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

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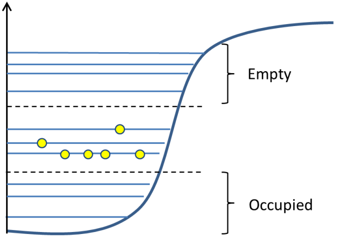
Plan

1. Introduction
2. Formalism: *ab-initio* effective *sd*-shell Hamiltonian from the **NCSM** solution for $A = 18$ via Okubo-Lee-Suzuki similarity transformation
3. **Theory (NCSM) & Theory (Valence-space)**:
   - Comparison of the NCSM with Daejeon16 versus valence-space calculations for $A > 18$
   - Construction of effective $E2$ and $M1$ operators and comparison of NCSM versus valence-space results
4. **Theory & Experiment**: Analysis of TBMEs: monopole corrections and comparison to phenomenological interactions and USDB
5. Summary and prospects

Nuclear Shell Model

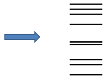
$$H = \sum_{i=1}^{A} \left(\frac{\vec{p}_i^{\,2}}{2m} + U(\vec{r}_i) \right) + \sum_{i<j=1}^{A} V(\vec{r}_i - \vec{r}_j) - \sum_{i=1}^{A} U(\vec{r}_i)$$



Solution of the eigenproblem by diagonalization of the Hamiltonian matrix:

- $\Psi_p = \sum_k a_{kp} \Phi_k$
- $\sum_{k=1}^{n} H_{lk} a_{kp} = E_p a_{lp}$
- Input: ϵ_j, $\langle ij | V_{res} | kl \rangle_{JT}$

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & \cdots & H_{nn} \\ H_{21} & H_{22} & \cdots & \cdots & H_{2n} \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ H_{n1} & H_{n2} & \cdots & \cdots & H_{nn} \end{pmatrix}$$



Phenomenological Hamiltonians: Cohen-Kurath (p-shell), USD (sd-shell), KB3G, GXPF1A (pf-shell), . . . provide excellent spectroscopy at low energies.

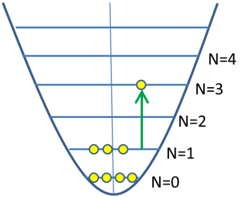
Motivation: towards microscopic effective interactions

- Many-body Perturbation Theory (MBPT)
  - G matrix *Bertsch (1965); Kuo, Brown, Nucl. Phys. 85 (1966); . . .;*
    Hjorth-Jensen, Kuo, Osnes, Phys. Rep. 261, 125 (1995)
    Coraggio, Covello, Gargano, Itaco, Kuo, Prog. Part. Nucl. Phys. 62, 135 (2009)
  - $V_{\mathrm{low-k}}$ $(NN + 3N)$
    Bogner, Kuo, Coraggio, Covello, Itaco, PRC65 (2002);
    Bogner, Kuo, Schwenk, Phys. Rep. 386 (2003); Simonis et al, PRC93 (2016)
  - V_{SRG} $(NN + 3N)$
    Holt, Menendez, Schwenk, EPJA49 (2013)
  - bare V $(NN + 3N)$
    Fukui, De Angelis, Ma, Coraggio, Cargano, Itaco, Xu, PRC98, 044305 (2018);
    Ma, Coraggio, De Angelis, Fukui, Cargano, Itako, Xu, PRC100, 034324 (2019)
- Valence-space IMSRG $(NN + 3N)$
  Stroberg, Calci, Hergert, Holt, Bogner, Roth, Schwenk, PRL118, 032502 (2017)
- Coupled-cluster effective interaction method $(NN + 3N)$
  Jansen et al, PRC94, 011301(R) (2016)
  Sun, Morris, Hagen, Jansen, Papenbrock, PRC98, 054320 (2018)
- OLS transformation of the NCSM solution
  Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC91, 064301 (2015)
  Smirnova, Barrett, Kim, Shin, Shirokov, Dikmen, Maris, Vary, PRC100, 054329 (2019)

Formalism: OLS transformation the **NCSM** solution

Ab-initio No-Core-Shell Model (NCSM)

$$H = \sum_{i<j=1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2Am} + \sum_{i<j=1}^{A} V_{ij}^{NN} \left(+ \sum_{i<j<k=1}^{A} V_{ijk}^{NNN} \right)$$



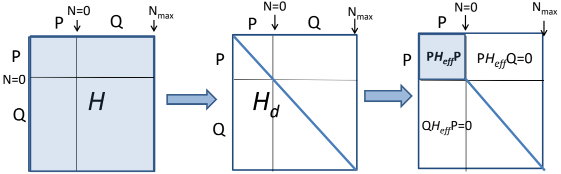
Diagonalization of the A-nucleon Hamiltonian in the harmonic oscillator basis

- Basis: $\hbar\Omega$ and $N_{\max}$ (cut-off)
- $N_{\min} \leq \sum_{i=1}^{A} (2n_i + l_i) \leq N_{\min} + N_{\max}$
- Bare or effective V_{ij}^{NN}

For review: Barrett, Navratil, Vary, Progr. Part. Nucl. Phys. 60, 131 (2013)

Ab-initio effective interaction 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

- NCSM for ^{18}F at $N_{\max}$
- H_{eff} for ^{18}F at $N = 0$ (OLS)
- ^{16}O at $N_{\max}$ (core energy)
- ^{17}O, ^{17}F at $N_{\max}$ (one-body terms)
- ϵ_j, $\langle ij | V_{\text{eff}} | kl \rangle_{JT}$

Okubo, Progr. Theor. Phys. 12 (1954); Suzuki, Lee, Prog. Theor. Phys. 68 (1980)
Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC91, 064301 (2015)

Smirnova, Barrett, Kim, Shin, Shirokov, Dikmen, Maris, Vary, PRC100, 054329 (2019)

Ab-initio effective interaction from the NCSM

Present results obtained from the NCSM

- $N_{max} = 4, 6$
- $\hbar\Omega = 14$ MeV ($\hbar\Omega = 12$ MeV – 20 MeV)
- ^{18}F $\Rightarrow$ $T = 0, 1$ TBMEs in *sd* shell (charge-independent)
- ^{18}O, ^{18}F, ^{18}Ne $\Rightarrow$ pp,nn, pn ($T = 0, 1$) TBMEs in *sd* shell (charge-dependent)
- MFDn code (*Vary, Maris et al, Iowa SU*)

NN potentials

- χN^{3}LO

  Entem, Machleidt, PRC91, 041001 (2003)

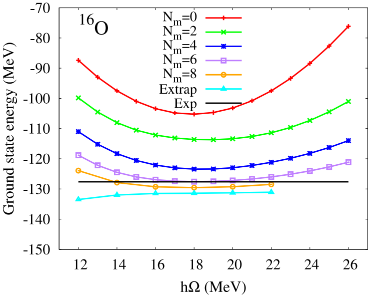
- *J*-matrix Inverse Scattering Potential (JISP16 + PET)

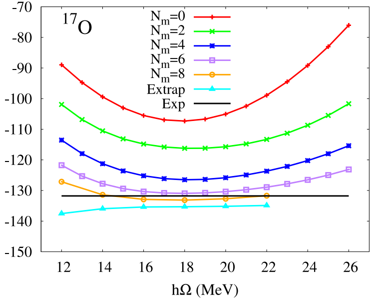
  Shirokov, Vary, Mazur, Weber, PLB644, 33 (2007)

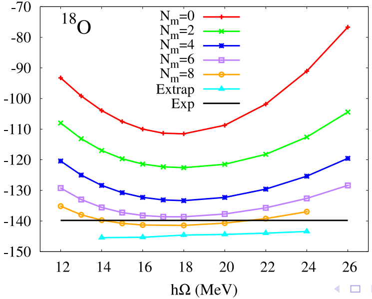
- Daejeon16 *NN* potential (SRG-evolved chiral N^{3}LO + phase-equivalent transformations to adjust for light nuclei)

  Shirokov, Shin, Kim, Sosonkina, Maris, Vary, PLB761, 81 (2016)

NCSM calculations for the g.s. $^{16-18}$O with Daejeon16



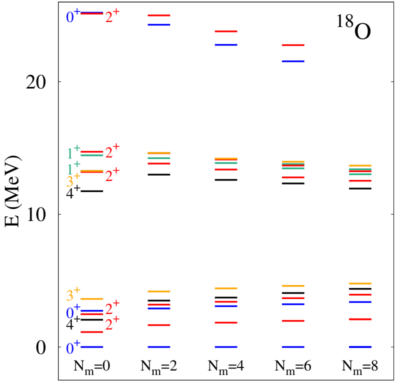




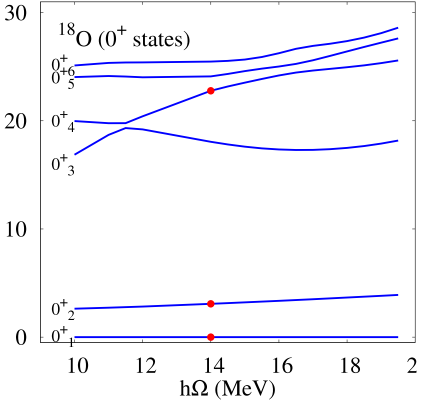
NCSM calculations for the excitation spectrum of ^{18}O with Daejeon16 with largest $N = 0$ component

State selection

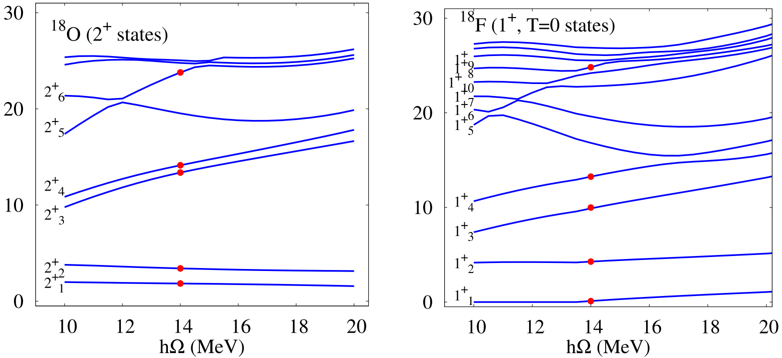
$\hbar\Omega = 14$ MeV



$N_{\text{max}} = 4$

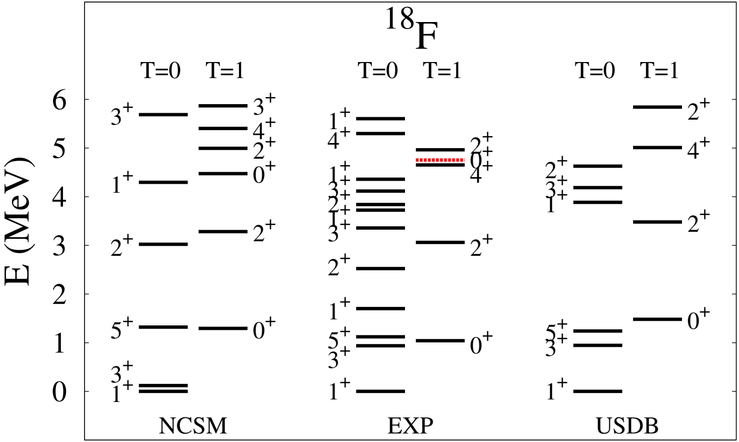


Intruder state problem (illustrated for $N_{\text{max}} = 4$)



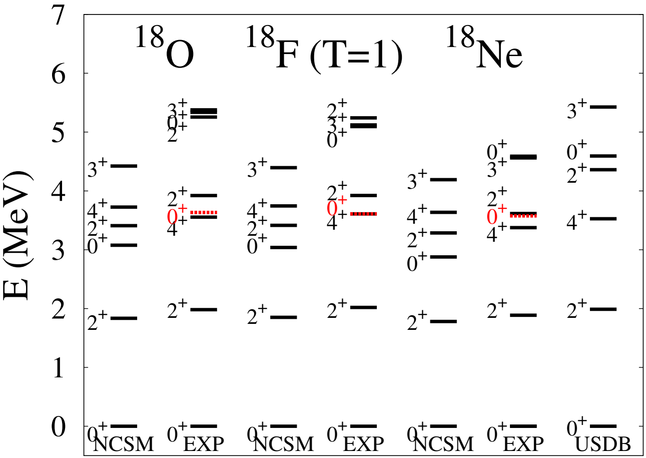
^{18}F from Daejeon16 at $N_{\max} = 6$

For $A = 18$ the valence-space calculations exactly reproduce the NCSM states by construction



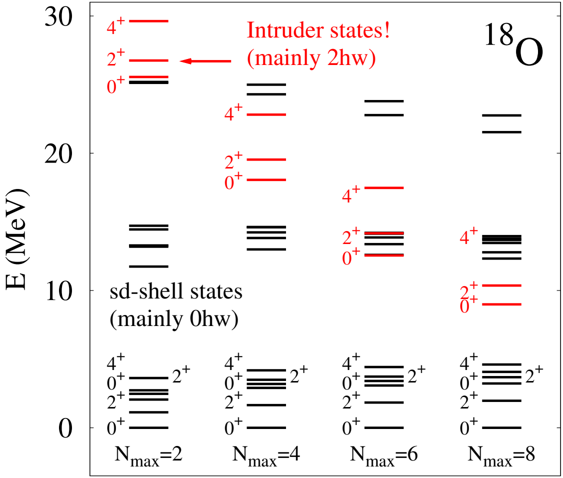
^{18}O, ^{18}F ($T = 1$) and ^{18}Ne from Daejeon16

The charge dependence (from two-body Coulomb interaction in the NCSM) is small.



Position of intruder states in ^{18}O from Daejeon16

Position of the lowest intruder states with respect to the lowest *sd*-shell states.

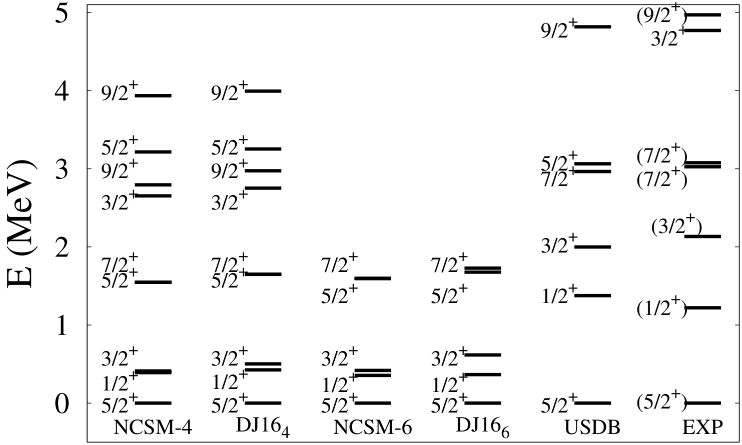


Theory (NCSM) versus Theory (valence-space)

Comparison of NCSM and valence space SM results

For $A > 18$ the valence-space spectra are very close to the NCSM results

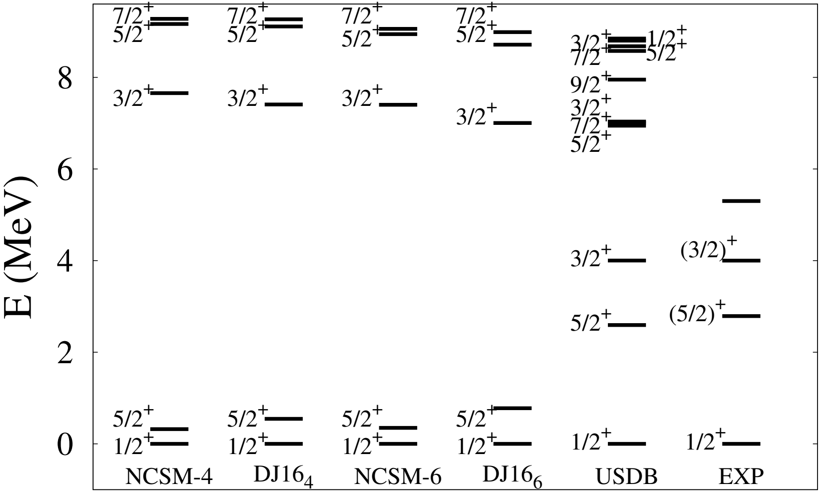
^{21}O (rms error for 12 lowest states is 125 keV)



Comparison of NCSM and valence space SM results

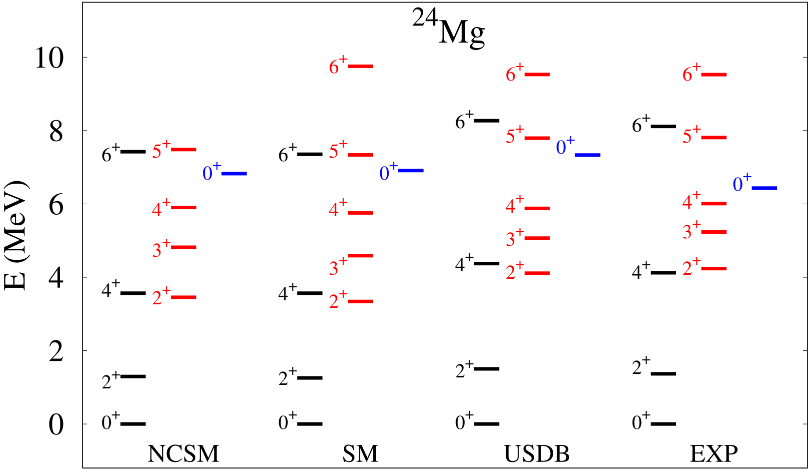
For $A > 18$ the valence-space spectra are very close to the NCSM results

^{23}O (rms error for 14 lowest states is 63 keV)



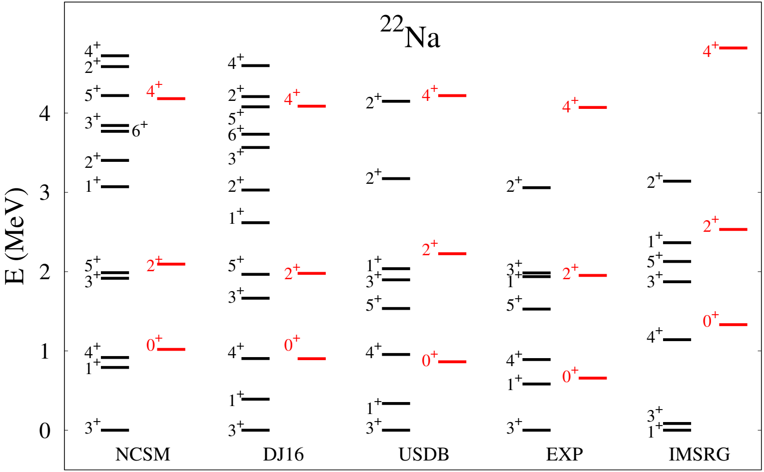
Comparison of NCSM and valence space SM results

^{24}Mg: NCSM versus valence-space SM (rms error 225 keV)



Comparison of NCSM and valence space SM results

^{22}Na: NCSM versus valence-space SM (rms error 220 keV)



Effective electromagnetic operators

We require that the valence-space single-particle $E2$ and $M1$ matrix elements reproduce the NCSM results for ^{17}O and ^{17}F obtained in a large N_{max} space.

Effective $E2$ operator in the sd shell

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

$$\hat{O}(E2) = \sum_{k=1}^{A} e_k r_k^2 \hat{Y}_2(\hat{r}_k) \quad (e_n = 0, e_p = e)$$

Effective $M1$ operator in the sd shell

$$g^s_{n/p}(a,b)\langle b||\mu_N\,\vec{s}\,||a\rangle = \langle J_f||\hat{O}(M1)_{\text{spin}}||J_i\rangle \quad (\text{from } {}^{17}\text{O}/{}^{17}\text{F})$$

$$g^l_{n/p}(a,b)\langle b||\mu_N\,\vec{l}\,||a\rangle = \langle J_f||\hat{O}(M1)_{\text{orbit}}||J_i\rangle \quad (\text{from } {}^{17}\text{O}/{}^{17}\text{F})$$

$$\hat{O}(M1) = \sum_{k=1}^{A} \mu_N\left[g^s_k\vec{s}_k + g^l_k\vec{l}_k\right] \quad (g^s_n{=}-3.826, g^s_p{=}5.586, g^l_n{=}0, g^l_p{=}1)$$

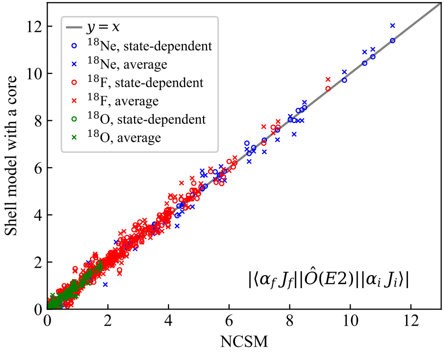
Effective electromagnetic operators

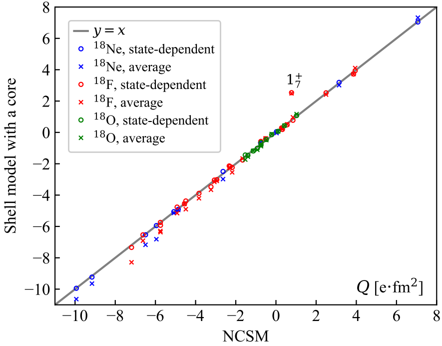
State-dependent effective charges/g-factors

(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

$E2$ data for $A = 18$: comparison of NCSM and valence-space SM results

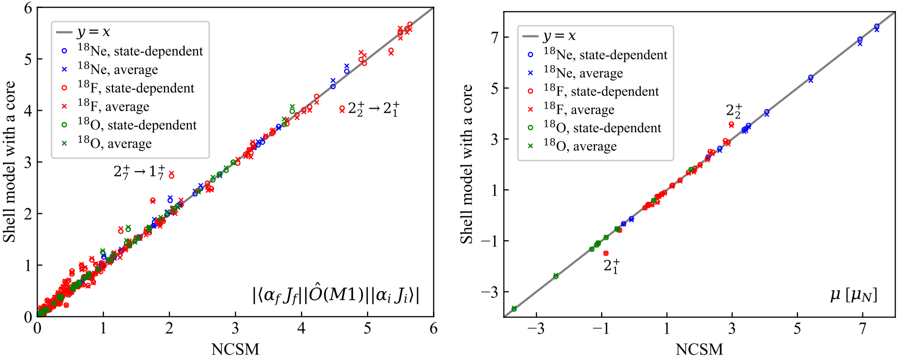
^{18}O : rms(RME) $\approx$ 0.07 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2
^{18}F : rms(RME) $\approx$ 0.11 e.fm^2 (269 data), rms(Q)$\approx$ 0.37 e.fm^2
^{18}Ne : rms(RME)$\approx$ 0.22 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2





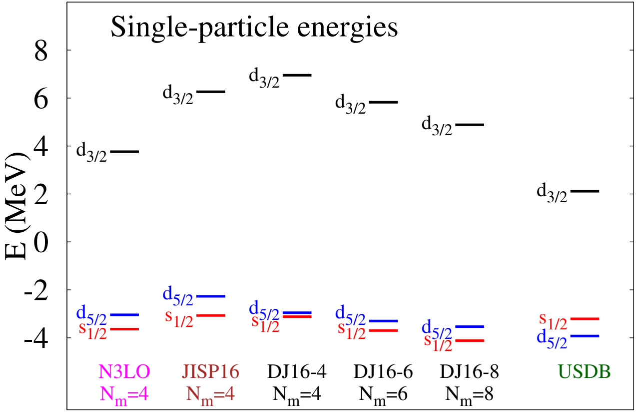
$M1$ data: comparison of NCSM and valence-space SM results

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



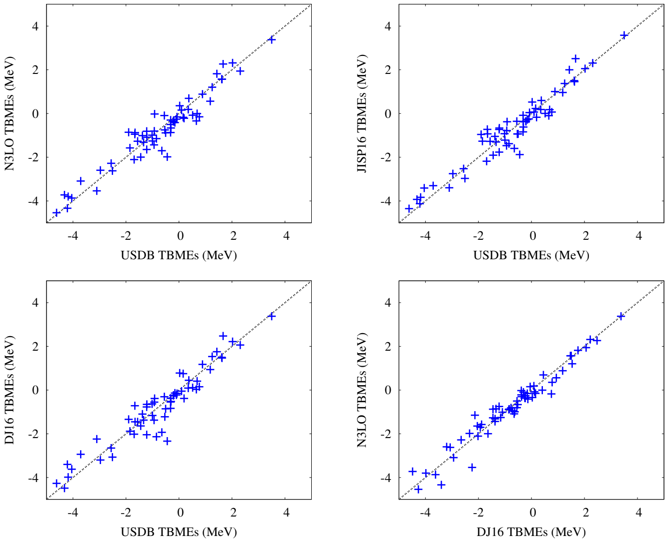
Theory (valence-space) versus Experiment

Single-particle energies (theory & phenomenology)



We adopt USDB s.p. energies and impose the mass dependence $A^{-1/3}$ on TBMEs.

How to compare various sets of TBMEs?



Multipole form of the valence-space Hamiltonian

In a particular (harmonic-oscillator) basis:

$$\hat{H} = \sum_i \epsilon_i a_i^+ a_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_l a_k \qquad i \equiv (n_i l_i j_i m_i), \ldots$$

Re-write the two-body interaction in the multipole form:

$$\hat{H} = \sum_i \epsilon_{\nu_i} \hat{n}_{\nu_i} + \sum_i \epsilon_{\pi_i} \hat{n}_{\pi_i} + \sum_{ij} \overline{V}_{ij}^{\nu\pi} \hat{n}_{\nu_i} \hat{n}_{\pi_j} + \sum_{i \le j} \frac{\hat{n}_{\nu_i}(\hat{n}_{\nu_j} - \delta_{ij})}{1 + \delta_{ij}} \overline{V}_{ij}^{\nu\nu} + \ldots$$

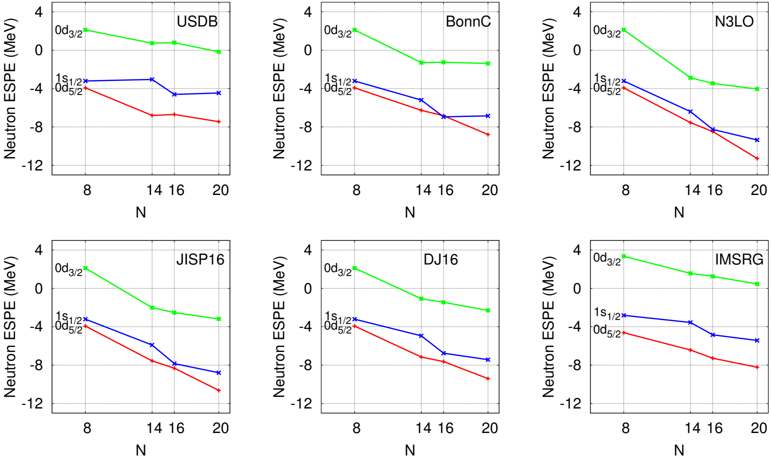
$$\overline{V}_{ij}^{\rho\rho'} = \frac{\sum_J \langle ij|V|ij\rangle_J (2J+1)}{\sum_J (2J+1)} \qquad i \equiv (n_i l_i j_i), \ldots$$

- Monopole part:
  - shell formation $\Rightarrow$ *spherical mean field*;
  - dominant contribution to the *nuclear binding*.
- Higher-multipole part: nucleonic *correlations* (quadrupole-quadrupole, etc).

Poves, Zuker (1981); Dufour, Zuker (1995); Caurier et al, RMP77 (2005)

Neutron Effective SPEs in O-isotopes

$$\tilde{\epsilon}_{\nu_i}(A) = \epsilon_{\nu_i}(A_0) + \sum_j \overline{V}_{ij}^{\nu\nu}\ n_{\nu_j}$$



BonnC: *Hjorth-Jensen, Kuo, Osnes, PR261 (1995)*; IMSRG: *Stroberg et al, PRL118 (2017)*

Neutron Effective SPEs in O-isotopes

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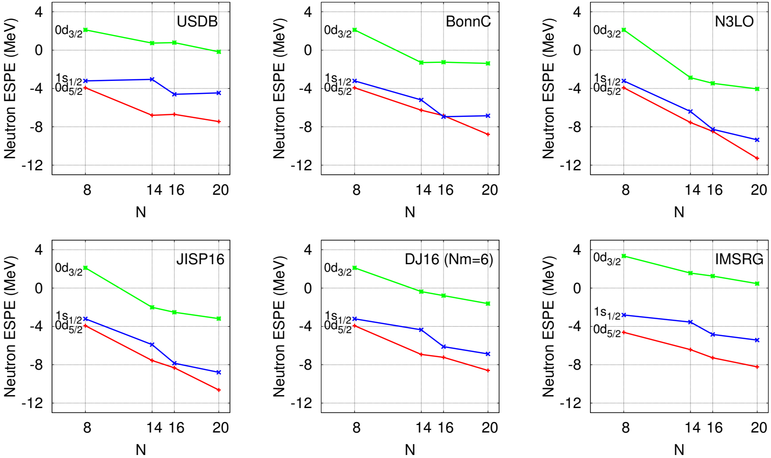
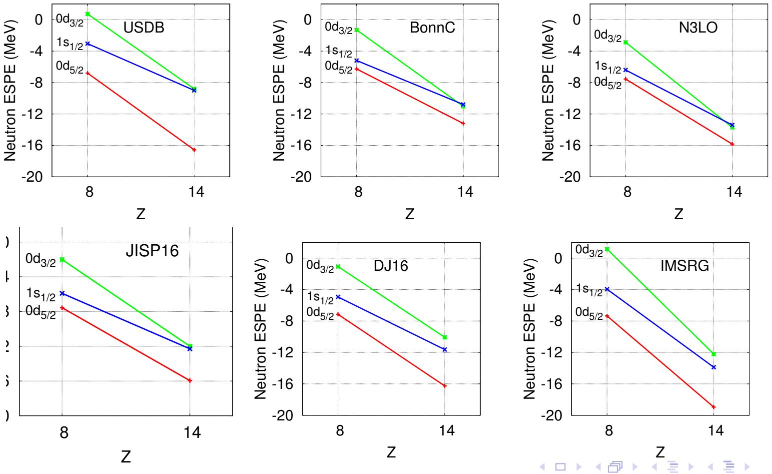


BonnC: *Hjorth-Jensen, Kuo, Osnes, PR261 (1995)*; IMSRG: *Stroberg et al, PRL118 (2017)*

Neutron ESPEs in $N = 14$ isotones (from ^{22}O to ^{28}Si)

$$\tilde{\epsilon}_{\nu_i}(A) = \epsilon_{\nu_i}(A_0) + \sum_j \overline{V}_{ij}^{\nu\pi}\, n_{\pi_j}$$



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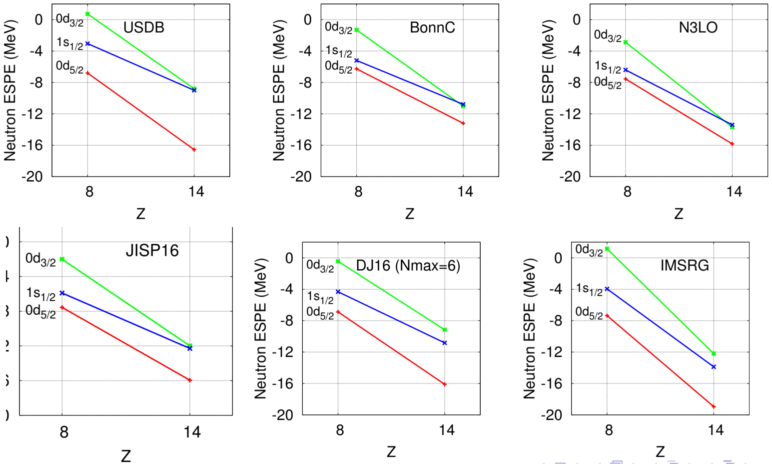
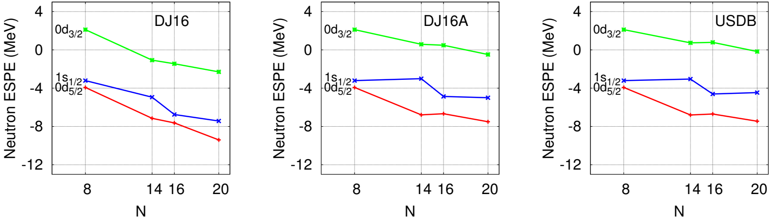


Monopole-modified V_{eff} from Daejeon16

Modifications of the centroids

$N_{\max} = 4$	$N_{\max} = 6$
$\Delta V^{T=1}_{d_{5/2}d_{5/2}} = +80$ keV	$\Delta V^{T=1}_{d_{5/2}d_{5/2}} = +20$ keV
$\Delta V^{T=1}_{d_{5/2}s_{1/2}} = +350$ keV	$\Delta V^{T=1}_{d_{5/2}s_{1/2}} = +230$ keV
$\Delta V^{T=1}_{d_{5/2}d_{3/2}} = +300$ keV	$\Delta V^{T=1}_{d_{5/2}d_{3/2}} = +210$ keV
$\Delta V^{T=1}_{d_{3/2}s_{1/2}} = +200$ keV	$\Delta V^{T=1}_{d_{3/2}s_{1/2}} = +100$ keV
$V^{T=0}_{d_{5/2}d_{5/2}} = -80$ keV	$V^{T=0}_{d_{5/2}d_{5/2}} = -100$ keV
$V^{T=0}_{d_{5/2}s_{1/2}} = +100$ keV	$V^{T=0}_{d_{5/2}s_{1/2}} = +50$ keV



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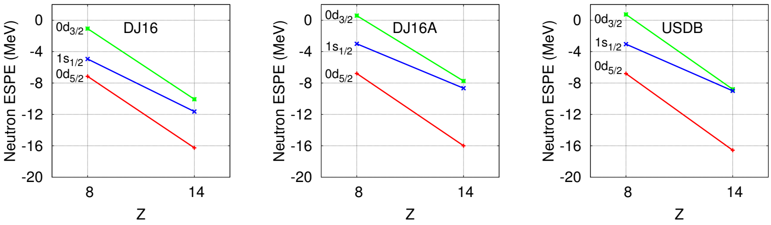
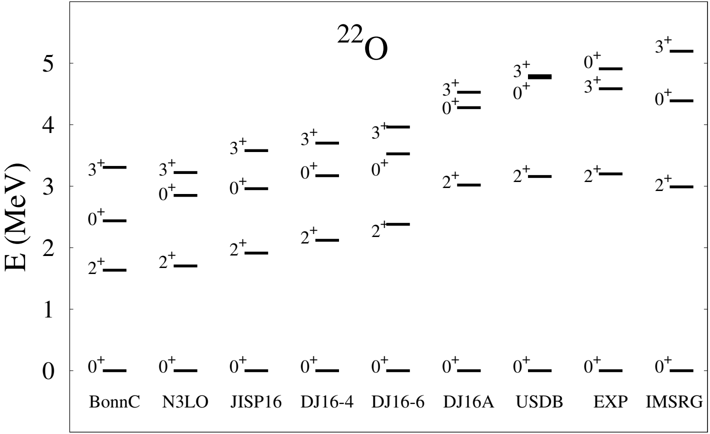
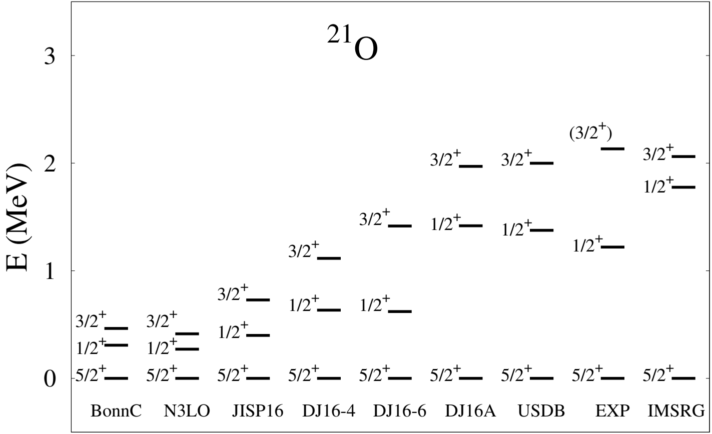
$\Delta V^{T=1}_{d_{5/2}s_{1/2}} = +350$ keV	$\Delta V^{T=1}_{d_{5/2}s_{1/2}} = +230$ keV
$\Delta V^{T=1}_{d_{5/2}d_{3/2}} = +300$ keV	$\Delta V^{T=1}_{d_{5/2}d_{3/2}} = +210$ keV
$\Delta V^{T=1}_{d_{3/2}s_{1/2}} = +200$ keV	$\Delta V^{T=1}_{d_{3/2}s_{1/2}} = +100$ keV
$V^{T=0}_{d_{5/2}d_{5/2}} = -80$ keV	$V^{T=0}_{d_{5/2}d_{5/2}} = -100$ keV
$V^{T=0}_{d_{5/2}s_{1/2}} = +100$ keV	$V^{T=0}_{d_{5/2}s_{1/2}} = +50$ keV



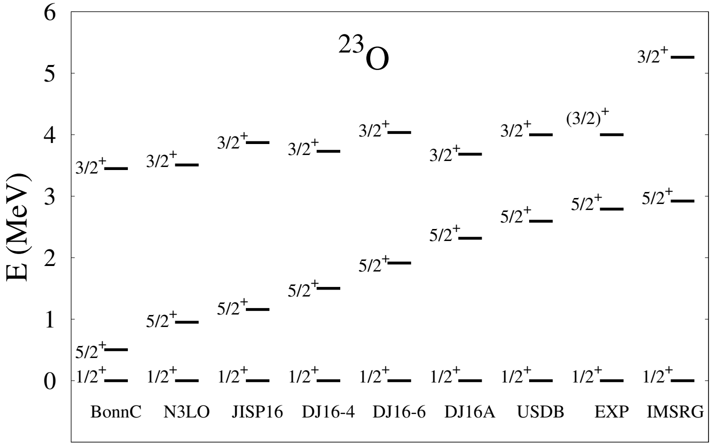
Spectrum of ^{22}O



Spectrum of ^{21}O

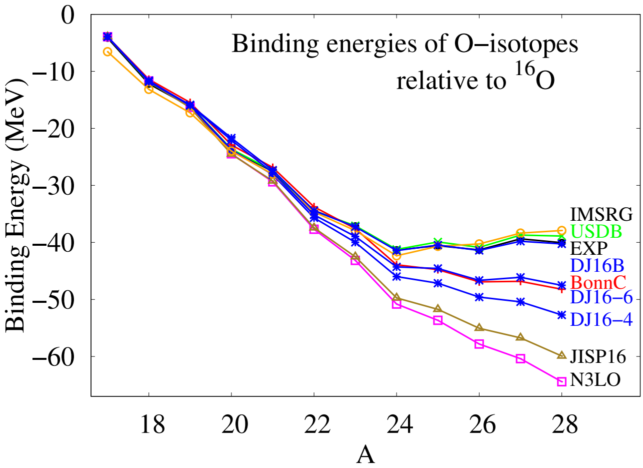


Spectrum of ^{23}O

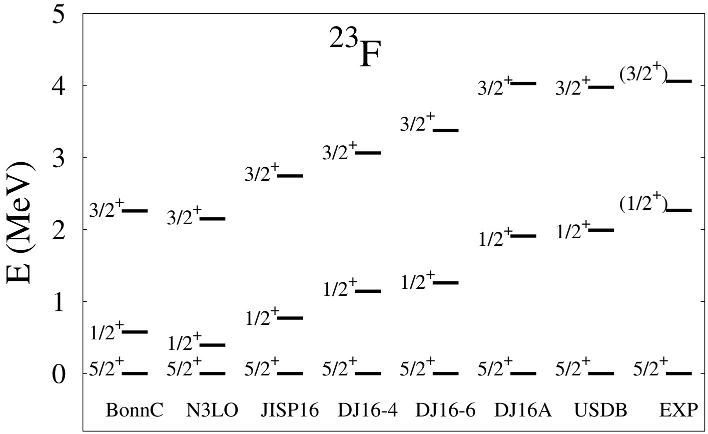


Binding energies of O-isotopes

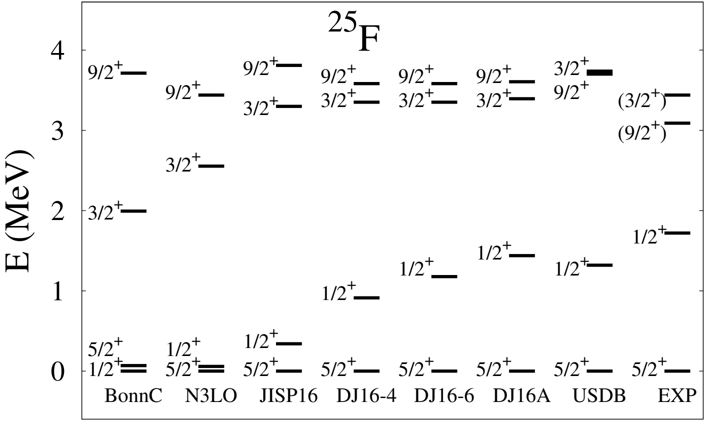
rms(DJ16-6) ≈ 3671 keV; rms(DJ16B) ≈ 235 keV; rms(USDB) ≈ 467 keV



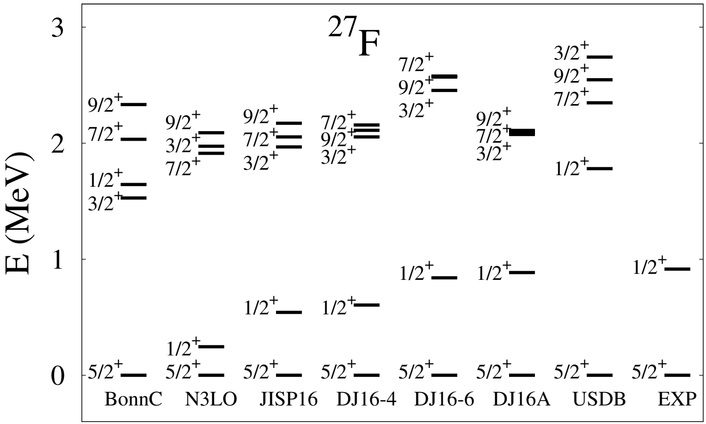
Spectrum of ^{23}F



Spectrum of ^{25}F

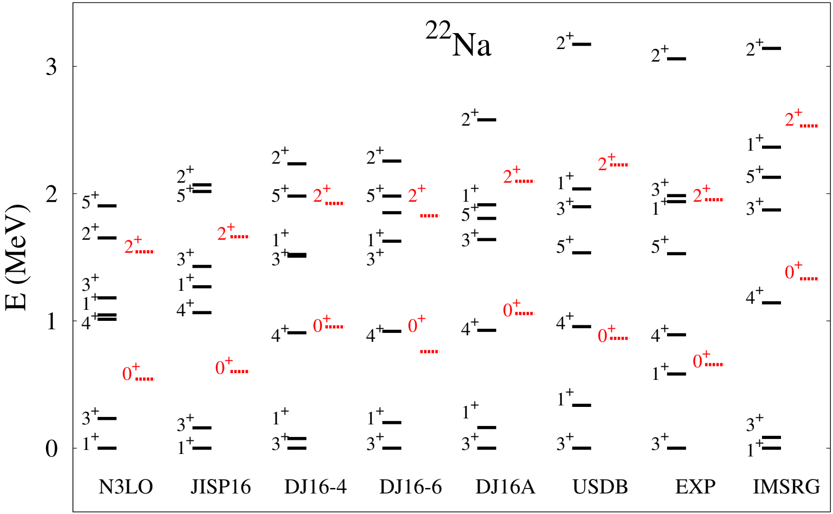


Spectrum of ^{27}F

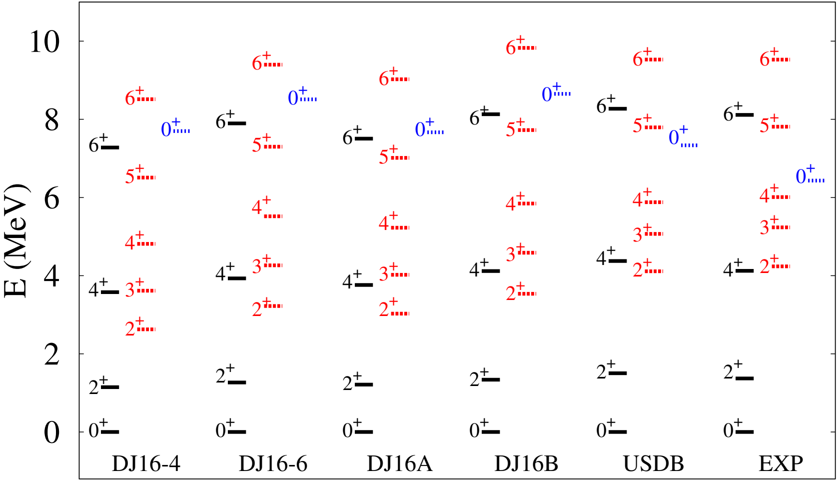


Experiment: P. Doornenbal et al, PRC95, 041301 (2017)

Spectrum of ^{22}Na



Collective properties: ^{24}Mg



^{24}Mg: $E2$ transition rates

Standard effective charges: $e_p = 1.5e$, $e_n = 0.5e$

	Exp	USDB	BonnC	N3LO	JISP16	DJ16
^{24}Mg						
$B(E2; 2_1^+ \to 0_1^+)$ (e^2fm^4)	88(4)	95	108	107	106	104
$B(E2; 4_1^+ \to 2_1^+)$ (e^2fm^4)	160(16)	124	143	140	138	138
$B(E2; 6_1^+ \to 2_1^+)$ (e^2fm^4)		115	140	135	133	135
$Q(2_1^+)$ (e fm^2)	$-16.6(6)$	-19.3	-18.3	-18.8	-19.1	-19.7

Charge-dependence of the valence-space Hamiltonian

Charge-dependent valence-space interaction derived from the NCSM with Daejeon16

- DJ16 *NN* potential (charge-independent) + Coulomb
- Different proton and neutron single-particle energies
- ^{18}O, ^{18}F, ^{18}Ne $\Rightarrow$ pp,nn, pn ($T = 0, 1$) TBMEs in *sd* shell

Valence-space INC interaction (including classes Coulomb and effective CSB and CIB *NN* forces)

- We consider an isospin-symmetry non-conserving term

$$\hat{V}_{INC} = \underbrace{\lambda_C \hat{V}_C}_{Coulomb} + \underbrace{\lambda_1 \hat{V}^{(1)}}_{CSB} + \underbrace{\lambda_2 \hat{V}^{(2)}}_{CIB} + \underbrace{\hat{H}_0^{IV}}_{\sum_\alpha(\varepsilon_\alpha^p - \varepsilon_\alpha^n)}$$

- Within perturbation theory:

$$\langle \Psi_{TT_z} | \hat{V}_{INC} | \Psi_{TT_z} \rangle = E^{(0)}(\alpha, T) + E^{(1)}(\alpha, T) T_z + E^{(2)}(\alpha, T) \left[3T_z^2 - T(T+1) \right]$$

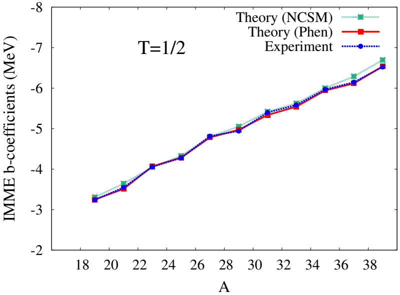
- Wigner's Isobaric Mass Multiplet Equation (IMME):

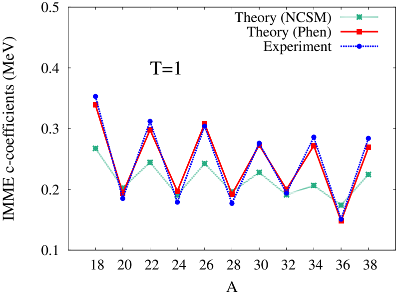
$$M(\alpha, T, T_z) = a(\alpha, T) + b(\alpha, T) T_z + c(\alpha, T) T_z^2 \,,$$

Ab-initio effective interaction from the NCSM

Present results obtained from the NCSM

- DJ16 *NN* potential (charge-independent) + Coulomb
- ^{18}O, ^{18}F, ^{18}Ne $\Rightarrow$ pp,nn, pn ($T = 0, 1$) TBMEs in *sd* shell





- *b*-coefficients: rms (NCSM) $\approx$ 86 keV, rms (phen) $\approx$ 30 keV
- *c*-coefficients: rms (NCSM) $\approx$ 51 keV, rms (phen) $\approx$ 11 keV

Lam, Smirnova, Caurier, PRC87 (2013).

Summary and Perspectives

- *Ab-initio* effective *sd*-shell interactions from the **NCSM** via OLS transformation: robust mapping procedure $\Rightarrow$ spectra and (state-dependent) electromagnetic transition operators
- NN potential versus $NN + (3N)$: Daejeon16
- Monopole part (Daejeon16): some deficiencies in $T = 1$ part (improving at $N_{max} = 6$), although robust proton-neutron centroids. Small monopole modifications allow to visibly improve the spectroscopy of O and F-isotopes
- Multipole part (Daejeon16): still to explore
- Charge-dependence: robust agreement with the data regarding Coulomb. Need for CSB and CIB NN terms.
- Heavier nuclei (*pf*-shell): challenging
- Possibility to explore $1\hbar\Omega$, ...

Thank you for your attention !