Standard Shell-Model Effective Interactions from the No Core Shell Model calculations

Alexander Lisetskiy

Bruce Barrett

Michael Kruse

Erdal Dikmen

Petr Navratil

James Vary

THE UNIVERSITY OF ARIZONA.
Arizona's First University.

Motivation

Goal: Describe nuclei as systems of nucleons interacting via realistic forces

How to choose: Appropriate Finite Shell Model Space ???
Corresponding Effective Interaction & Operators ???

Way A: No Core Shell Model – consistent procedure to derive effective interaction from bare realistic NN & NNN potentials for the requested space and nucleus
Problem: intractable spaces are needed for A > 12 to get converged result

Way B: Traditional Core Shell Model – powerful phenomenologically renormalized G-matrix type interactions :: USD(05), GXPF(1,2) :: A < 132
Problem: local, links to fundamental interactions are lost

Way C: use NCSM Formalism (Way A) to get tools for CSM (Way B)

No Core Shell Model

Starting Hamiltonian

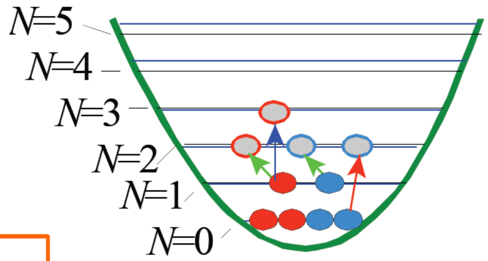
$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

Realistic NN and NNN potentials

Coordinate space –	Argonne V18, AV18',	NNN Tucson - Melbourne
Momentum space –	CD-Bonn, chiral N³LO,	NNN chiral N²LO

Binding center-of-mass HO potential (Lipkin 1958)

$$\frac{1}{2} A m \Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m \Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$



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

$\langle HO | V_{NN}(\Omega, A) | HO \rangle$

Two-body cluster approximation

$$H_2^{\Omega} = \sum_{i=1}^{2} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{2} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

NCSM & effective Hamiltonian

Solving $H_2^{\Omega}\Psi_2 = E\,\Psi_2$ in "infinite space" 2n+l = 350 relative coordinates

Unitary Transformation using Ψ_2

$$H_{\text{eff}}^{\Omega} = \frac{(P + P\omega^{\dagger}Q)}{\sqrt{P+\omega^{\dagger}\omega}} H_2^{\Omega} \frac{(Q\omega P + P)}{\sqrt{P+\omega^{\dagger}\omega}}$$

Criteria:

$$H: \quad E_1, E_2, E_3, \dots E_{d_P}, \dots E_{\infty}$$

$$H_{\text{eff}}: \quad E_1, E_2, E_3, \dots E_{d_P}$$

P – model space projector operator , P+Q = 1

To calculate matrix elements of ω **operator** Ψ_2 **= |k> is needed**

$$P|k\rangle = \sum_{p=1}^{d_P} A_{pk}|\alpha_p\rangle \qquad Q|k\rangle = \sum_{q=d_P+1}^{\text{full}} B_{qk}|\alpha_q\rangle$$

$$\langle\alpha_q|\omega|\alpha_p\rangle = \sum_{k=1}^{d_P} B_{qk}[A^{-1}]_{kp}$$

Two ways of convergence:

- For $P \rightarrow 1$ $\quad H^{(n)}_{\text{eff}} \rightarrow H$
- For $n \rightarrow A$ and fixed P: $H^{(n)}_{\text{eff}} \rightarrow H'$

NCSM & effective Hamiltonian

$$H_{\rm diag} = UHU^\dagger$$

$$H_{\rm diag} = \begin{pmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & E_{max} \end{pmatrix} \qquad U = \begin{pmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,max} \\ a_{2,1} & a_{2,2} & \dots & a_{2,max} \\ \dots & \dots & \dots & \dots \\ a_{max,1} & a_{max,2} & a_{max,3} & a_{max,max} \end{pmatrix}$$

$$H^p_{\rm diag} = \begin{pmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & E_{p_{max}} \end{pmatrix} \qquad U_p = \begin{pmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,p_{max}} \\ a_{2,1} & a_{2,2} & \dots & a_{2,p_{max}} \\ \dots & \dots & \dots & \dots \\ a_{p_{max},1} & a_{p_{max},2} & a_{p_{max},3} & a_{p_{max},p_{max}} \end{pmatrix}$$

Effective Hamiltonian can be constructed

$$H_{\rm eff} = \frac{U_p^\dagger}{\sqrt{U_p^\dagger U_p}} H^p_{\rm diag} \frac{U_p}{\sqrt{U_p^\dagger U_p}}.$$

From NCSM to CSM in 0hΩ space

NCSM : effective interaction is constructed for $N_{max}h\Omega$ space with $\Delta N = 0, 2, \ldots, N_{max}$ cross shell excitations

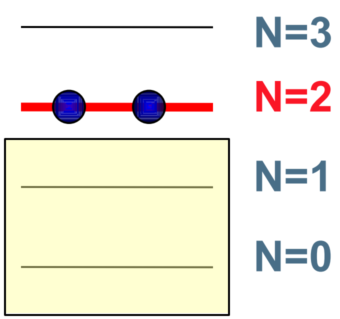
Relation between NCSM and CSM effective interactions $N_{max} = 0$ for ^{18}F

NCSM	CSM
0 SPE	3 SPE
332 TBME	63 sd-shell TBME
	Core Energy

$$\epsilon_j = \sum_{j_{oc}} (2j_{oc}+1) \frac{V_{\rm mon}^{T=0}(jj_{oc}) + 3V_{\rm mon}^{T=1}(jj_{oc})}{4}$$

$$V_{\rm mon}^{T}(jj_{oc}) = \frac{\sum_J (2J+1)\langle jj_{oc};JT|V_{eff}|jj_{oc};JT\rangle}{\sum_J (2J+1)}$$

$$E_{\rm core} = \sum_{j_{oc}<j'_{oc},J,T} (2J+1)(2T+1)\langle j_{oc}j'_{oc};JT|V|j_{oc}j'_{oc};JT\rangle$$

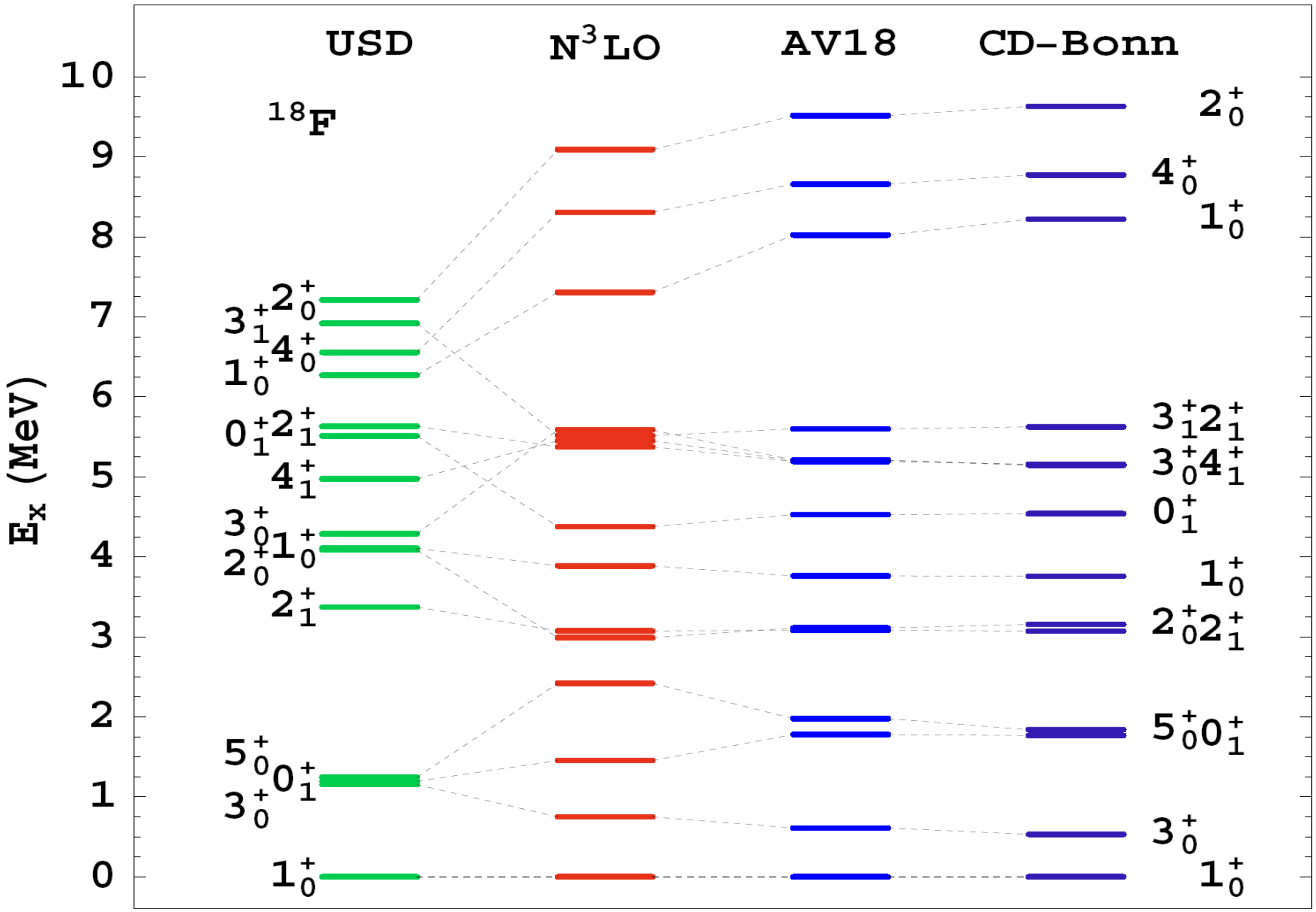


1-step: UT of bare H to 0hΩ
2-step: UT of 0hΩ H to sd H

→ The same set of E

4hΩ NCSM with chiral N^{3}LO, AV18, CD-Bonn for ^{18}F

Step 1: NCSM calculation in 4hΩ space for ^{18}F



H(N_{max}=4,A=18)

$$H_{\text{diag}} = U H U^{\dagger}$$

E_k(A=18)

ANTOINE SM code:
E. Caurier & F. Nowacki,
Acta. Phys. Pol.
B30 (1999) 705.

- A. Lisetskiy

From 4hΩ NCSM to sd CSM for ^{18}F

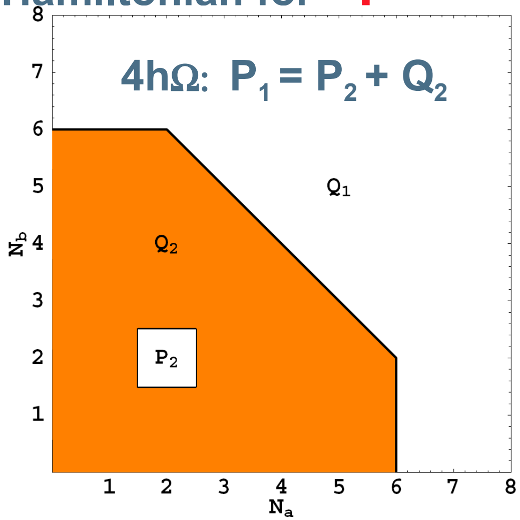
Petr Navrátil, Michael Thoresen, and Bruce R. Barrett, Phys. Rev. C 55, R573 (1997)

Step 2: Projection of 18-body 4hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{18}F

$H_{eff}([sd]^2) = \Sigma_k \, |k,N_{max}=4,A=18> E_k \, (A=18) < \overline{k,N_{max}=4,A=18)}|$

$|k,N_{max}=4,A=18> = U_{k,kp2}|k_{p2}[0h\Omega,18]> + U_{k,kq2}|k_{q2}[2+4h\Omega,18]>$

$\dim(P_1) = 6\,706\,870$ $\quad \dim(P_2)=28$ $\quad \dim(Q_2) = 6\,706\,842$



$$H_{\rm diag} = U H U^\dagger$$

$E_k(A=18)$ $\quad H(N_{max}=4, A=18)$

$$U = \begin{pmatrix} U_{PP} & U_{PQ} \\ U_{QP} & U_{QQ} \end{pmatrix}$$

$$H_{\rm eff} = \frac{U_p^\dagger}{\sqrt{U_p^\dagger U_p}} H^p_{\rm diag} \frac{U_p}{\sqrt{U_p^\dagger U_p}}.$$

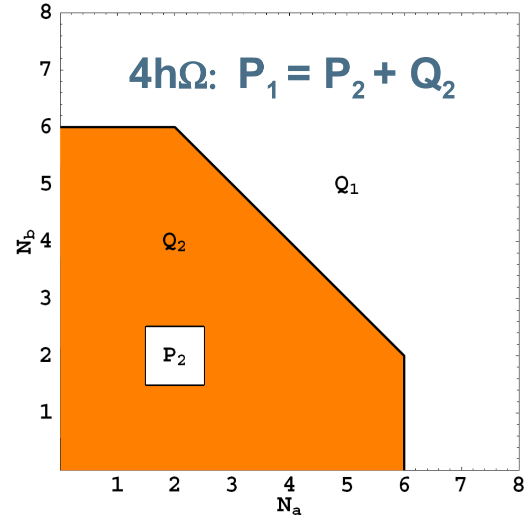
$H_{eff} = H_{eff}(1b) + H_{eff}(2b) + H_{eff}(3b) + H_{eff}(4b) + \ldots$

From 4hΩ NCSM to sd CSM for ^{18}F

Step 2: Projection of 18-body 4hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{18}F

$H_{eff}([sd]^2) = \Sigma_k \, |k,N_{max}=4,A=18 > E_k\,(A=18) < \overline{k,N_{max}=4,A=18)|}$

$|k,N_{max}=4,A=18> = U_{k,kp2}|k_{p2}[0h\Omega,18]> + U_{k,kq2}|k_{q2}[2+4h\Omega,18]>$



$\dim(P_1) = 6\,706\,870$ $\dim(P_2)=28$ $\dim(Q_2) = 6\,706\,842$

$$H_{\rm diag} = U H U^\dagger$$

$E_k(A=18)$ $H(N_{max}=4,A=18)$

$$U = \begin{pmatrix} U_{PP} & U_{PQ} \\ U_{QP} & U_{QQ} \end{pmatrix}$$

$$H_{\rm eff} = \frac{U_p^\dagger}{\sqrt{U_p^\dagger U_p}} H^p_{\rm diag} \frac{U_p}{\sqrt{U_p^\dagger U_p}}.$$

$H_{eff} = H_{eff}(1b) + H_{eff}(2b)$

Separation of one-body & two-body parts

Step 3: Projection of 17-body 4hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{17}F

17-body H constructed using 4AV18 for A=18 !

$$H_{eff}(j;17) = E_{core}(16) + H_{eff}(j;1b)$$

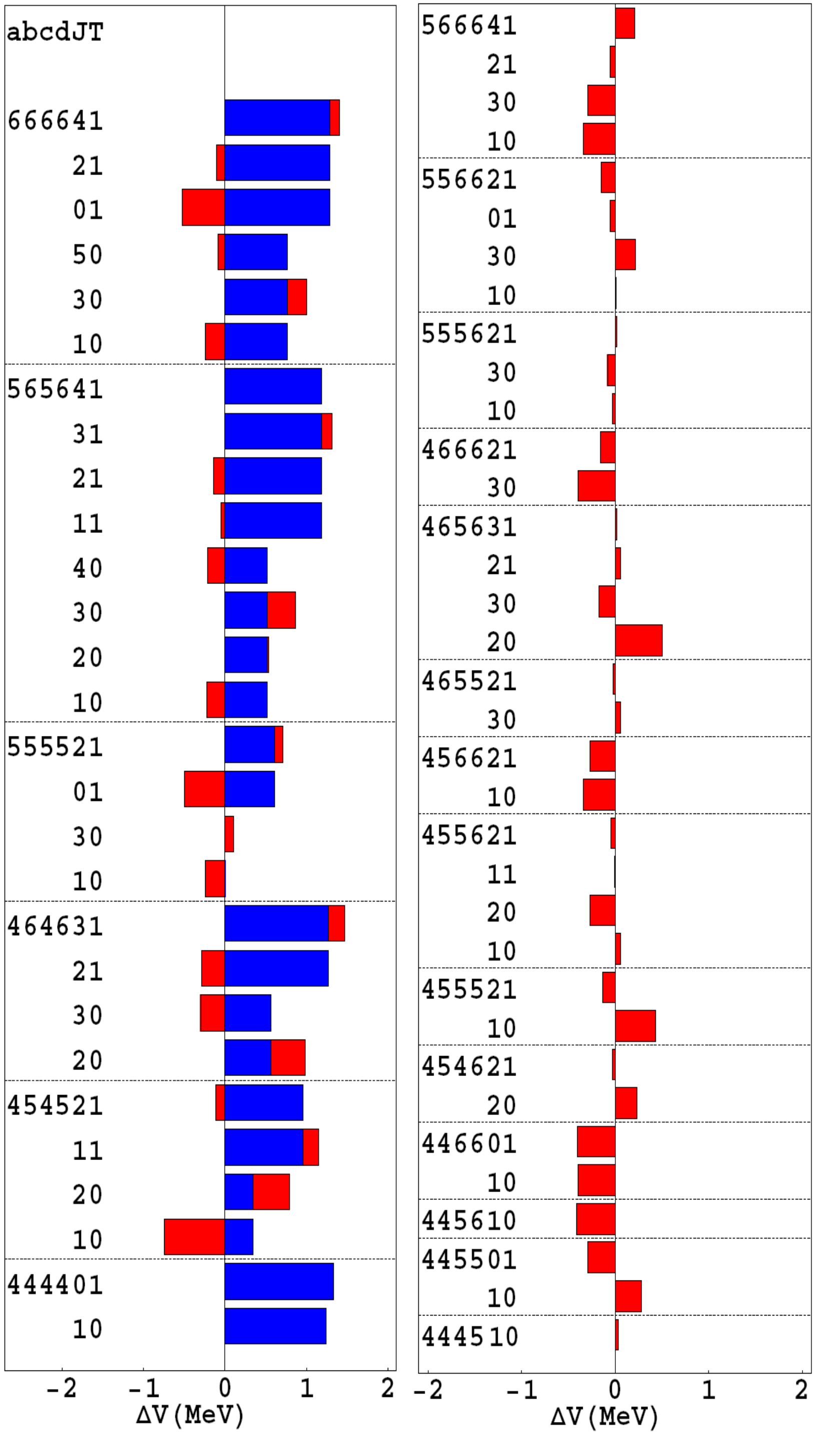
$$\varepsilon(j) = H_{eff}(j;1b) - H_{eff}(s_{1/2})$$

$s_{1/2}$	0.000
$d_{5/2}$	0.402
$d_{3/2}$	8.310

$$H_{eff}(s_{1/2}) = E_g(^{17}F;USD)$$

$$E_{core}(16) = E_g(^{18}F;4AV18) - E_g(^{18}F;USD)$$

$$V_{eff}(abcd;JT) = H_{eff}(A=18) - \varepsilon(a) - \varepsilon(b)$$



Comparison of 4AV18SD & sd-part of 4AV18

$\Delta V(abcd;JT) =$

$V_{eff}(4AV18SD) - V(4AV18) - \Delta V_{mon}(55,T=0)$

$\Delta V(abcd;JT) =$

$\Delta V_{mon}(ab,T) + \Delta V_{res}(abcd;JT) - \Delta V_{mon}(55,T=0)$

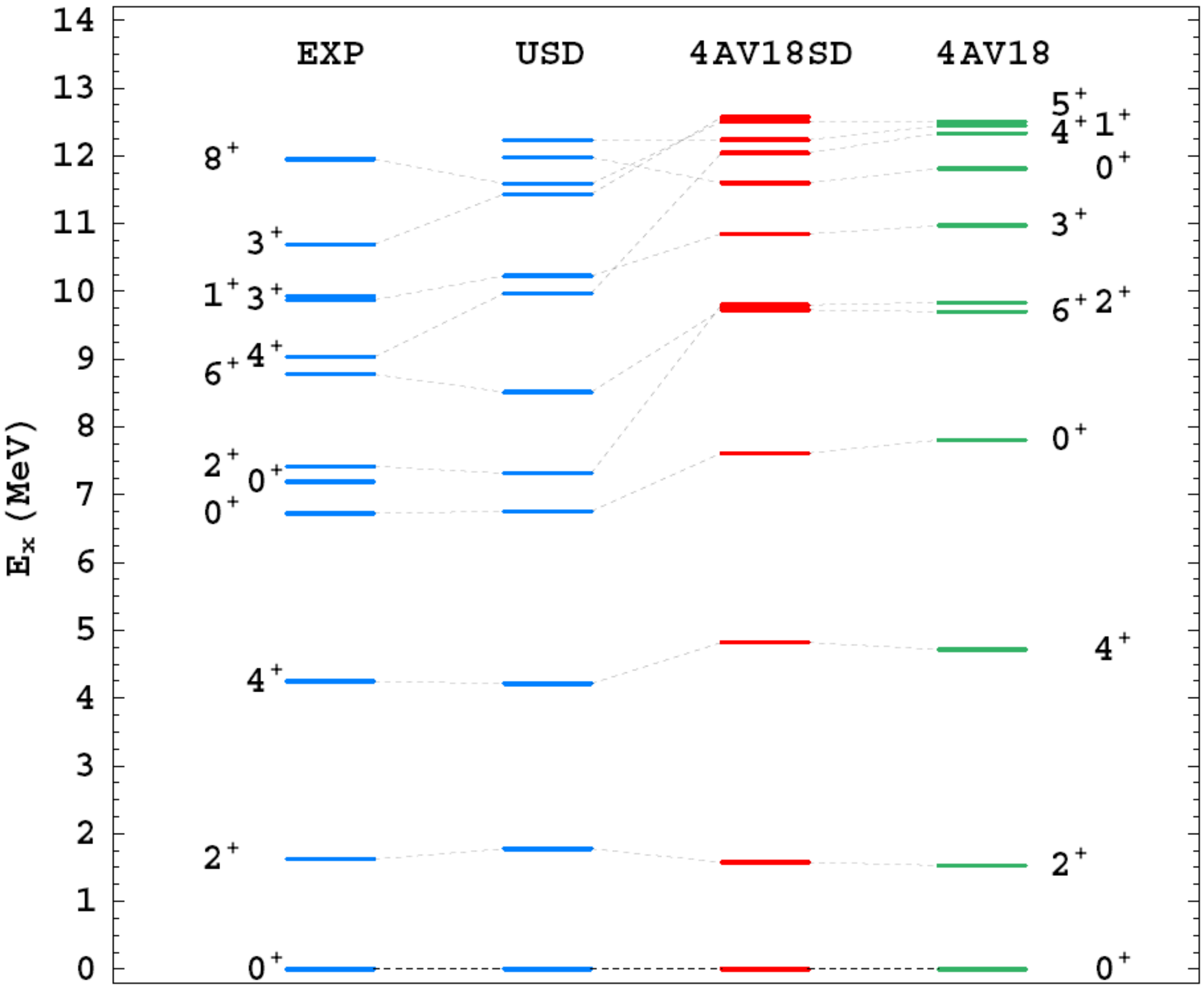
Next steps

Testing different methods to derive interactions directly: 4AV18SD is exact mapping of the 4AV18

Testing 4AV18SD interaction for other sd-shell nuclei

$4 - s_{1/2}$ $5 - d_{3/2}$ $6 - d_{5/2}$

CSM(4AV18SD) & NCSM(4AV18) results for ^{20}Ne



Dimensions: ^{20}Ne

sd-space: 640

2hΩ-space: 542 072

4hΩ-space: 74 668 421

Dimensions: ^{22}Ne

sd-space: 4 206

2hΩ-space: 3 108 957

4hΩ-space: 415 227 419

???

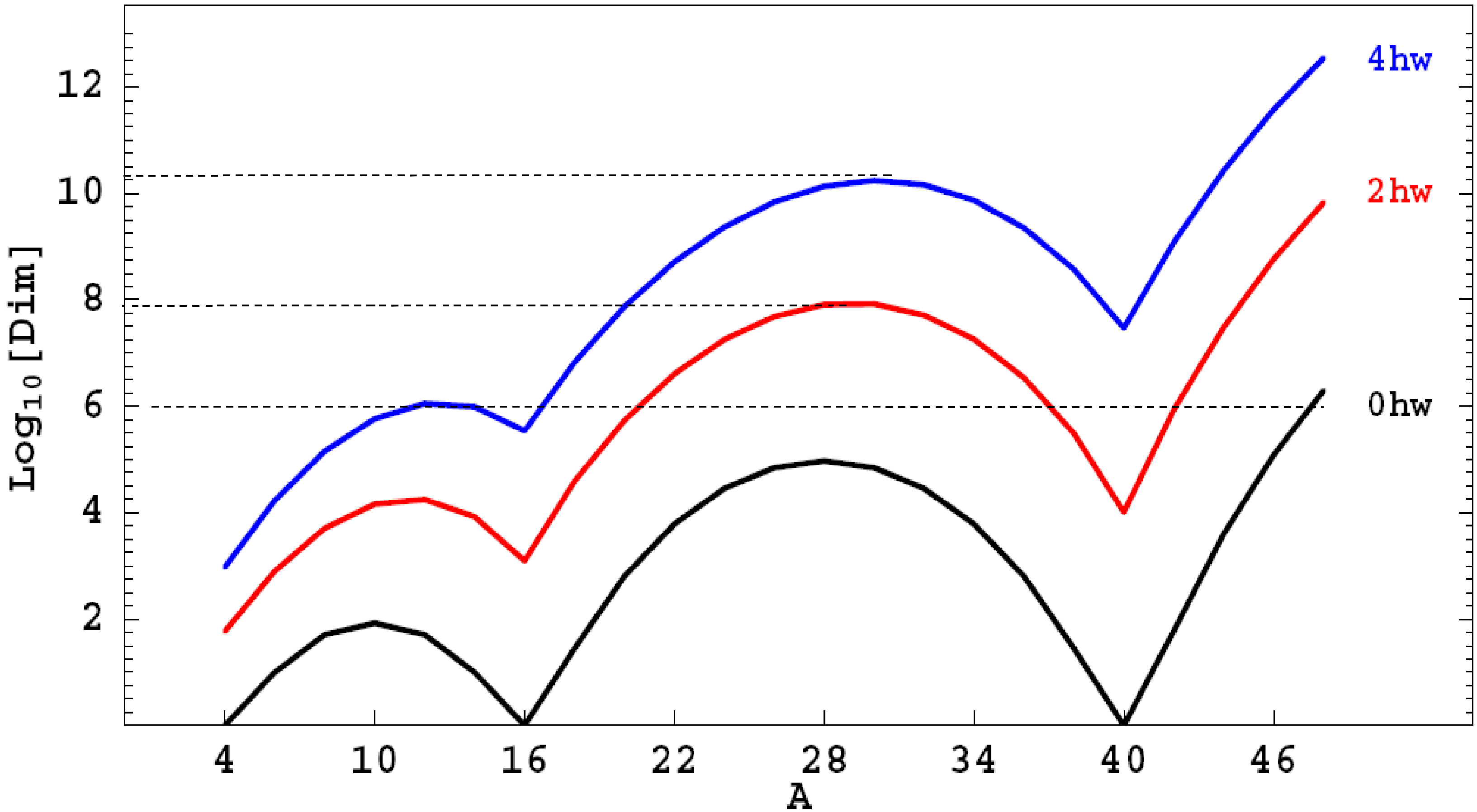
Dimensions: ^{24}Ne

4hΩ-space:1 000 618 679

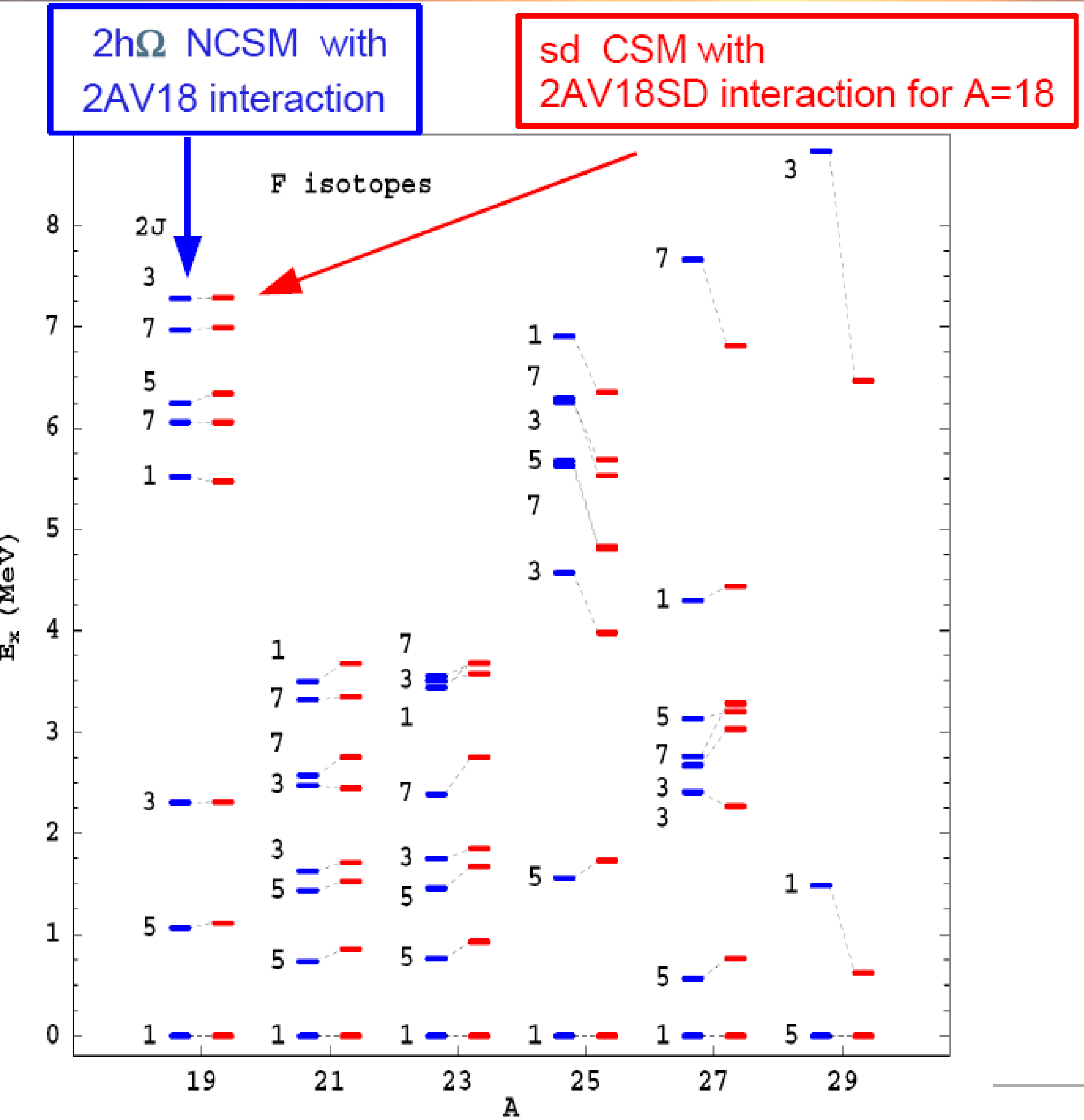
???

Test in 2hΩ space is possible for many cases

Space dimension



Testing effective 2AV18SD interaction for Fluorine isotopes in 2hΩ space



Maximum dimension

^{23}F

sd-space: 1 469

2hΩ-space: 1 725 000

Sources of difference:
a) many-body correlations
b) mass dependence

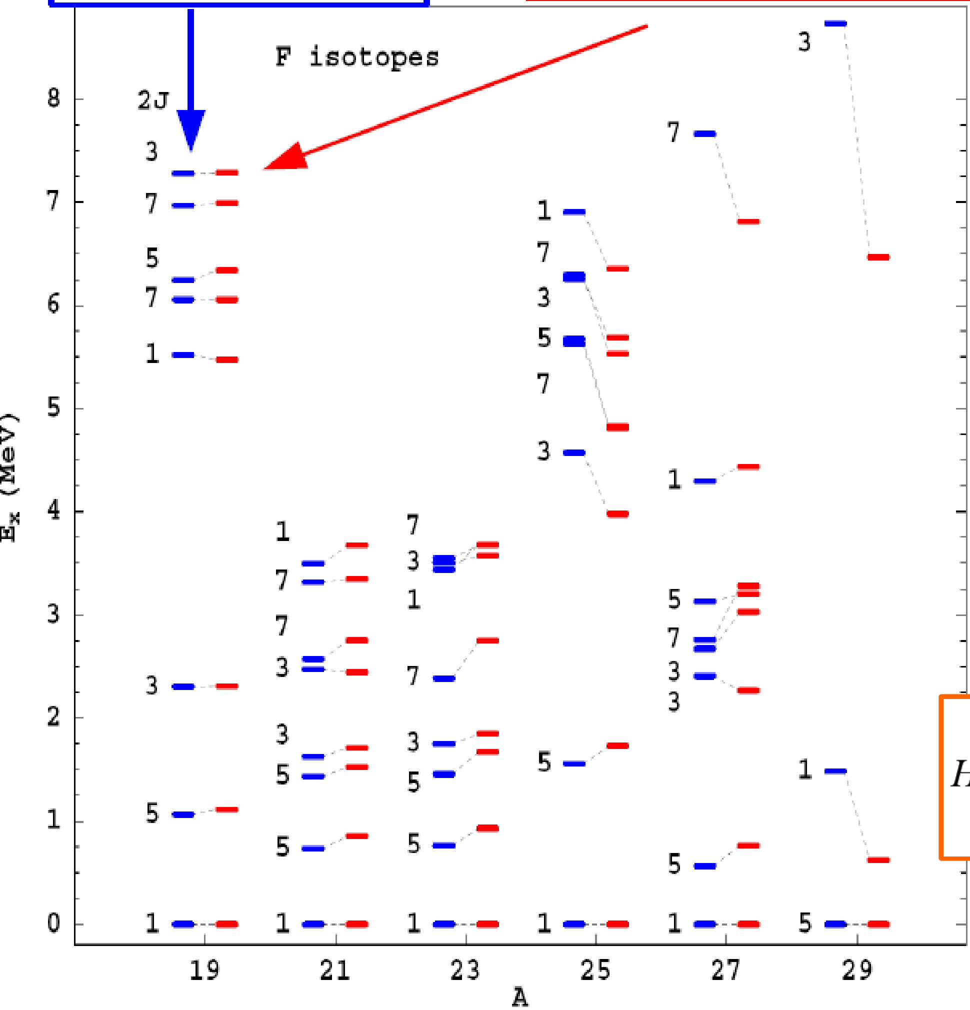
NCSM 2AV18 is A-dependent
CSM 2AV18SD is for A=18

Source b) can be eliminated by deriving 2AV18SD interaction for specific mass A

Testing effective 2AV18SD interaction for Fluorine isotopes in 2hΩ space

2hΩ NCSM with 2AV18 interaction

sd CSM with 2AV18SD interaction for A=18



Maximum dimension

^{23}F

sd-space: 1 469

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Sources of difference:
a) many-body correlations
b) mass dependence

NCSM 2AV18 is A-dependent
CSM 2AV18SD is for A=18

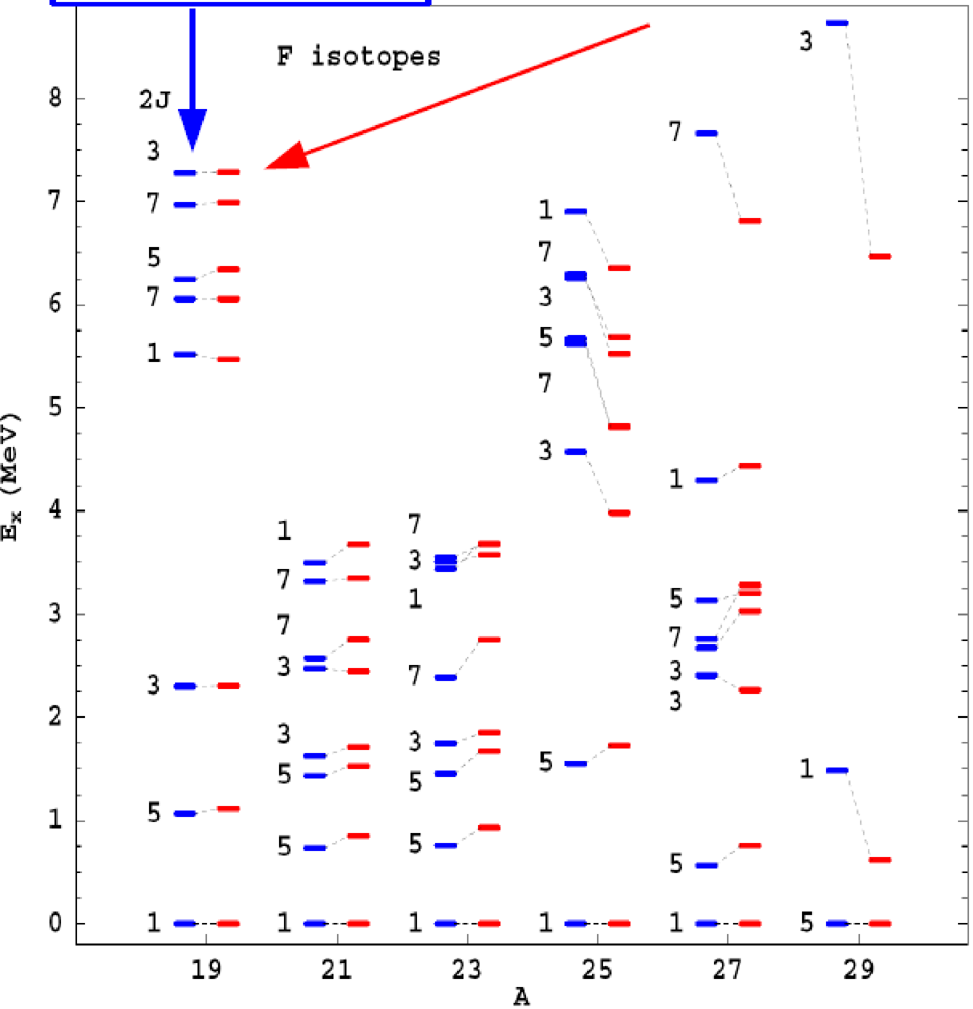
$$H_2^{\Omega} = \sum_{i=1}^{2} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{2} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

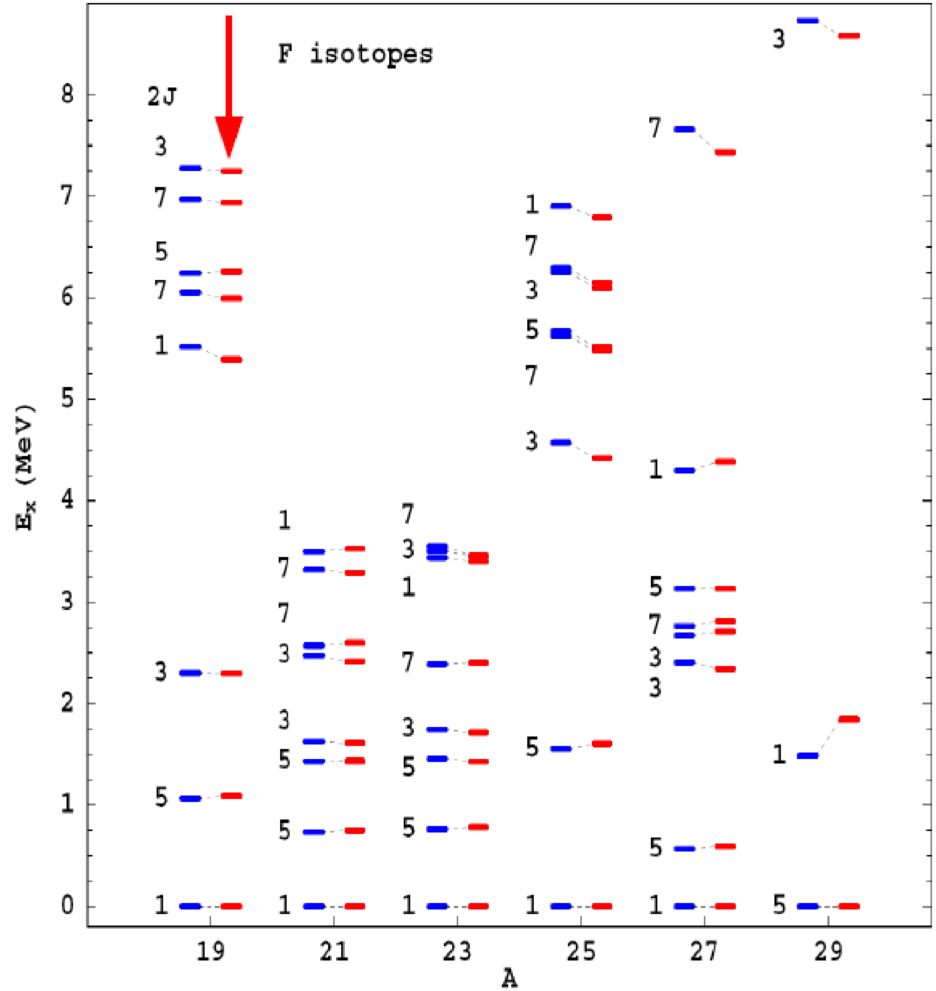
Testing effective 2AV18SD interaction for Fluorine isotopes in 2hΩ space

2hΩ NCSM with 2AV18 interaction

sd CSM with 2AV18SD interaction for A=18

sd CSM with 2AV18SD interaction for specific A



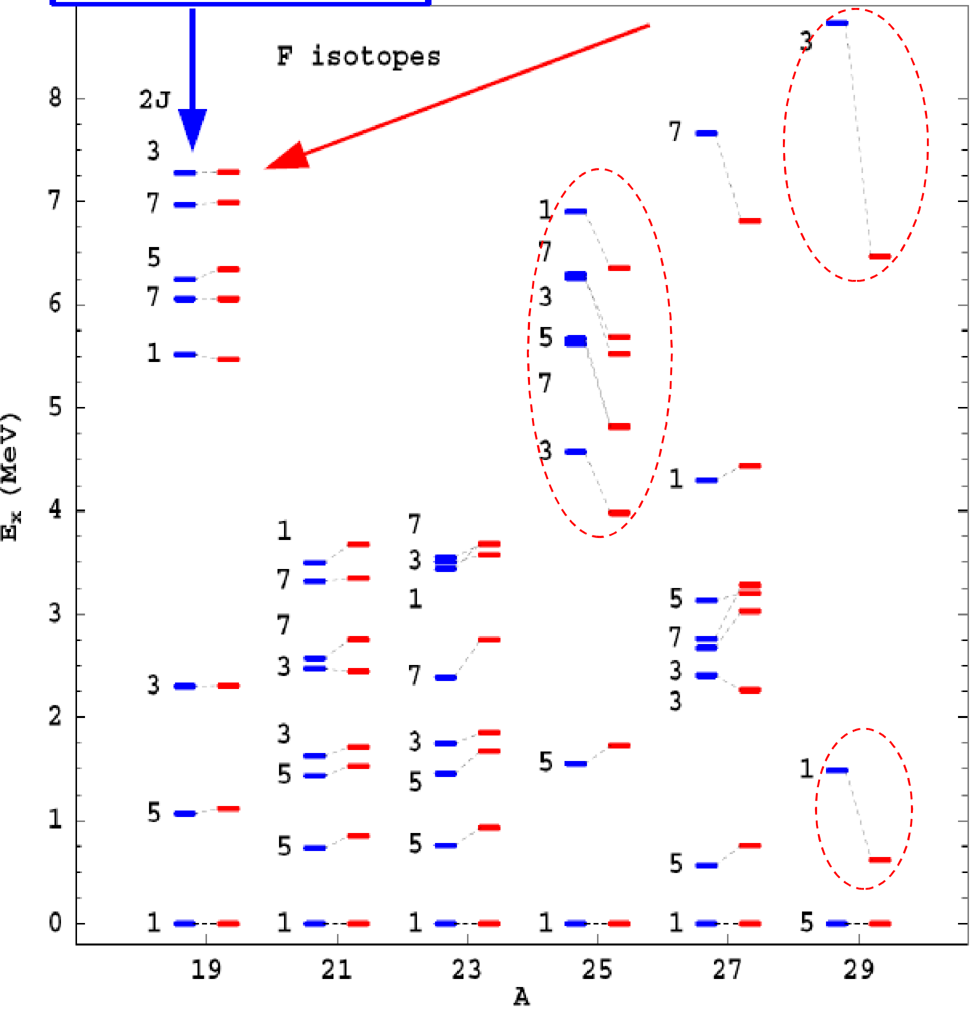


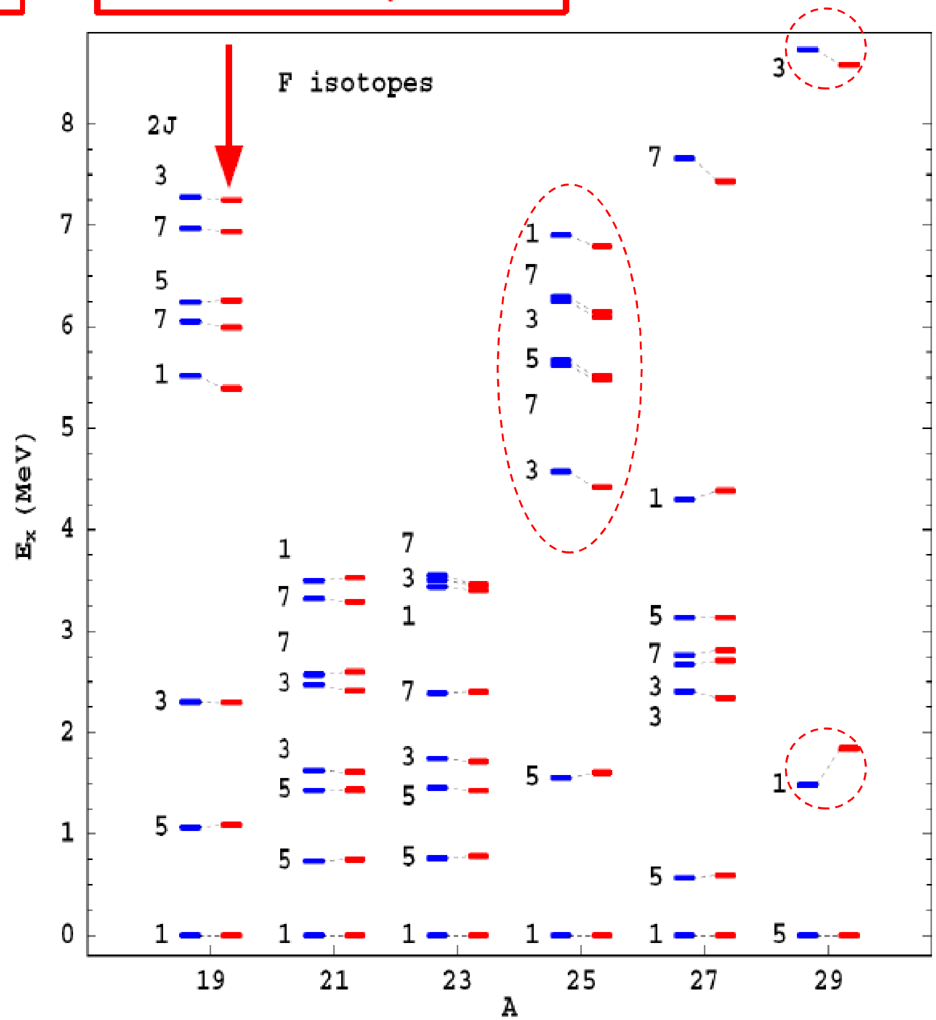
Testing effective 2AV18SD interaction for Fluorine isotopes in 2hΩ space

2hΩ NCSM with 2AV18 interaction

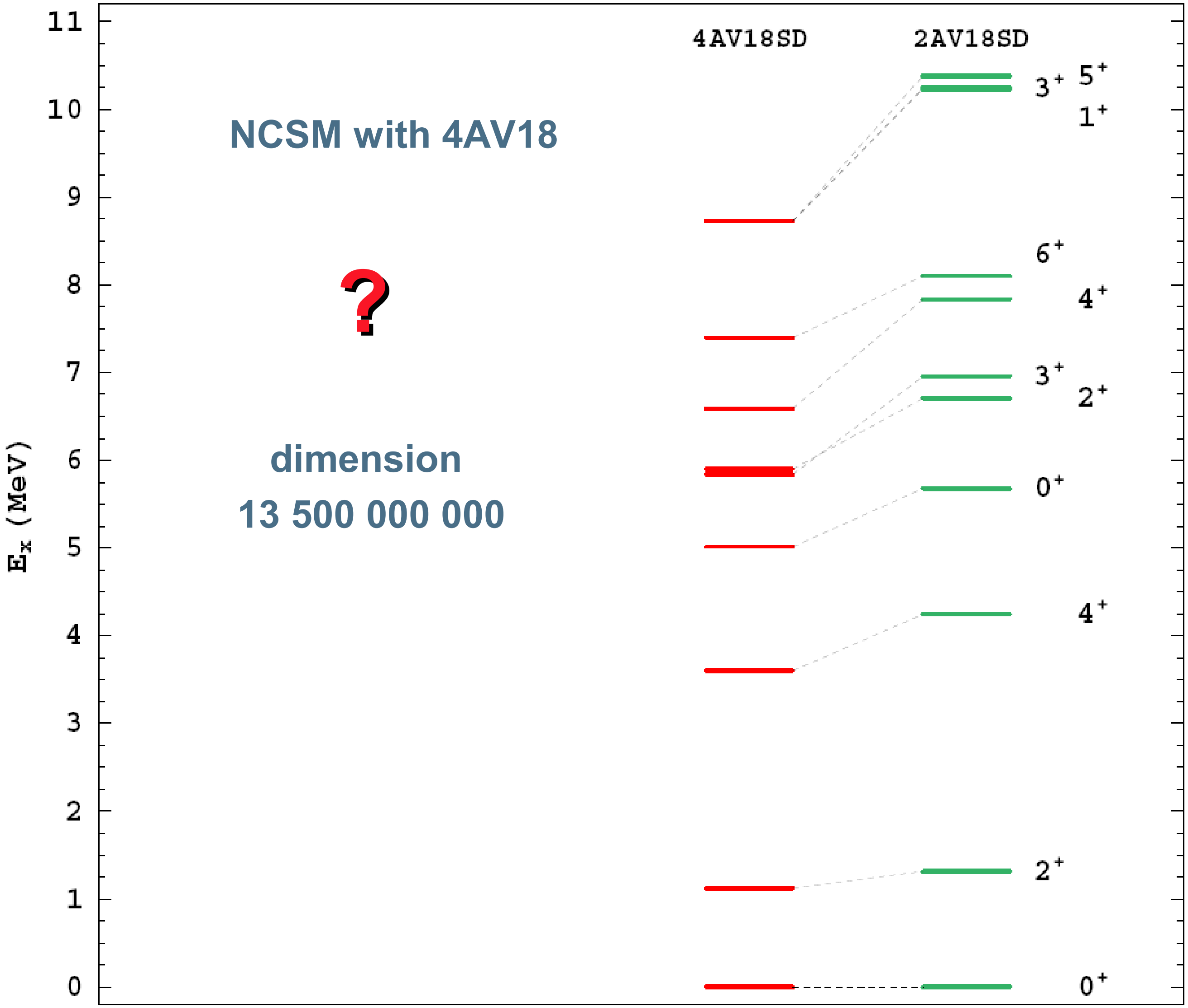
sd CSM with 2AV18SD interaction for A=18

sd CSM with 2AV18SD interaction for specific A





CSM(2AV18SD & 4AV18SD) results for ^{28}Si



From 2hΩ NCSM to pf CSM for ^{42}Sc

Projection of 42-body 2hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{42}Sc

$$H_{eff}([pf]^2) = \Sigma_k \, |k,N_{max}=2,A=42 > E_{\,k} \,(A=42) < \overline{k,N_{max}=2,A=42)|}$$

$$|k,N_{max}=4,A=42 > = U_{k,kp2}|k_{p2}[0h\Omega,42]> + \; U_{k,kq2}|k_{q2}[2h\Omega,42]>$$

2hΩ: $P_1 = P_2 + Q_2$

$\dim(P_1) = 856\,722$ $\quad$ $\dim(P_2)=60$ $\quad$ $\dim(Q_2) = 856\,662$

$$H_{\rm diag} = U H U^{\dagger}$$

$$U = \begin{pmatrix} U_{PP} & U_{PQ} \\ U_{QP} & U_{QQ} \end{pmatrix}$$

$E_k(A=42)$ $\quad$ $H(\,N_{max}=2,A=42)$

$$H_{\rm eff} = \frac{U_p^{\dagger}}{\sqrt{U_p^{\dagger} U_p}} H^{p}_{\rm diag} \frac{U_p}{\sqrt{U_p^{\dagger} U_p}}.$$

$$H_{eff} = H_{eff}(1b) + H_{eff}(2b) + H_{eff}(3b) + H_{eff}(4b) + \ldots$$

Separation of one-body & two-body parts

Step 3: Projection of 41-body 2hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{41}Sc

41-body H constructed using 2AV18 for A=42 !

$$H_{eff}(j;17) = E_{core}(16) + H_{eff}(p_{3/2}) + \varepsilon(j)$$

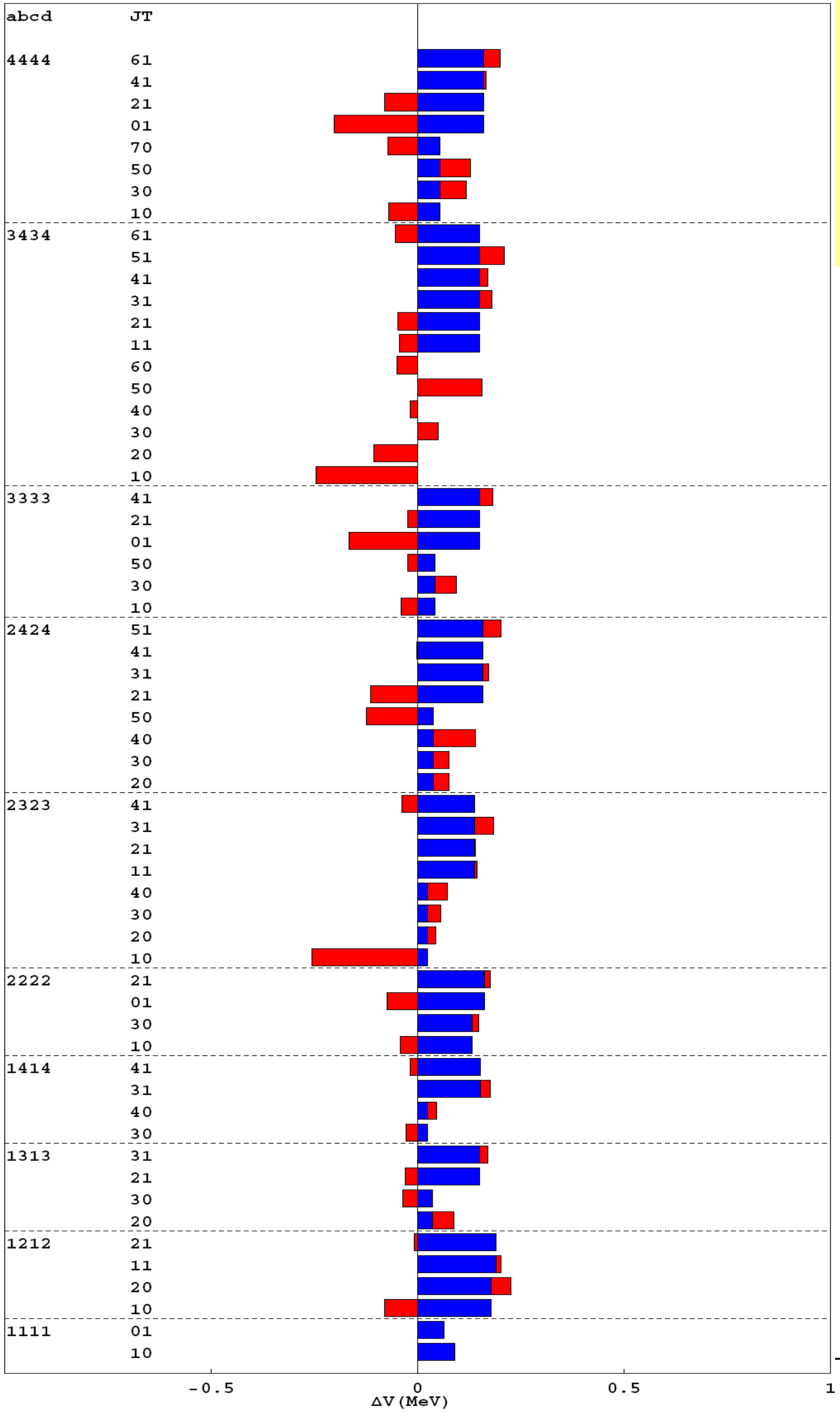
$$\varepsilon(j) = H_{eff}(j;1b) - H_{eff}(p_{3/2})$$

$p_{3/2}$	0.000
$f_{7/2}$	1.676
$p_{1/2}$	1.820
$f_{5/2}$	6.576

$$H_{eff}(p_{3/2}) = E_g(^{41}Sc;GXPF1)$$

$$E_{core}(40) = E_g(^{41}Sc;4AV18) - E_g(^{41}Sc;GXPF1)$$

$$V_{eff}(abcd;JT) = H_{eff}(A=42) - \varepsilon(a) - \varepsilon(b)$$



Comparison of 2AV18PF & pf-part of 2AV18 diagonal part

$$\Delta V(abcd;JT) =$$
$$V_{eff}(4AV18F) - V(4AV18) - \Delta V_{mon}(34,T=0)$$

$$\Delta V(abcd;JT) =$$
$$\Delta V_{mon}(ab,T) + \Delta V_{res}(abcd;JT) - \Delta V_{mon}(34,T=0)$$

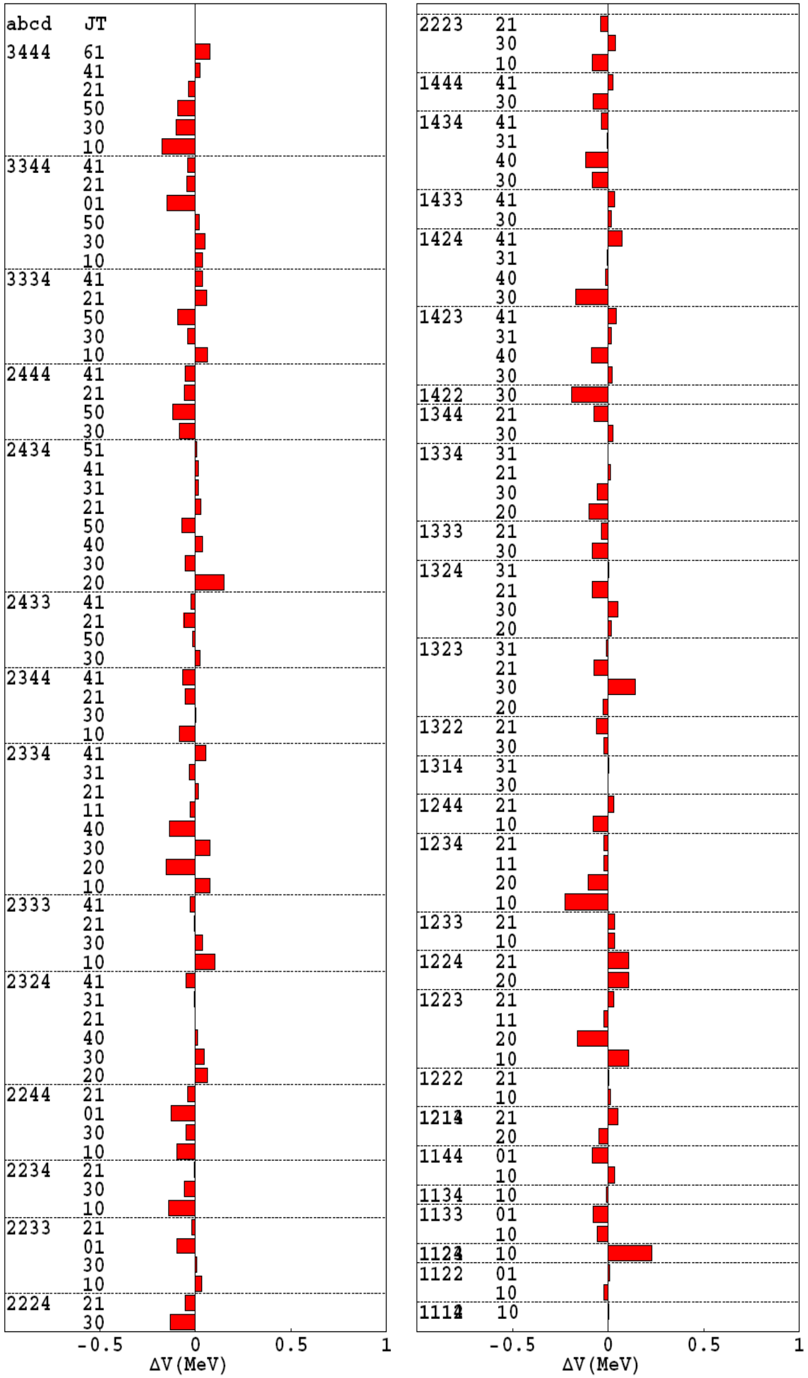
Next steps

→ **Testing different methods to derive interactions directly: 2AV18PF is exact mapping of the 2AV18 for ^{42}Sc**

→ **Testing 2AV18PF interaction for other sd-shell nuclei**

1 - $p_{1/2}$ 2 - $p_{3/2}$ 3 - $f_{5/2}$ 4 – $f_{7/2}$

Comparison of 2AV18PF & pf-part of 2AV18 nondiagonal part



$\Delta V(abcd;JT) =$

$V_{eff}(4AV18SD) - V(4AV18) - \Delta V_{mon}(34,T=0)$

$\Delta V(abcd;JT) =$

$\Delta V_{mon}(ab,T) + \Delta V_{res}(abcd;JT) - \Delta V_{mon}(34,T=0)$

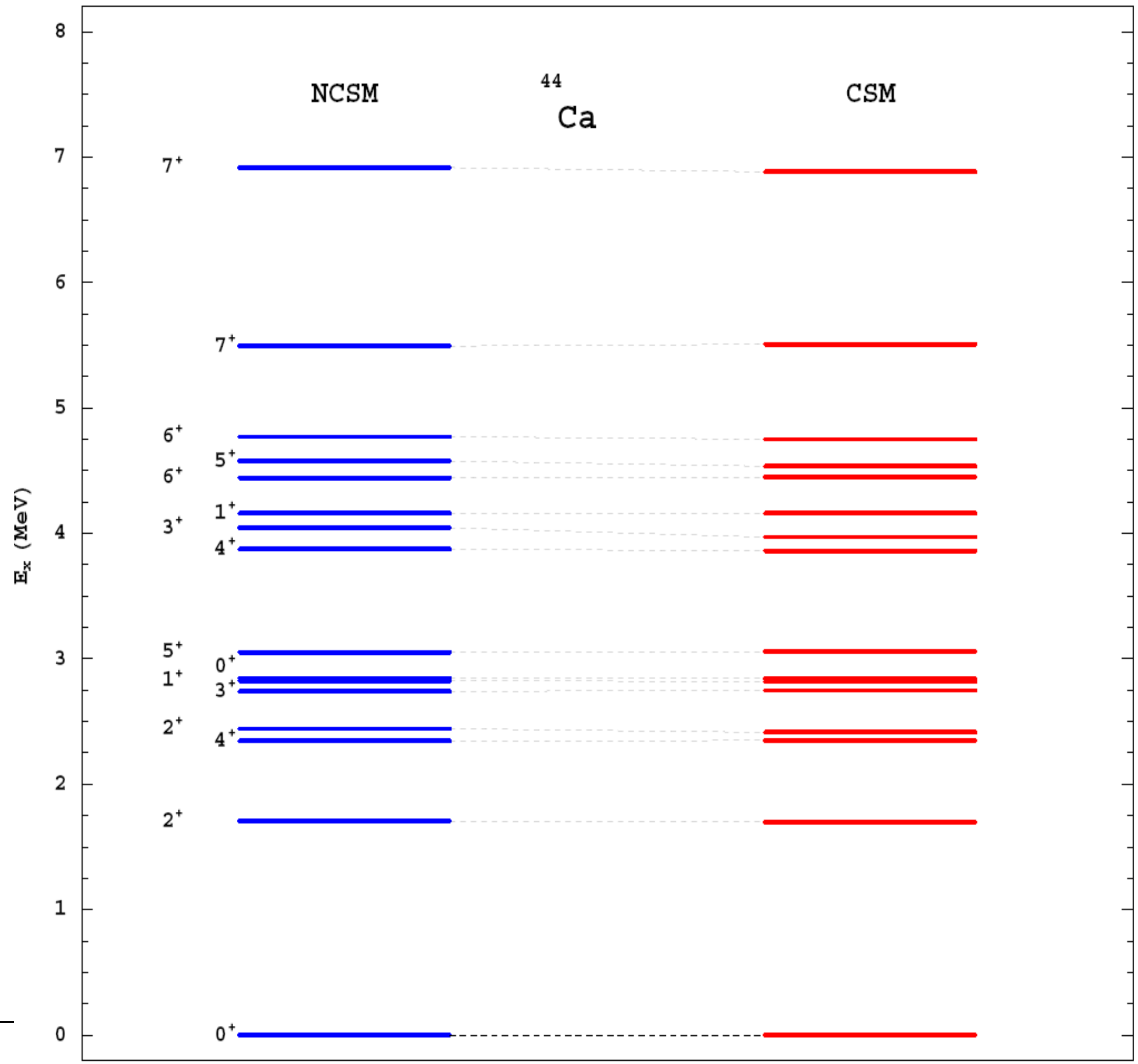
Next steps

Testing different methods to derive interactions directly: 2AV18PF is exact mapping of the 2AV18 for ^{42}Sc

Testing 2AV18PF interaction for other sd-shell nuclei

1 - $p_{1/2}$ 2 - $p_{3/2}$ 3 - $f_{5/2}$ 4 – $f_{7/2}$

CSM(2AV18PF) & NCSM(2AV18) results for ^{44}Ca

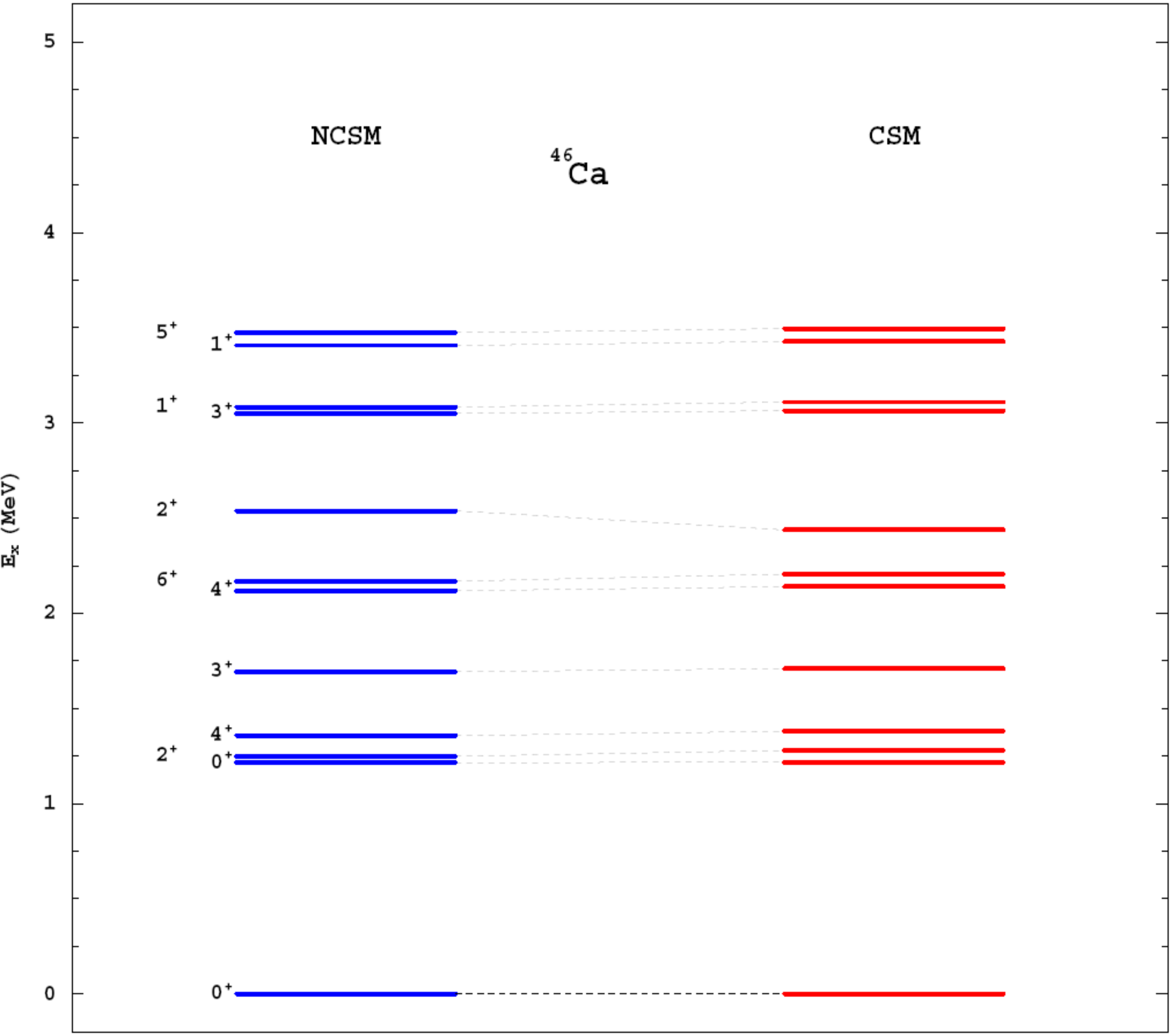


Dimensions: ^{44}Ca

pf-space: 565

2hΩ-space: 10 545 125

CSM(2AV18PF) & NCSM(2AV18) results for ^{46}Ca



Dimensions: ^{46}Ca

pf-space: 3 952

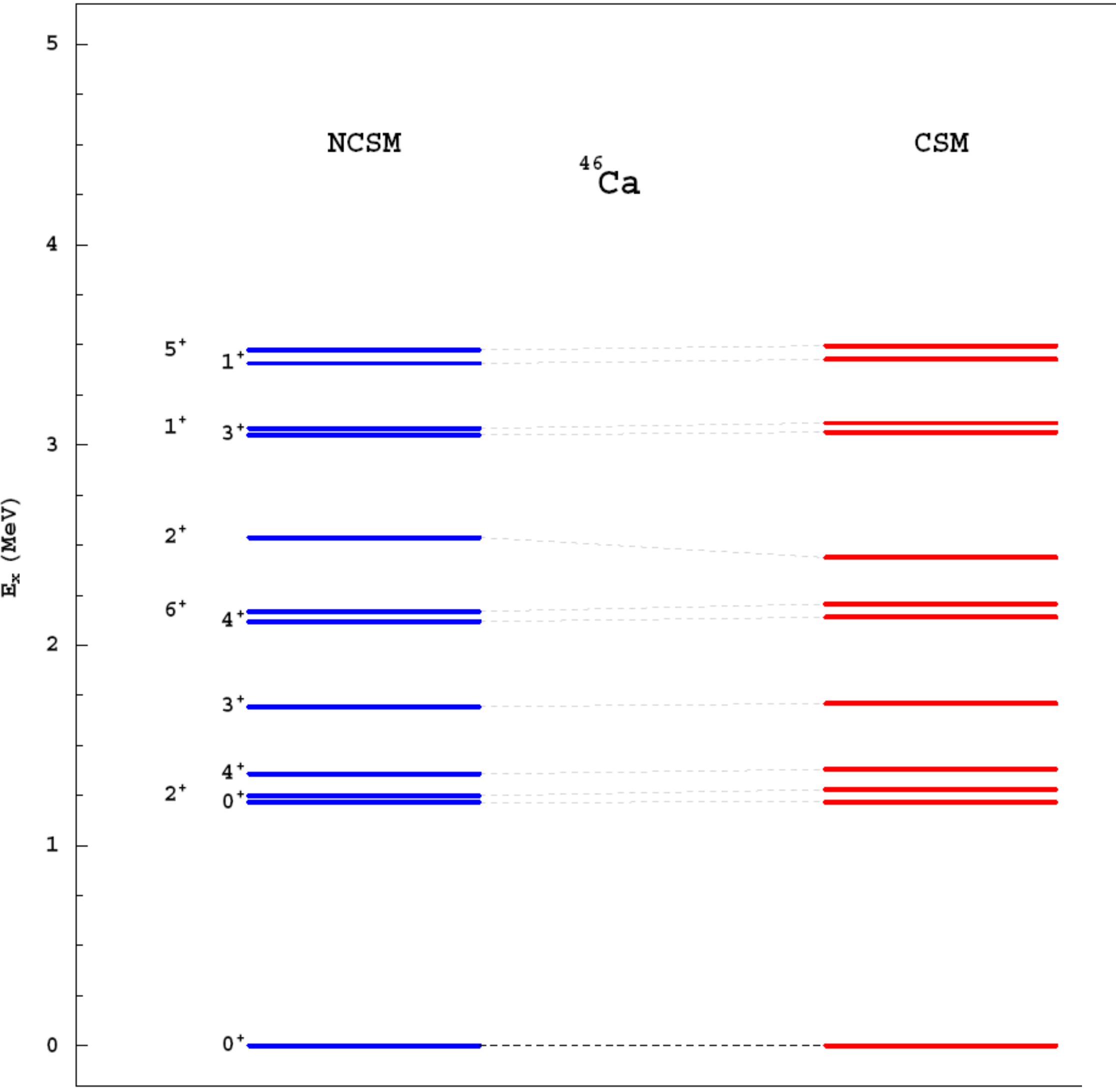
2hΩ-space: 70 213 163

Dimensions: ^{48}Ca

pf-space: 12 022

2hΩ-space: 214 664 244

CSM(3AV18PF) & NCSM(3AV18) results for ^{46}Ca



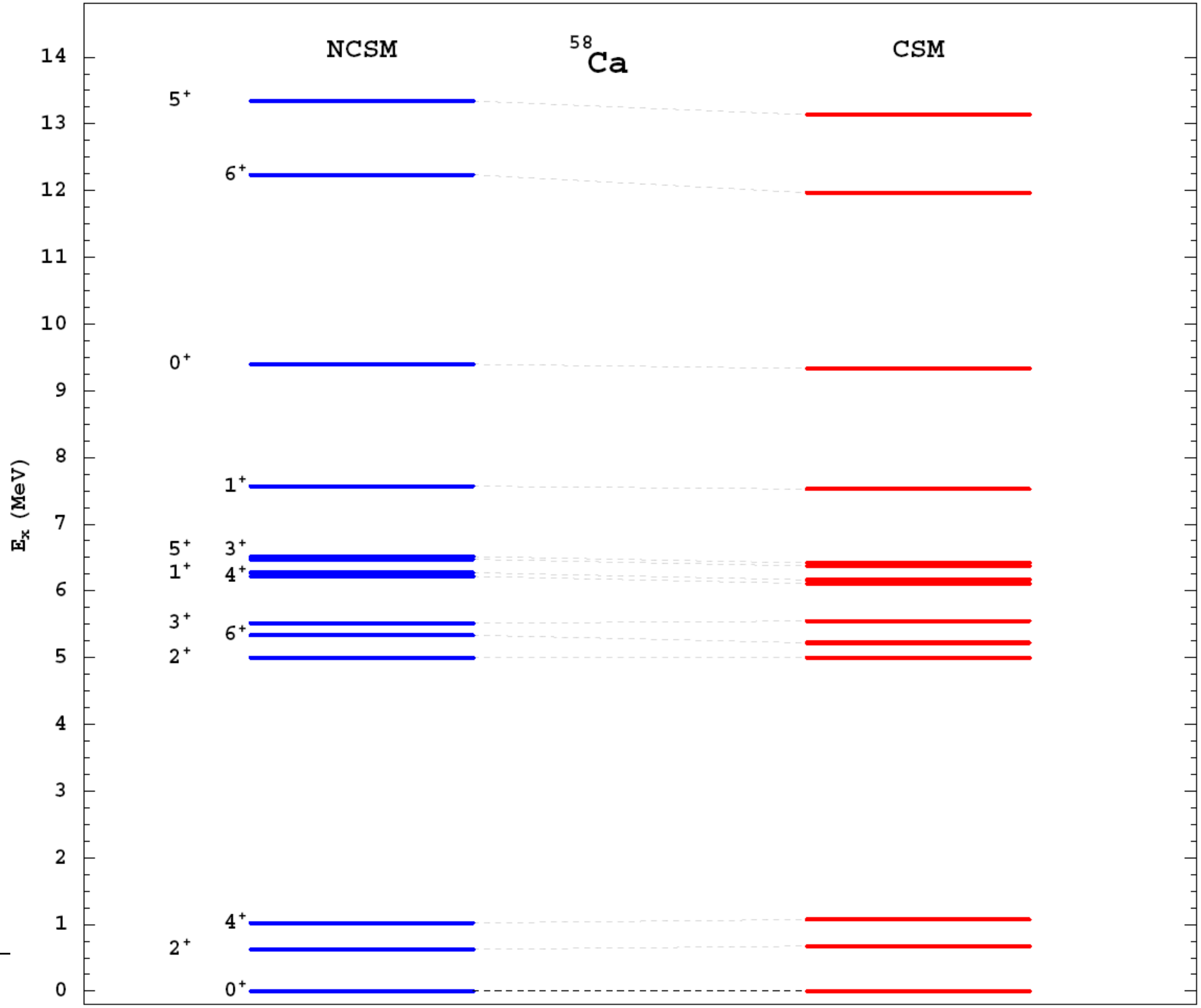
Dimensions: ^{46}Ca

pf-space: 3 952

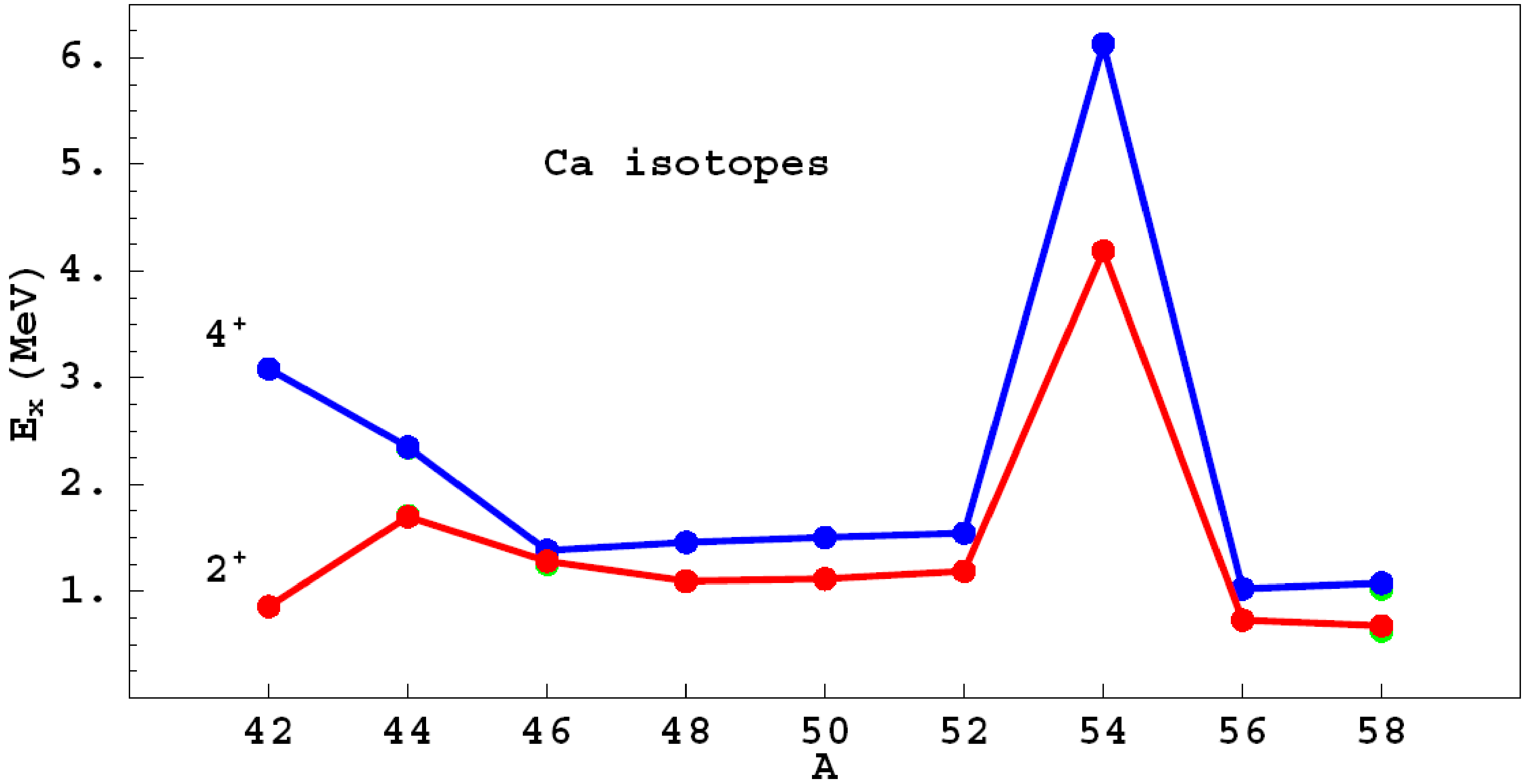
2hΩ-space: 70 213 163

Nuclei	NCSM	CSM
Ca42	623,931	30
Ca44	10,545,125	565
Ca46	70,213,163	3952
Ca48	214,664,244	12022
Ca50	323,752,656	17276
Ca52	246,605,270	12022
Ca54	93,356,454	3952
Ca56	16,503,967	565
Ca58	1,186,633	30

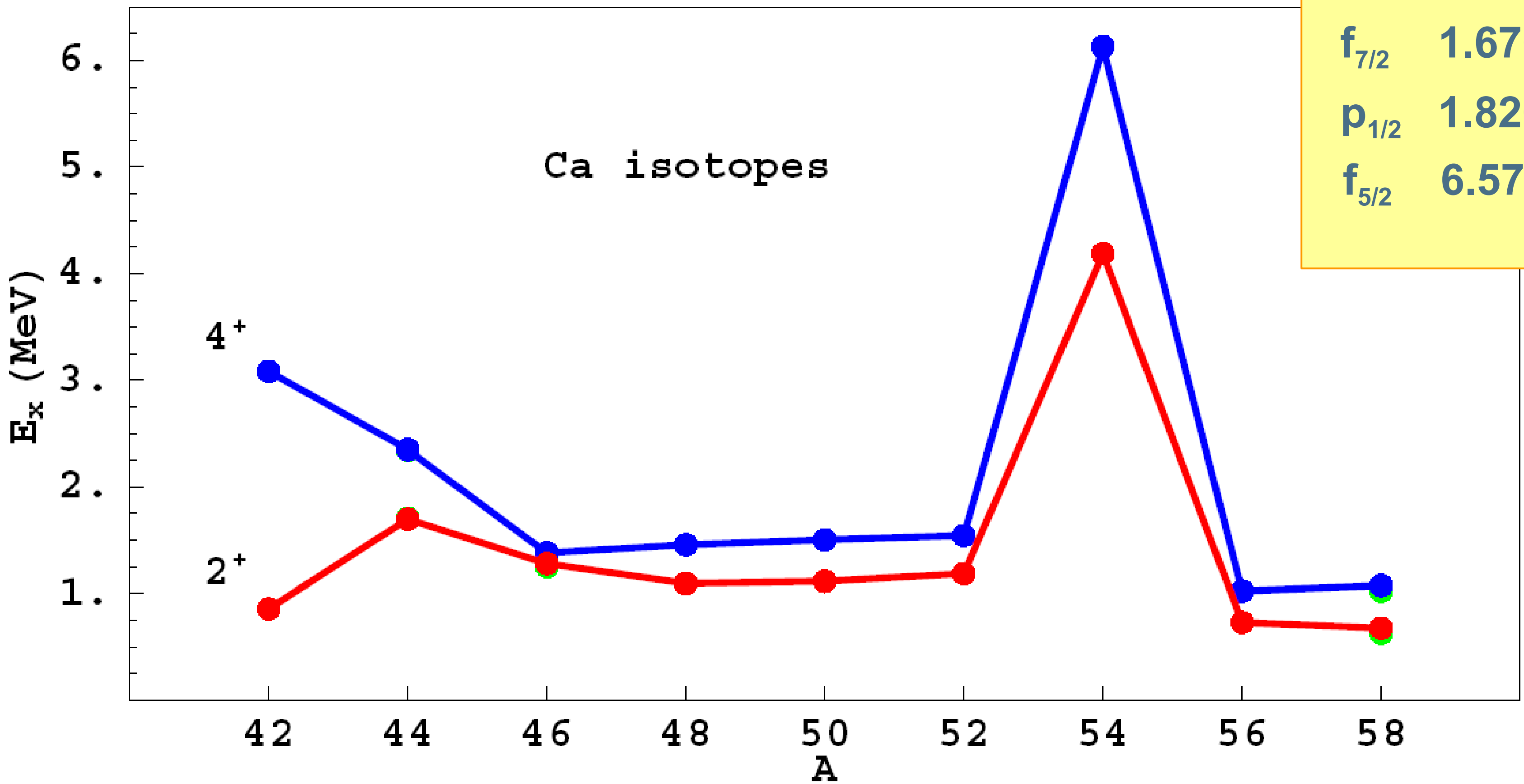
CSM(2AV18PF) & NCSM(2AV18) results for ^{58}Ca



CSM(2AV18PF) & NCSM(2AV18) results for Ca isotopes



CSM(2AV18PF) & NCSM(2AV18) results for Ca isotopes



$p_{3/2}$	0.000
$f_{7/2}$	1.676
$p_{1/2}$	1.820
$f_{5/2}$	6.576

Summary

1) 2-step construction procedure of H_{eff} is introduced:

   # 1 standard 2-body UT (2-body cluster approximation)

   # 2 A-body UT + 2-body projection

2) sd-shell 2-body H_{eff} are derived from 18-body $2h\Omega$ ($4h\Omega$) Hamiltonians constructed using AV18, N^3LO and CD-Bonn NN potentials

3) pf-shell 2-body H_{eff} are derived from 42-body $2h\Omega$ Hamiltonians constructed using AV18 potential

4) Major modification of the original H (after step #1) reduces to 1-body corrections and monopole corrections of TBME - to be explored further - to find an approach to generate H best matching exactly projected one without doing NCSM calculation

5) Effective 2-body interactions "predict" the large scale NCSM spectra for sd- & pf-shell nuclei with good precision - efficient tool to test NCSM performance in the case of intractable dimensions

6) Missing higher-order (>2) correlations in sd- & pf- spaces do not play important role for low-energy spectra -- binding energy to be explored

7) Issues to be addressed: effective operators, increased "small" space, negative parity spectra, 3-body sd Hamiltonian effects for spectra & binding energies

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