Perspectives of the Ab Initio No-Core Shell Model

No-core Monte Carlo shell model in light nuclei

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Outline

- Motivation
- Recent Development s of MCSM
  - Acceleration of TBMEs Computation
  - Energy-variance Extrapolation
- Benchmark Results
- Error Assignment of Extrapolation
- Summary & Outlook

Introduction

- Current motivation for the nuclear structure theory

  - Understand the nuclear structures from the first principle of nuclear theory by *ab-initio* calc w/ realistic nuclear forces

→ Machine power: one of the main limitations for the large-scale computation

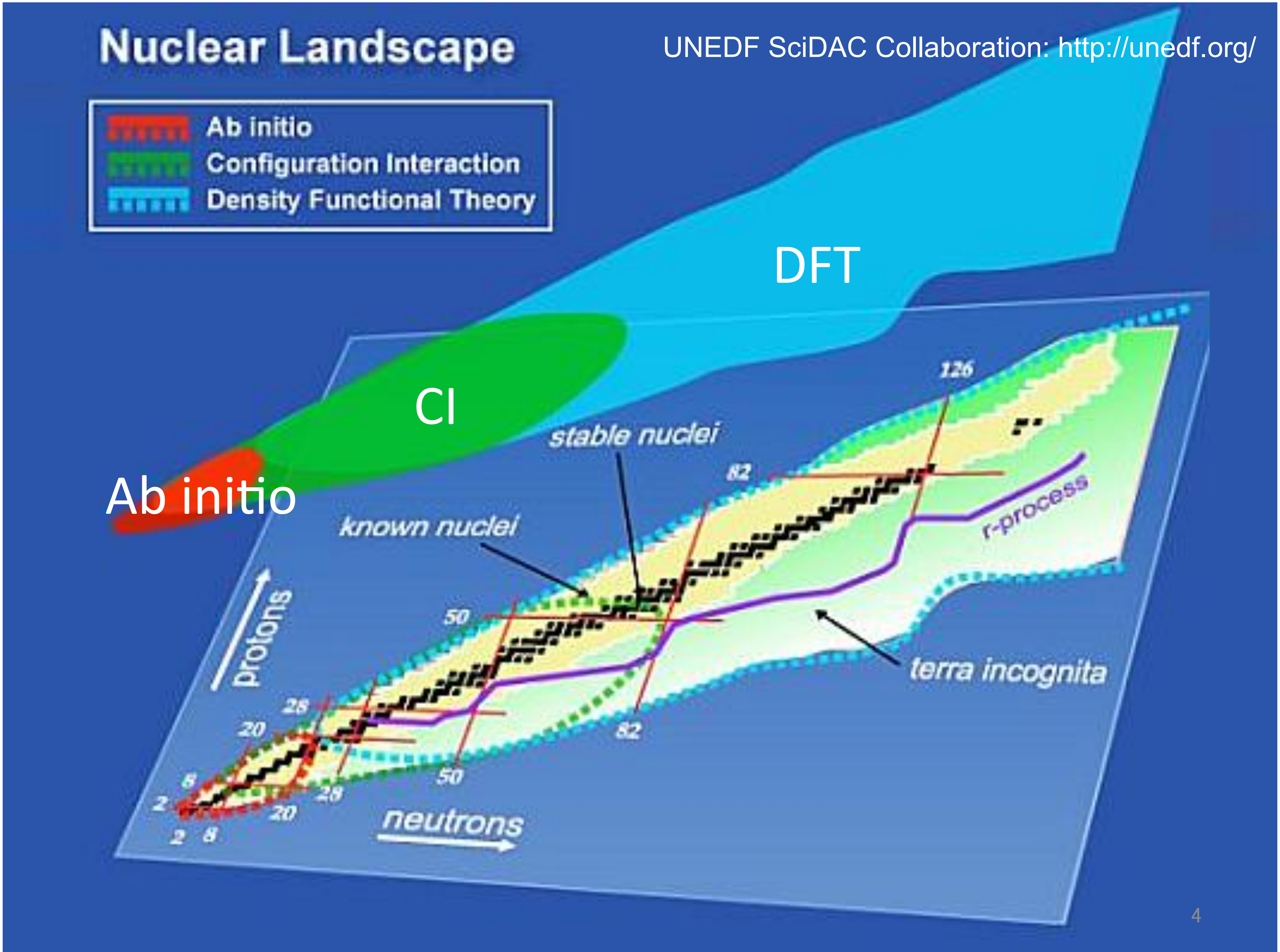
- Necessity of *ab-initio*(-like) method compared w/ GFMC, NCSM, (up to ~ A = 12-16), CC(closed shell +/- 1,2)

→ No-core Monte Carlo shell model

- Choice of the nuclear forces (interactions) efficient for the MCSM calculation

→ JISP16 NN int.

Open the way to understand nuclear structures from the realistic nuclear forces


Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
DFT
CI
Ab initio
stable nuclei
known nuclei
r-process
terra incognita
protons
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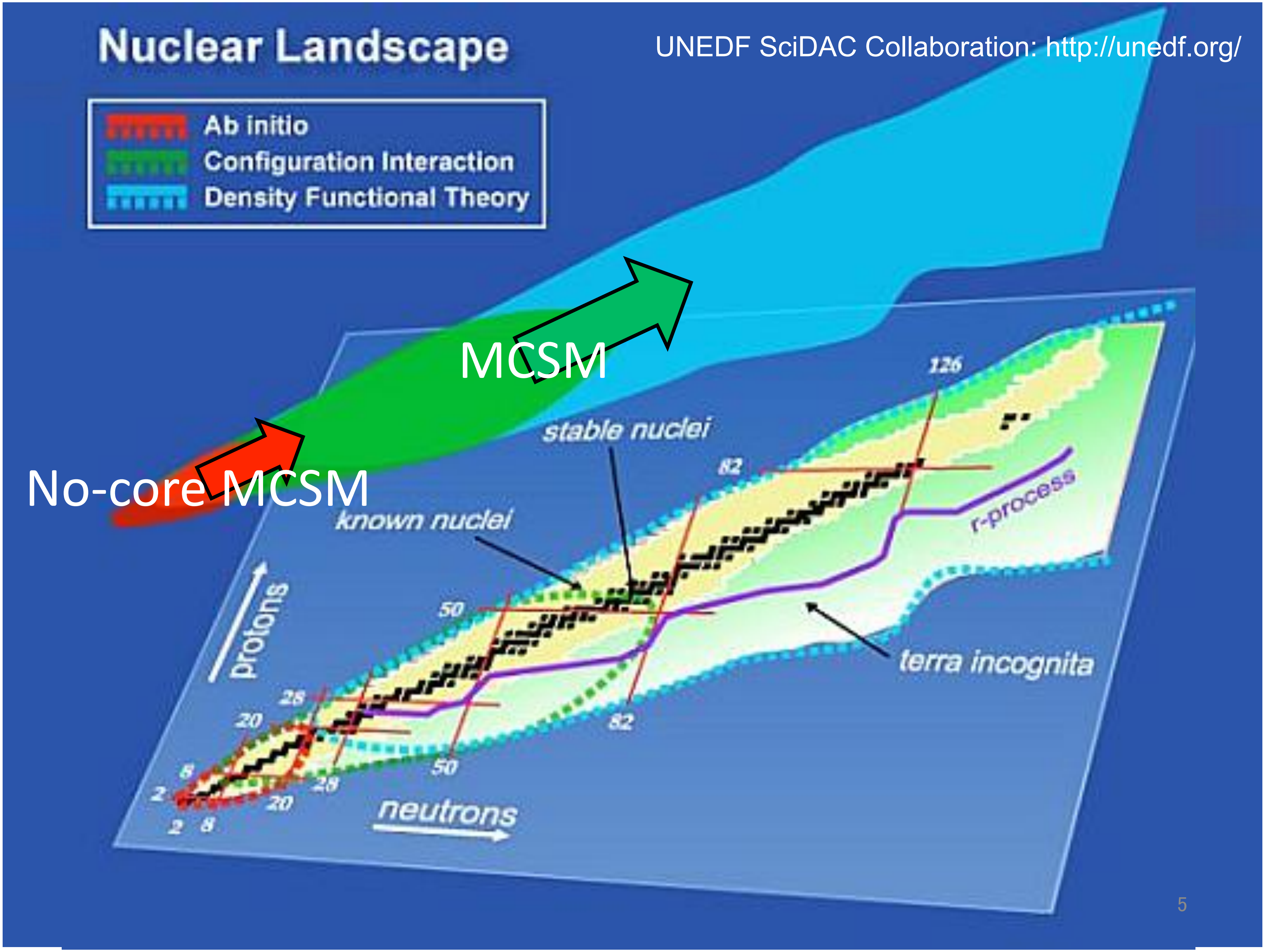
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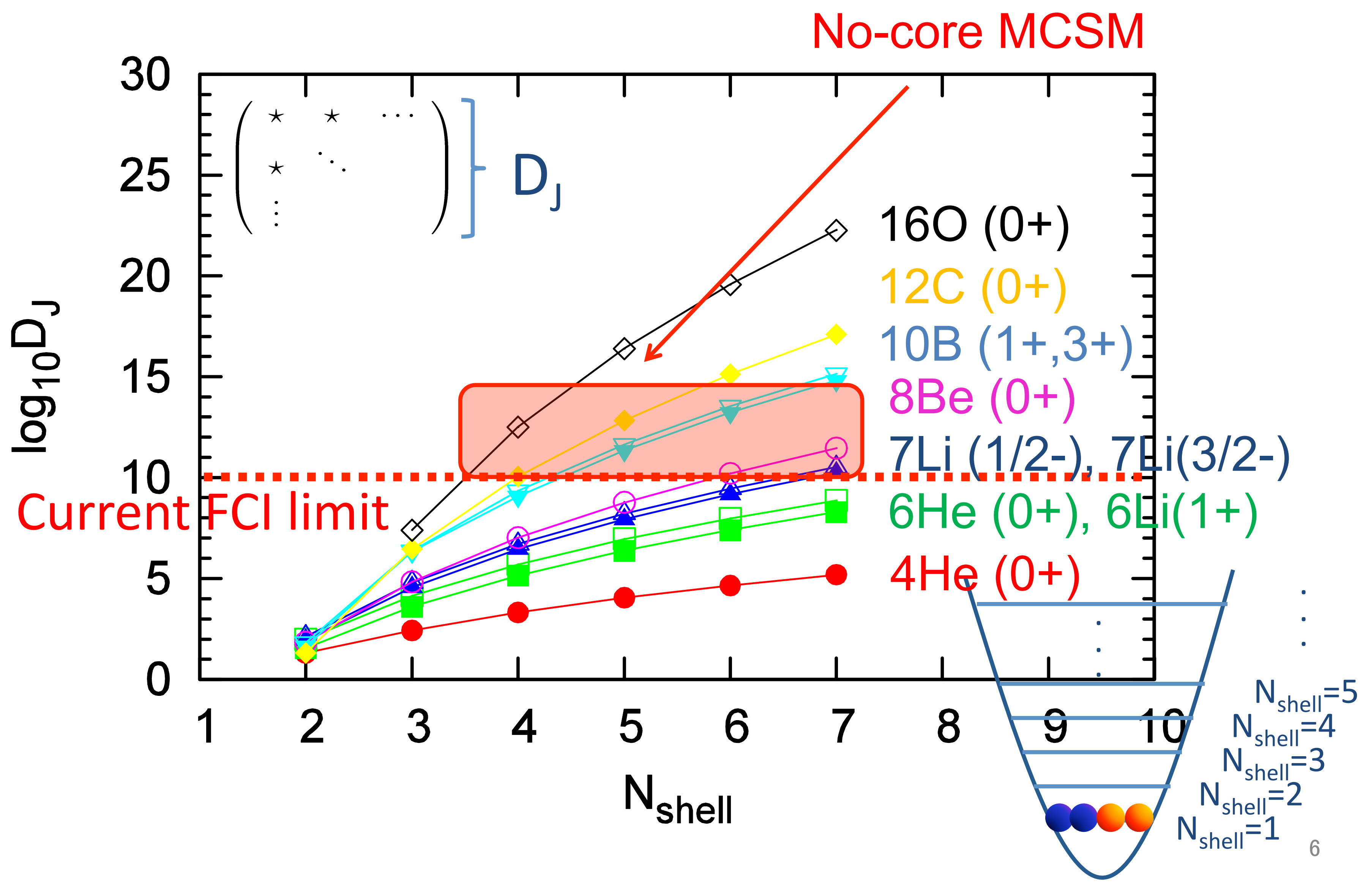
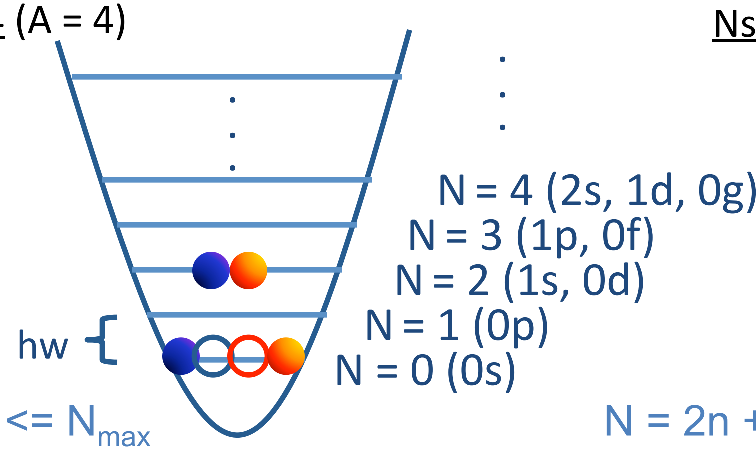
J-scheme dimension



Truncations of the Model Space in NCSM & FCI

- **Nmax (NCSM, NCFC, IT-NCSM, …)**
  - ➢ Max. # of HO quanta of many-body basis

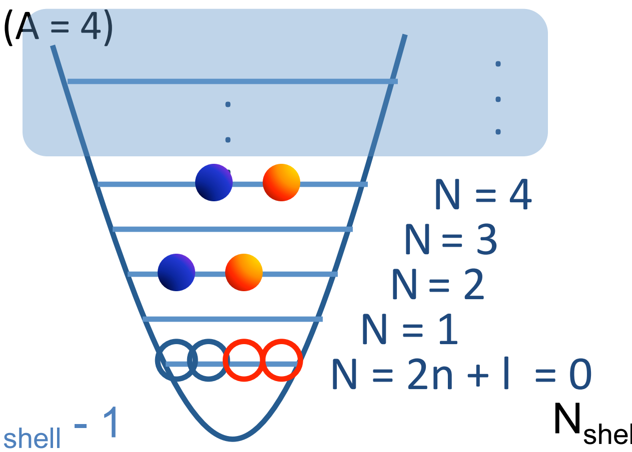
Nmax = 4 (A = 4)



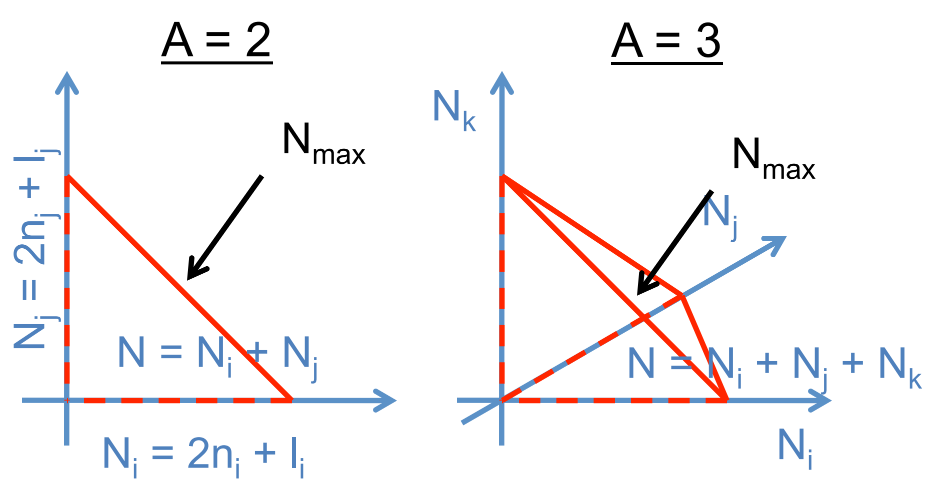
$N = \sum_i 2n_i + l_i <= N_{max}$

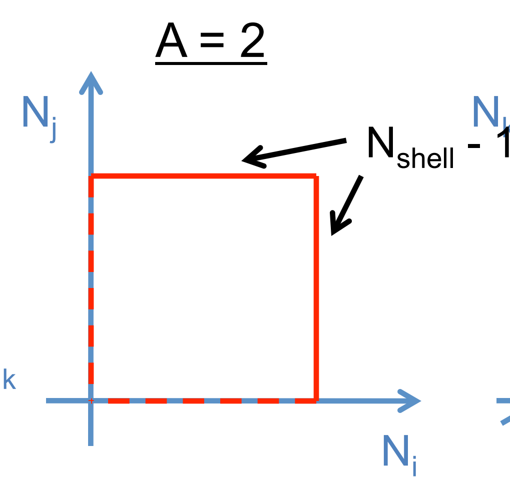
- **Nshell (FCI, MCSM, IT-CI, …)**
  - ➢ Max. # of HO quanta of single-particle basis

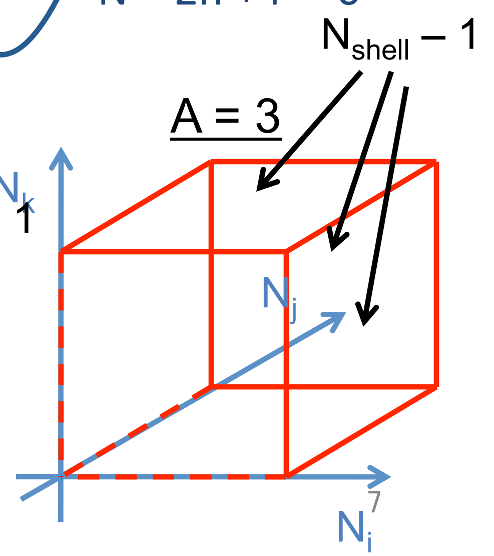
Nshell = 5 (A = 4)



$N = 2n + l <= N_{shell} - 1$







NCSM, FCI, NCFC, MCSM

	Truncation	Interaction
NCSM	Nmax	Bare/Effective
FCI	Nshell	Bare
NCFC	Nmax	Bare
MCSM	Nshell	Bare/Effective

- ✓ NCSM,FCI,NCFC does exact diagonalization of large Hamilotonian matrices, while MCSM utilizes the diagonalization of smaller matrices w/ importance-truncated bases.
- ✓ NCSM,NCFC uses Nmax truncation, while FCI, MCSM does Nshell truncation.
- ✓ Nmax is the sum of the HO excitation quanta from the reference state.
- ✓ Nshell is the # of major shells included as the model space.
- ✓ NCSM usually employs effective interactions for getting faster convergence wrt the model space.
- ✓ FCI,NCFC employs bare interactions & extrapolates into the infinite model space (Nshell, Nmax -> ∞).
- ✓ Treatment of spurious CM effect is exact in NCSM,NCFC , while it is approximate in FCI,MCSM (by using Gloeckner-Lawson method).

JISP16 NN interaction

- JISP16: J-matrix Inverse Scattering Potential tuned B.E.s up to 16O with phase-shift-equivalent unitary transformation

$$V = \sum_{\Gamma,\Gamma'} \sum_{n=0}^{N_\Gamma} \sum_{n'=0}^{N_{\Gamma'}} |n,\Gamma\rangle V_{n,n'}^{\Gamma,\Gamma'} \langle n',\Gamma'|$$

  - Small matrix of the NN int. in the oscillator basis
  - High quality description of NN potential thru. p-shell nuclei
    -> Reproduce the phase shift, deuteron properties, & B.E.s of some light nuclei
    -> In this sense, JISP16 is the “bare” interaction
  - JISP16 NN int. seems to minimize 3N (many-body) int.

→ realistic large-scale computation of nuclear structures w/o genuine 3N force

<u>References</u>

JISP16: A. M. Shirokov, J.P. Vary, A. I. Mazur, T.A. Weber, Phys. Lett. B644, 33 (2007)
NCFC calc of light nuclei w/ JISP16: P. Maris, J.P. Vary, A.M. Shirokov, Phys. Rev. C 79, 014308 (2009)

Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

Monte Carlo shell model (MCSM)

$$|\psi(\sigma)\rangle = \prod e^{\Delta\beta h(\sigma)}|\phi\rangle$$

- Importance truncation

$$|\phi\rangle = \prod_{\alpha=1}^{N}\left(\sum_{i=1}^{N_{sp}} c_i^{\dagger} D_{i\alpha}\right)|-\rangle$$

<u>Standard shell model</u>

$$H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix} \Rightarrow \begin{pmatrix} E_0 & & & & 0 \\ & E_1 & & & \\ & & E_2 & & \\ & & & \ddots & \\ 0 & & & & \end{pmatrix}$$

Diagonalization

All Slater determinants

$$|\Psi\rangle = \sum_{i=1}^{d_{MCSM}} c_i \mathrm{P}^{\mathrm{J},\Pi}|\psi_i(\sigma)\rangle$$

<u>Monte Carlo shell model</u>

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \Rightarrow \begin{pmatrix} E_0' & & 0 \\ & E_1' & \\ 0 & & \ddots \end{pmatrix}$$

Diagonalization

Important bases stochastically selected

$d_{MCSM} \sim O(10\text{-}100)$

New MCSM code

Original MCSM code

since 1995 for conventional large-scale shell-model calc.

Useful even nowadays, but …

- Fortran 77
- PVM (less popular now)
- Isospin-conserving interaction only
- Developed on Alpha chip

→ difficult to run it on state-of-the-art supercomputers with minor modification

New MCSM code since 2010

written from scratch

- Not only for shell-model calc. with core, but also for no-core calc.
- Fortran 95
- MPI (+OpenMP hybrid parallel)
- Isospin-breaking interaction
- Developed on Intel chip
- New algorithm to evaluate Hamiltonian matrix elements in Slater det. Basis
- Improved sampling algorithm
- Extrapolation by energy variance

Ref. T. Otsuka, T. Mizusaki, and M. Honma: Phys. Rev. Lett. 75 1284 (1995)

not yet : 3-body force

Recent developments in MCSM

- Acceleration of the computation of two-body matrix elements

$$\langle \phi | \hat{V} | \phi' \rangle = \frac{1}{2} \sum_{i,k} \rho_{ki} \left(\sum_{j,l} v_{ij\,kl} \rho_{lj} \right) = \frac{1}{2} \sum_{(ki)} \rho_{(ki)} \left(\sum_{j\,l} v_{(ki),(lj)} \rho_{(lj)} \right)$$

Matrix product is performed by DGEMM subroutine in BLAS library

800 % performance improvement from the original MCSM code

- Extrapolation method by the energy variance

$$\langle H \rangle = E_0 + E_1 \langle \Delta H^2 \rangle + E_2 \langle \Delta H^2 \rangle^2 + \cdots \qquad \langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

$$\frac{\langle \phi | \hat{H}^2 | \psi \rangle}{\langle \phi | \psi \rangle} = \sum_{i<j,\alpha<\beta} \left(\sum_{k<l} v_{ijkl} ((1-\rho)_{k\alpha} (1-\rho)_{l\beta} - (1-\rho)_{l\alpha} (1-\rho)_{k\beta}) \right) \left(\sum_{\gamma<\delta} v_{\alpha\beta\gamma\delta} (\rho_{\gamma i} \rho_{\delta j} - \rho_{\delta i} \rho_{\gamma j}) \right)$$
$$+ \mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho) + \left(\mathrm{Tr}(\rho(t + \frac{1}{2}\Gamma)) \right)^2$$

(naively) 8-fold loops -> (effectively) 6-fold loops by the factorization

N. Shimizu, Y. Utsuno, T.Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

Acceleration of TBMEs Computation

New algorithm for the MCSM code

Hot spot: compute the matrix element of two-body interaction between two deformed Slater determinants, $|\phi\rangle = \prod_{\alpha=1}^{N}\left(\sum_{i=1}^{N_{sp}} c_i^\dagger D_{i\alpha}\right)|-\rangle$

sparse two-body matrix elements in *m*-scheme

real, block diagonal

complex

$$\langle\phi|\hat{V}|\phi'\rangle = \sum_{i<j,k<l} v_{ijkl}\langle\phi|c_i^\dagger c_j^\dagger c_l c_k|\phi'\rangle$$

$$= \sum_{i<j,k<l} v_{ijkl}\left(\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li}\right) = \frac{1}{2}\sum_{i,k}\rho_{ki}\left(\sum_{j,l} v_{ijkl}\rho_{lj}\right)$$

Original code:

```
do n=1,nmax
   i  = ind(1,n)
   j  = ind(2,n)
   k = ind(3,n)
   l  = ind(4,n)
   x = x + v(n)*(rho(k,i)*rho(l,j)-rho(k,j)*rho(l,i))
end do
```

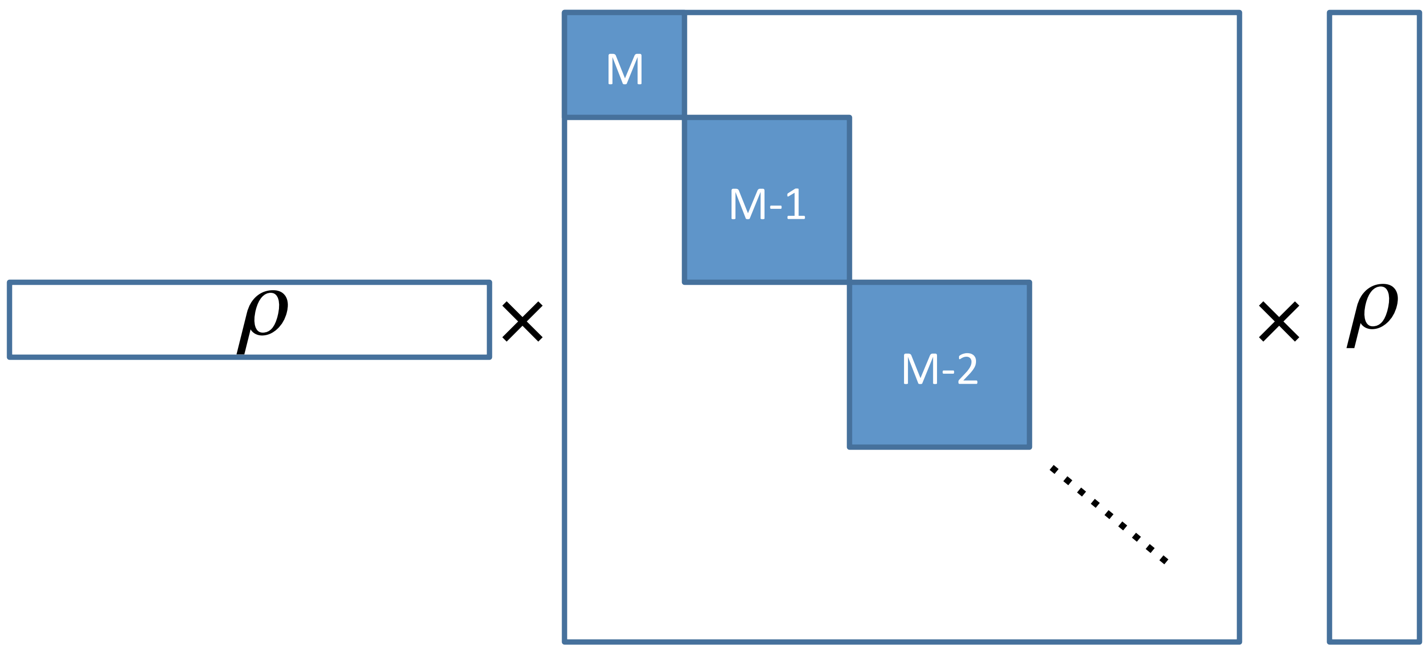
New code (concept):

```
do ki=1,ijmax
     y = 0.
    do jl=1,jlmax
        y  = y +v(ki, jl) *rho(jl)
     end do
     x = x + rho(ki) * y
end do
```

(Matrix) x (Vector)

$$\langle \phi | \hat{V} | \phi' \rangle = \frac{1}{2} \sum_{i,k} \rho_{ki} \left(\sum_{j,l} v_{ij\,kl} \rho_{lj} \right) = \frac{1}{2} \sum_{(ki)} \rho_{(ki)} \left(\sum_{jl} v_{(ki),(lj)} \rho_{(lj)} \right)$$

$$M = m_k - m_i$$



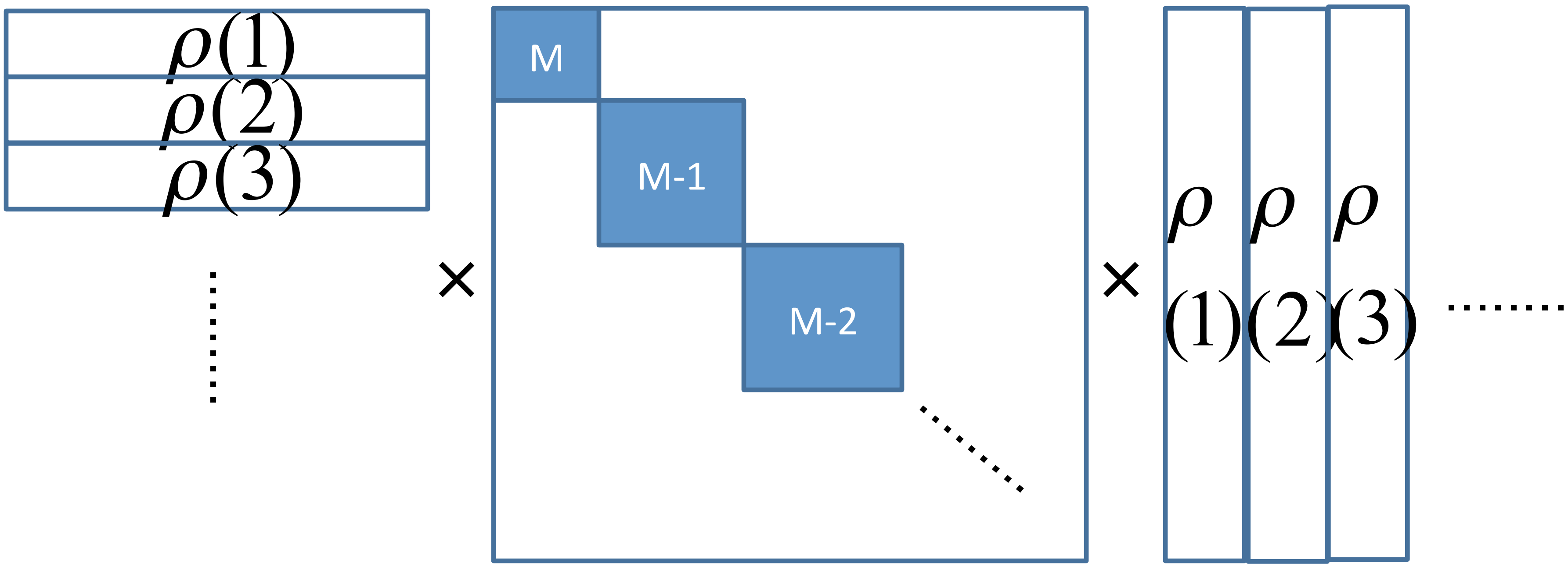
$v_{i,j,k,l} = v_{(ki),(lj)}$ is block diagonal thanks to the symmetries of Jz, parity, and isospin

Non-zero matrix elements: $j_z(i)+j_z(j)=j_z(k)+j_z(l)$ -> $j_z(j)-j_z(k)=-(j_z(j)-j_z(l))$

(Matrix) x (Matrix)

$$\langle \phi | \hat{V} | \phi' \rangle = \frac{1}{2} \sum_{i,k} \rho_{ki} \left(\sum_{j,l} v_{ij\,kl} \rho_{lj} \right) = \frac{1}{2} \sum_{(ki)} \rho_{(ki)} \left(\sum_{jl} v_{(ki),(lj)} \rho_{(lj)} \right)$$

$$M = m_k - m_i$$



Matrix product is performed by DGEMM subroutine in BLAS library

DGEMM/BLAS is always highly tuned for TOP500 list

Energy-variance Extrapolation

Obstacle: computation time

The expectation value of general four-body operator in deformed Slater determinants is obtained by Wick's theorem :

$$\hat{V} = \sum_{i<j,k<l} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \qquad \rho_{ij} = \frac{\langle \phi | c_j^\dagger c_i | \phi' \rangle}{\langle \phi | \phi' \rangle}$$

$$\begin{aligned}
\frac{\langle \phi | \hat{V}^2 | \phi' \rangle}{\langle \phi | \phi' \rangle} = \frac{1}{16} \sum_{ijkl\alpha\beta\gamma\delta} \overline{v}_{ijkl} \overline{v}_{\alpha\beta\gamma\delta} \\
\Big((1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma i}\rho_{\delta j} - (1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma j}\rho_{\delta i} \\
-(1-\rho)_{l\alpha}(1-\rho)_{k\beta}\rho_{\gamma i}\rho_{\delta j} + (1-\rho)_{l\alpha}(1-\rho)_{k\beta}\rho_{\gamma j}\rho_{\delta i} \\
+\rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\delta j} - \rho_{\gamma\alpha}(1-\rho)_{k\beta}\rho_{li}\rho_{\delta j} \\
-\rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{kj}\rho_{\delta i} + \rho_{\gamma\alpha}(1-\rho)_{k\beta}\rho_{lj}\rho_{\delta i} \\
-\rho_{\delta\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\gamma j} + \rho_{\delta\alpha}(1-\rho)_{k\beta}\rho_{li}\rho_{\gamma j} \\
+\rho_{\delta\alpha}(1-\rho)_{l\beta}\rho_{lj}\rho_{\gamma i} - \rho_{\delta\alpha}(1-\rho)_{k\beta}\rho_{lj}\rho_{\gamma i} \\
-\rho_{\gamma\beta}(1-\rho)_{l\alpha}\rho_{ki}\rho_{\delta j} + \rho_{\gamma\beta}(1-\rho)_{k\alpha}\rho_{li}\rho_{\delta j} \\
+\rho_{\gamma\beta}(1-\rho)_{l\alpha}\rho_{kj}\rho_{\delta i} - \rho_{\gamma\beta}(1-\rho)_{k\alpha}\rho_{lj}\rho_{\delta i} \\
+\rho_{\delta\beta}(1-\rho)_{l\alpha}\rho_{ki}\rho_{\gamma j} - \rho_{\delta\beta}(1-\rho)_{k\alpha}\rho_{li}\rho_{\gamma j} \\
-\rho_{\delta\beta}(1-\rho)_{l\alpha}\rho_{lj}\rho_{\gamma i} + \rho_{\delta\beta}(1-\rho)_{k\alpha}\rho_{lj}\rho_{\gamma i} \\
+\rho_{ki}\rho_{lj}\rho_{\gamma\alpha}\rho_{\delta\beta} - \rho_{ki}\rho_{lj}\rho_{\delta\alpha}\rho_{\gamma\beta} - \rho_{li}\rho_{kj}\rho_{\gamma\alpha}\rho_{\delta\beta} + \rho_{li}\rho_{kj}\rho_{\delta\alpha}\rho_{\gamma\beta} \Big)
\end{aligned}$$

Factorization

- Extrapolation method by the energy variance

$$\langle H\rangle = E_0 + E_1\langle \Delta H^2\rangle + E_2\langle \Delta H^2\rangle^2 + \cdots$$

$$\langle \Delta H^2\rangle = \langle H^2\rangle - \langle H\rangle^2$$

$$\frac{\langle\phi|\hat{H}^2|\psi\rangle}{\langle\phi|\psi\rangle} = \sum_{i<j,\alpha<\beta}\left(\sum_{k<l} v_{ijkl}((1-\rho)_{k\alpha}(1-\rho)_{l\beta} - (1-\rho)_{l\alpha}(1-\rho)_{k\beta})\right)\left(\sum_{\gamma<\delta} v_{\alpha\beta\gamma\delta}(\rho_{\gamma i}\rho_{\delta j} - \rho_{\delta i}\rho_{\gamma j})\right)$$
$$+\mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho) + \left(\mathrm{Tr}(\rho(t+\frac{1}{2}\Gamma))\right)^2$$

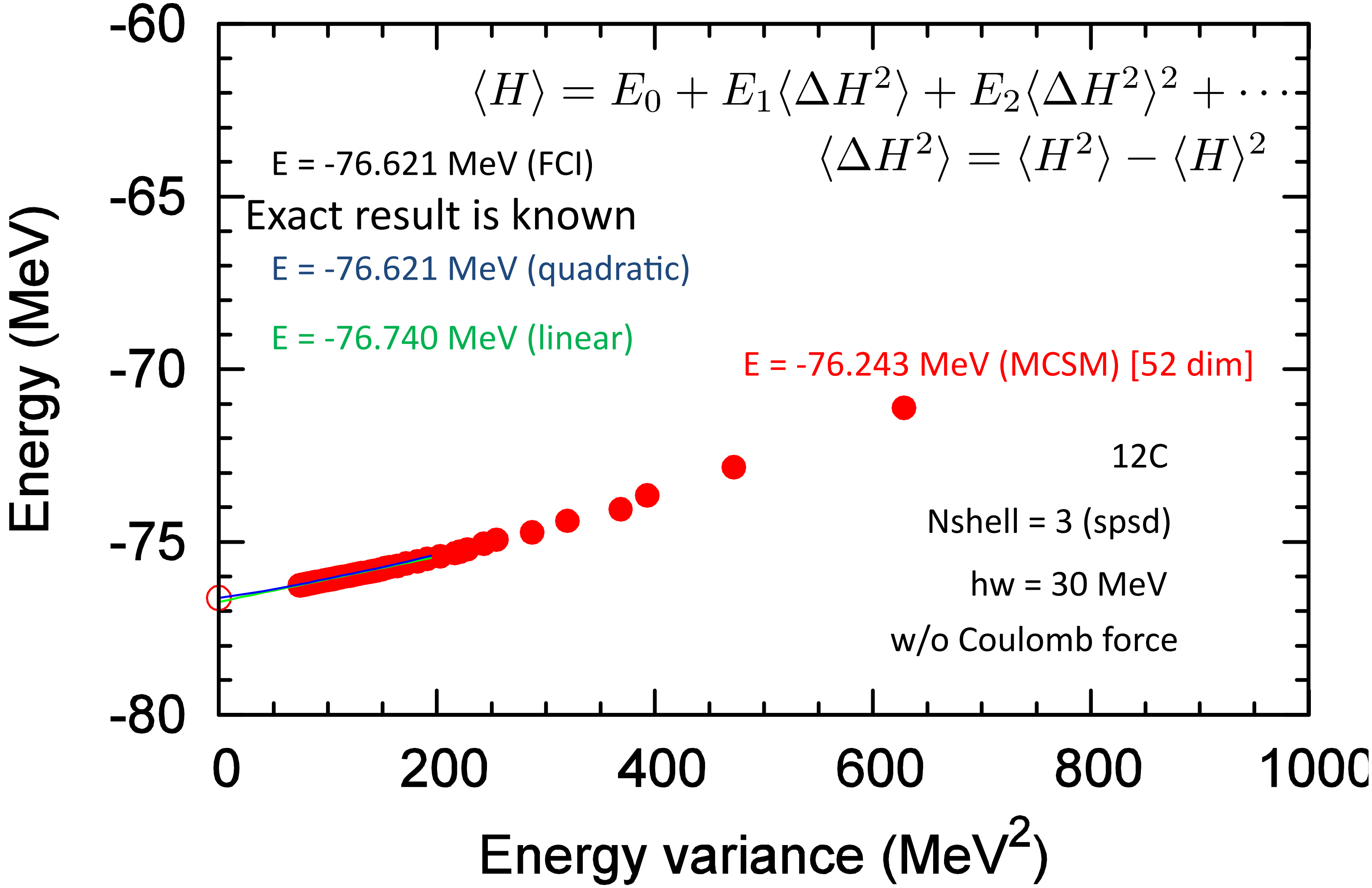
$$\Gamma_{ik} = \sum_{jl} v_{ijkl}\rho_{lj}$$

(naively) 8-fold loops -> (effectively) 6-fold loops by the factorization

N. Shimizu, Y. Utsuno, T.Mizusaki, T. Otsuka, T. Abe, & M. Honma, Phys. Rev. C82, 061305(R) (2010)

Extrapolation of B.E.s of 12C

D_J =2,936,582 = 2.9 x 10^6



Benchmark Results

What we have calculated as Benchmark

- Nuclei (JP): s- & p-shell nuclei
  - 4He(0+)
  - 6He(0+)
  - 6Li(1+)
  - 7Li(1/2-, 3/2-)
  - 8Be(0+)
  - 10B(1+, 3+)
  - 12C(0+)
- Observables
  - BE
  - Point-particle RMS radius
  - Q-moment
  - μ-moment

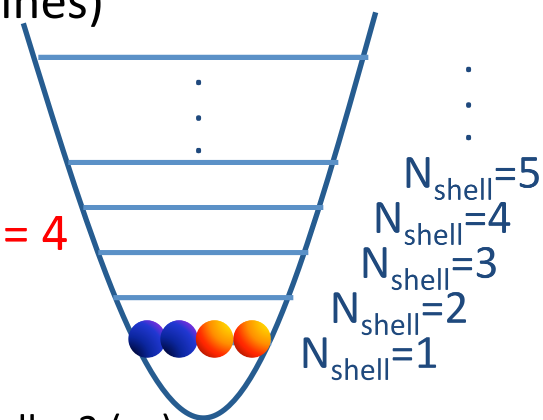
Model space: Nshell = 2, 3, 4
NN Interaction: JISP16
w/o Coulomb
w/o Gloeckner-Lawson prescription

MCSM: Abe, Otsuka, Shimizu, Utsuno (Tokyo)
T2K (Tokyo, Tsukuba), BX900 (JAEA)
FCI: Maris, Vary (Iowa)
Jaguar, Franklin (NERSC, DOE)

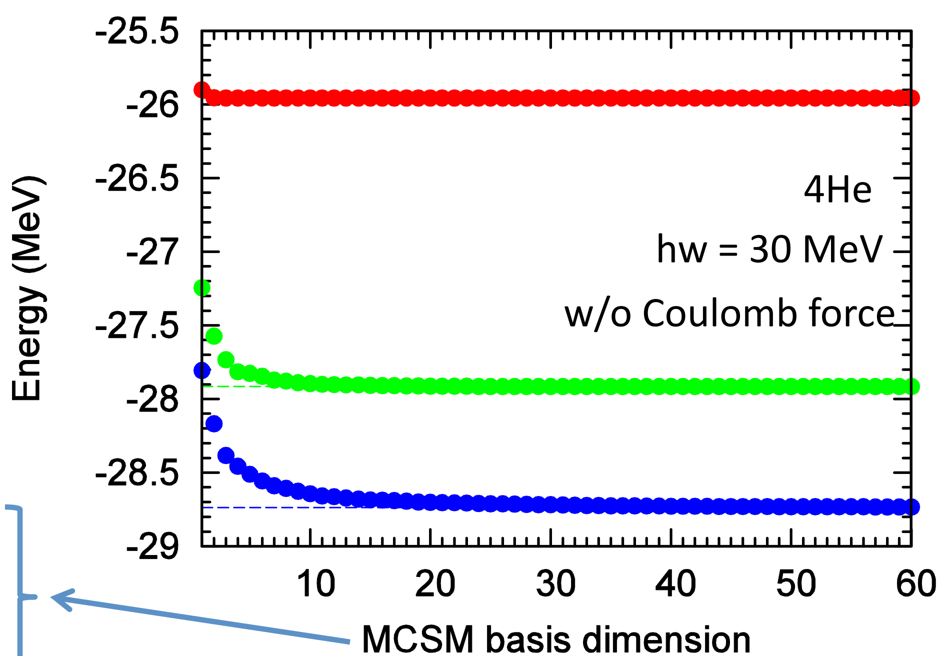
Convergence pattern of the 4He B.E.s w.r.t. MCSM basis dimension

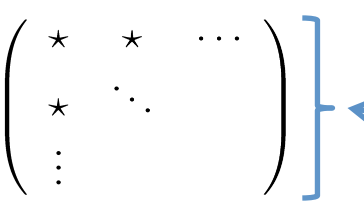
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)

Good agreement w/ FCI within a few keV up to Nshell = 4



H = Hint + β Hcm, (β = 0)





Nshell = 2 (sp)
-25.956 MeV (MCSM)
-25.956 MeV (FCI)

Nshell = 3 (spsd)
-27.914 MeV (MCSM)
-27.914 MeV (FCI)

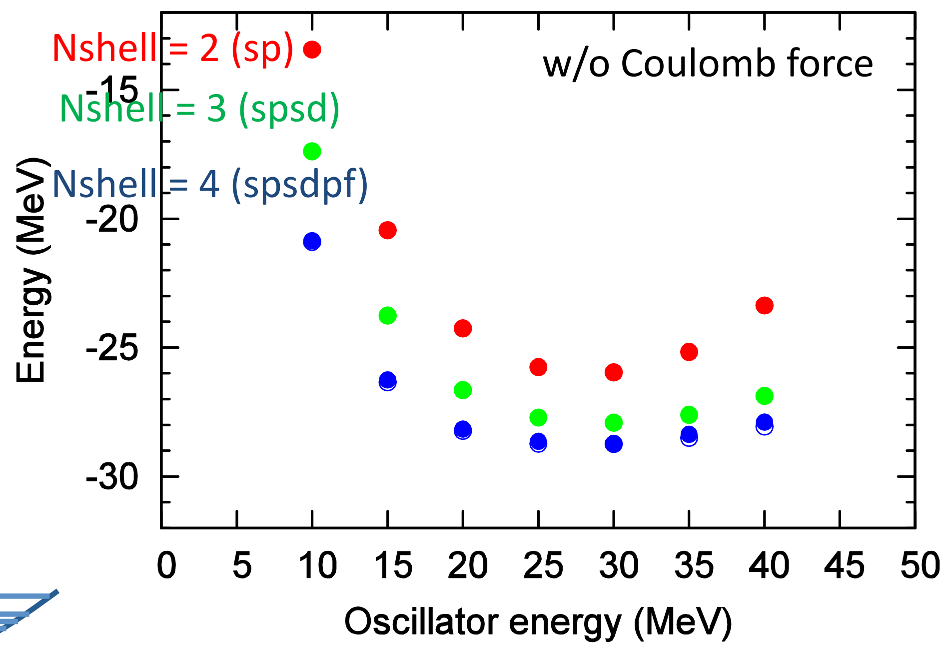
Nshell = 4 (spsdpf)
-28.733 MeV (MCSM)
-28.738 MeV (FCI)

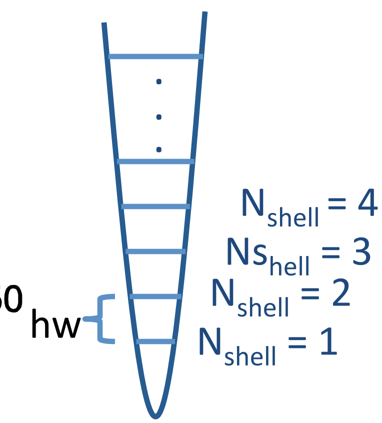
hw dependence of 4He B.E.s

- Comparison of MCSM (solid symbols) w/ FCI (open symbols) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)

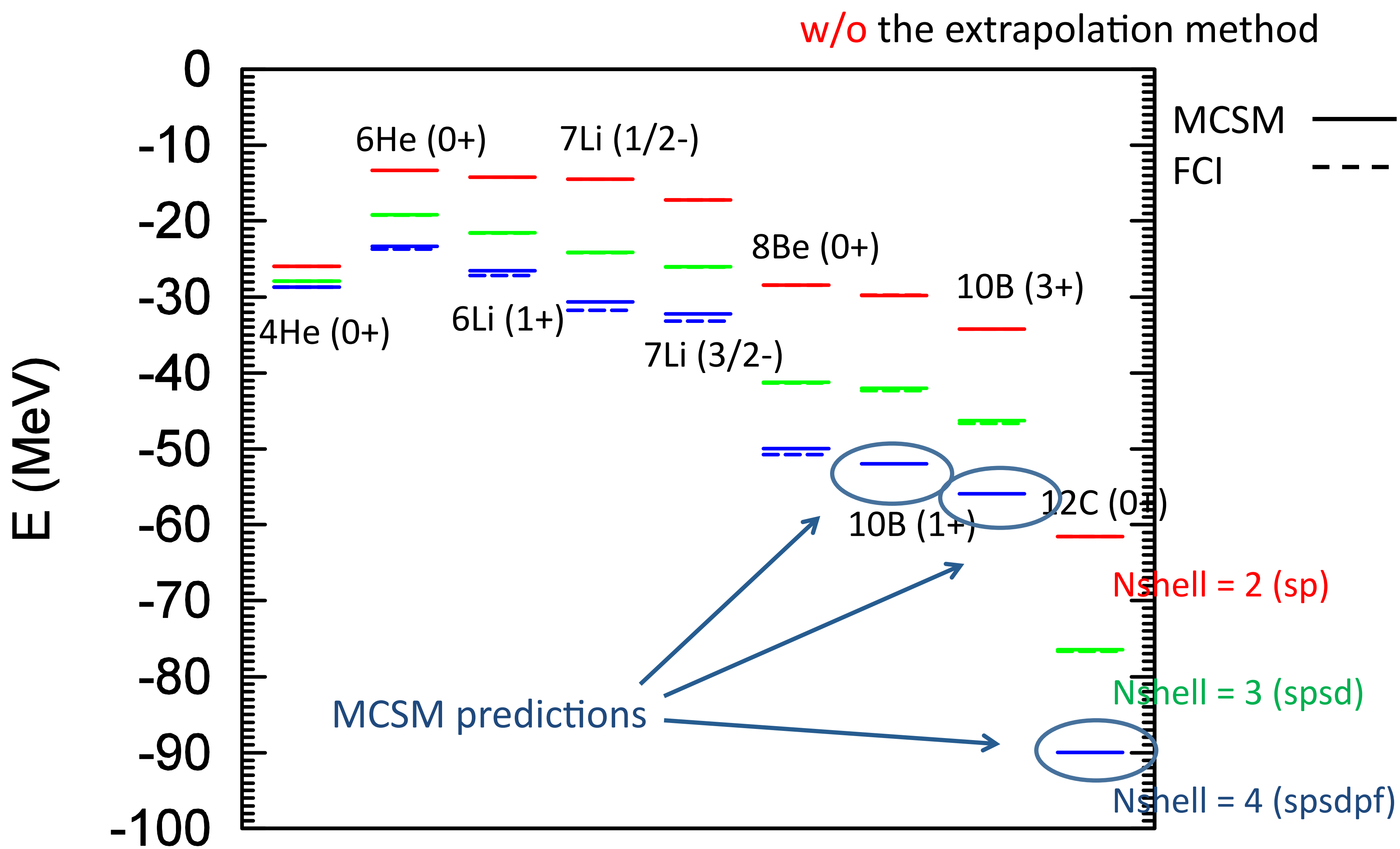
Good agreement w/ FCI results within a few keV

H = Hint + β Hcm, (β = 0)

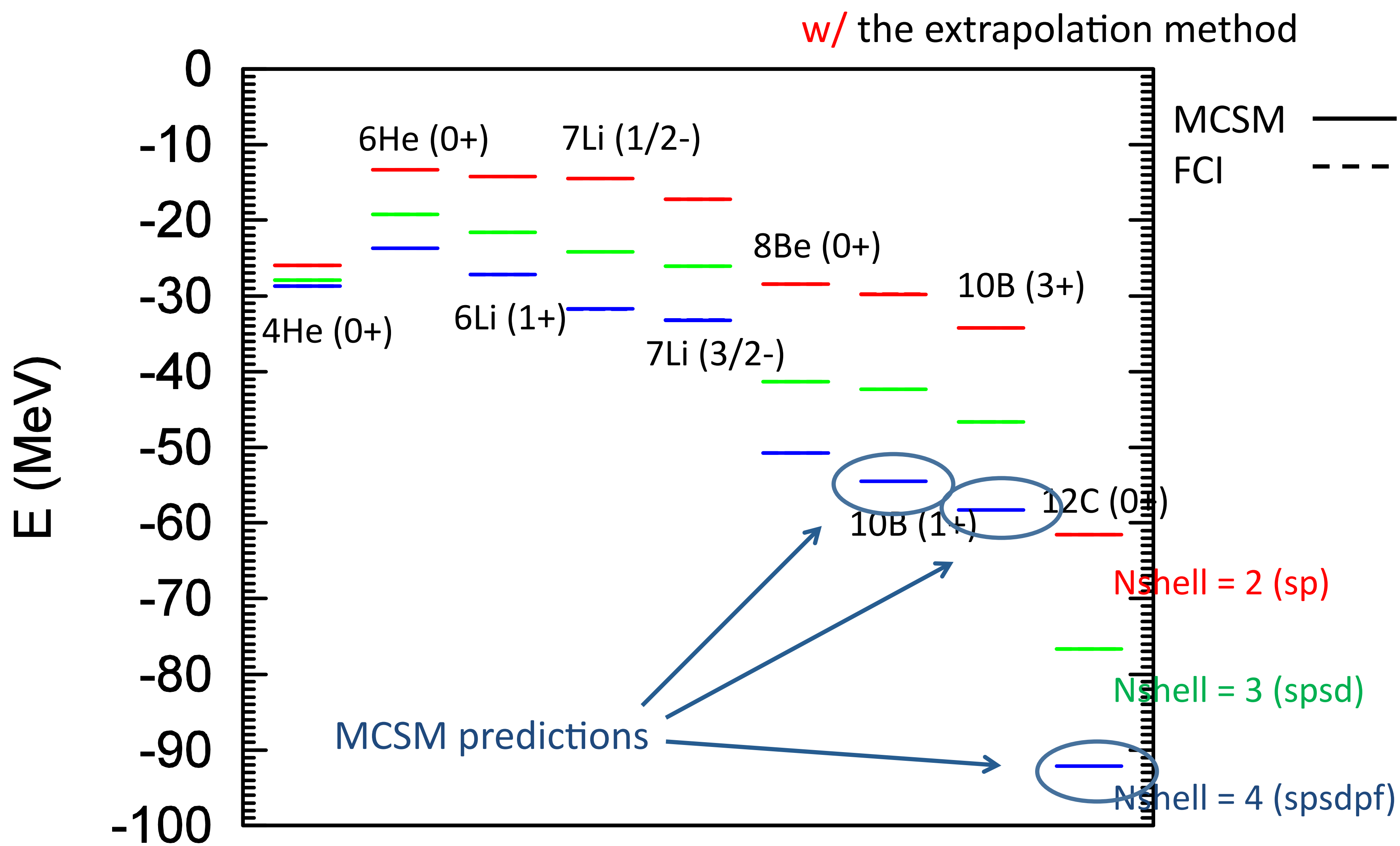




Binding Energy of Light Nuclei

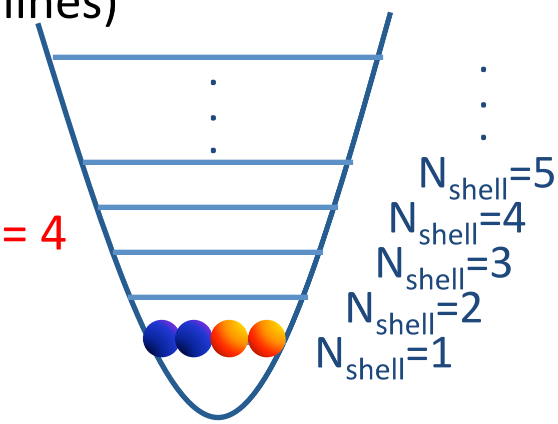


Binding Energy of Light Nuclei



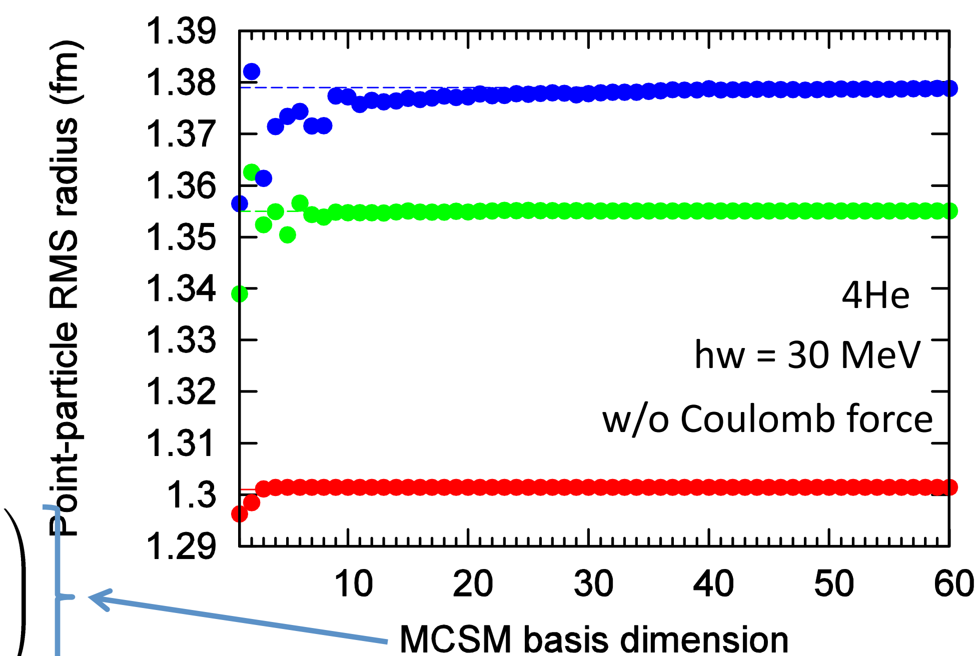
Convergence pattern of the 4He point-particle RMS radius w.r.t. MCSM basis dimension

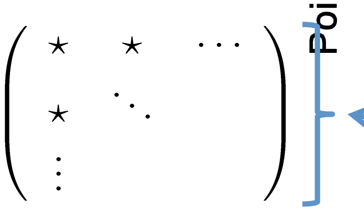
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)



Good agreement w/ FCI within 0.001 fm up to Nshell = 4

H = Hint + β Hcm, (β = 0)



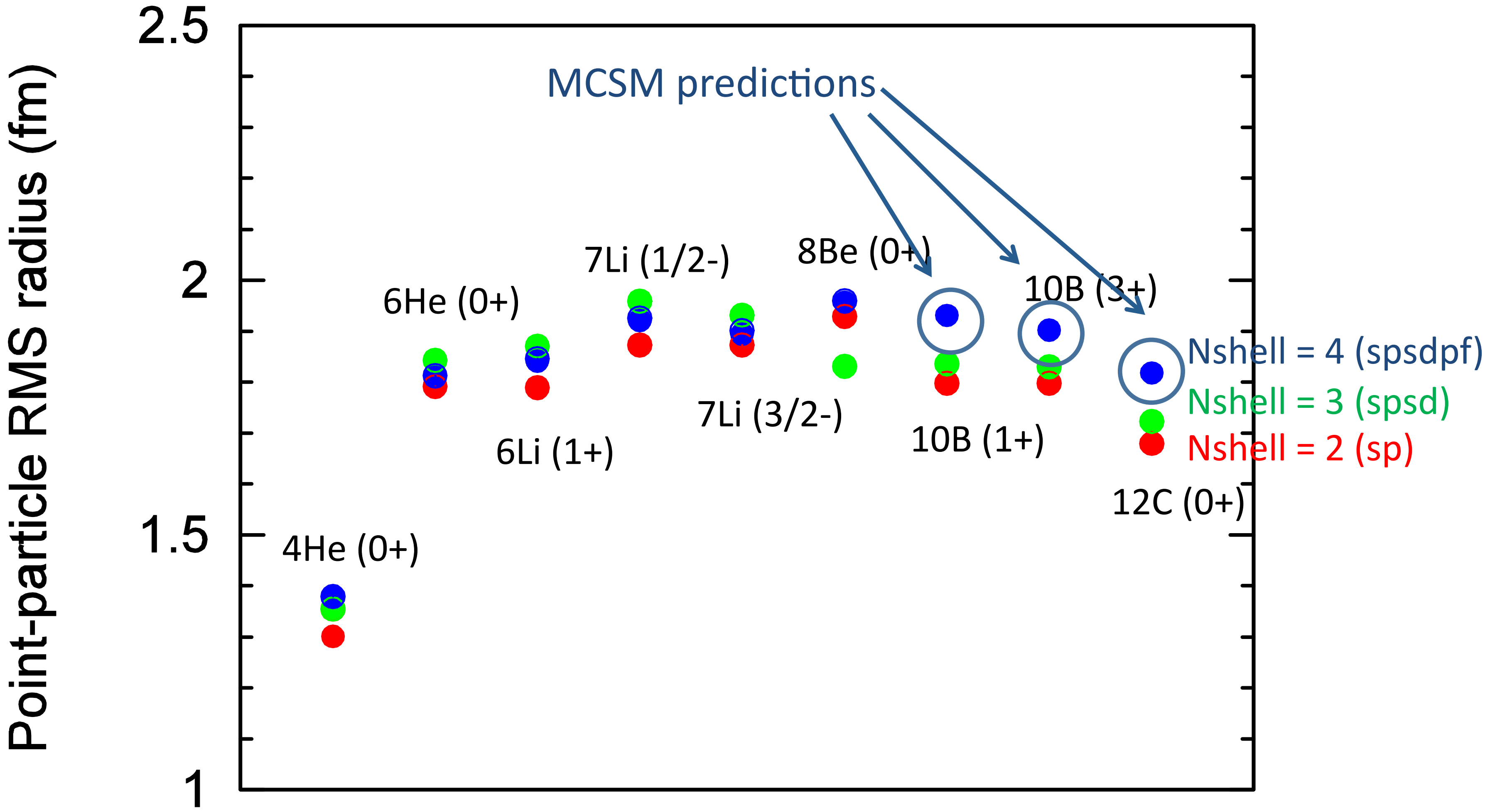


Nshell = 4 (spsdpf)
1.379 fm (MCSM)
1.379 fm (FCI)

Nshell = 3 (spsd)
1.355 fm (MCSM)
1.355 fm (FCI)

Nshell = 2 (sp)
1.301 fm (MCSM)
1.301 fm (FCI)

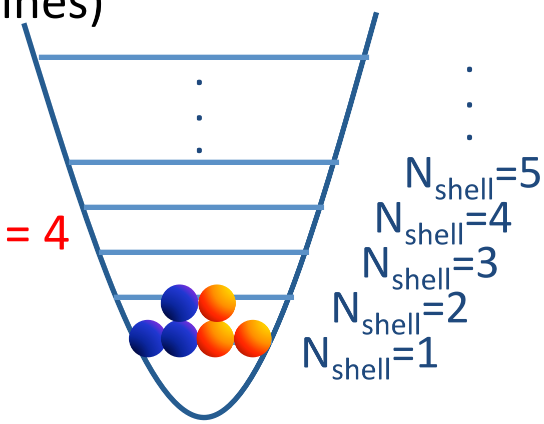
Point-particle RMS Radius of Light Nuclei



Convergence pattern of the 6Li Q-moment w.r.t. MCSM basis dimension

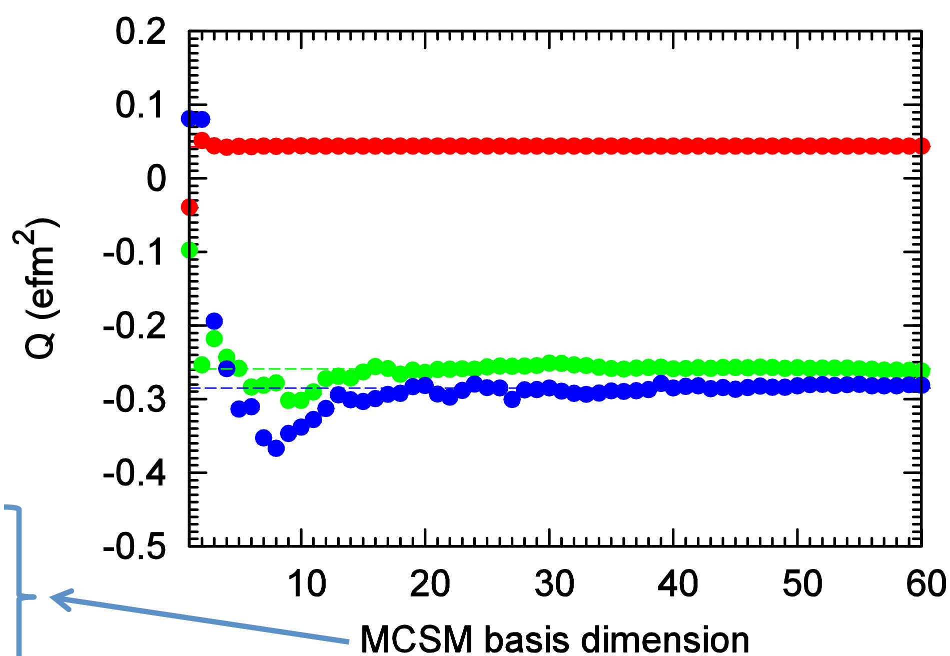
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)

Good agreement w/ FCI within 0.01 efm^2 up to Nshell = 4



H = Hint + β Hcm, (β = 0)

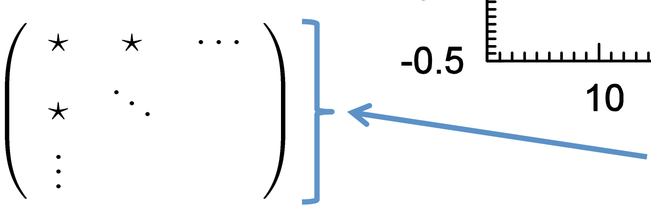
w/o Coulomb force



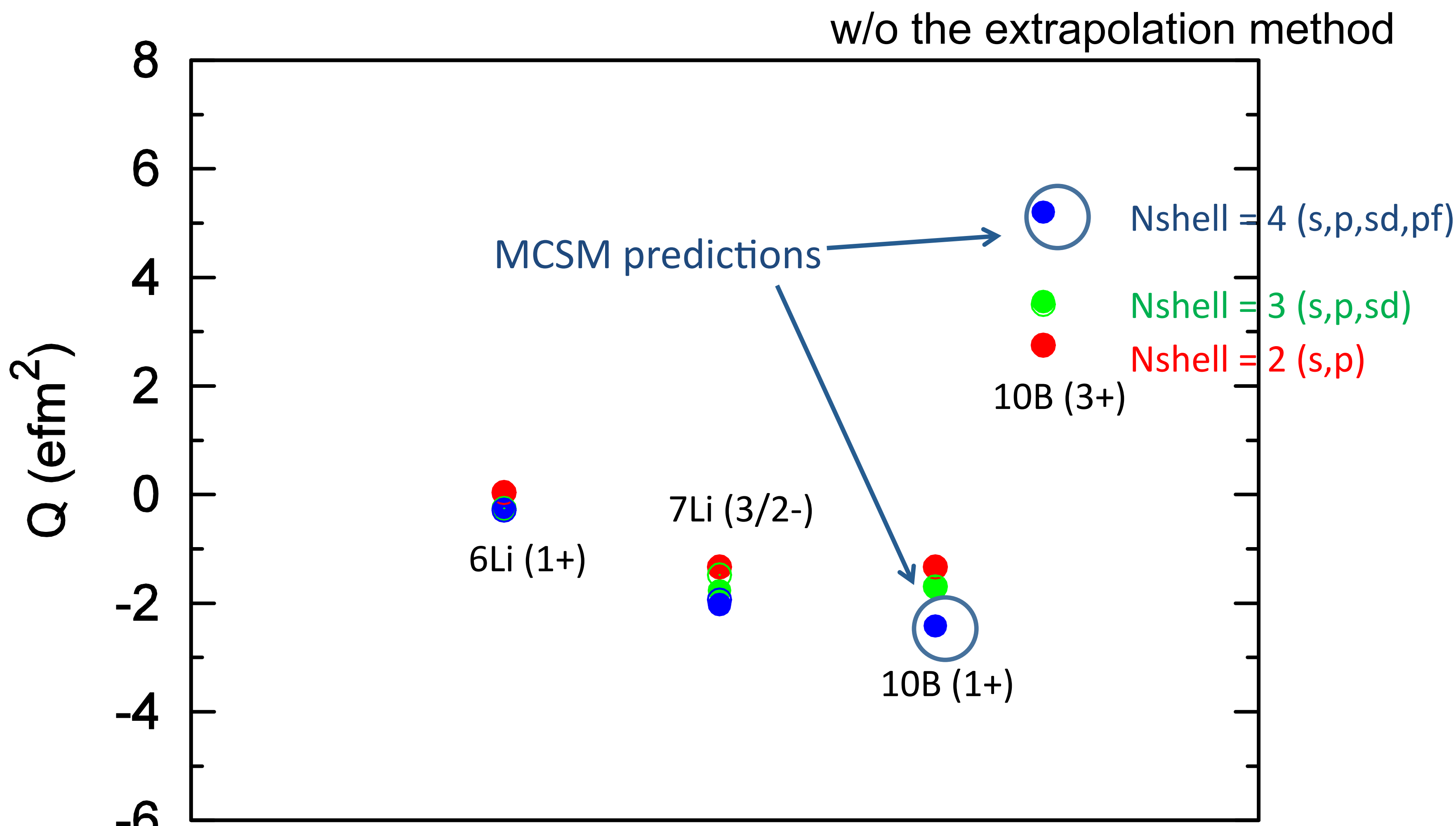
N_{shell} = 2 (s,p)
0.044 efm^2 (MCSM)
0.043 efm^2 (FCI)

N_{shell} = 3 (s,p,sd)
-0.260 efm^2 (MCSM)
-0.259 efm^2 (FCI)

N_{shell} = 4 (s,p,sd,pf)
-0.280 efm^2 (MCSM)
-0.285 efm^2 (FCI)

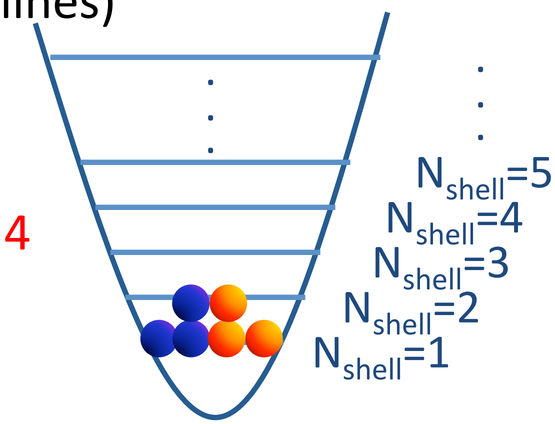


Q-moment of Light Nuclei



Convergence pattern of the 6Li μ-moment w.r.t. MCSM basis dimension

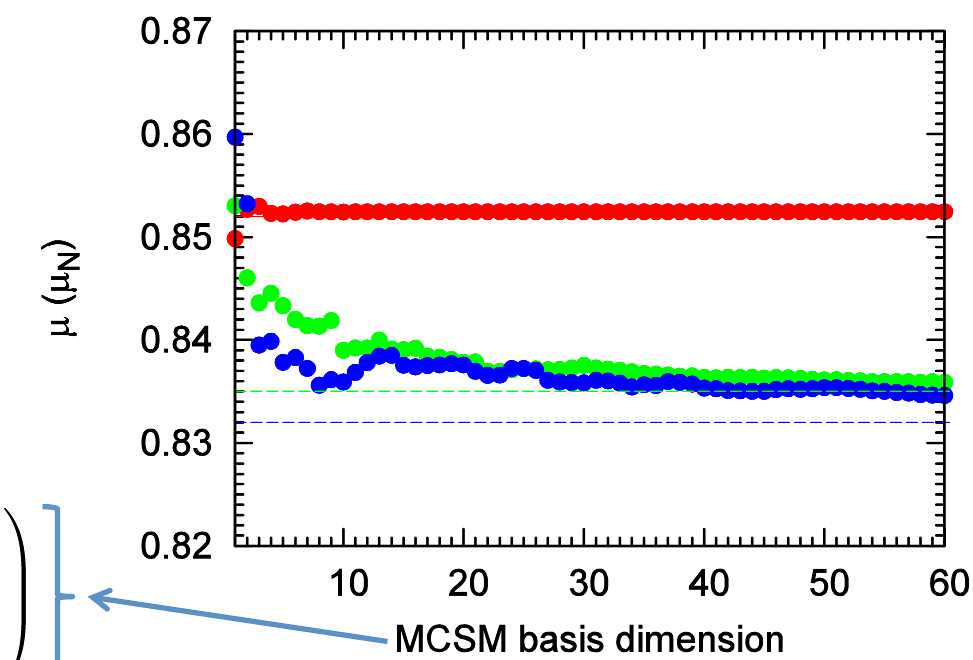
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines)
  @ Nshell = 2 (s,p), 3 (s,p,sd), & 4 (s,p,sd,pf)

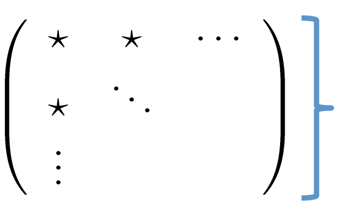


Good agreement w/ FCI within 0.01 μ_N up to Nshell = 4

H = Hint + β Hcm, (β = 0)

w/o Coulomb force





Nshell = 2 (sp)

0.852 μN (MCSM)

0.852 μN (FCI)

Nshell = 3 (spsd)

-0.836 μN (MCSM)

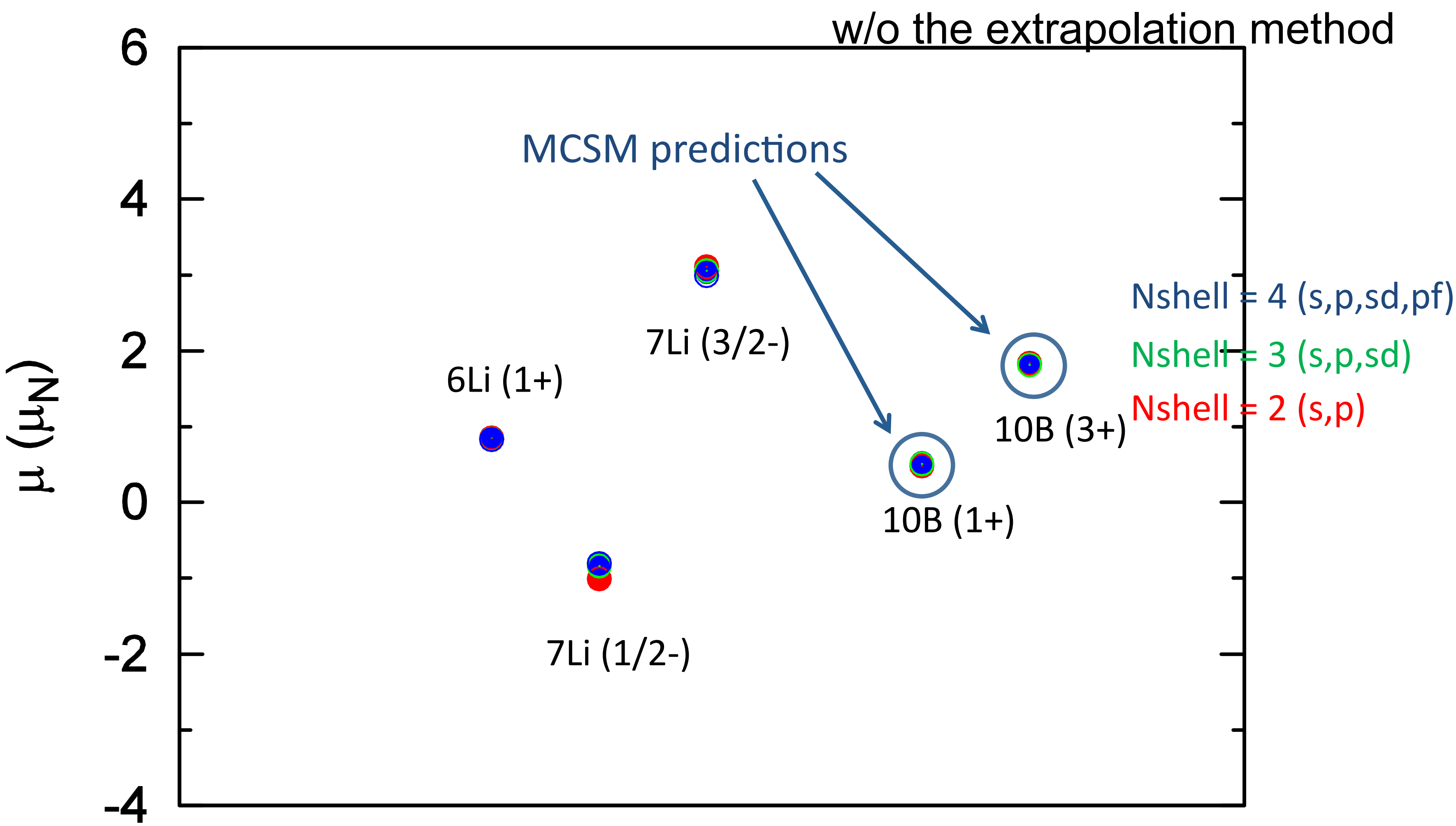
-0.833 μN (FCI)

Nshell = 4 (spsdpf)

-0.835 μN (MCSM)

-0.832 μN (FCI)

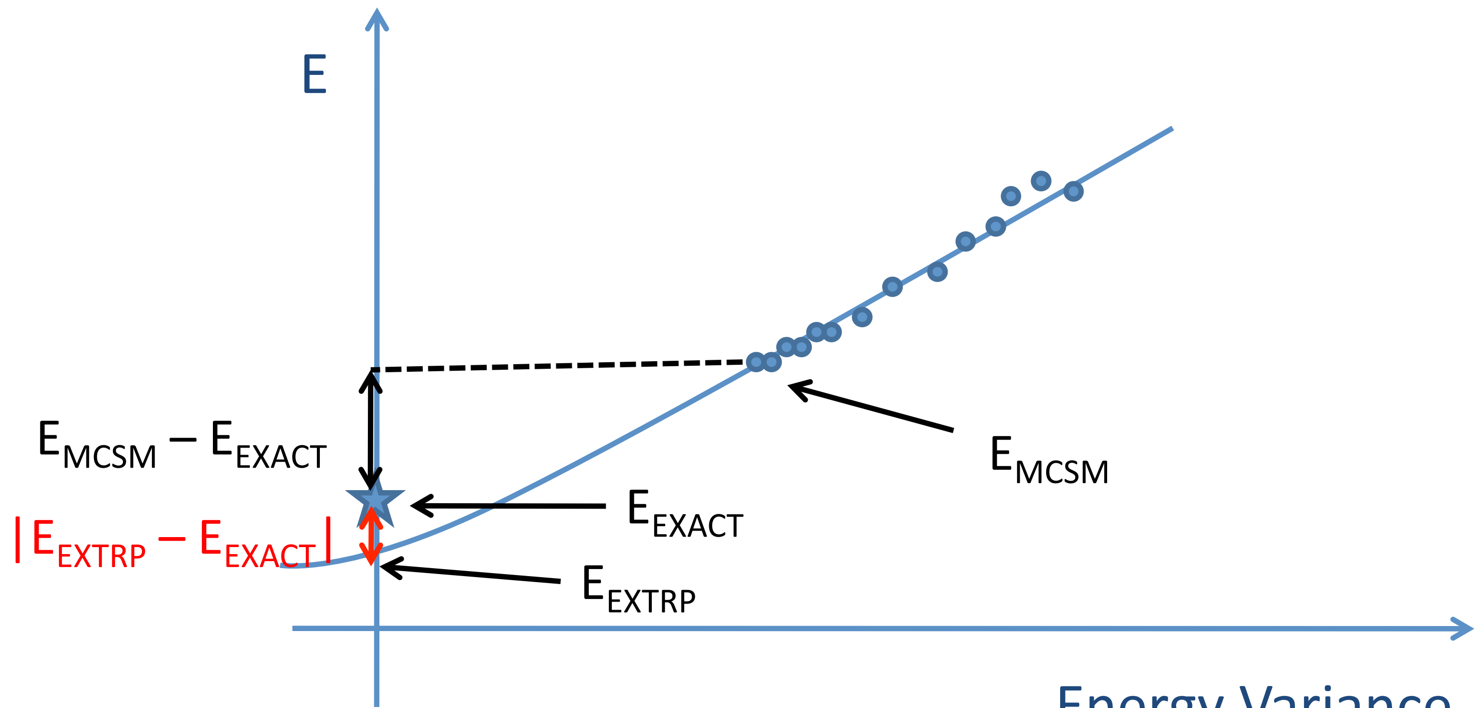
μ-moment of Light Nuclei



Error Assignment of Extrapolation

Error estimate of extrapolation

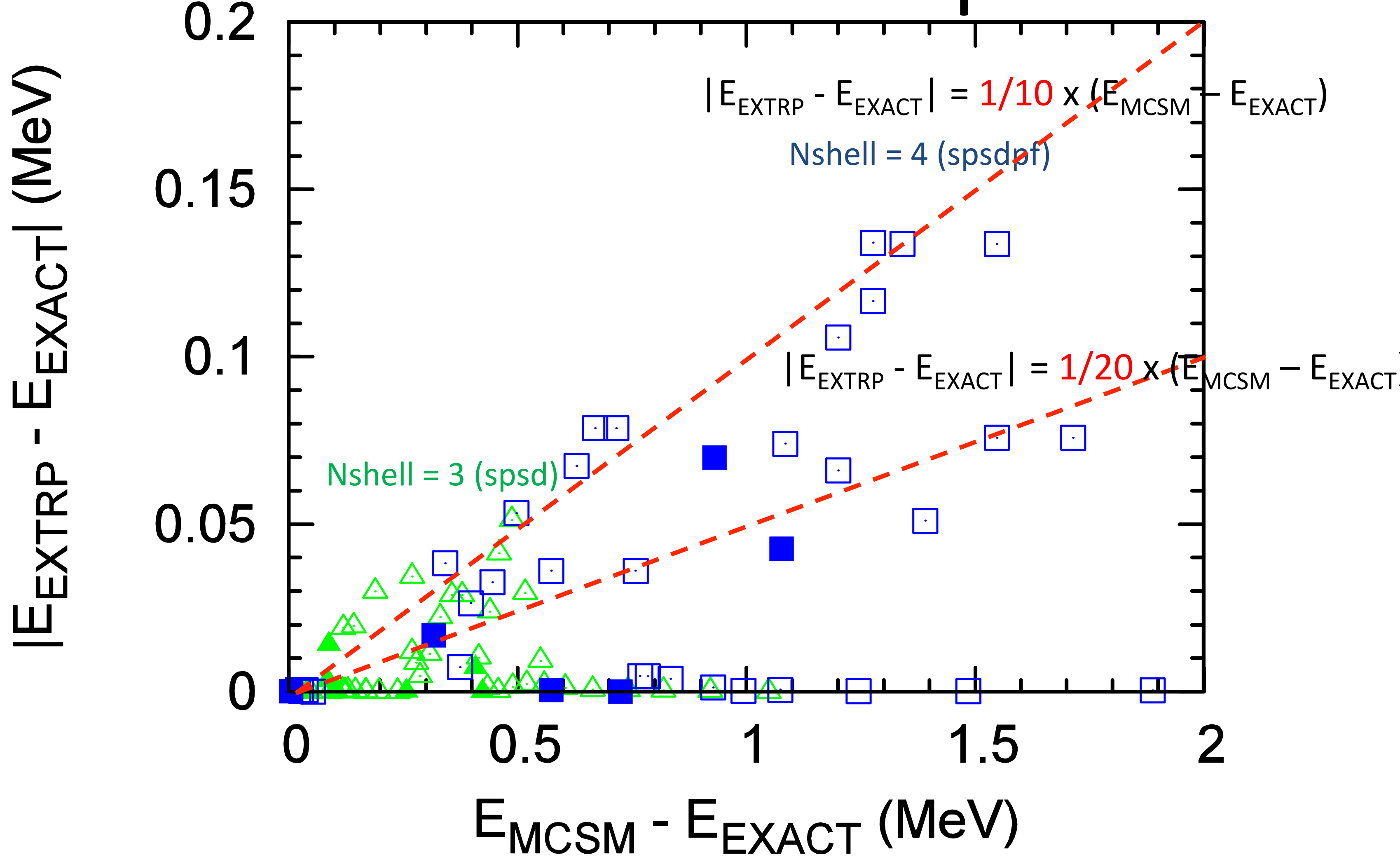
- Rough estimate



- From my experience,

  $|E_{EXTRP} - E_{EXACT}| \sim 1/10 - 1/20 \times (E_{MCSM} - E_{EXACT})$

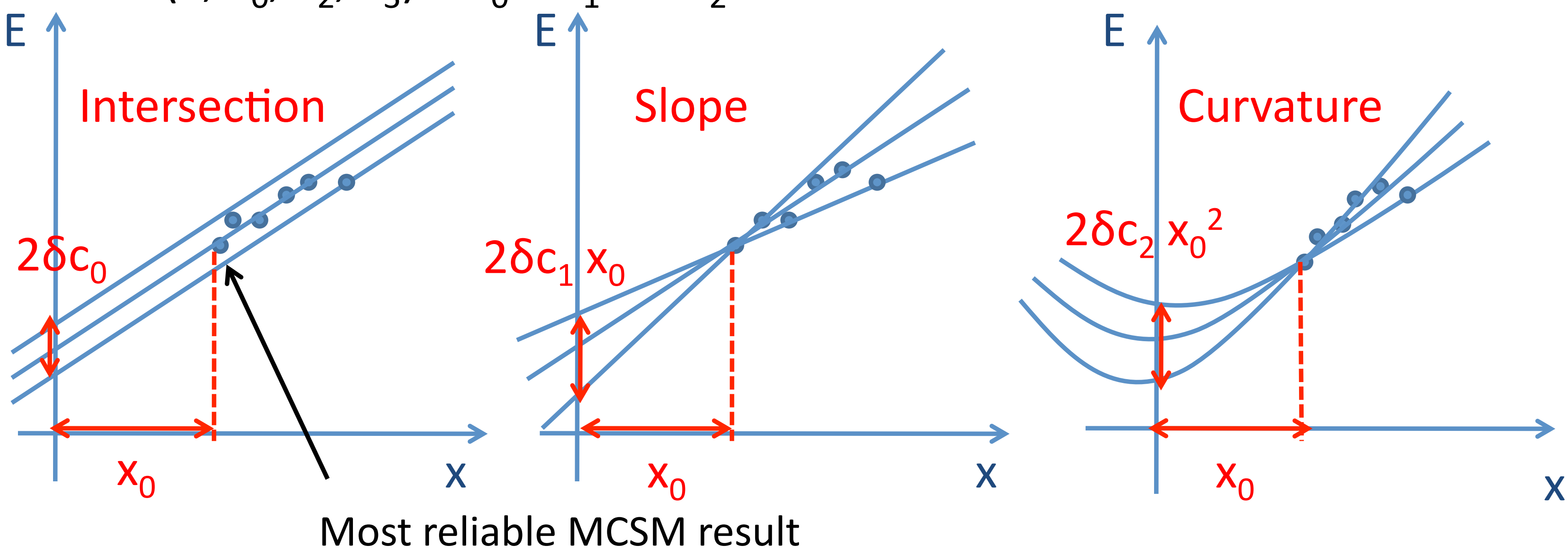
Error estimate for extrapolation



1 σ of the naïve error estimate gives the slope of 1/10 ~ 1/20

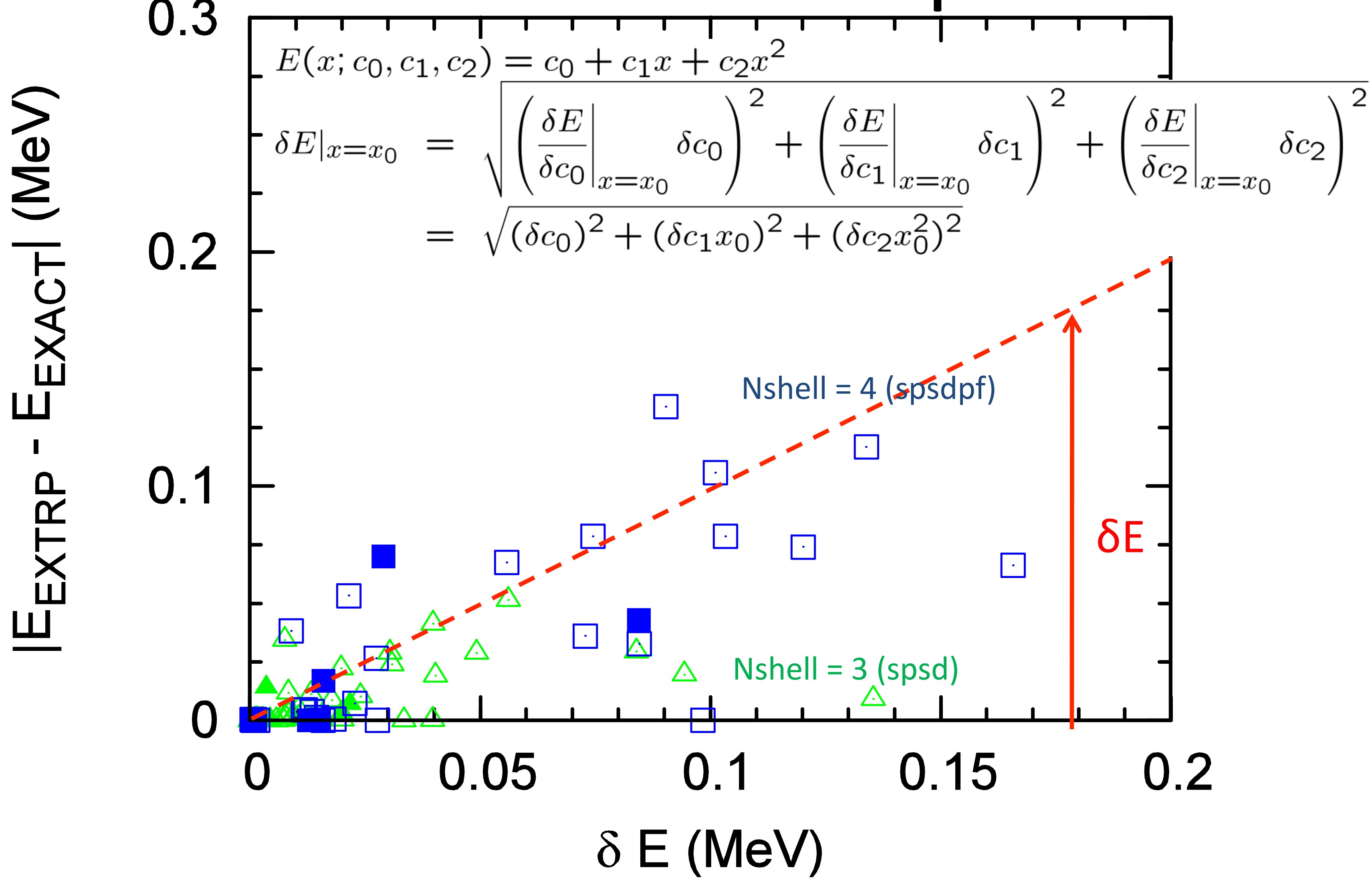
Error estimate of extrapolation

- More precise estimate
- $E(x; c_0, c_2, c_3) = c_0 + c_1 x + c_2 x^2$



- $\delta E = [(\delta c_0)^2 + (\delta c_1 x_0)^2 + (\delta c_2 x_0^2)^2]^{1/2}$

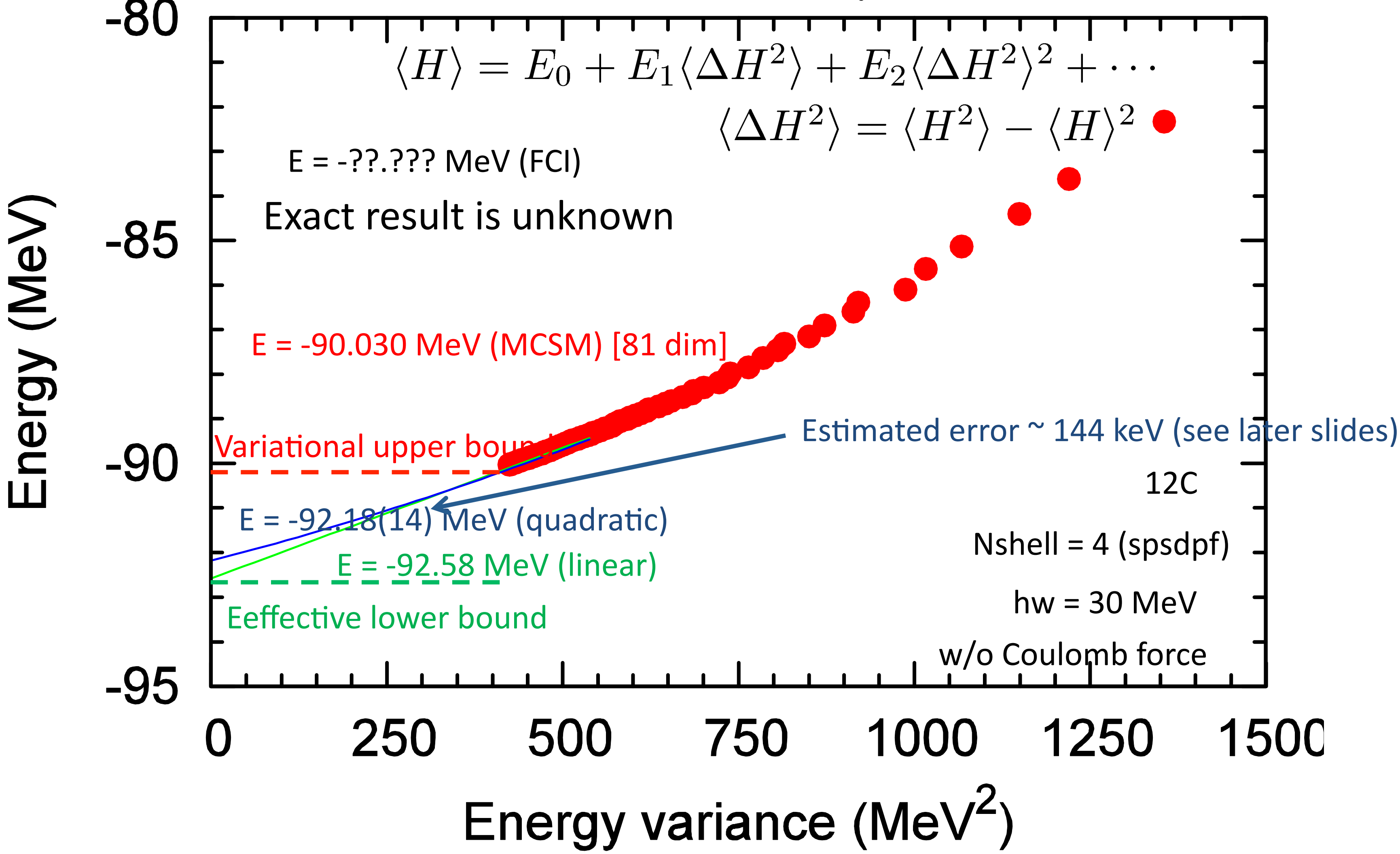
Error estimate for extrapolation



Equation above gives good error estimate of the extrapolation

Extrapolation of B.E.s of 12C

D_J = 11,384,214,614 ~ 1.1 x 10^{10}



Summary & Outlook

- Summary

  - Most obs for s- & p-shell nuclei will be able to be reproduced by no-core MCSM calc. w/ JISP16 NN int up to Nshell = 4 (spsdpf) model space by new code & extrapolation method.

- Outlook

  - Check the convergence wrt Nshell
  - Clarify advantages/disadvantages of Nshell truncation to Nmax truncation
  - Do Physics

END