Effective interaction and effective operators from the No-Core Shell Model

N. A. Smirnova, Zhen Li, *LP2IB, CNRS/IN2P3 – University of Bordeaux, France*
I.J.Shin, Y. Kim, *LP2IB, IBS, Republic of Korea*
A.M. Shirokov, *SINP, Moscow State University, Russia*
B.R. Barrett, *Arizona State University, USA*
J.P. Vary, P. Maris, *Iowa State University, USA*

Effective interaction and effective operators from the No-Core Shell Model

- **Introduction** (see also talks by Prof. R.V. Jolos and Prof. J.P. Vary on Monday)

- **Formalism**: *ab-initio* effective sd-shell Hamiltonian from the NCSM solution for A=18 via Okubo-Lee-Suzuki similarity transformation

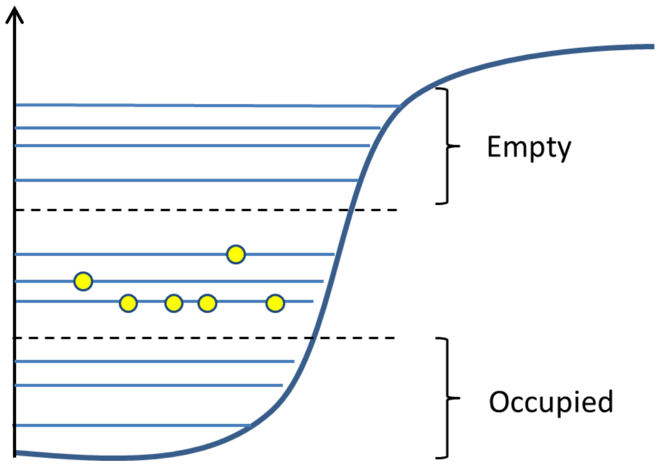
- **Theory & Theory**:
  - comparison of the NCSM solution with Daejeon16 with valence-space calculations for A>18 ;
  - construction of effective electromagnetic operators for A=18.

- **Theory & Experiment**: Analysis of TBMEs, monopole corrections and comparison with experiment and with phenomenological USDB interaction

- **Conclusions and prospects**

Shell model (full configuration-interaction approach)

Resolution of the nuclear many-body problem by Hamiltonian matrix diagonalization



$$H = \sum_i T_i + \sum_{i<j} V_{ij} = \underbrace{\sum_i T_i + \sum_i U_i}_{\text{Independent particle Hamiltonian}} + \underbrace{\sum_{i<j} V_{ij} - \sum_i U_i}_{\text{residual interaction}} = H_0 + V_{res}$$

Independent particle Hamiltonian

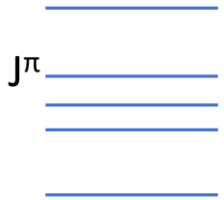
residual interaction

$$H|\Psi_p\rangle = E_p|\Psi_p\rangle$$

$$|\Psi_p\rangle = \sum c_{kp}\,|\Phi_k\rangle$$

$$H_0|\Phi_k\rangle = E_k^0|\Phi_k\rangle \qquad \langle\Phi_k|\Phi_l\rangle = \delta_{kl}$$

$$\sum_{k=1}^{d} \langle\Phi_l|H|\Phi_k\rangle\, c_{kp} = E_p c_{lp} \;\Rightarrow\; \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1d} \\ H_{21} & H_{22} & \cdots & H_{2d} \\ \vdots & & \ddots & \\ H_{d1} & H_{d2} & \cdots & H_{dd} \end{pmatrix} \;\Rightarrow$$



Avantages of the theoretical approach:

- Conservation of symmetries of the full Hamiltonian (rotational, translation invariance, parity, particle number, etc)
- Precise information on low-energy states and transitions
- Excellent description with appropriate interactions and in suitable model space

Challenges :

- Basis dimensions !

Large-scale diagonalization

Basis construction (for example, in M-scheme)

$$\Phi(1,2,\ldots,A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{\alpha_1}(\vec{r}_1) & \phi_{\alpha_1}(\vec{r}_2) & \ldots & \phi_{\alpha_1}(\vec{r}_A) \\ \phi_{\alpha_2}(\vec{r}_1) & \phi_{\alpha_2}(\vec{r}_2) & \ldots & \phi_{\alpha_2}(\vec{r}_A) \\ \vdots & & & \\ \phi_{\alpha_A}(\vec{r}_1) & \phi_{\alpha_A}(\vec{r}_2) & \ldots & \phi_{\alpha_A}(\vec{r}_A) \end{vmatrix}$$

$$\alpha = (nljm)$$

$$\mathrm{Dim} = \binom{D_N}{N} \cdot \binom{D_Z}{Z}$$

Computational challenges :

- (Lowest) eigenvalues of geant, but sparse matrices -> Lanczos algorithm
- Storage of the Hamiltonian matrix elements (if stored, otherwise in-fly computation)

High-performance codes (up to 10^{12} x 10^{12})

- ANTOINE, NATHAN (Strasbourg)
- MFDn (Iowa State U.)
- NushellX (Oxford-MSU)
- Mshell , Kshell (Tokyo)
- Bigstick (St-Diego SU – LLNL-…)
- …

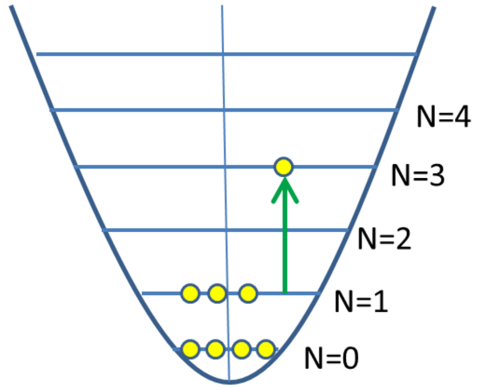
Basis truncation techniques :

- Importance truncated (NC)SM (Darmstadt)
- Symmetry adapted basis (LSU)
- Monte-Carlo SM (Tokyo)
- Generalized seniority approximation,

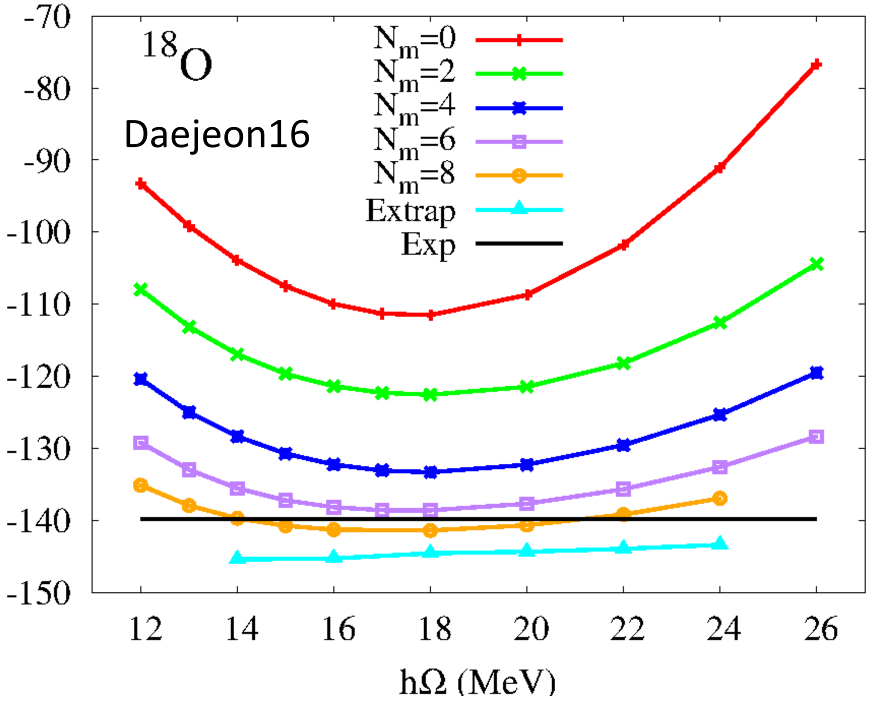
interacting boson approximation …

No-Core Shell Model (for light nuclei)

A nucleons in a (harmonic-oscillator) potential well in a large model space defined by hΩ and Nmax.



$$H = \sum_{i<j} \frac{(\vec{p_i} - \vec{p_j})^2}{2mA} + \sum_{i<j}^{A} V_{ij} + \sum_{i<j<k}^{A} V_{ijk}$$



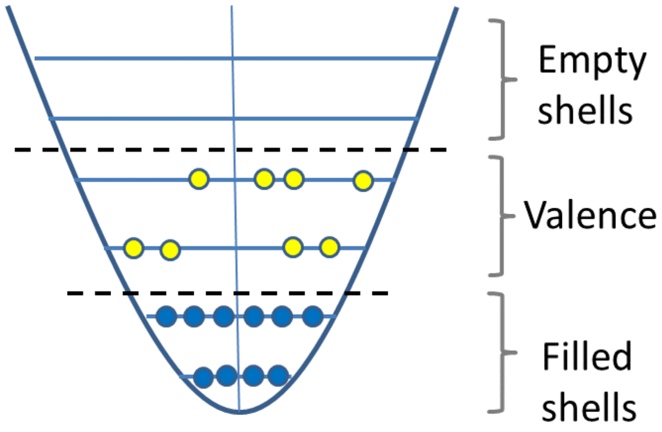
- **Current status :**
  - Calculations with (bare) nucleon-nucleon forces (NN + 3NF)
  - Ground state, excitation spectra, transition probabilities
    => benchmark for nuclear theory
  - Reach *sd* shell nuclei in a large basis (up to A~18)
  - Bridging with reaction theory

MFDn code, P. Maris, J. P. Vary et al, Iowa State University

B.R. Barrett, P. Navratil, J.P. Vary, Ab initio no core shell model, ***PPNP 69****, 131 (2013).*

Valence-space shell model (heavier nuclei)

Restricted model space



Effective operators

$$H|\Psi_p\rangle = E_p|\Psi_p\rangle \quad \rightarrow \quad H_{eff}|\Psi_p^M\rangle = E_p|\Psi_p^M\rangle$$

$$H = T + V = (T + U) + (V - U) = H_0 + V_{res}$$

$(T+U)$: *exactly solvable*; $(V-U)$: *residual interaction*

$$H = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V_{res}|\delta\gamma\rangle\, a_\alpha^\dagger a_\beta^\dagger\, a_\gamma\, a_\delta$$

ε_α: *Empirical*

$\langle\alpha\beta|V_{res}|\delta\gamma\rangle$: *Microscopic*; *Semi-microscopic (microscopic, constrained by the data)*; *Empirical*

- **Current status :**
- Excellent description with empirical (phenomenological) interactions
- Microscopic interactions -> recent progress and challenges

Effective Interactions : monopole-multipole decomposition

Multipole decomposition :

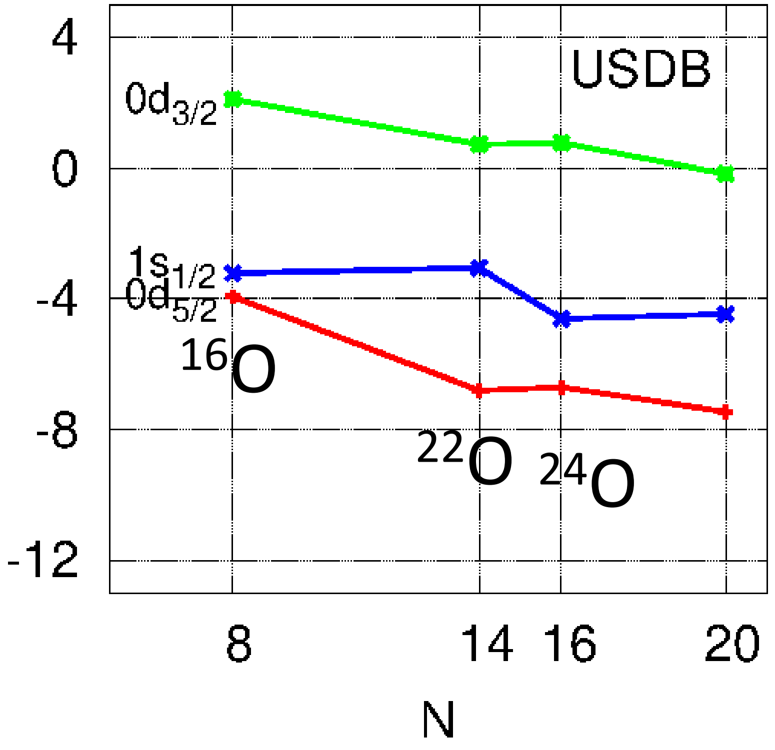
$$H = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4}\sum_{ijkl,\lambda} w_{ijkl,\lambda} [\, a_i^\dagger \tilde{a}_j \,]^{(\lambda)} [\, a_k^\dagger \tilde{a}_l \,]^{(\lambda)} + \cdots$$

$$H = \underbrace{\sum_i \varepsilon_i n_i + \sum_{i<j} \bar{V}_{ij} \frac{n_i(n_j - \delta_{ij})}{1+\delta_{ij}}} + \underbrace{V_{pair} + V_{quad} + \cdots}$$

Monopole part (spherical mean-field)

Multipole part (correlations)

Neutron ESPEs in O-isotopes (from monopole part)



USDB – universal sd interaction: W.A. Richter, B.A.Brown, PRC74 (2006)

- **Important to understand the nature of nuclear excitations (competition between sphericity and deformation)**
- **Only a physically meaningful combination of these ingredients will results in a successful description !**

E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, A. Zuker, RMP77,427 (2005)

Microscopic approaches to valence space interactions

$$H|\Psi_p\rangle = E_p|\Psi_p\rangle$$

$$\langle\Psi_f|O|\Psi_i\rangle = O_{fi}$$

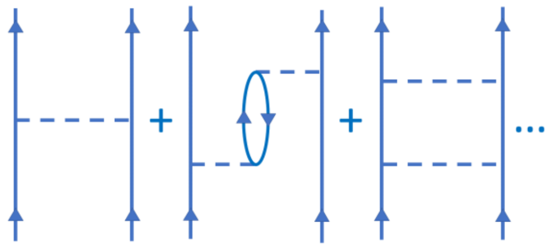
Effective operators

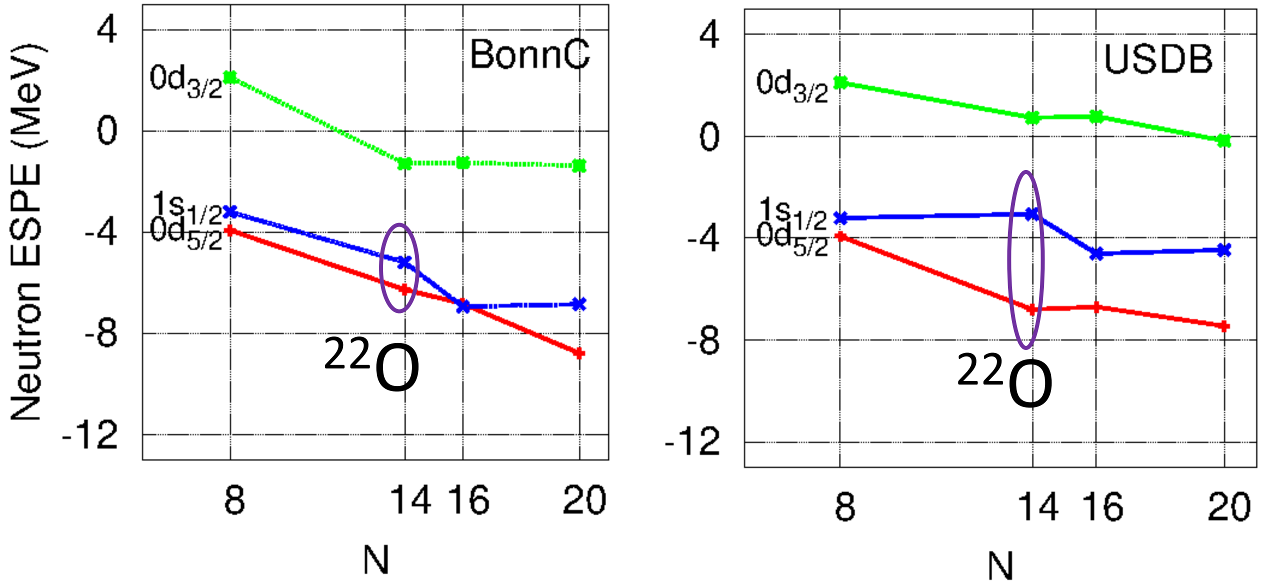
$$H_{eff}|\Psi_p^M\rangle = E_p|\Psi_p^M\rangle$$

$$\langle\Psi_f^M|\, O_{eff}|\Psi_i^M\rangle = O_{fi}$$

Theoretical approach: **Many-body perturbation theory** based on the G-matrix (NN)

G.F. Bertsch, T.T.S. Kuo, G.F. Brown, B.R.Barrett, M.Kirson, et al. (from 60's)
M. Hjorth-Jensen, T.T.S. Kuo, E. Osnes, PR261, 126 (1995)

Veff =




Poor description of the monopole term (spherical mean-field)

Missing 3N forces

Conjectured : A.Poves, A.P. Zuker, PR70, 71 (1981)
A.P. Zuker, PRL90, 042502 (2003)
Confirmed : T. Otsuka et al (2010), J. Holt et al (2014); L. Coraggio et al (2018 – 2020), etc.

Microscopic approaches to valence space interactions

Non-perturbative approaches :

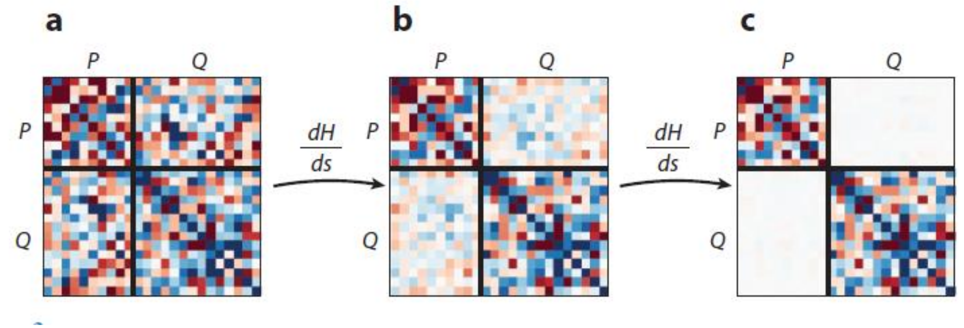
Review : S. R. Stroberg, H. Heigert, S.K. Bogner, J.D. Holt, ***ARNPS 69,*** *307 (2019).*

- **Valence-space In-Medium Similarity Renormalization Group – IMSRG** (NN + 3N)

  S.R. Stroberg et al, PRC93, 051301 (2016); PRL118, 032502

  $$H(s) = U(s)H(0)U^{\dagger}(s),$$

  $$dH(s)/ds = [\eta(s), H(s)]$$



- **OLS transformation applied to NCSM results**

  $$PH_{eff}Q = QH_{eff}P = 0$$

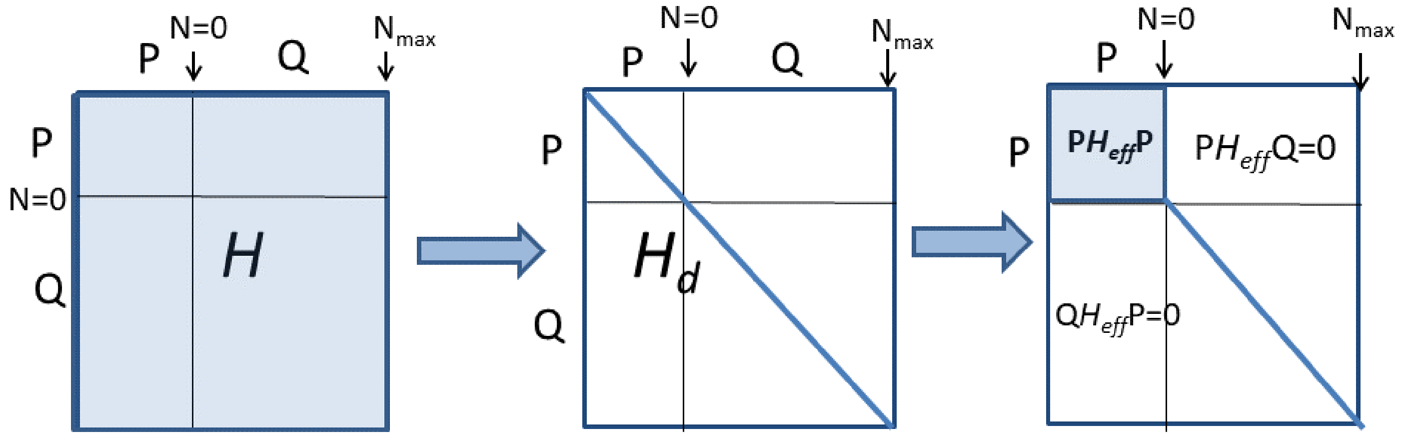
  E.Dikmen et al, PRC94 (2015); N. Smirnova, B.R. Barrett et al, PRC100 (2019)

- **Coupled-cluster theory** $(NN + 3N)$

  G.R. Jansen et al, PRC94, 011301 (2016); Z.H. Sun, T.D. Morris, G. Hagen et al, PRC98 (2018)

Ab-initio effective Hamiltonian from the NCSM

Okubo-Lee-Suzuki (OLS) similarity transformation
of the NCSM solution



$$H_d = UHU^\dagger \qquad H_{eff} = \frac{U_P^\dagger}{\sqrt{U_P U_P^\dagger}} H_d \frac{U_P}{\sqrt{U_P U_P^\dagger}}$$

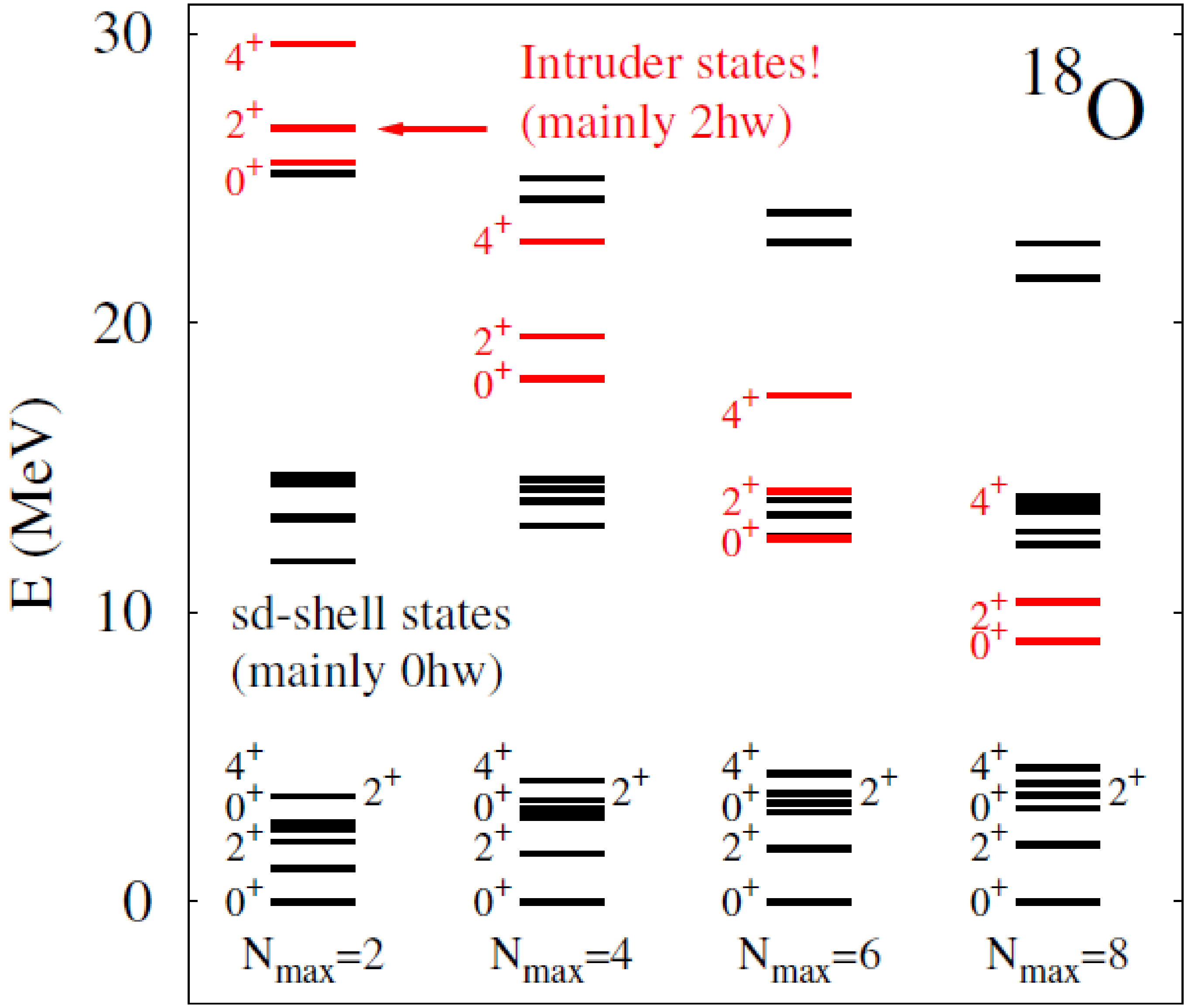
FLOW

- ❑ ^{18}F from the NCSM at N_{max}
- ❑ H_{eff} for ^{18}F at N=0
- ❑ ^{16}O from the NCSM at N_{max}
  - → Core energy
- ❑ ^{17}O, ^{17}F from the NCSM at N_{max}
  - → One-body terms
- ❑ Single-particle energies ε_i

two-body matrix elements V_{ijkl}

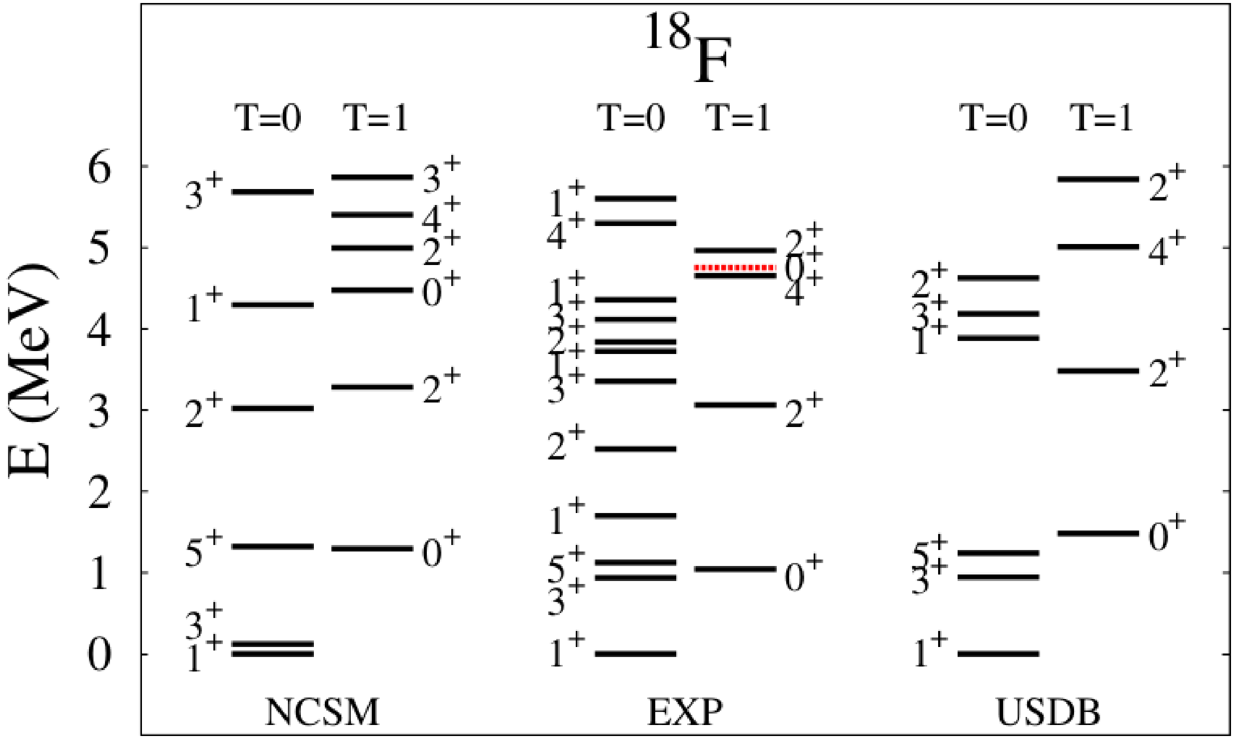
S. Okubo, Prog. Theor. Phys. 12 (1954); K. Suzuki, S. Lee, Prog. Theor. Phys. 68 (1980)
E. Dikmen, A. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
J.P. Vary , R. Basili, W.Du, M. Lockner, P. Maris, S.Pal, S.Sarker PRC98, 065502 (2018)
N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100 (2019)

Low-energy spectrum of ^{18}O from the NCSM with Daejeon16

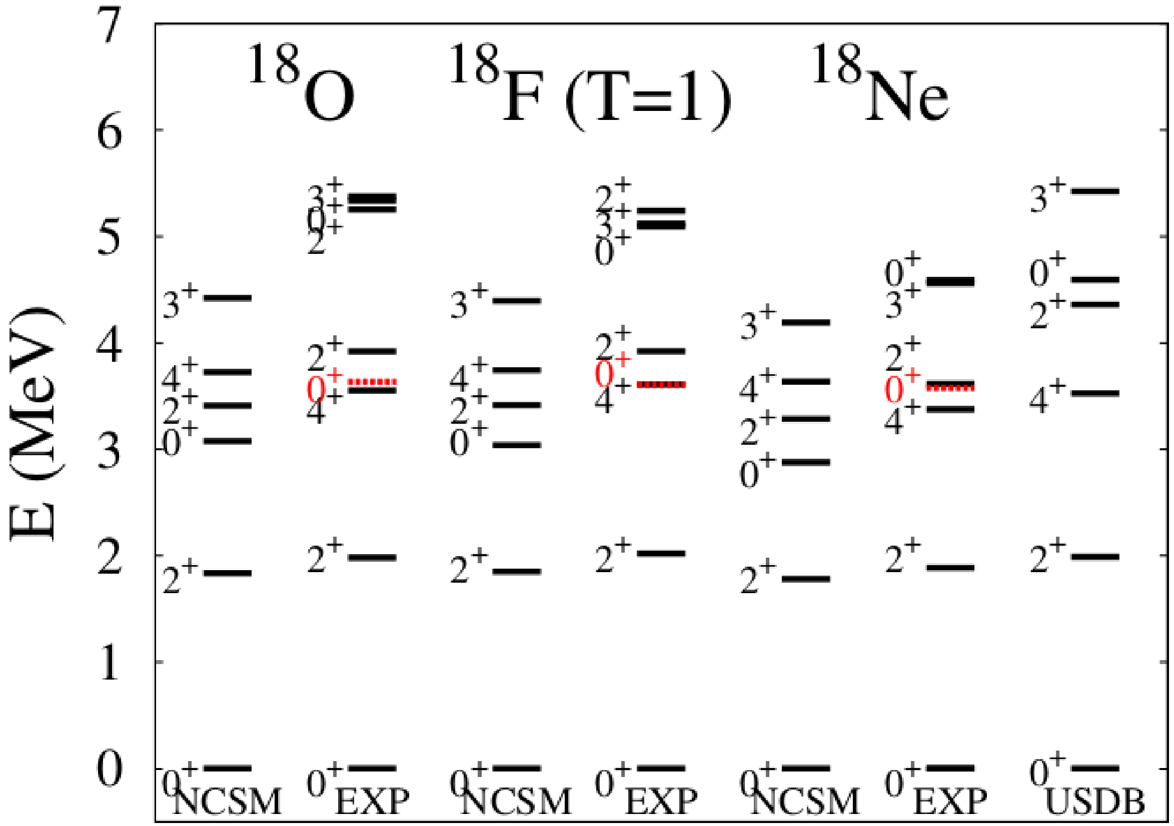


- Contrary to the states dominated by sd-shell components, the energies of intruder states are not converged yet !
- Intruder states are identified experimentally by large E2 matrix elements

Ab-initio effective Hamiltonian from the NCSM with Daejeon16

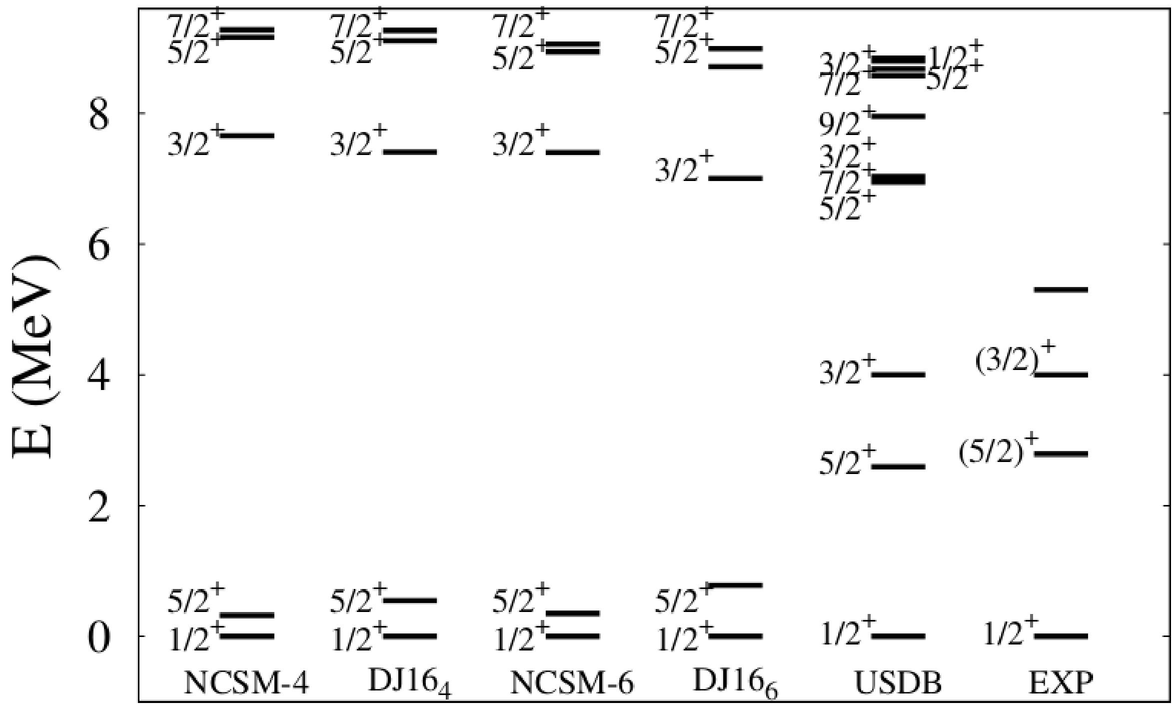


By construction, valence-space two-nucleon calculation reproduces NCSM results



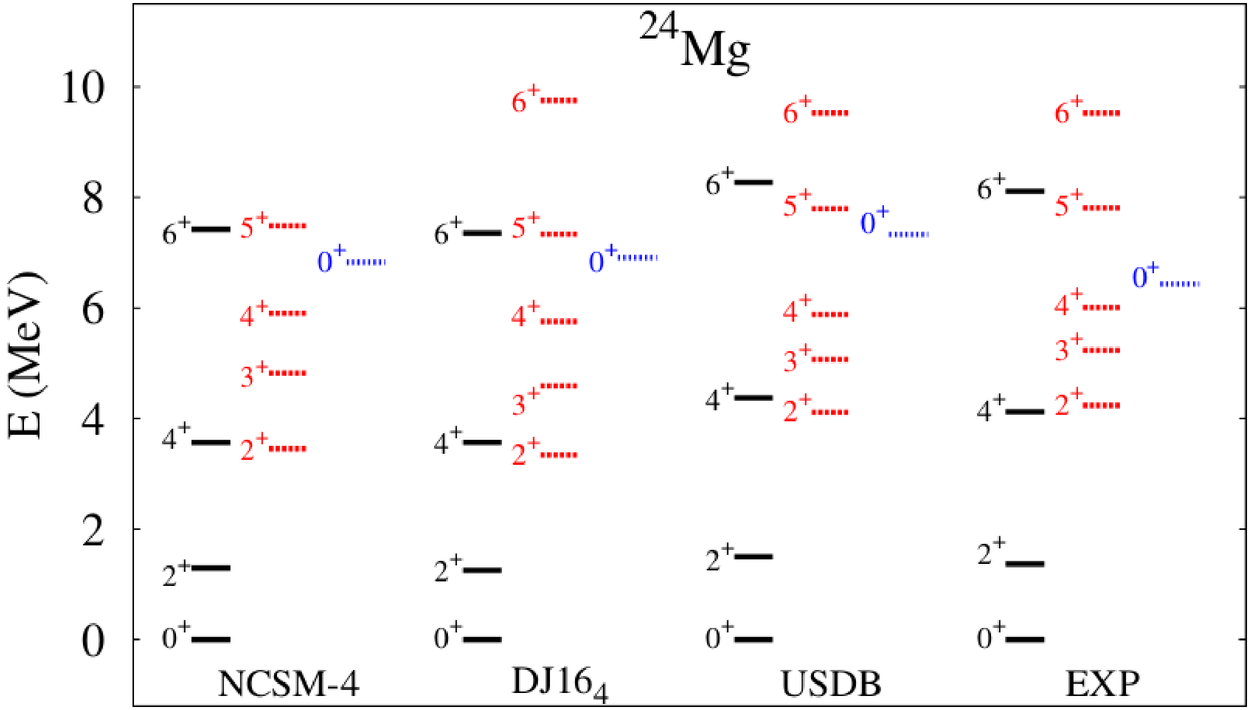
Ab-initio effective Hamiltonian from the NCSM : A>18 nuclei

^{23}O



14 states : rms error 63 keV

9 states : rms error 225 keV



Electromagnetic transition operators from the NCSM

Effective $E2$ operator in the sd shell

$$e_{n/p}(a,b)\langle b||r^2\hat{Y}_2(\hat{r})||a\rangle = \langle J_f||\hat{O}(E2)||J_i\rangle \quad (\text{from } ^{17}\text{O}/^{17}F)$$

sd-shell single-particle matrix elements

from the NCSM

$$\hat{O}(E2) = \sum^{A} e_k r_k^2 \hat{Y}_2(\hat{r}_k) \quad (e_n = 0, e_p = e)$$

Bare one-body operator

State-dependent effective charges/g-factors

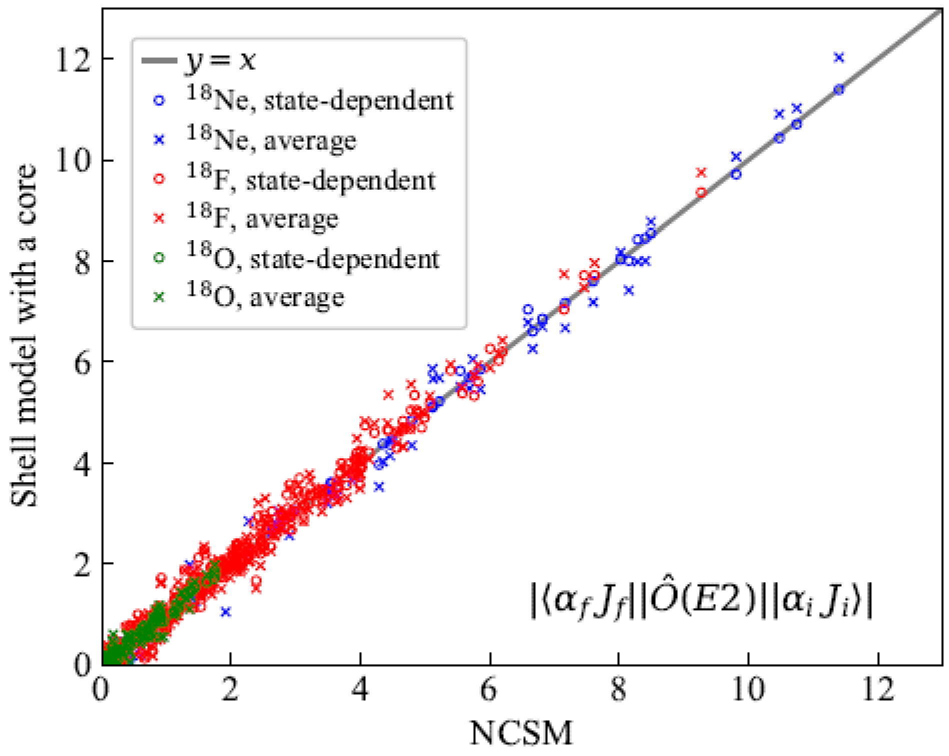
(a,b)	$e_n(a,b)$	$e_p(a,b)$	$g_n^s(a,b)$	$g_n^l(a,b)$	$g_p^s(a,b)$	$g_p^l(a,b)$
bare	0.0	1.0	-3.826	0.0	5.586	1.0
$(0d_{5/2},1s_{1/2})$	0.181	1.171				
$(0d_{5/2},0d_{3/2})$	0.281	1.236	-3.608	0.020	5.252	0.916
$(1s_{1/2},0d_{3/2})$	0.168	1.297				
$(0d_{5/2},0d_{5/2})$	0.179	1.060	-3.751	0.026	5.499	0.976
$(0d_{3/2},0d_{3/2})$	0.172	1.248	-3.690	0.033	5.332	0.957
$(1s_{1/2},1s_{1/2})$			-3.729		5.468	
	$\overline{e}_n$	$\overline{e}_p$	$\overline{g}_n^s$	$\overline{g}_n^l$	$\overline{g}_p^s$	$\overline{g}_p^l$
average	0.196	1.202	-3.695	0.026	5.388	0.950
typical	0.35	1.35	-3.826	0.0	5.586	1.0

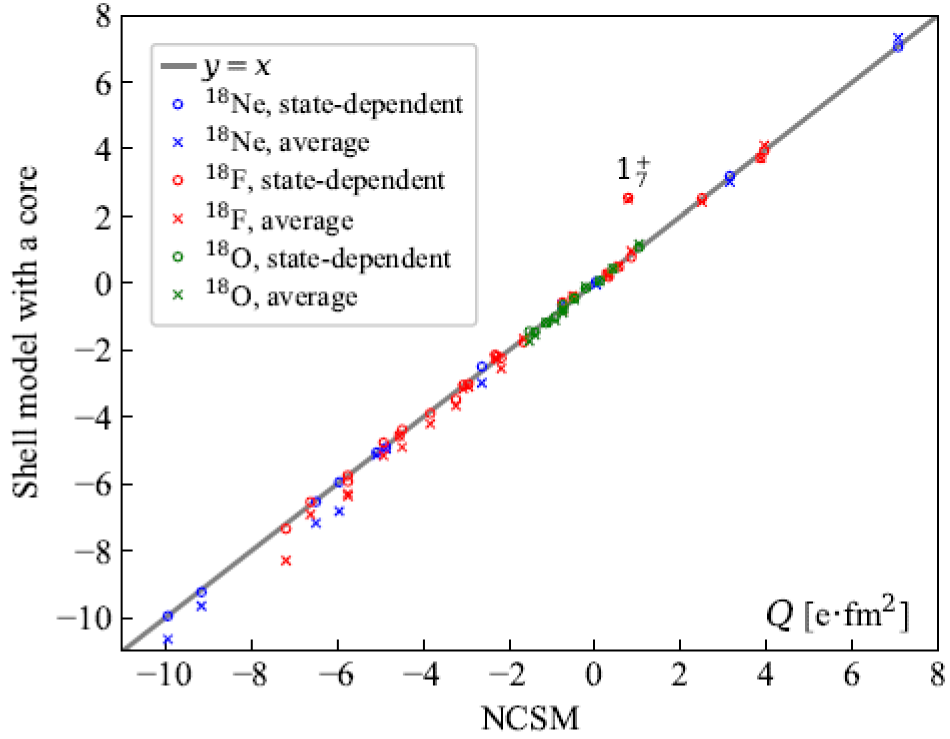
Idem for M1 operator =>
Effective g-factors

Effective one-body
state-dependent
transition operators !

E2 operator from the NCSM : transitions and moments in A=18

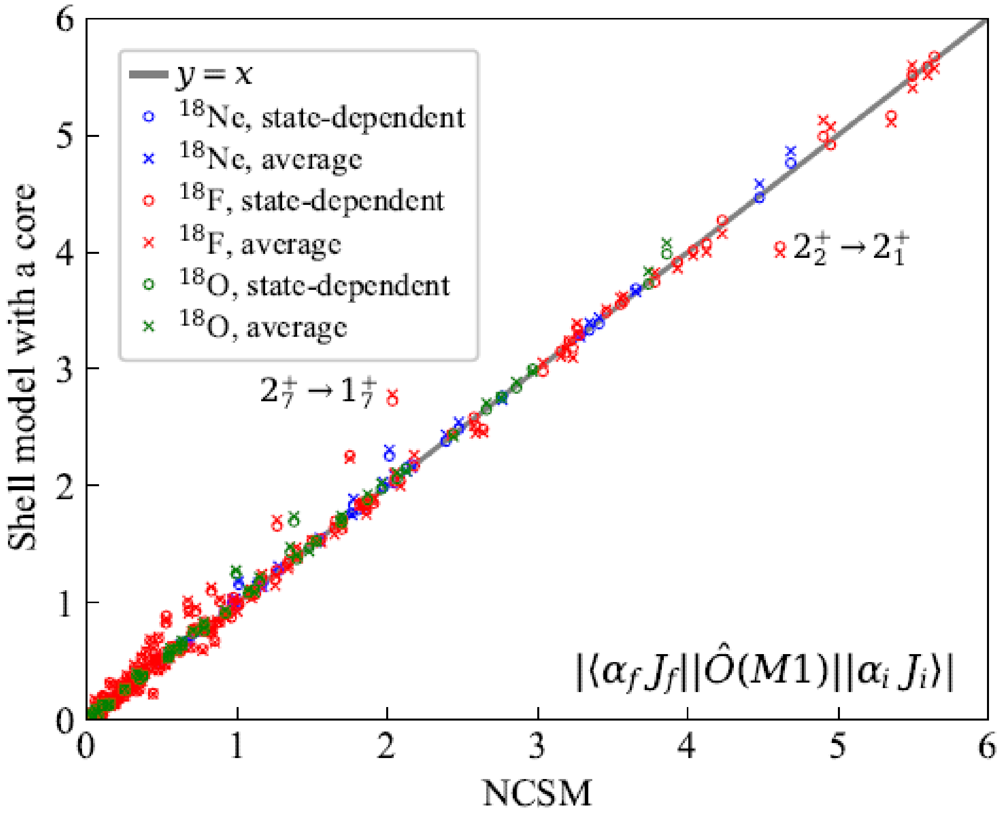
^{18}O : rms(RME) $\approx$ 0.07 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2
^{18}F : rms(RME) $\approx$ 0.11 e.fm^2 (269 data), rms(Q)$\approx$ 0.37 e.fm^2
^{18}Ne : rms(RME)$\approx$ 0.22 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2

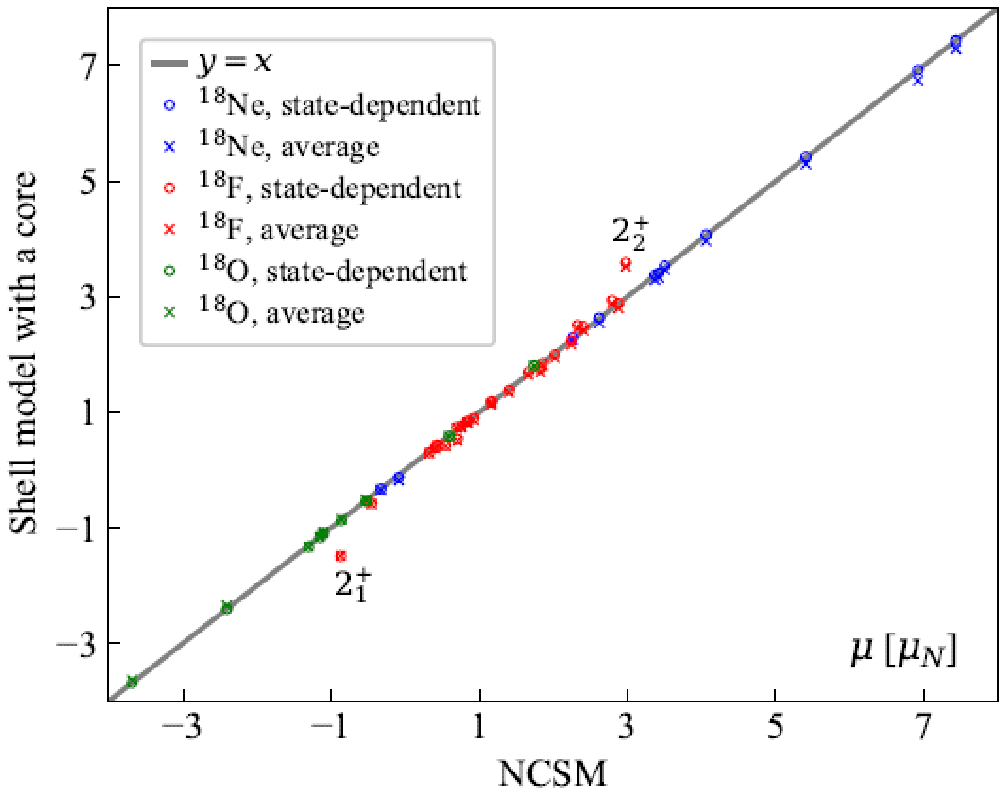




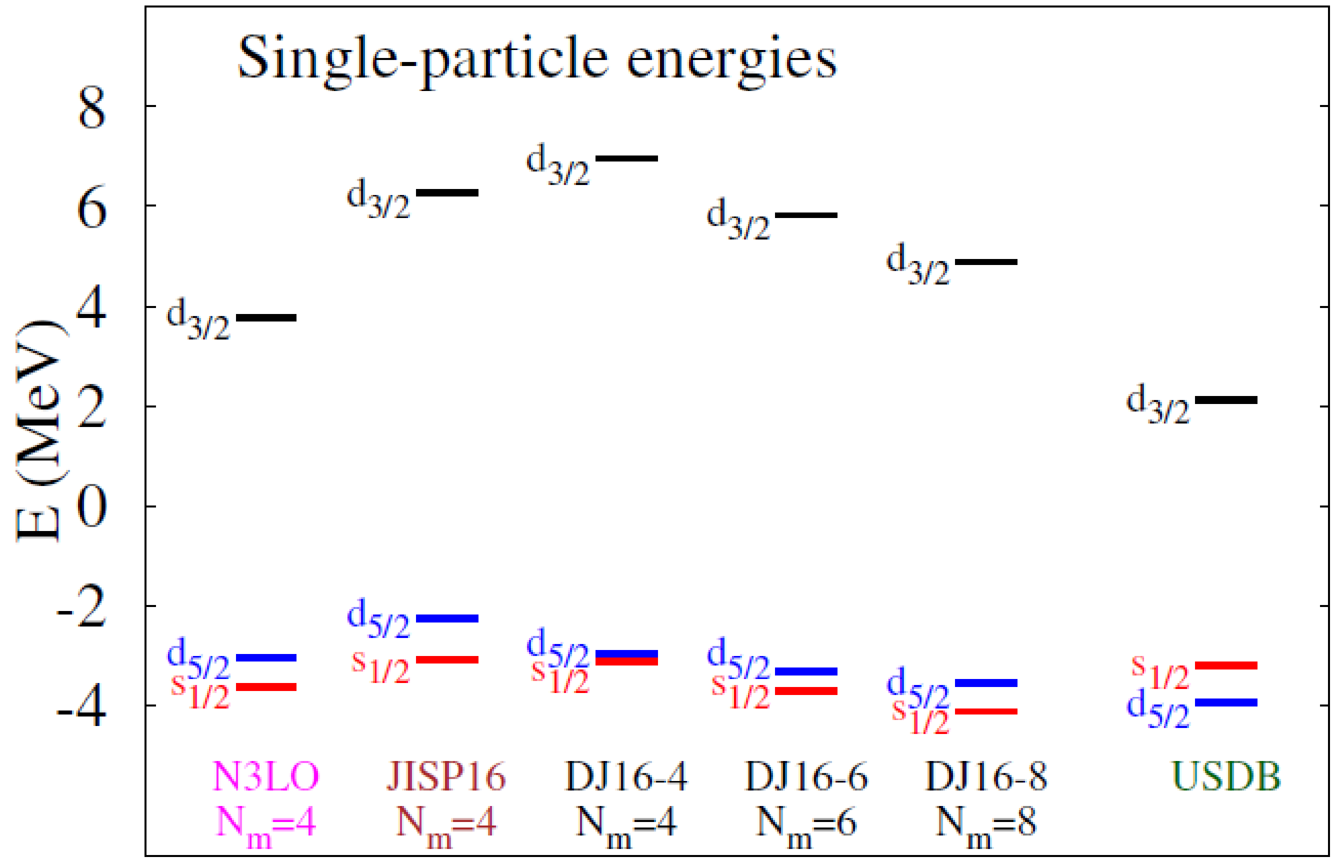
M1 operator from the NCSM : transitions and moments in A=18

^{18}O : rms(RME) $\approx$ 0.06 μ_N (43 data), rms(μ) $\approx$ 0.02 μ_N
^{18}F : rms(RME) $\approx$ 0.09 μ_N (212 data), rms(μ)$\approx$ 0.19 μ_N
^{18}Ne : rms(RME)$\approx$ 0.06 μ_N (43 data), rms(μ) $\approx$ 0.02 μ_N





Ab-initio effective Hamiltonian from the NCSM : Theory & Experiment



Drawbacks :

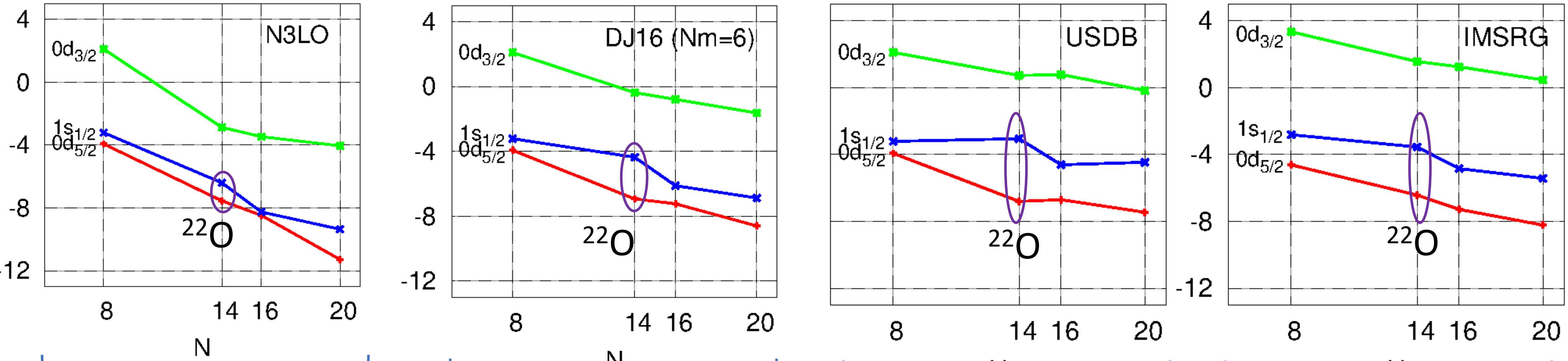
- *Inversion of s1/2 and d5/2 orbitals*
- *Too large d3/2 – d5/2 spin-orbit splitting*

We adopt USDB single-particle energies and impose an $A^{-1/3}$ mass dependence on TBMEs

N3LO : from chiral EFT by D.R.Entem, R.Machleidt, PRC68 (2003)
JISP16 : A.M. Shirokov et al, PRC70, 044005 (2004)
Daejeon16 : A.M. Shirokov et al, PLB761, 87 (2016) – based on N3LO + SRG evolved + phase-equivalently transformed

Comparison of monopole properties valence-space interactions

Neutron ESPEs in O-isotopes



From NN interaction

From Daejeon16 NN interaction

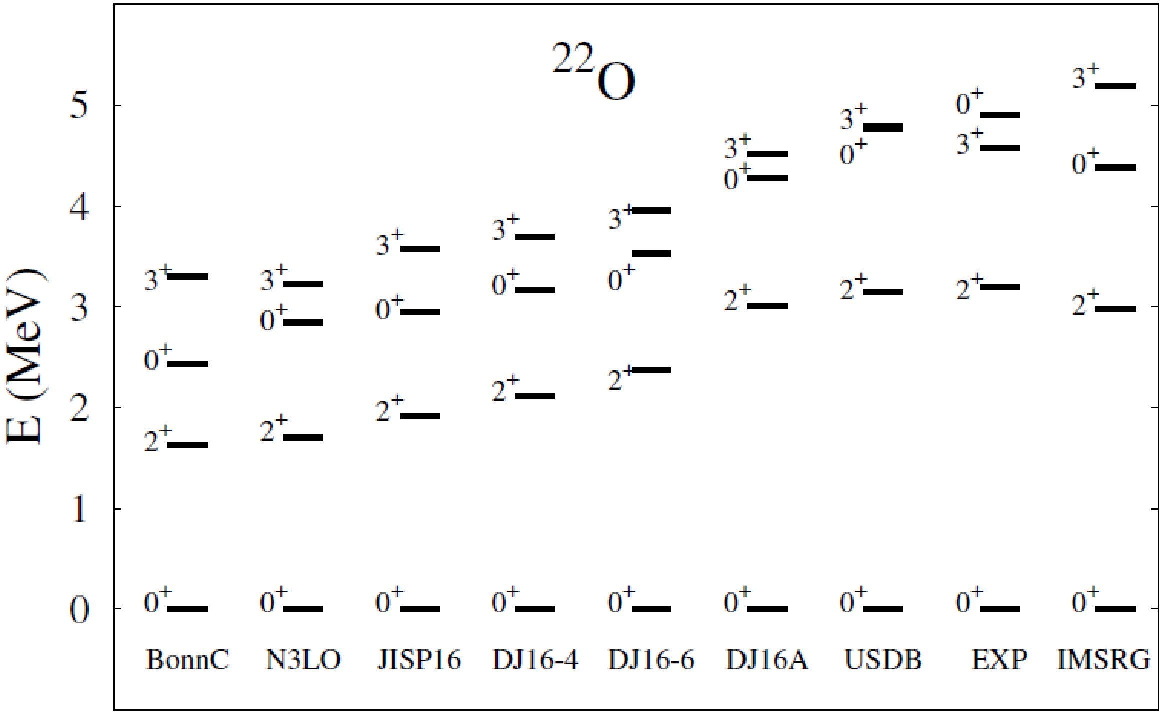
Empirical = experiment

From NN+3N interaction

Small monopole modifications to DJ16 (change of centroids by ~100-300 keV) can be useful !

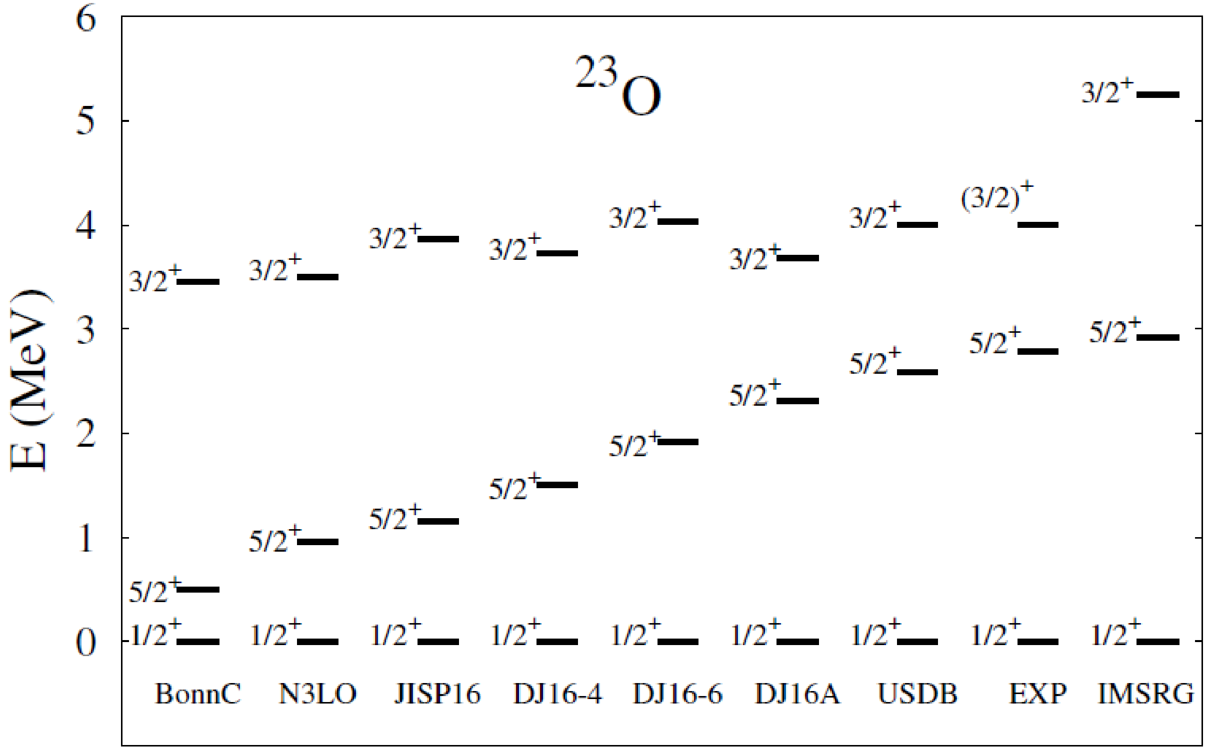
N. Smirnova, B.R. Barrett, Y. Kim, I.J. Shin, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, ***PRC100****, 054329 (2019) and in preparation*

Ab-initio effective Hamiltonian from the NCSM



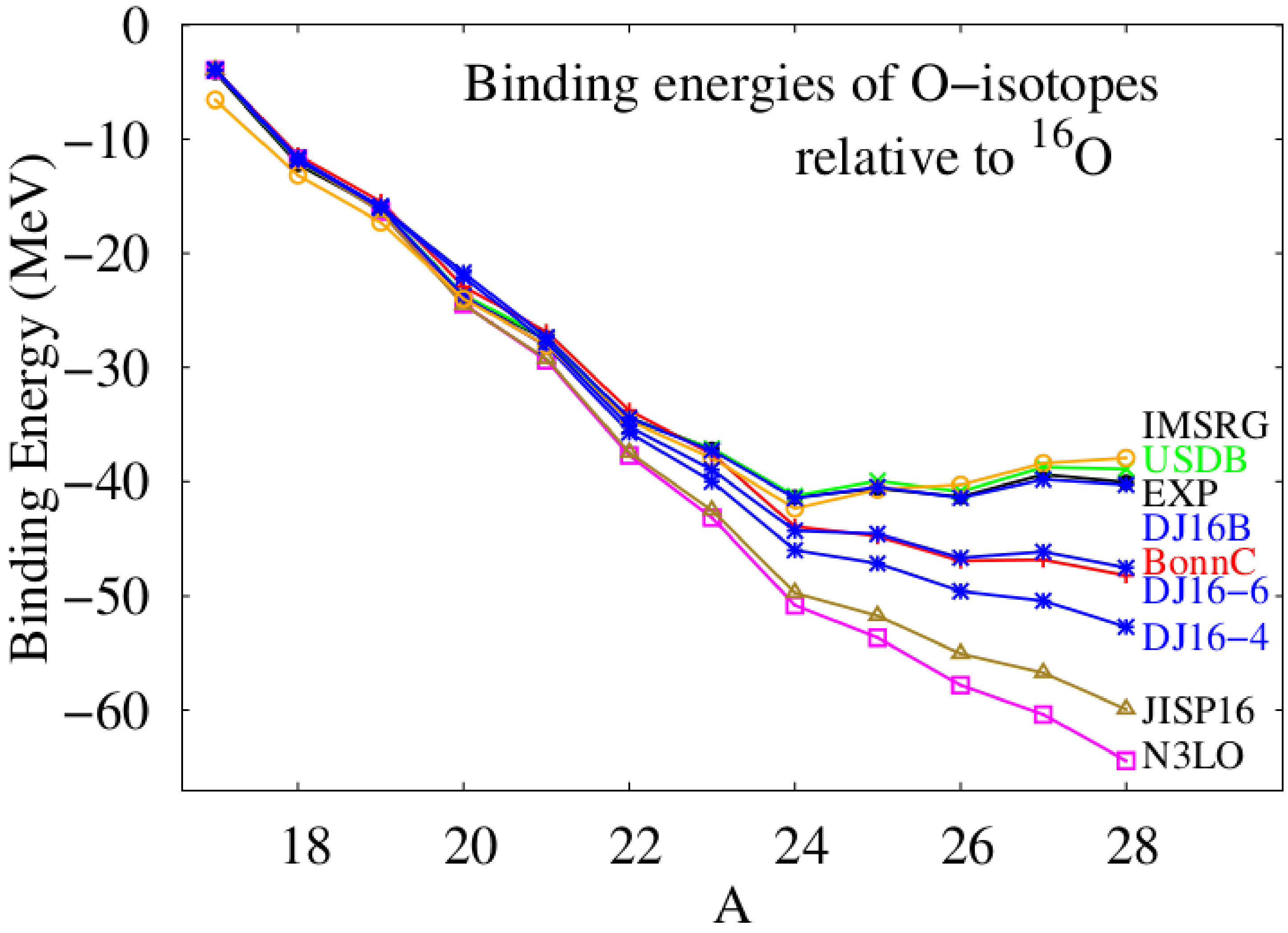
Increase of N=14 subshell gap

DJ16A is DJ16-4 with monopole modifications
DJ16B is DJ16-6 with monopole modifications



Increase of N=14 subshell gap

Ab-initio effective Hamiltonian from the NCSM

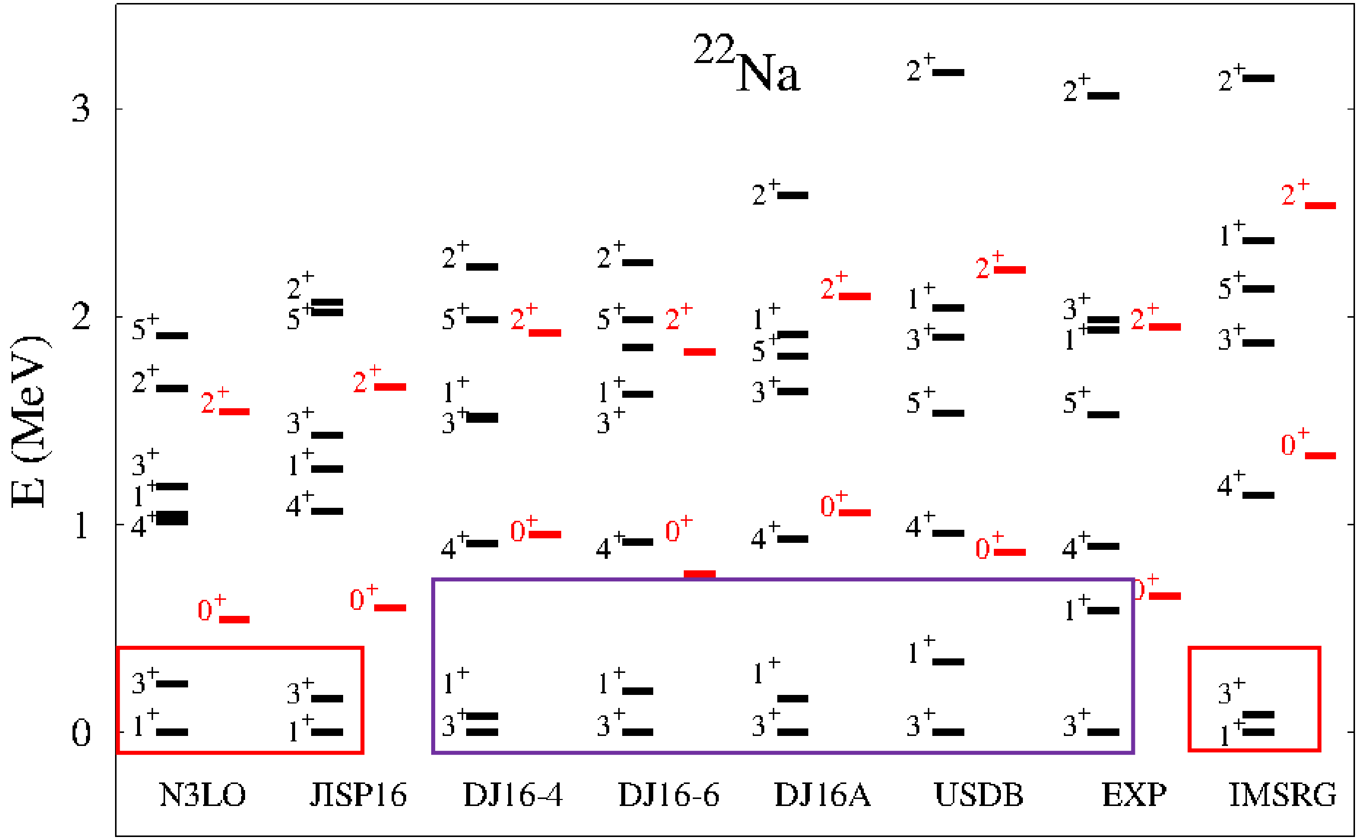


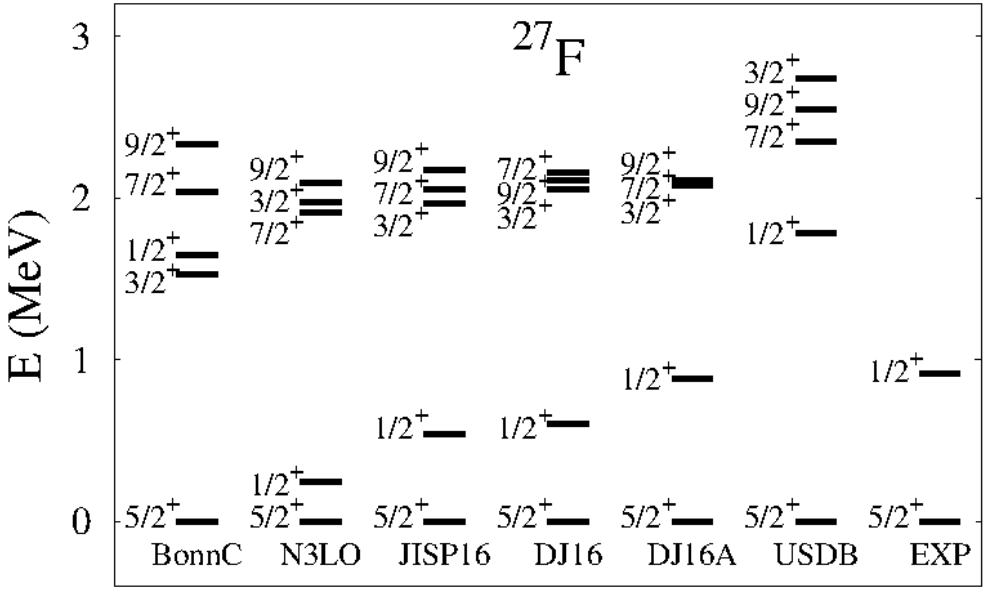
DJ16-6 : rms = 3671 keV

DJ16B (DJ16-6 with monopole modifications): rms = 235 keV

USDB : rms =467 keV

Microscopic effective interactions





RMS (microscopic) > RMS (phenomenological)

For detailed nuclear spectroscopy and applications - Experimentally constrained Interactions !

Conclusions and Perspectives

- Microscopic derivation of effective valence-space interaction for the nuclear shell model is still challenging, although it rapidly progresses

- OLS transformation of the NCSM solution gives encouraging results :

  further steps are foreseen towards larger NCSM spaces and/or larger valence-spaces (*p-sd-pf*).

- Effective interaction theory -> towards microscopic foundations of the model and link to the ab-initio nuclear theory

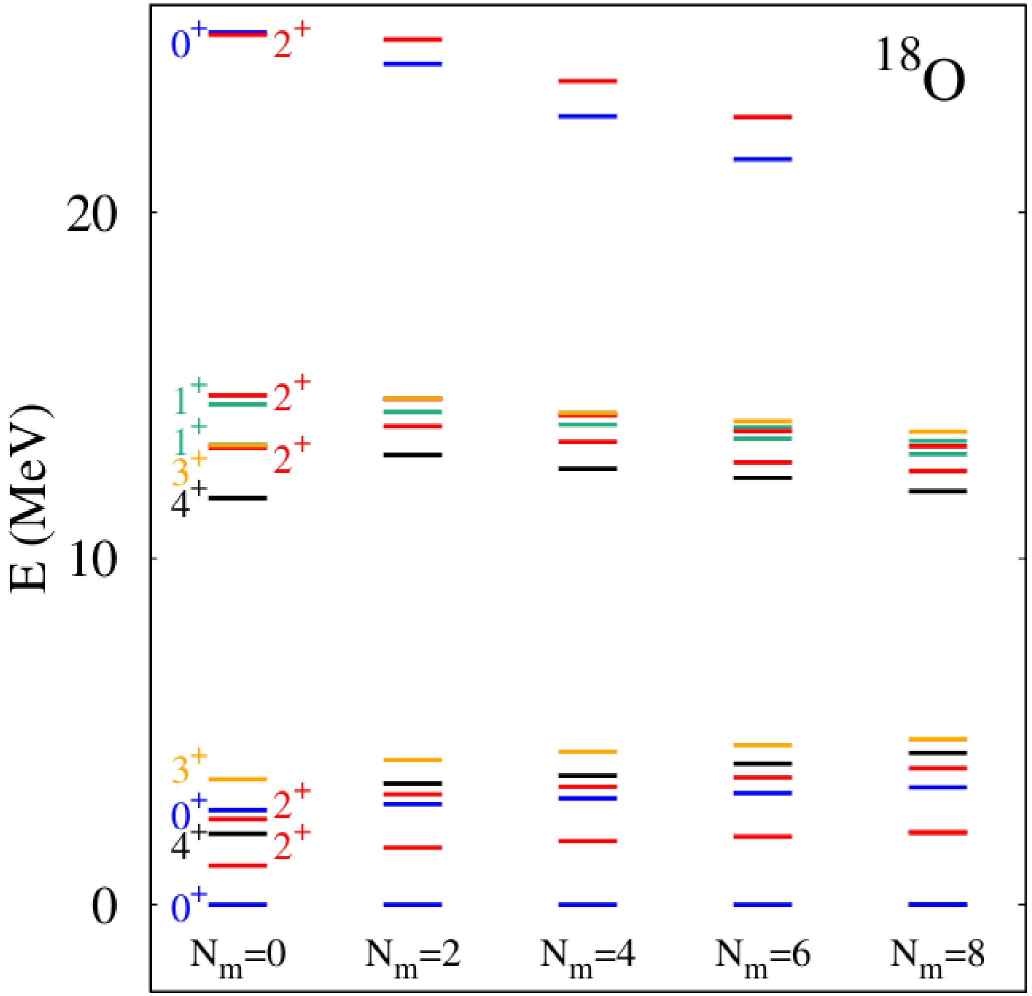
- Importance of further developments of microscopic approaches towards precision nuclear theory for spectroscopy of exotic nuclei, fundamental interaction studies and astrophysical applications

THANK YOU FOR YOUR ATTENTION !

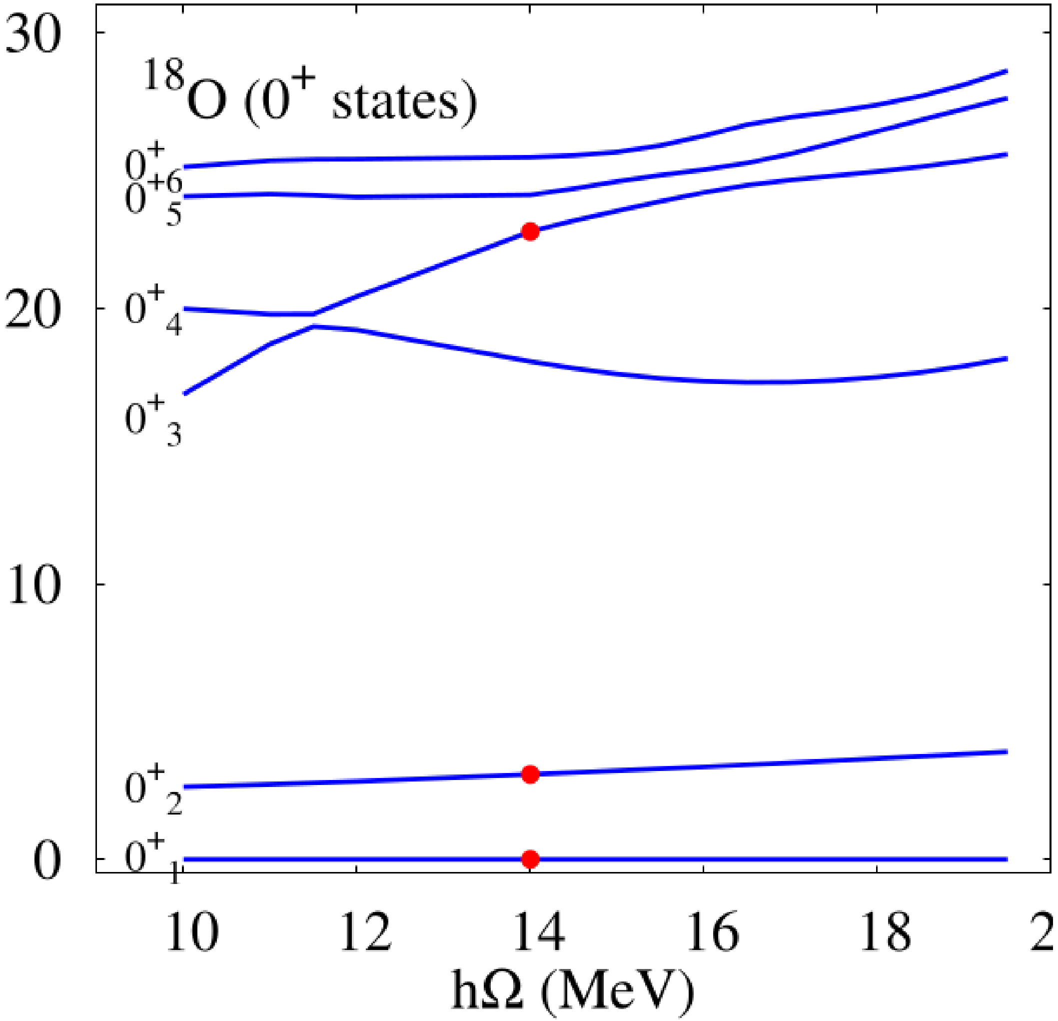
BACKUP SLIDES

Excitation spectrum and state selection for A=18

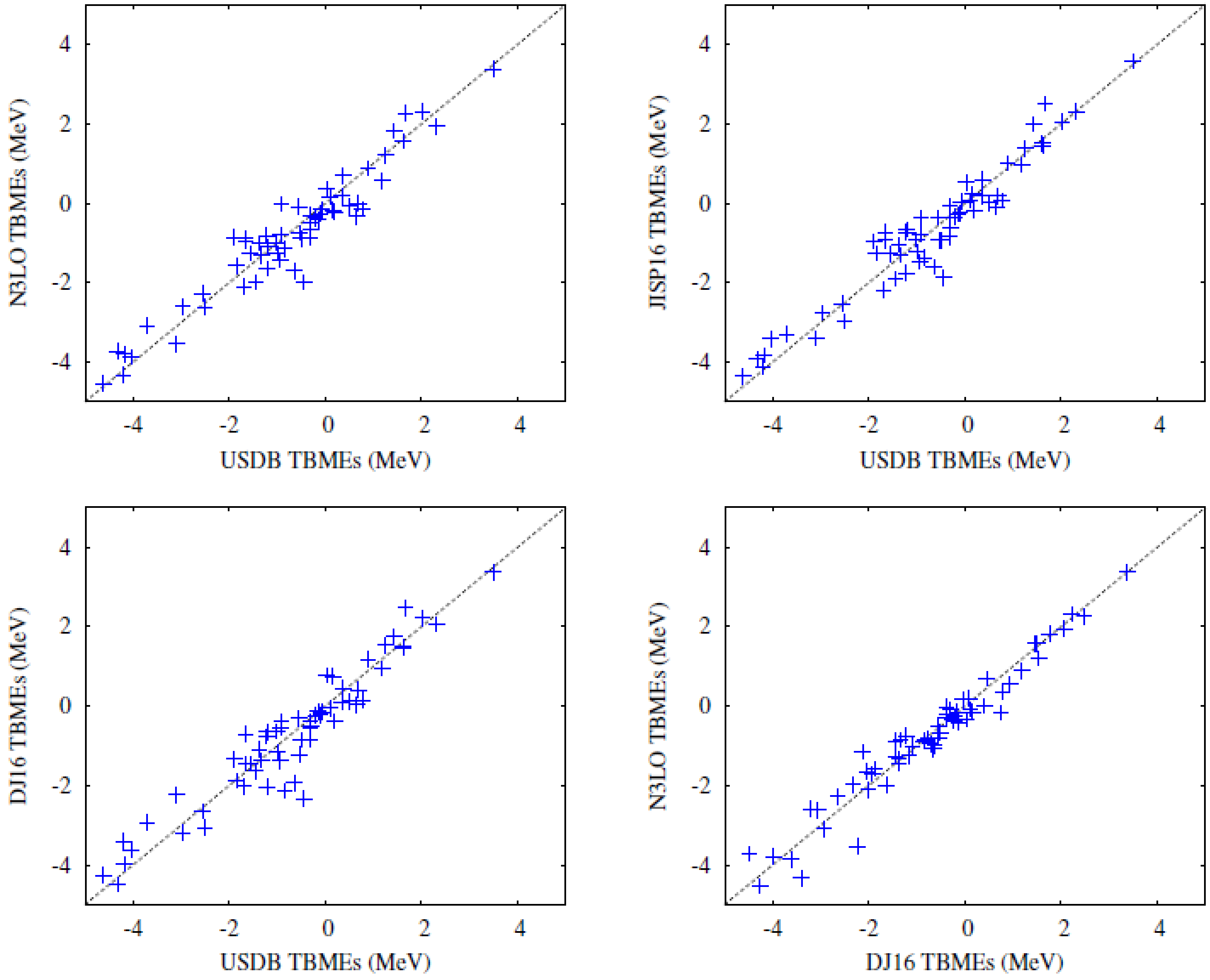
$\hbar\Omega = 14\ MeV$



$N_{max} = 4$



Comparison of TBMEs: microscopic & empirical (USDB)



Microscopic approaches to valence space interactions

χEFT

$\left(Q/_{\Lambda}\right)^{\nu}$, $Q \sim m_{\pi}$, $\Lambda \sim M_N$

$|V_{2N}| \gg |V_{3N}| \gg |V_{4N}|$

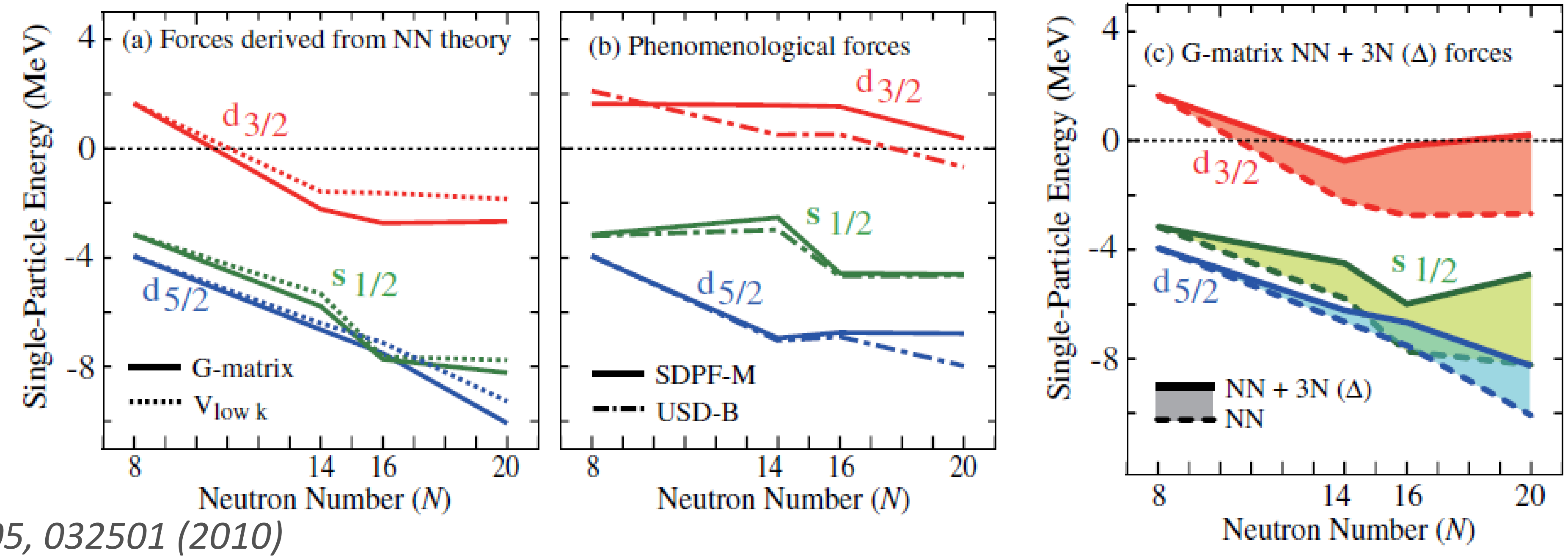
Modern theoretical approaches to effective interactions (with 3N forces)

- **Many-body perturbation theory with $V_{low\text{-}k}$ or V_{SRG}** (NN + 3N)

  T. Otsuka et al, PRL105, 032501 (2010); J.D. Holt et al, PRC90, 024312 (2014)

  Y.Z. Ma, L. Coraggio et al, PRC100, 034324 (2019); L. Coraggio et al, PRC102, 054326 (2020)

➢ **3N forces correct monopoles !**



From T. Otsuka et al, PRL105, 032501 (2010)

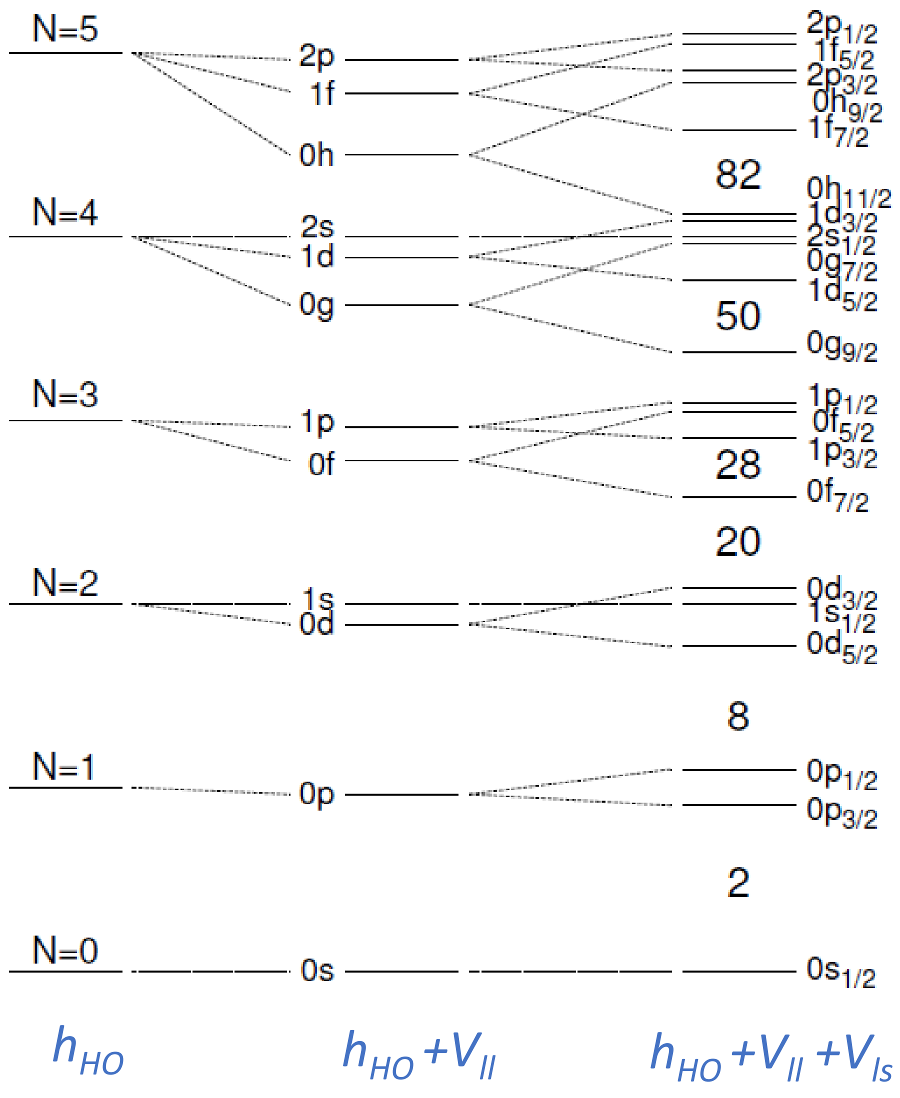
Independent-particle shell model

A spherically symmetry average potential + spin-orbit term

M. Goeppert-Mayer, PR75 (1949); PR78 (1950)
O.Haxel, J.H.D.Jensen, H.E.Suess, PR75 (1949)

For example, a harmonic-oscillator potential with orbital and spin-orbit terms

$$h = \underbrace{-\frac{\hbar^2}{2m}\triangle + \frac{1}{2}m\Omega^2 r^2}_{h_{HO}} + \underbrace{f_{ll}(r)\left(\vec{l}\cdot\vec{l}\right)}_{V_{ll}} + \underbrace{f_{ls}(r)\left(\vec{l}\cdot\vec{s}\right)}_{V_{ls}}$$



Capabilities :

- Magic numbers
- Spin and parities of g.s. of many odd-A nuclei known at that time

Challenges :

- Nuclear structure and decay in their complexity

➡ Need for accounting of the nucleon-nucleon interaction (realistic potential, residual interaction,..)