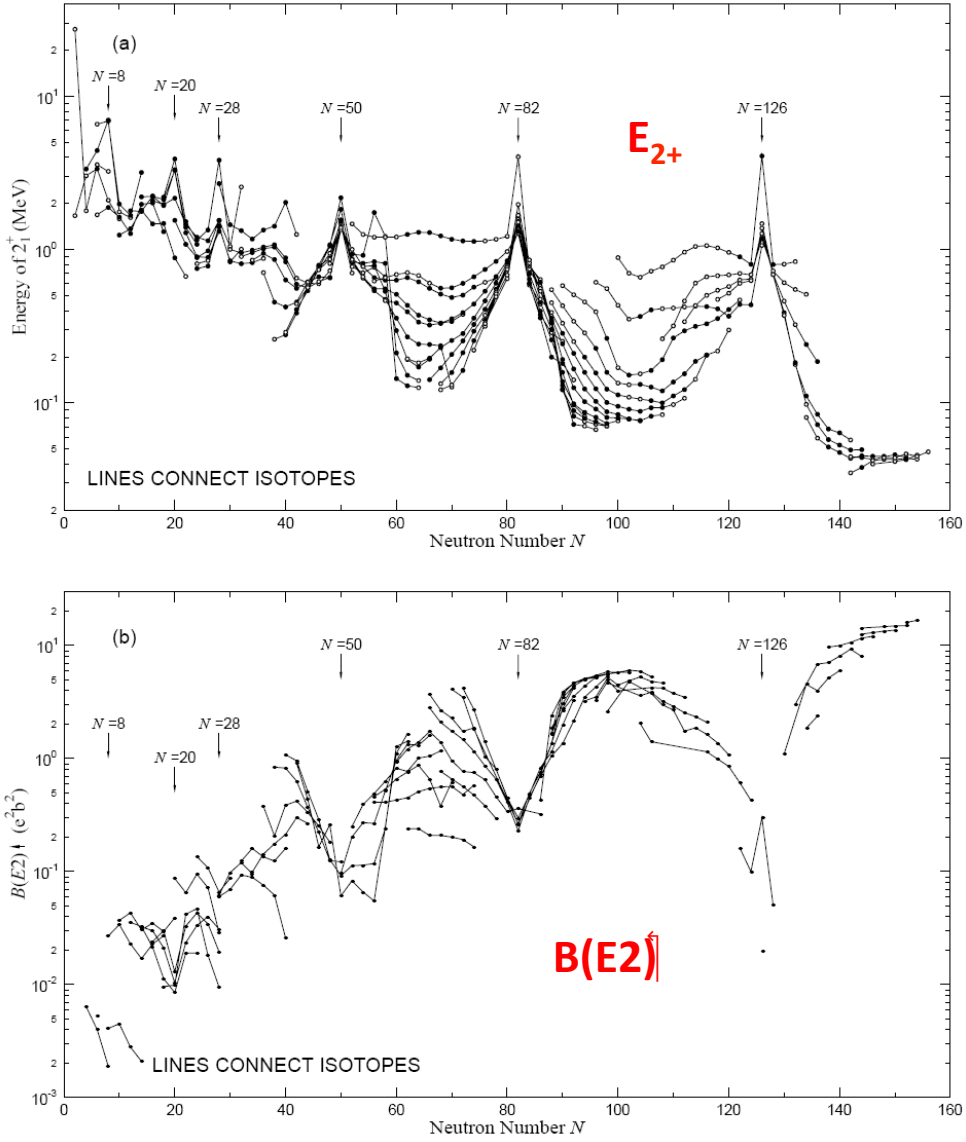
Mass differences: Liquid drop – experiment. Minima at closed shells.



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

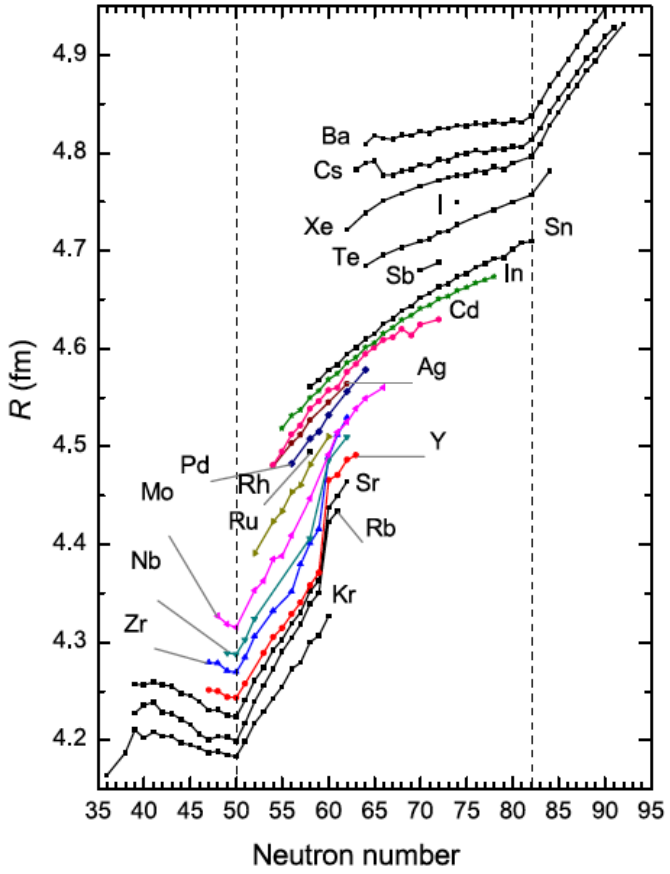
Bohr & Mottelson, Nuclear Structure.

Shell structure in nuclei



Nuclei with magic N :

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

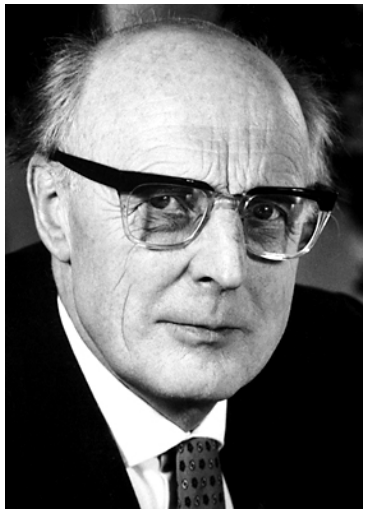


S. Raman et al, Atomic Data and Nuclear Data Tables 78 (2001) 1.

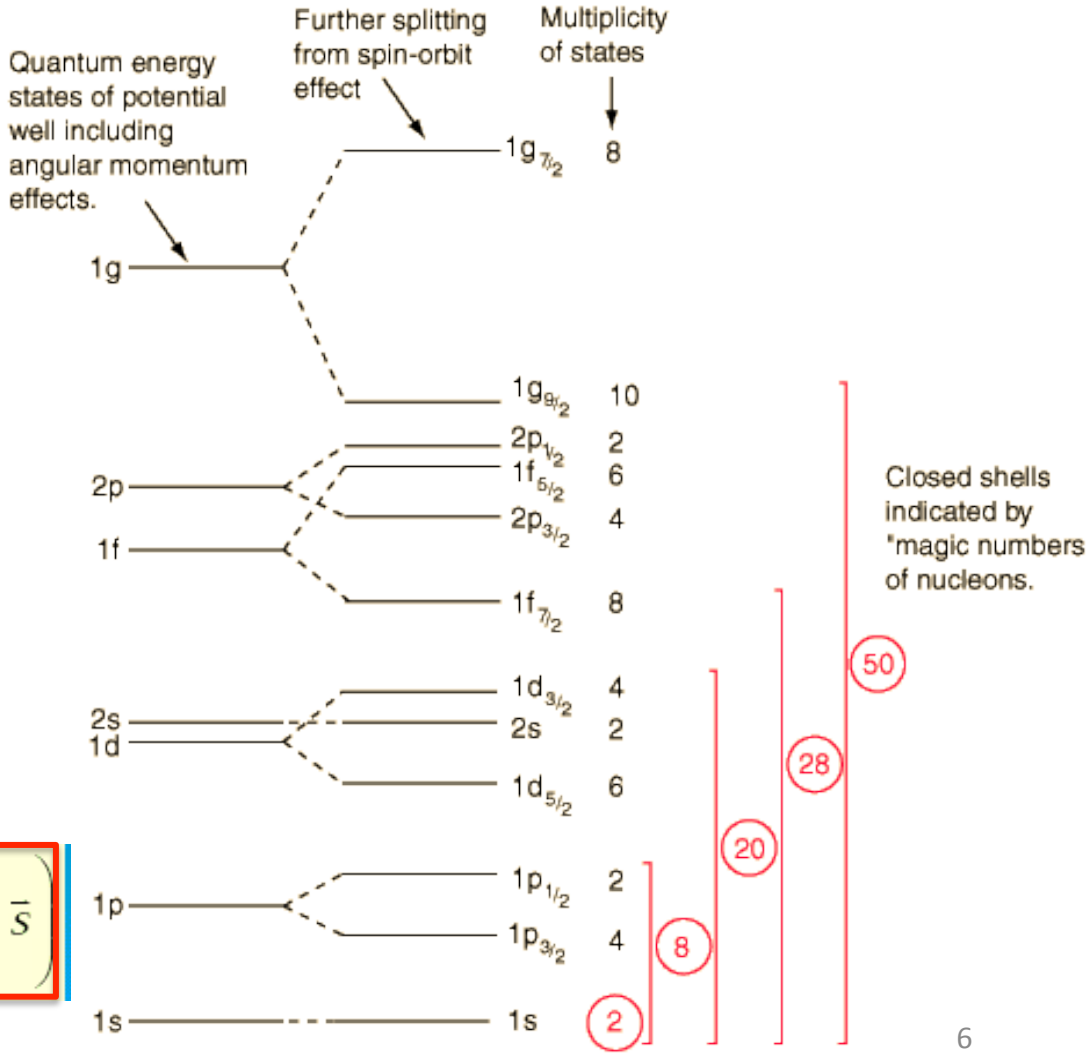
Magic numbers: 2, 8 20, 28, 50,82…

Nobel Prize 1963

Goeppert-Mayer



Jensen



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

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

Traditional shell model

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

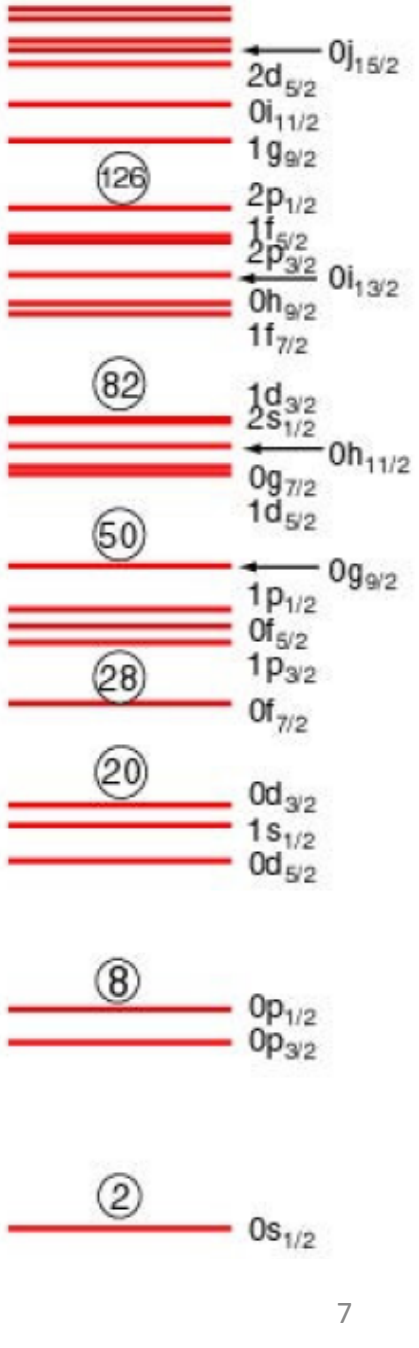
Nucleus (N,Z) = Double magic nucleus (N^*,Z^*)
+ valence nucleons (N-N^*, Z-Z^*)

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

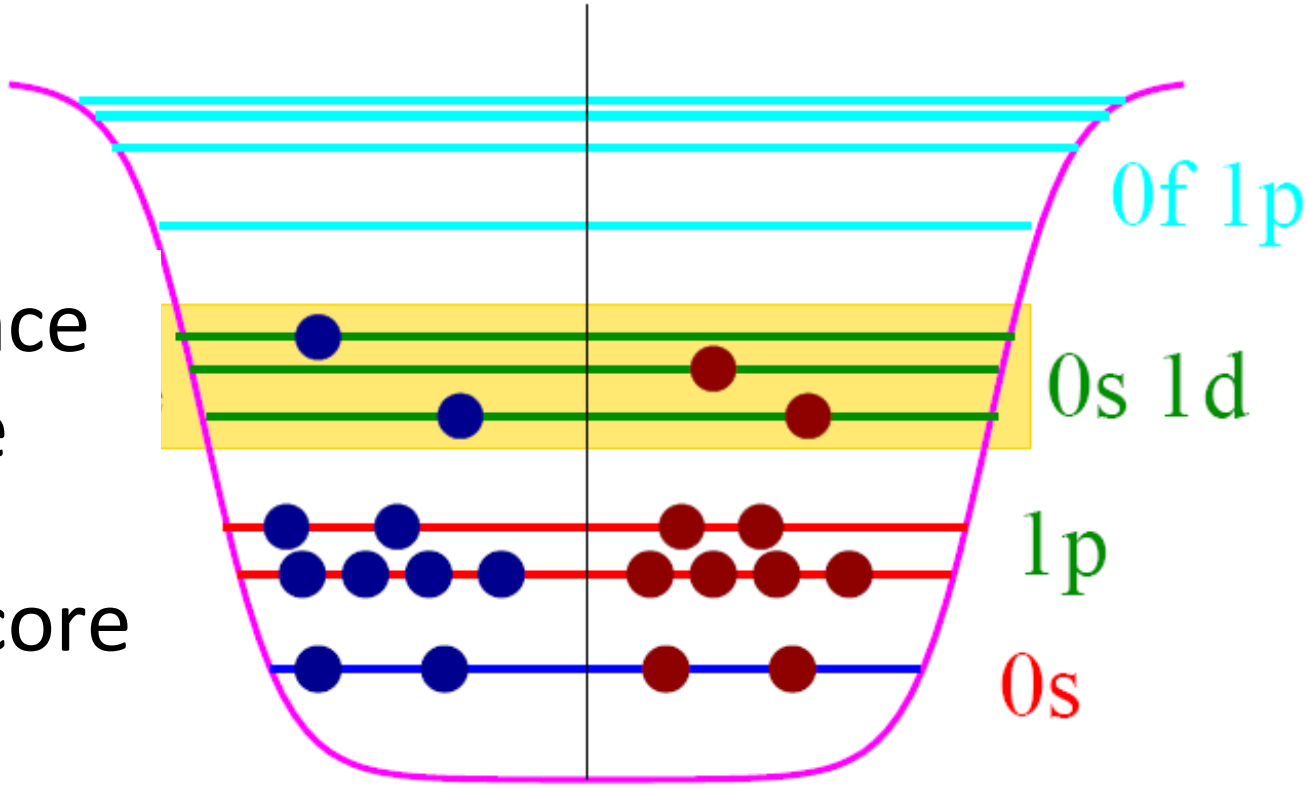
sd-shell nuclei: ^{16}O is doubly magic

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



Traditional shell model

Example: ^{20}Ne



Valence space

^{16}O core

Shell model Hamiltonian

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

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

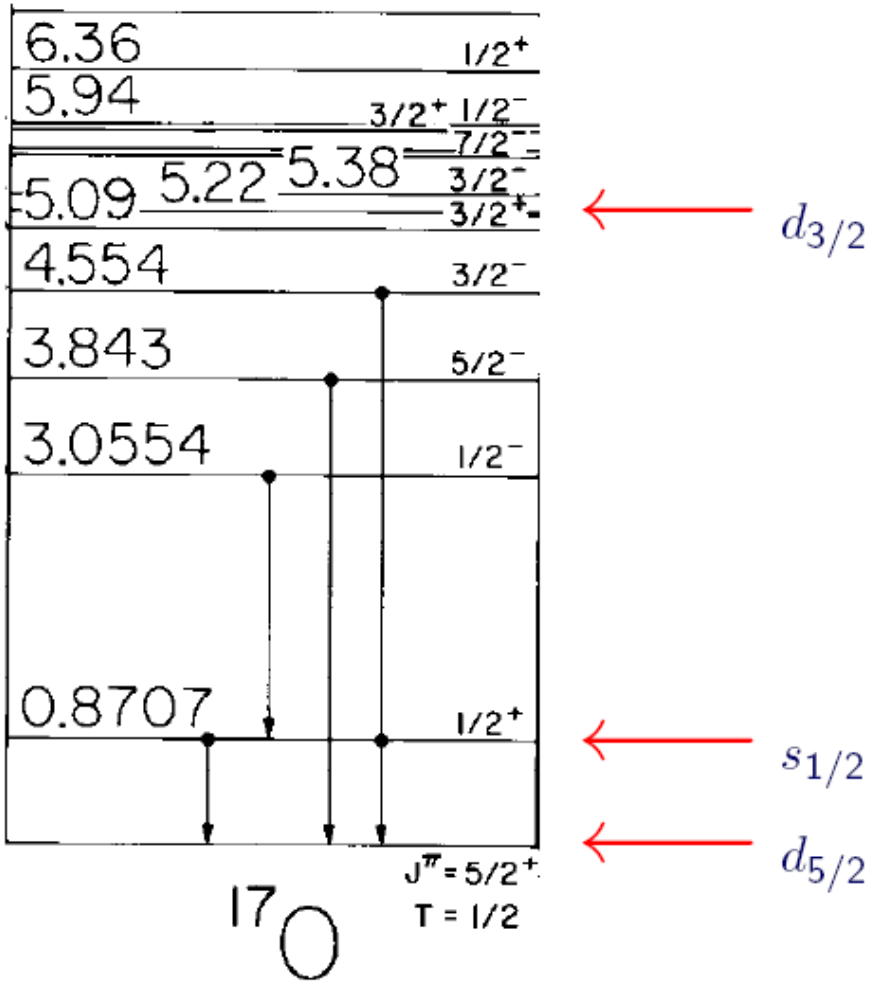
Single-particle energies (SPE)

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

Annihilates pair of fermions

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

Empirical determination of SPE and TBME



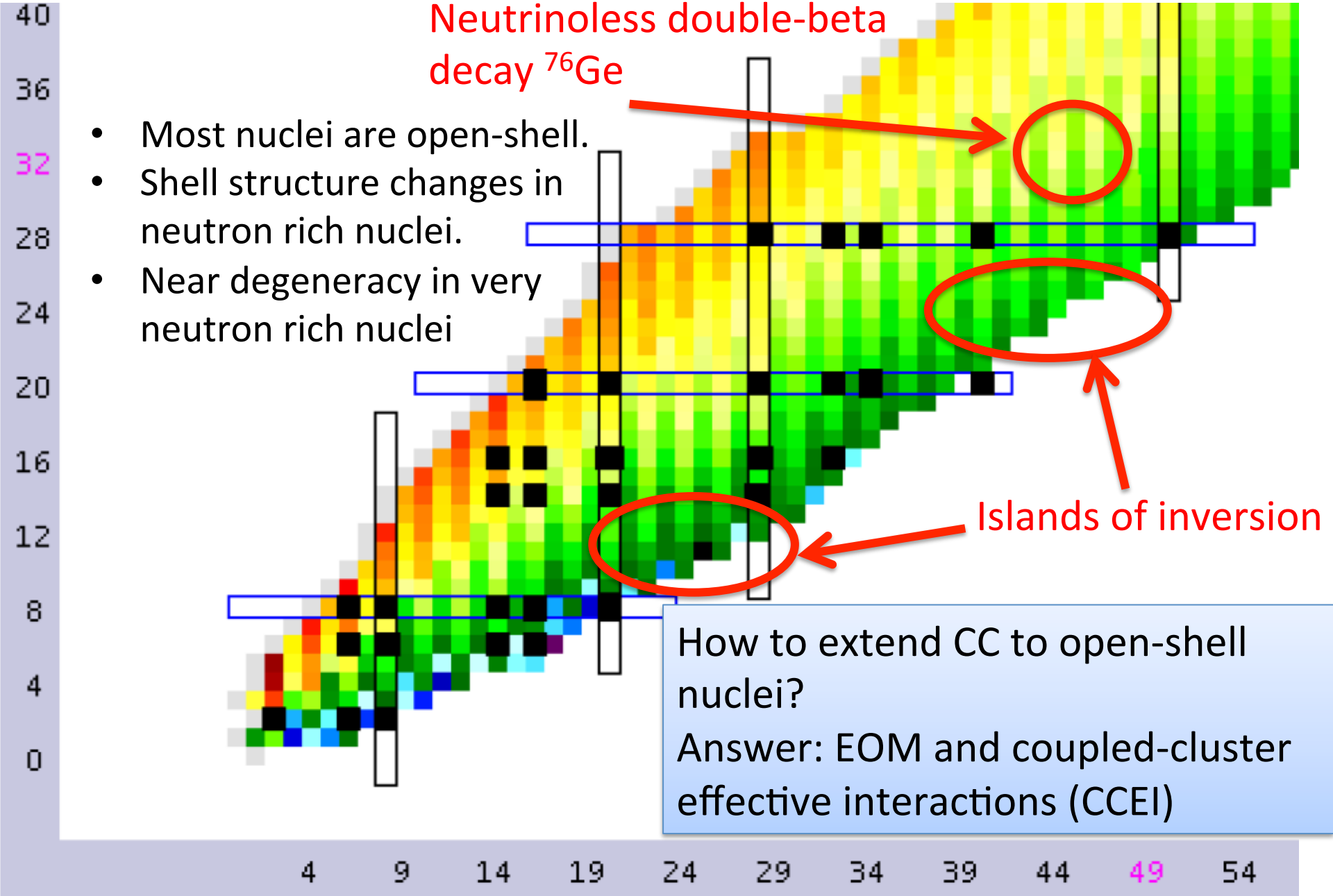
Determine SPE from neighbors of closed shell nuclei (A) having mass A +1

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



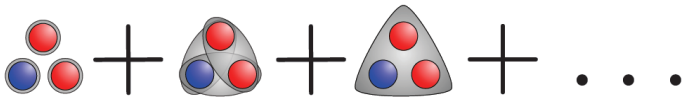
- Most nuclei are open-shell.
- Shell structure changes in neutron rich nuclei.
- Near degeneracy in very neutron rich nuclei

How to extend CC to open-shell nuclei?

Answer: EOM and coupled-cluster effective interactions (CCEI)

Going beyond closed shell nuclei with equation-of-motion techniques

Remember in coupled-cluster theory we deal with the similarity transformed Hamiltonian:

$$\overline{H} = e^{-T} H e^{T} \qquad \hat{T} = \text{  }$$

With *T* being the cluster amplitude (sum of 1p-1h, 2p-2h, 3p-3h, … excitations:

Structure of similarity-transformed Hamiltonian after the CCSD equations are solved

$$\bar{H}_{\mathrm{CCSD}} = \begin{array}{c} \begin{array}{ccc} \text{0p0h} & \text{1p1h} & \text{2p2h} \end{array} \\ \begin{pmatrix} E_{\mathrm{CCSD}} & \bar{H}_{0S} & \bar{H}_{0D} \\ 0 & \bar{H}_{SS} & \bar{H}_{SD} \\ 0 & \bar{H}_{DS} & \bar{H}_{DD} \end{pmatrix} \end{array} \begin{array}{l} \text{0p0h} \\ \text{1p1h} \\ \text{2p2h} \end{array}$$

We can diagonalize $\overline{H}$ in a sub-space of *n*-particle-*m*-hole to access other regions of Fock space

we can obtain excited states for the closed-shell systems by diagonalizing $\overline{H}$ in a sub-space 1p-1h and 2p-2h excitations

$$\left(\overline{H} R_\mu^A\right)_C |\Phi_0\rangle = \omega_u R_\mu^A |\Phi_0\rangle$$

$$R_\mu^A = \sum_{ia} r_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} r_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

Going beyond closed shell nuclei with equation-of-motion techniques

We can access the $A \pm 1$ Fock space by diagonalizing $\overline{H}$ in sub-space of one-particle (hole) and two-particle-one-hole (one-particle-two-hole) excitations:

$$\left(\overline{H} R_\mu^{A\pm1}\right)_C |\Phi_0\rangle = \omega_u R_\mu^{A\pm1} |\Phi_0\rangle$$

The $A \pm 1$ right eigenvectors are given by:

$$R_\mu^{A+1} = \sum_a r^a a_a^\dagger + \frac{1}{2}\sum_{iab} r_i^{ab} a_a^\dagger a_b^\dagger a_i \qquad R_\mu^{A-1} = \sum_i r_i a_i + \frac{1}{2}\sum_{ija} r_{ij}^a a_a^\dagger a_j a_i$$

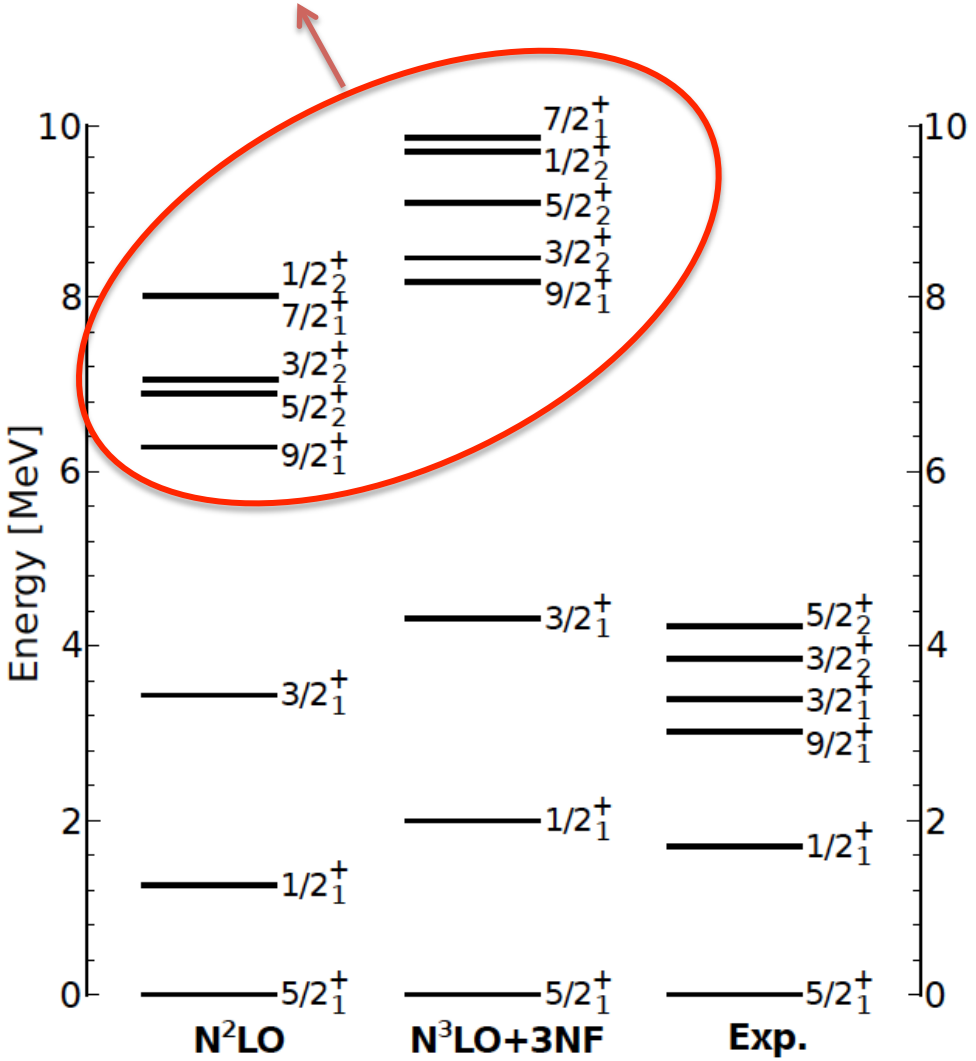
Note that since the similarity transformed Hamiltonian is non-Hermitian we need to compute the corresponding left eigenvectors if we want to compute expectation values and transition densities, i.e.

$$\langle \hat{O} \rangle = \langle L_\mu | \overline{O} | R_\mu \rangle$$

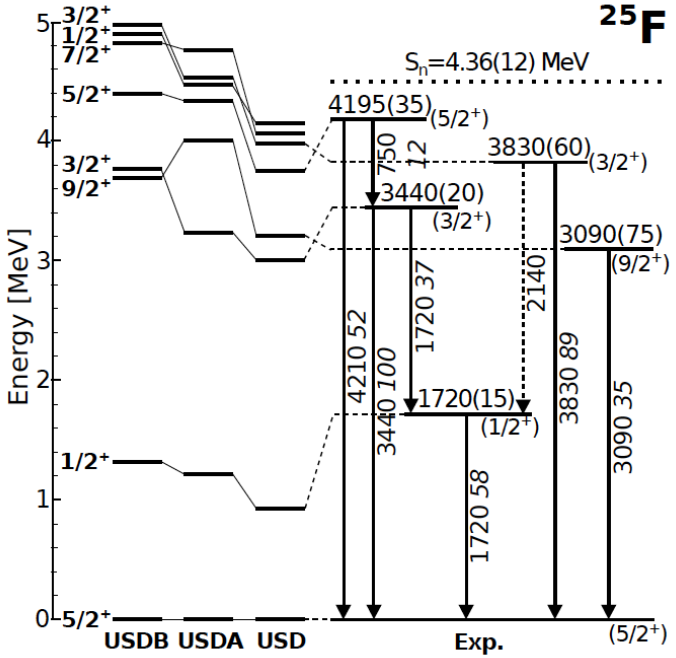
Particle attached equation-of-motion theory for nuclei :
J. R. Gour et al PRC 74 024310 (2006)

Computing nuclei with A+1
Example: proton-halo state in ^{25}F

States dominated by 3p-2h excitations



Zs. Vajta et al. PRC 89, 054323 (2014)



Excitation spectra of ^{25}F obtained with particle-attached equation-of-motion techniques. Here we included some 3p-2h excitations as well.

Going beyond closed shell nuclei with equation-of-motion techniques

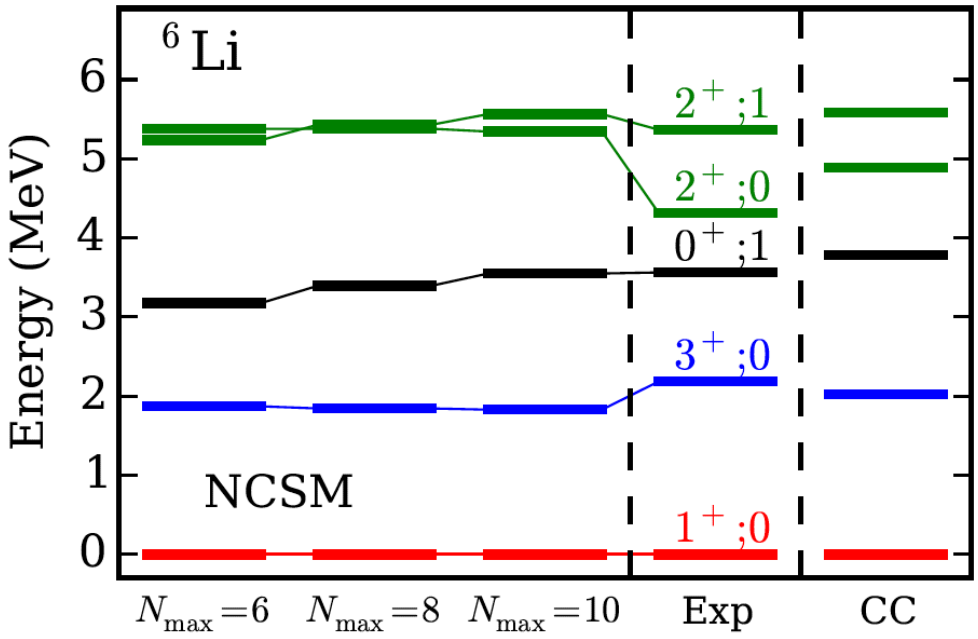
We can access the $A \pm 2$ Fock space by diagonalizing $\overline{H}$ in sub-space of two-particle (hole) and three-particle-one-hole (one-particle-three-hole) excitations:

$$\left(\overline{H} R_\mu^{A\pm 2}\right)_C |\Phi_0\rangle = \omega_u R_\mu^{A\pm 2} |\Phi_0\rangle$$

$$R_\mu^{A+2} = \frac{1}{2}\sum_{ab} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{iabc} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i$$

Two-particle attached equation-of-motion theory for nuclei :
G. Jansen et al PRC 2011, G. Jansen (2013), J. Shen and P. Piecuch J. Chem. Phys (2013)

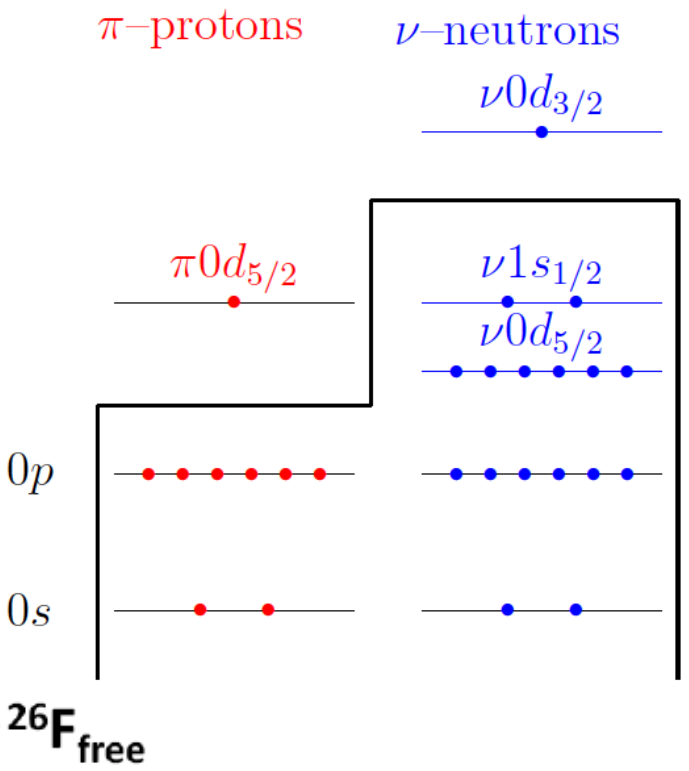
2PA-EOM compares well with NCSM for spectra in ^{6}Li (P. Navratil private communication)

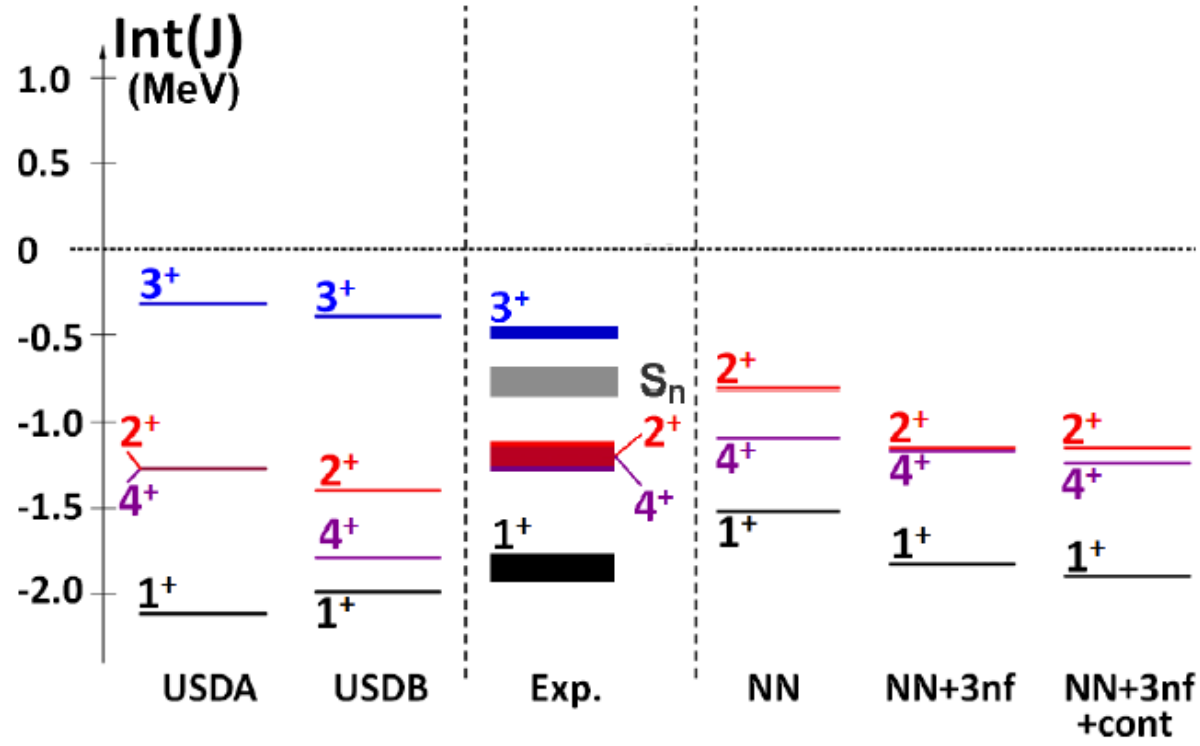


Computing nuclei with A+2: Example Fluorine-26

G. Jansen et al PRC 2011, J. Shen and P. Piecuch J. Chem. Phys (2013)

Experimental spectra in ^{26}F compared with phenomenological USD shell-model calculations and coupled-cluster calculations





A. Lepailleur et al PRL (2012)

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)

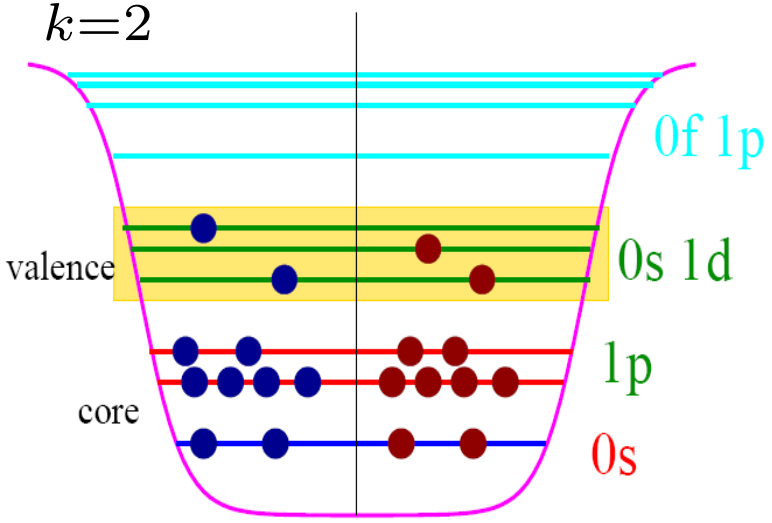
We start from the intrinsic Hamiltonian with NN and 3N forces:

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

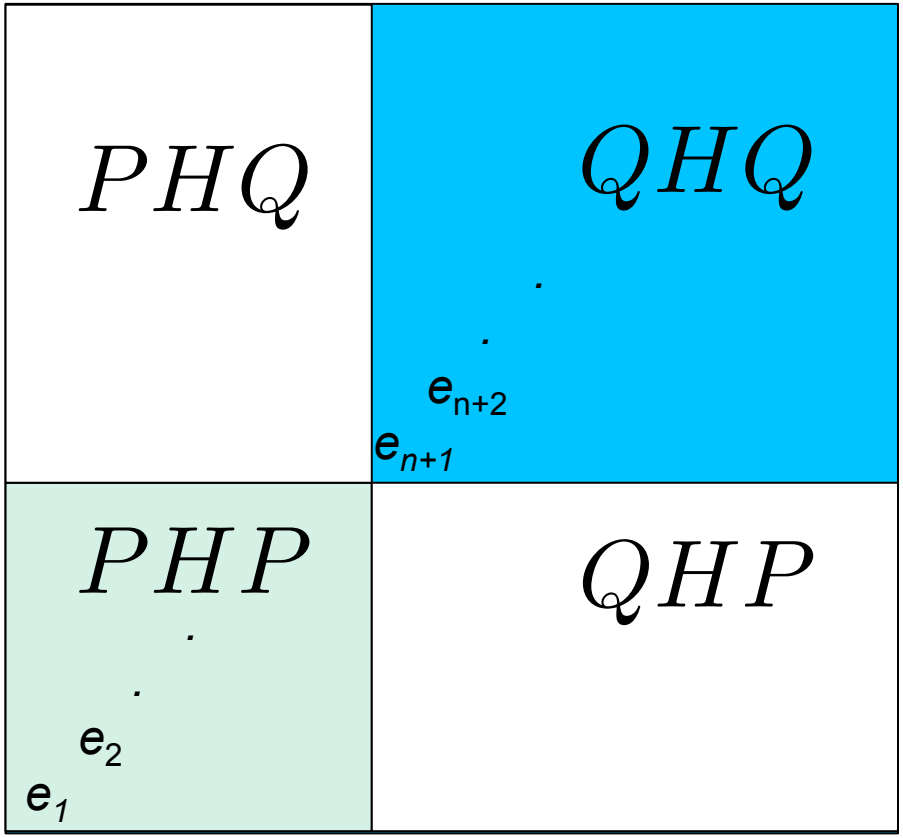
Write the intrinsic Hamiltonian as a valence cluster expansion:

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

- 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:

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

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

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

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

Effective eigenvectors are defined as (Bloch-Brandow): $|\psi_k^{\rm eff}\rangle \equiv P|\Psi_k\rangle$

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

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

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))

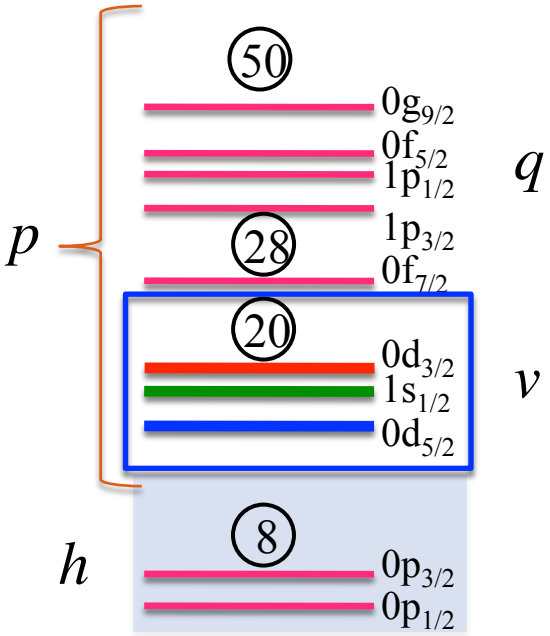
$$\left[S^\dagger S\right]^{1/2} \overline{H}_{\text{CCEI}}^{A} \left[S^\dagger S\right]^{-1/2}$$

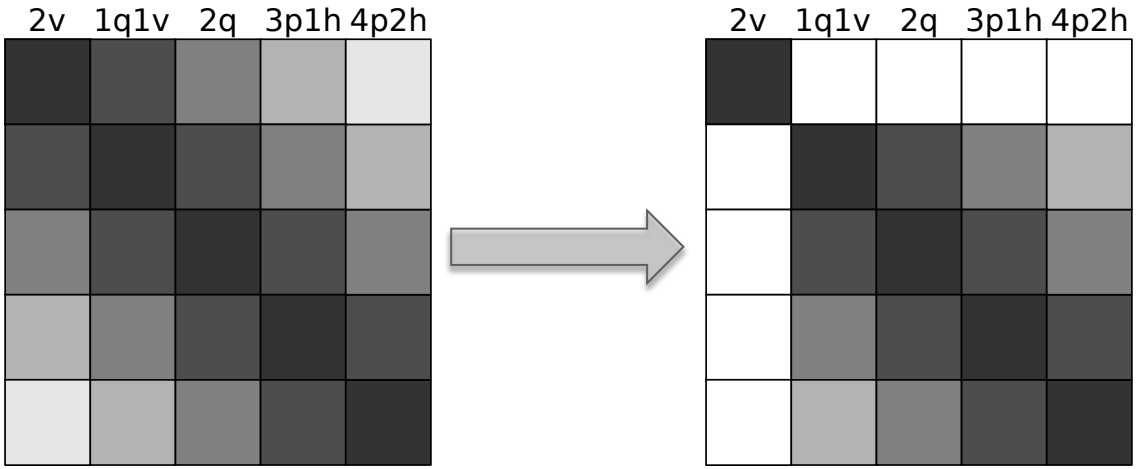
IM-SRG: Valence-Space Hamiltonians

Tsukiyama, Bogner, Schwenk, PRC (2012)
Bogner et al, PRL (2014).

Open-shell systems

Separate p states into valence states (v) and those above valence space (q)





$$H(s=0) \rightarrow H(\infty)$$

$$H(s) = U(s) H U^{\dagger}(s) \equiv H^{\mathrm{d}}(s) + H^{\mathrm{od}}(s) \rightarrow H^{\mathrm{d}}(\infty) \qquad \frac{\mathrm{d}H(s)}{\mathrm{d}s} = [\eta(s), H(s)]$$

$$\eta(s) \equiv (\mathrm{d}U(s)/\mathrm{d}s)\, U^{\dagger}(s) \qquad \eta_I(s) = \left[H^{\mathrm{d}}(s), H^{\mathrm{od}}(s)\right]$$

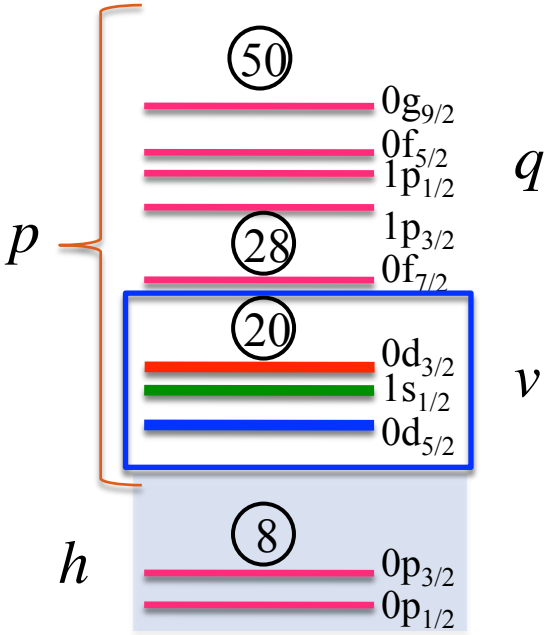
Define H^{od} to decouple valence space from excitations outside v

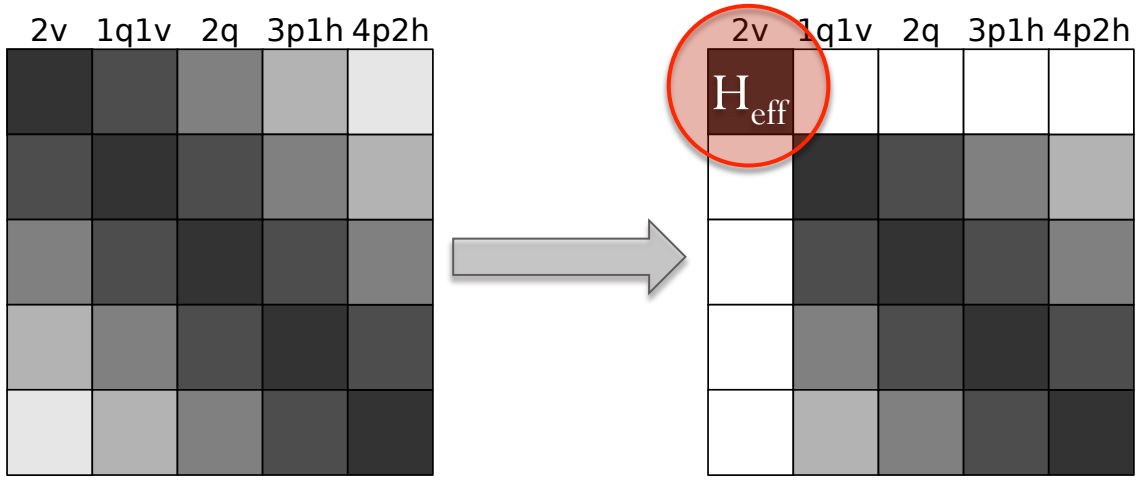
IM-SRG: Valence-Space Hamiltonians

Tsukiyama, Bogner, Schwenk, PRC (2012)
Bogner et al, PRL (2014).

Open-shell systems

Separate p states into valence states (v) and those above valence space (q)





$$H(s=0) \rightarrow H(\infty)$$

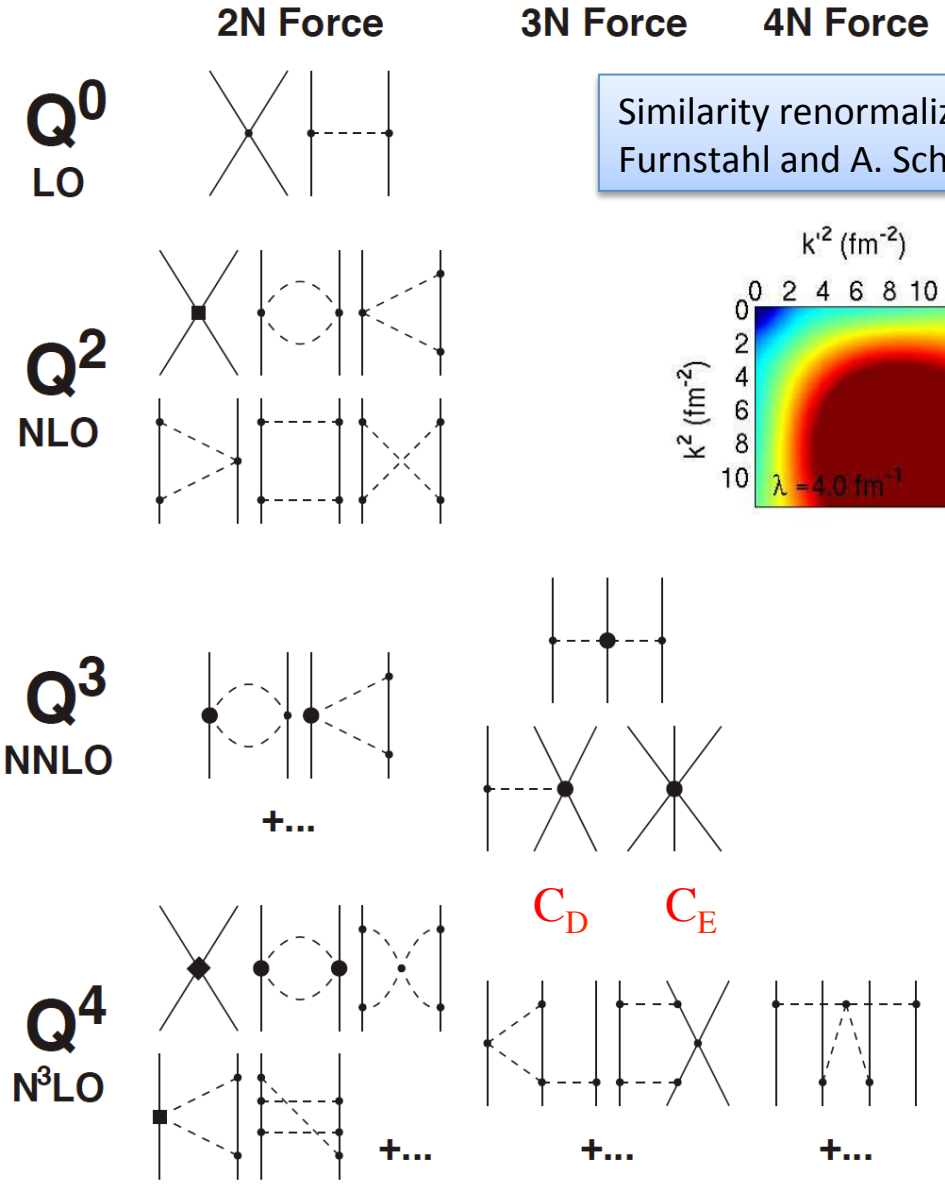
Core physics included consistently (**absolute energies, radii…**)

Inherently nonperturbative – no need for extended valence space

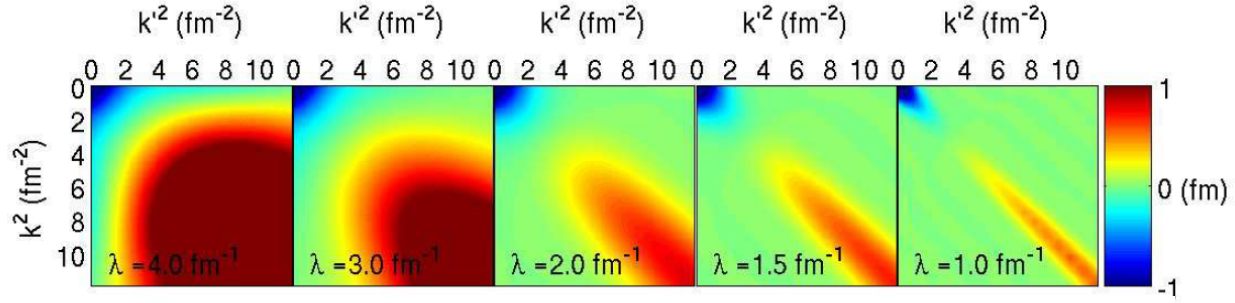
Non-degenerate valence-space orbitals

Nuclear forces from chiral effective field theory

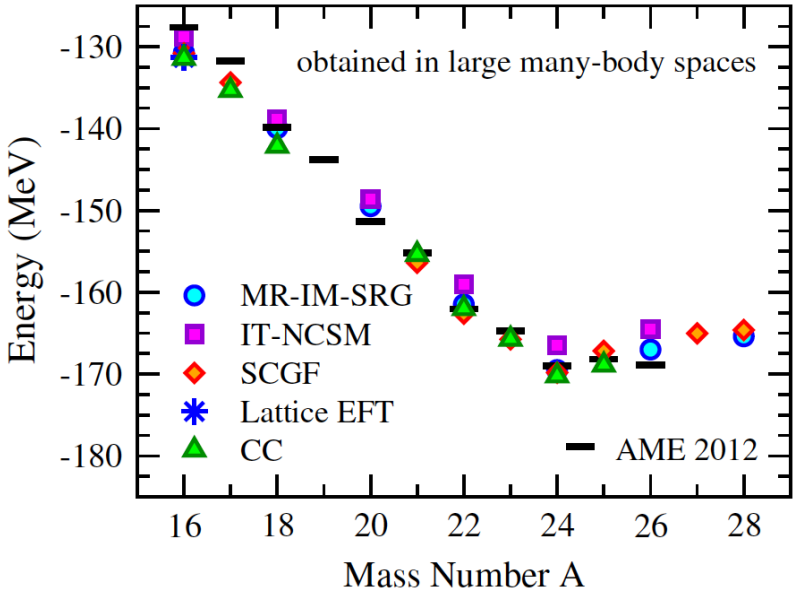
[Weinberg; van Kolck; Epelbaum *et al.*; Entem & Machleidt; …]



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

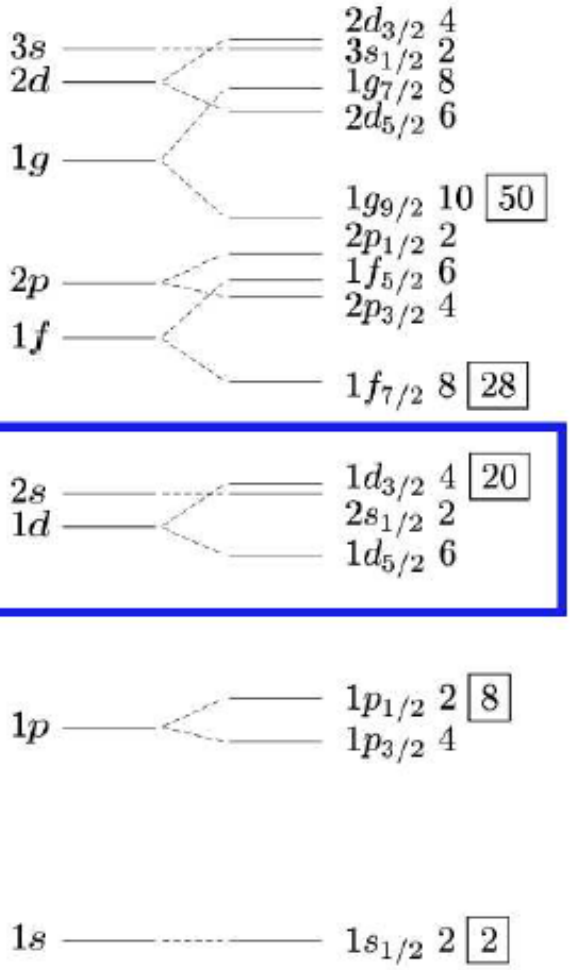


Hebeler, Holt, Menendez, Schwenk, Ann. Rev. Nucl. Part. Sci. in press (2015)



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

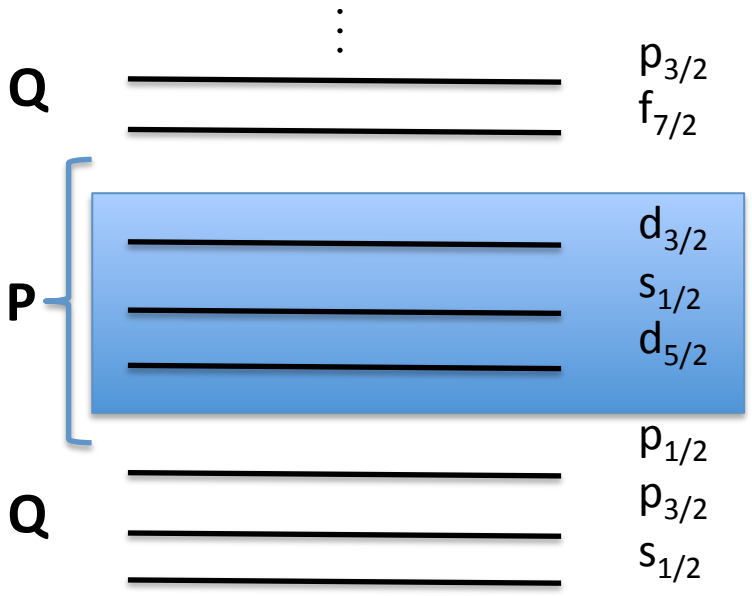


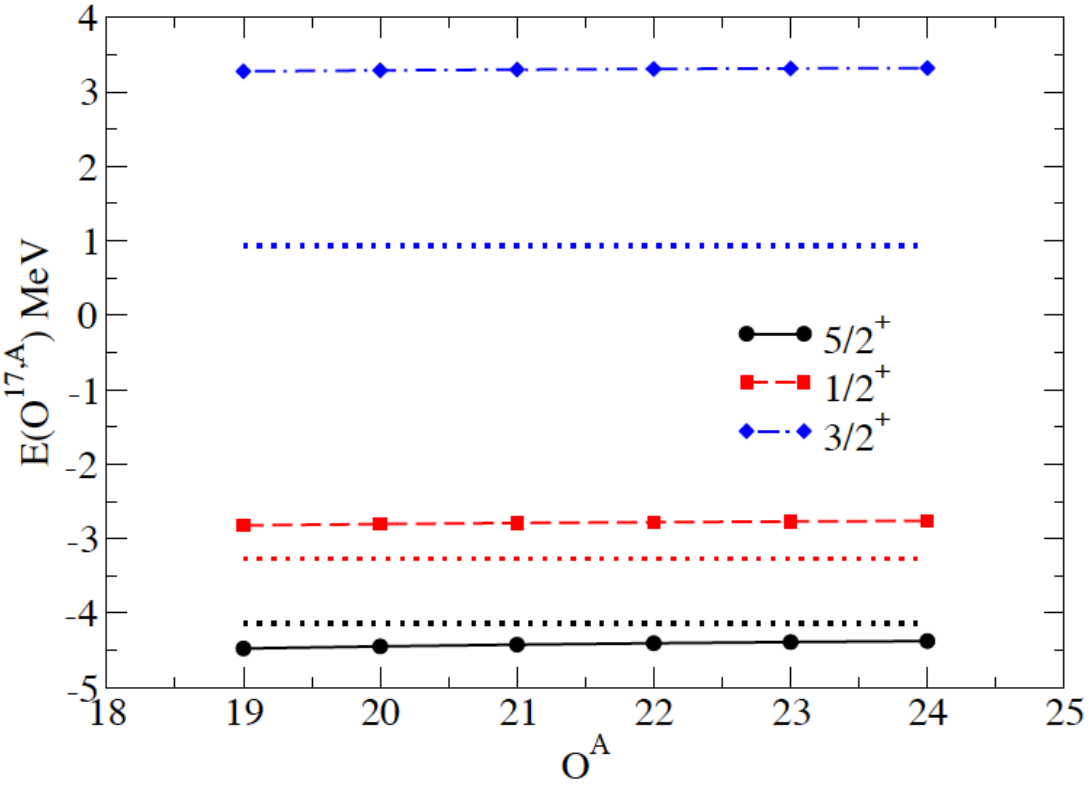
CCEI: Application to the oxygen chain

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

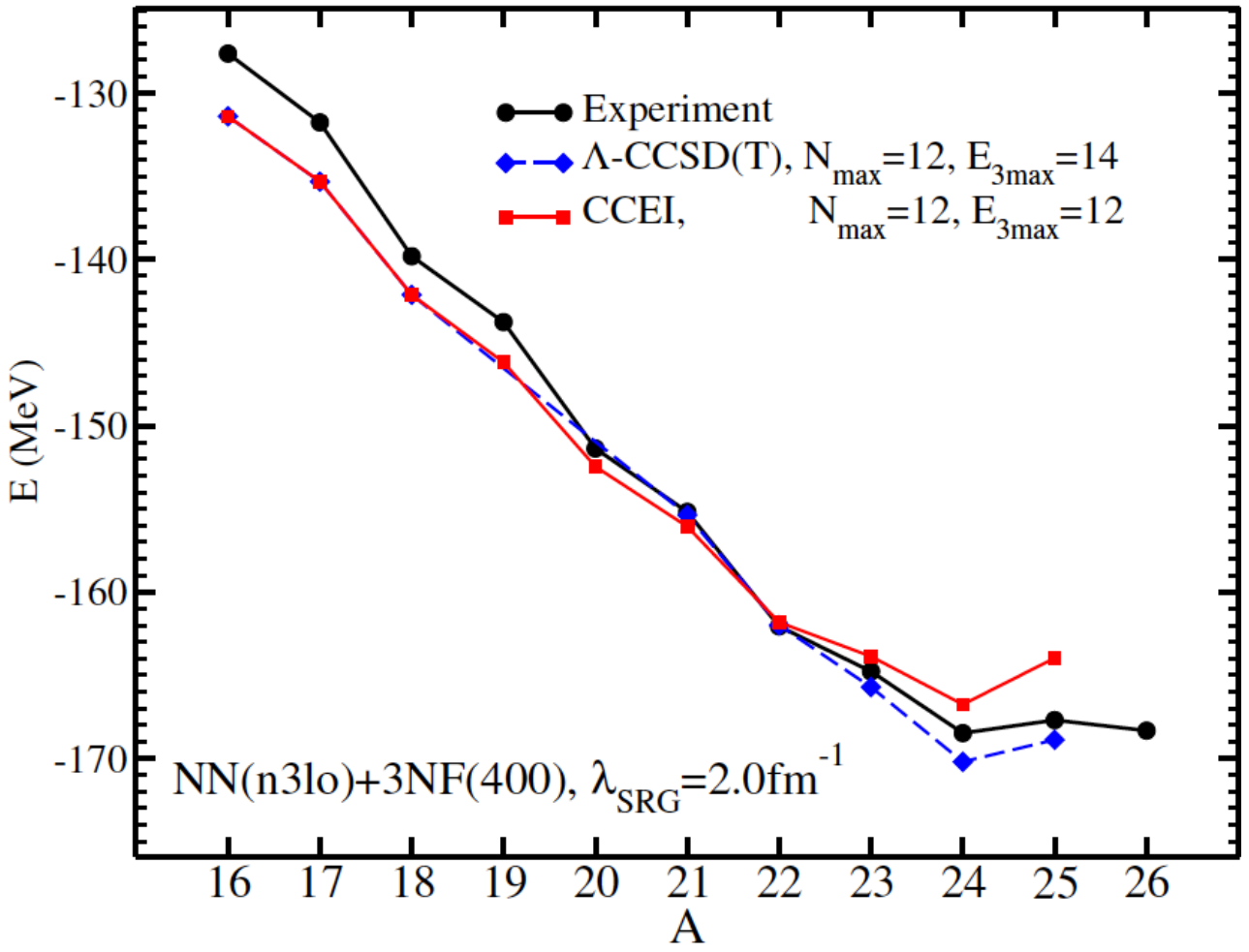
Low-lying states in ^{17}O as a function of A. These energies defines the single-particle energies of H_{eff}





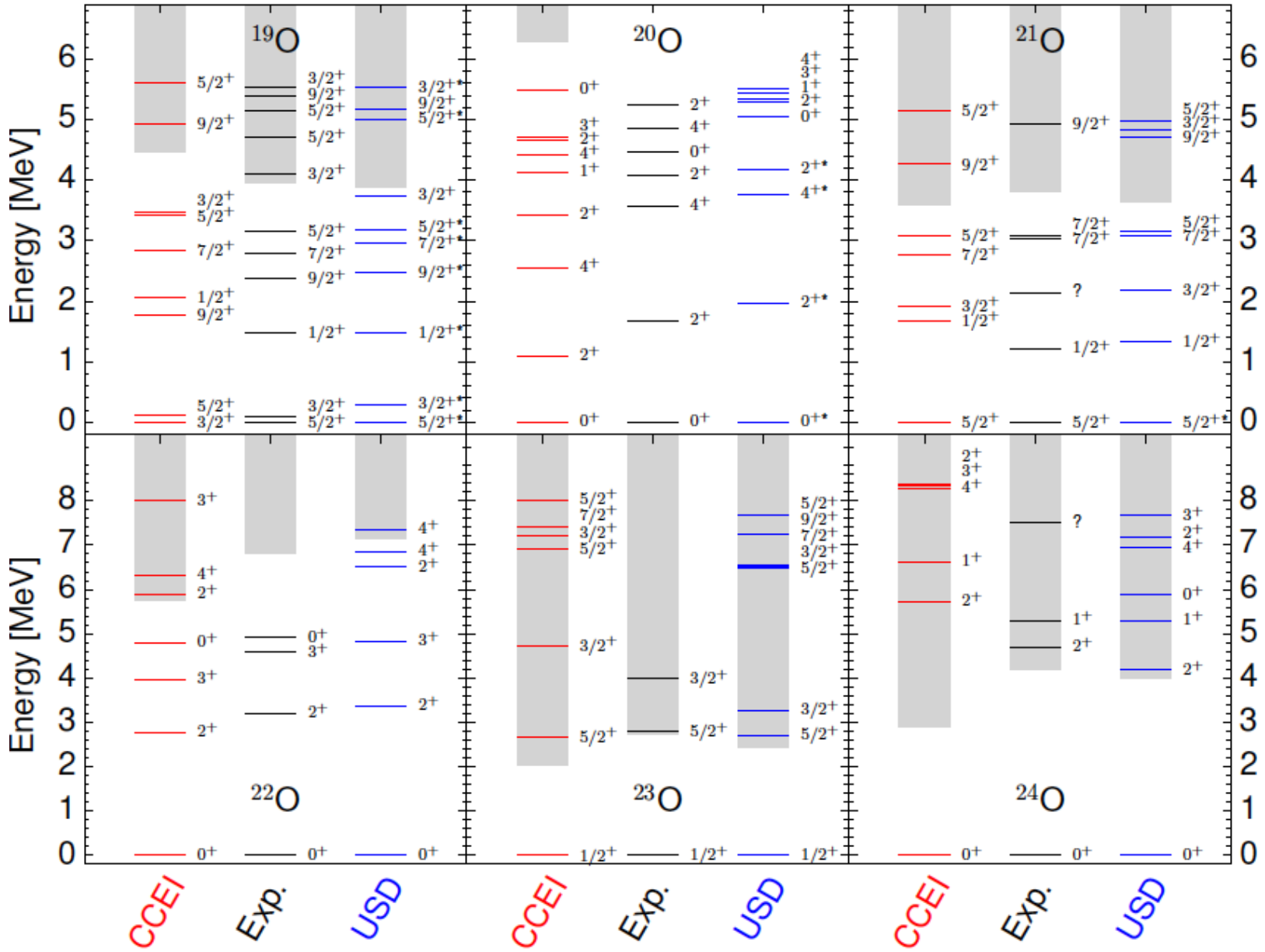
CCEI: Application to the oxygen chain

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

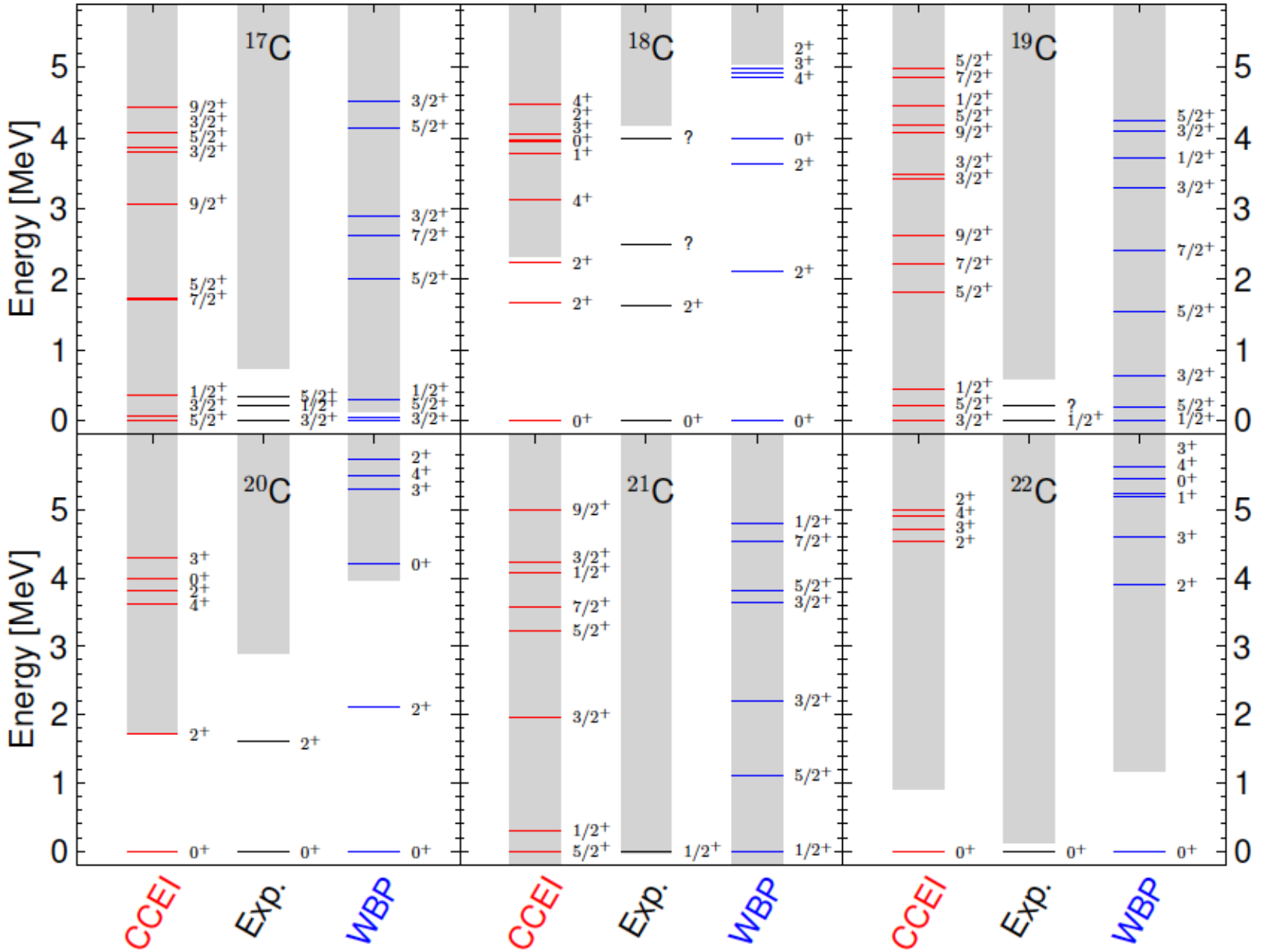


Comparison between coupled-cluster effective interaction (CCEI) and “exact” coupled-cluster calculation with inclusion of perturbative triples Λ-CCSD(T) (Talk by R. Bartlett).

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



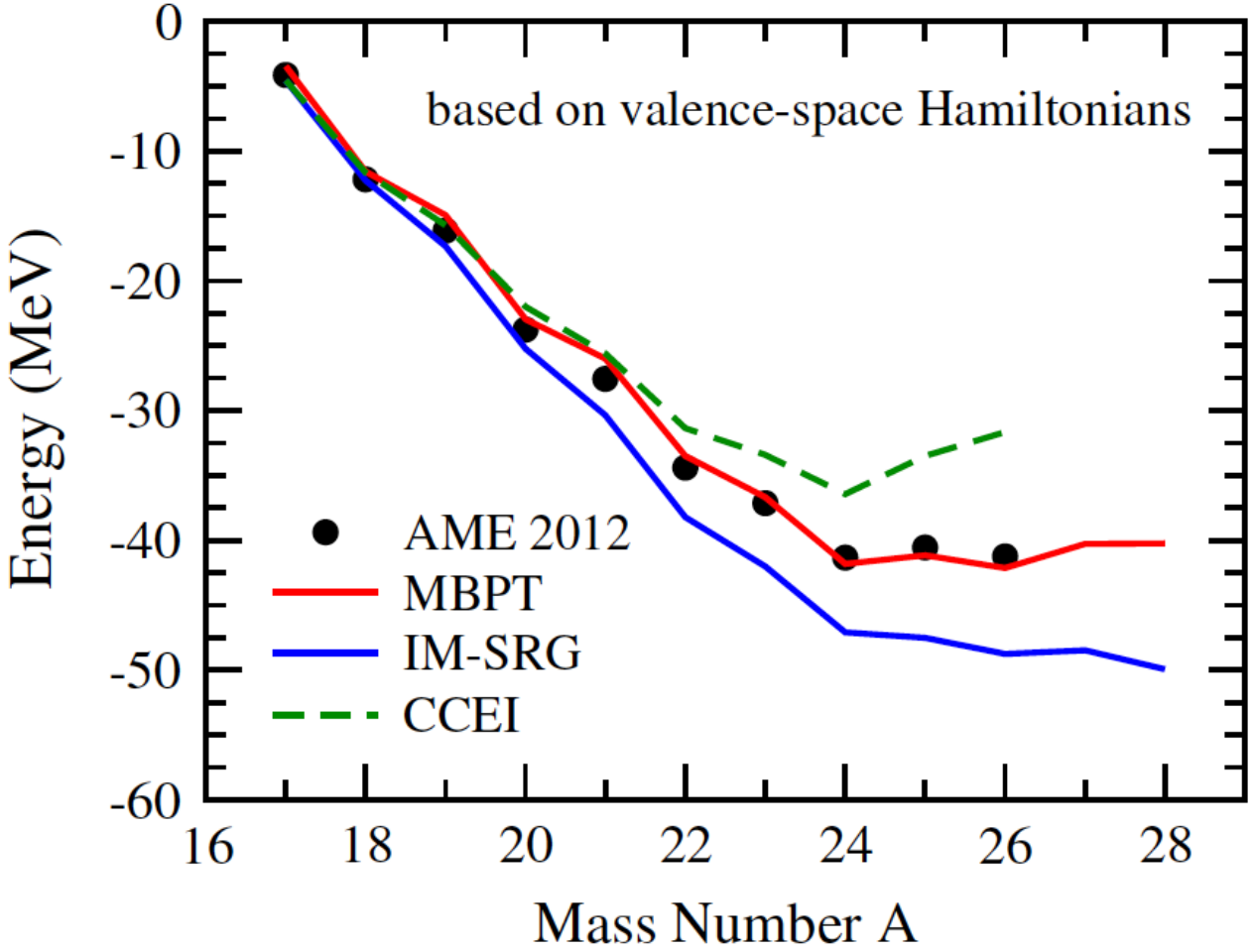
Coupled-cluster effective interactions for the shell model: Carbon isotopes



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

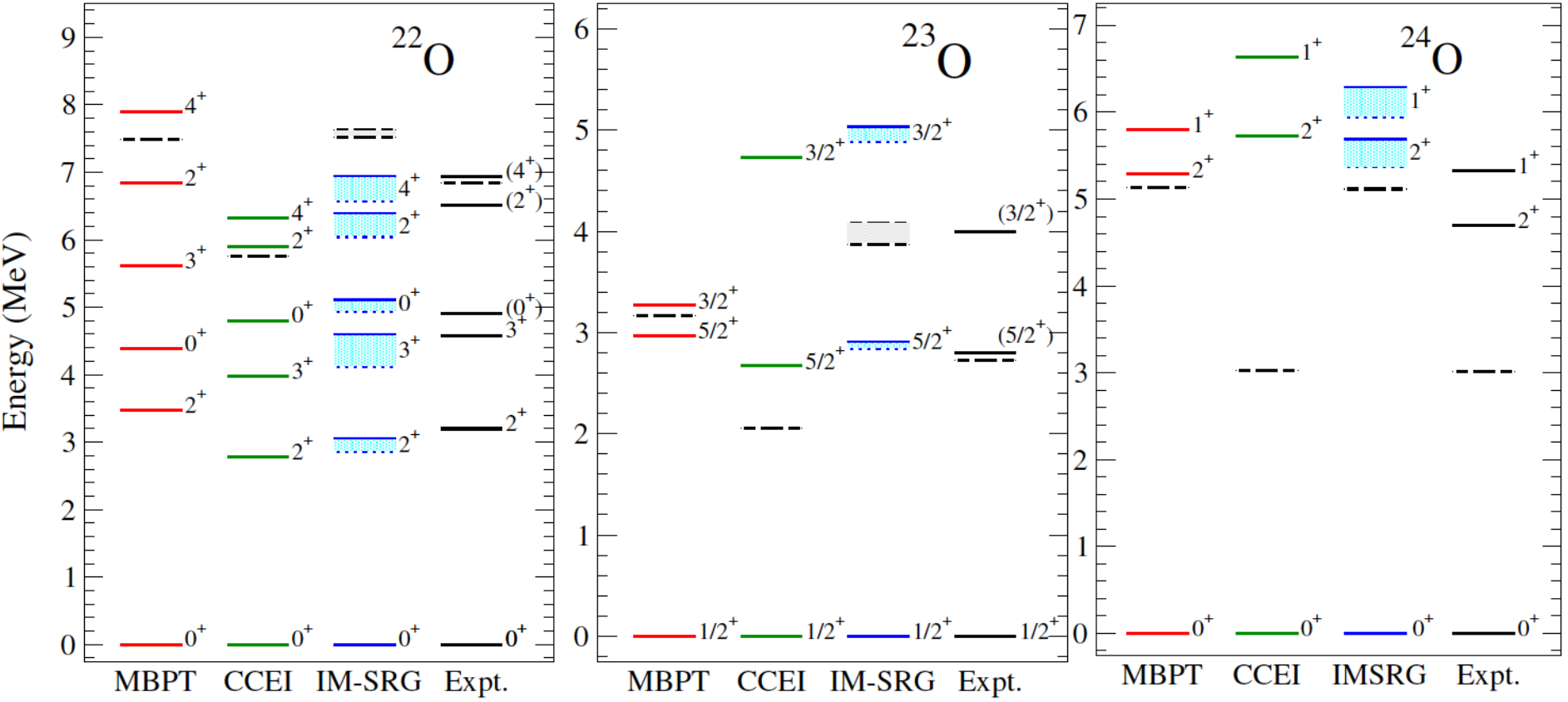
S. Bogner et al, Phys. Rev. Lett. 113, 142501 (2014)

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

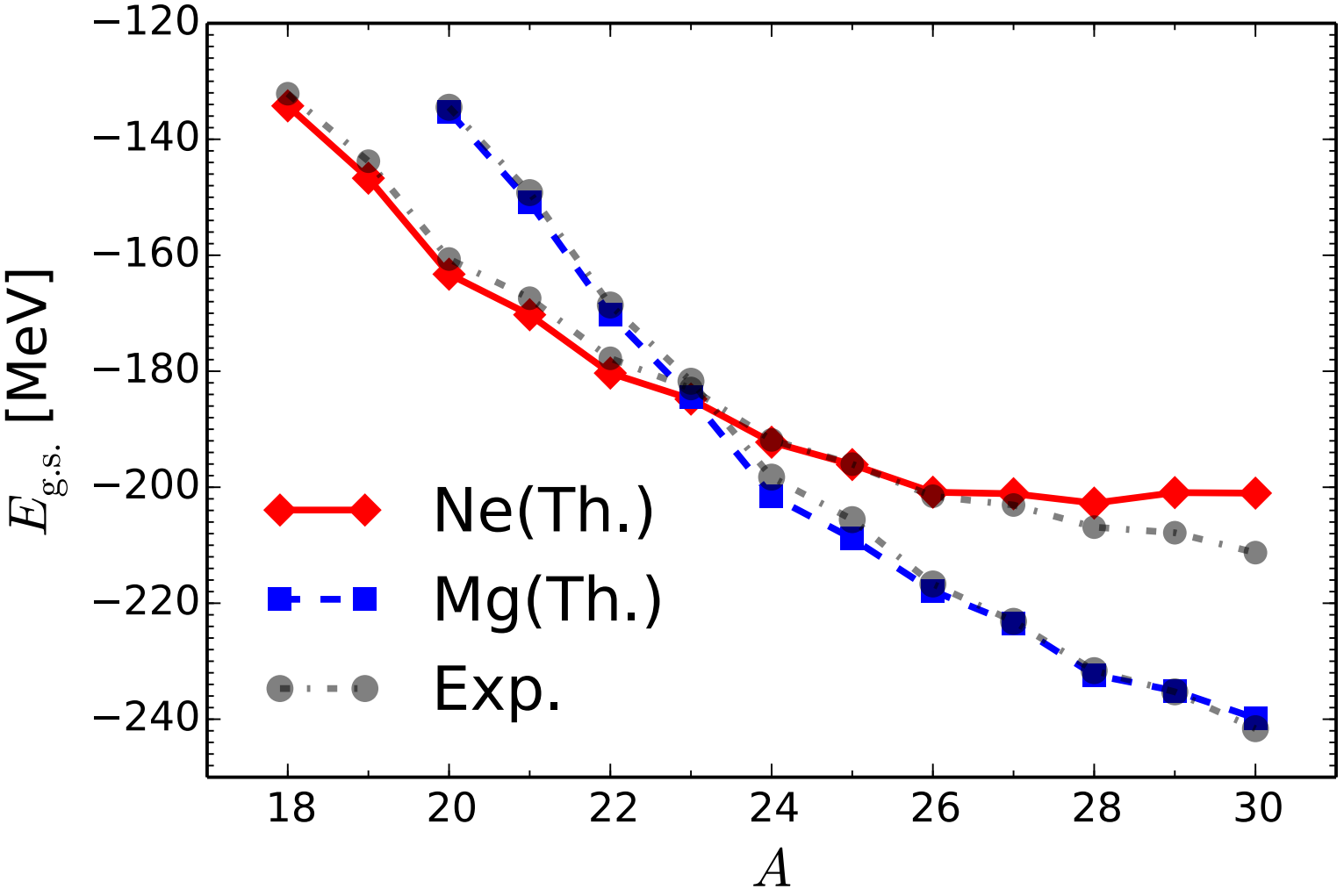
Coupled-Cluster Effective Interactions

G. R. Jansen et al,

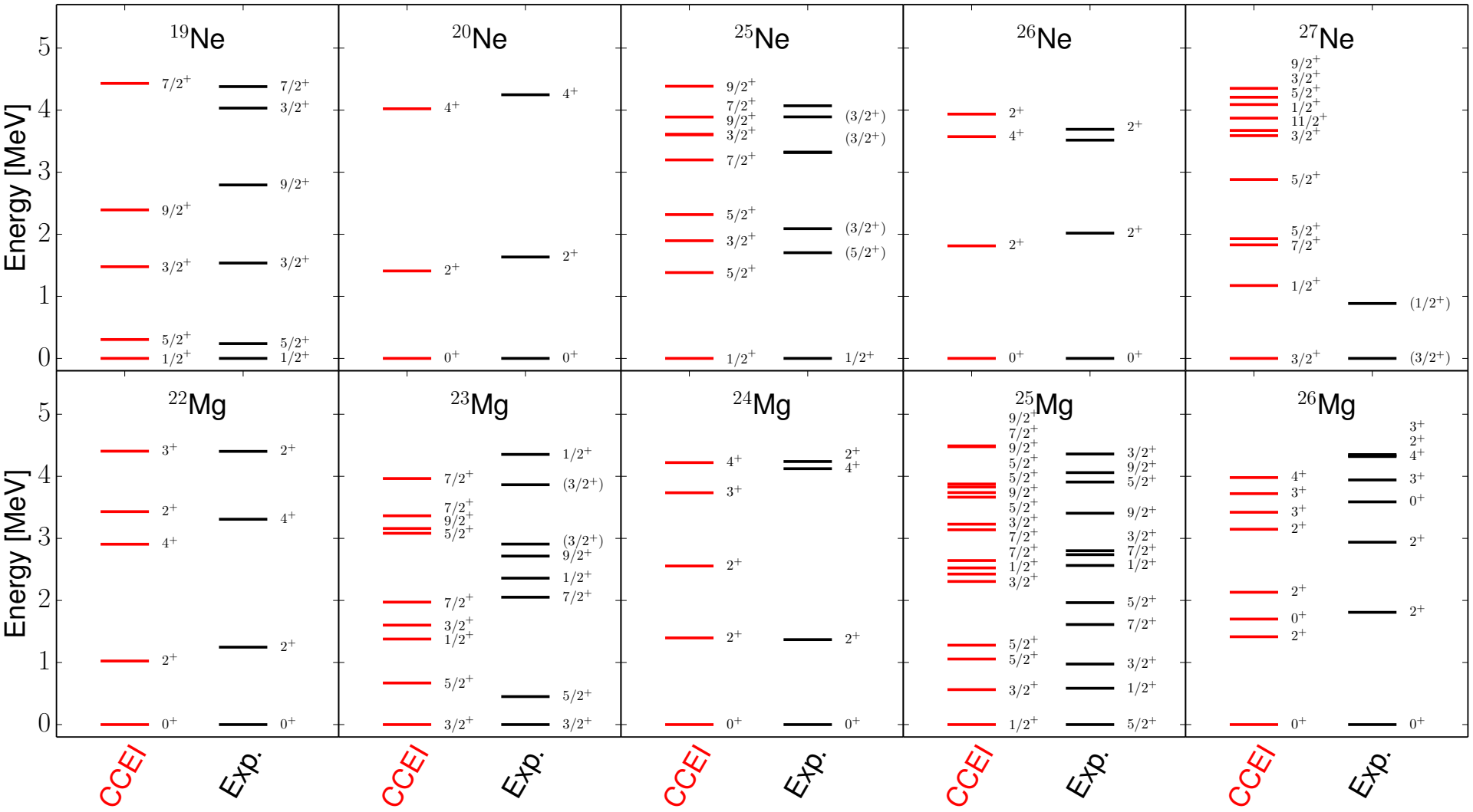
Phys. Rev. Lett. 113, 142502 (2014)



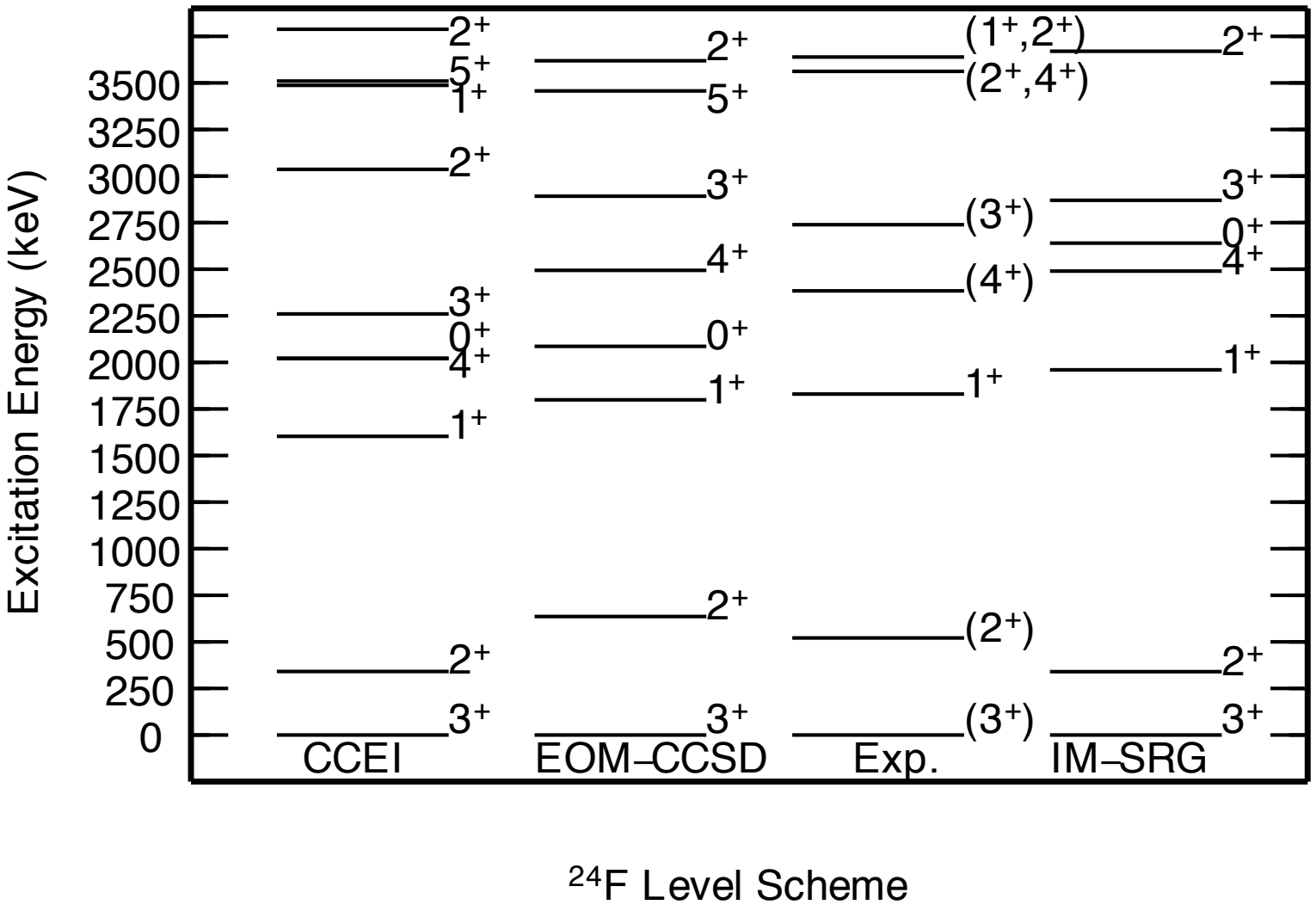
Extending CCEI to nuclei with protons and neutrons in valence space



CCEI for nuclei with protons and neutrons in valence space: Ne and Mg isotopes



Benchmarking different methods in ^{24}F



^{24}F Level Scheme

IM-SRG: L. Caceres et al arXiv:1501.01166 (2015)