素核宇宙融合　レクチャーシリーズ

第4回「原子核殻模型の基礎と応用」

阿部　喬（東大CNS）
京大基研

2012年1月11,12日

目次

- 核子の一粒子運動と原子核での殻構造
- 閉殻を仮定する（芯のある）殻模型計算の基礎
- 閉殻を仮定しない（芯のない）殻模型による第一原理計算の概要
- モンテカルロ殻模型

原子核分野におけるHPCI戦略活動

清水@核理懇、日本物理学会（弘前、2011）

革新的ハイパフォーマンス・コンピューティング・インフラ（HPCI）の構築

次世代スーパーコンピュータ「京」を中核として、多様なユーザーニーズに応える革新的な計算環境を実現するHPCI(革新的ハイパフォーマンス・コンピューティング・インフラ)を構築するとともに、その利用を促進する。　今年度から5年間。

戦略分野及び戦略機関	＜戦略分野＞	＜戦略機関＞
分野1	予測する生命科学･医療および創薬基盤	理化学研究所
分野2	新物質･エネルギー創成	東大物性研（分子研、東北大金材研）
分野3	防災･減災に資する地球変動予測	JAMSTEC
分野4	次世代ものづくり	東大生産研（JAXA、JAEA）
分野5	物質と宇宙の起源と構造	筑波大（高エネ研、天文台）

計算基礎科学研究連携拠点（筑波大学CCS、KEK、天文台）

http://www.jicfus.jp/field5/jp/　　拠点長　青木慎也（筑波大）

		開発課題責任者
課題1	格子QCDによる物理点でのバリオン間相互作用の決定	（藏増嘉伸）
課題2	大規模量子多体計算による核物性の解明とその応用	（大塚孝治）
課題3	超新星爆発およびブラックホール誕生過程の解明	（柴田大）
課題4	ダークマターの密度ゆらぎから生まれる第1世代天体形成	（牧野淳一郎）
計算科学技術推進体制の構築		（橋本省二）

HPCI戦略分野5課題2
「大規模量子多体計算による核物性の解明とその応用」

清水@核理懇、日本物理学会（弘前、2011）

大塚　孝治 (開発課題責任者)

清水　則孝
阿部　喬
月山　幸志郎
江幡　修一郎
吉田　亨

東大CNSに
H23．4．1着任
HPCI専従

角田　直文　(東大理)
角田　佑介　(東大理)
本間　道雄　（会津大）
宇都野　穣　（JAEA)
中務　孝　　（理研）
鈴木　俊夫　(日大)
中田　仁　　(千葉大)
梶野　敏貴　(天文台)

^{12}Cなどの計算　吉田

軽い核の芯を仮定しない殻模型計算　阿部、大塚、清水

第一原理的、p殻核、^{4}He～^{12}C，sd殻核

殻模型計算コード開発
アルゴリズム

清水、宇都野、阿部、大塚

大規模計算に必要な有効相互作用　月山、角田

中重核の殻模型計算　清水、宇都野、本間、大塚、角田

芯を仮定した有効相互作用
Cr, Ni, Sn, Xe, Nd, ...
r-process, 二重ベータ崩壊, 原子力工学, ...

密度汎関数法　江幡、中務

Outline of this part

- Motivation
- Monte Carlo Shell Model (MCSM)
- Benchmark Results
- Summary & Outlook

Current status of ab inito approaches

- Major challenge of the nuclear structure theory

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

  - Standard approaches: GFMC, NCSM (up to A ~ 12-14), CC (closed shell +/- 1,2)

→ demand for extensive computational resources

✓ *ab-initio*(-like) approaches (which attempt to go) beyond standard methods

→ No-core Monte Carlo shell model (MCSM)

✓ Another approaches beyond standard NCSM:

- IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navratil (TRIUMF)
- Sp-NCSM: T. Dytrych, K.D. Sviratcheva, J.P. Draayer, C. Bahri, and J.P. Vary (Louisiana State U, Iowa State U)

Current status of some ab initio calc

- GFMC
- NCSM
- IT-NCSM
- CC

Current Status of Green's Function Monte Carlo (GFMC)

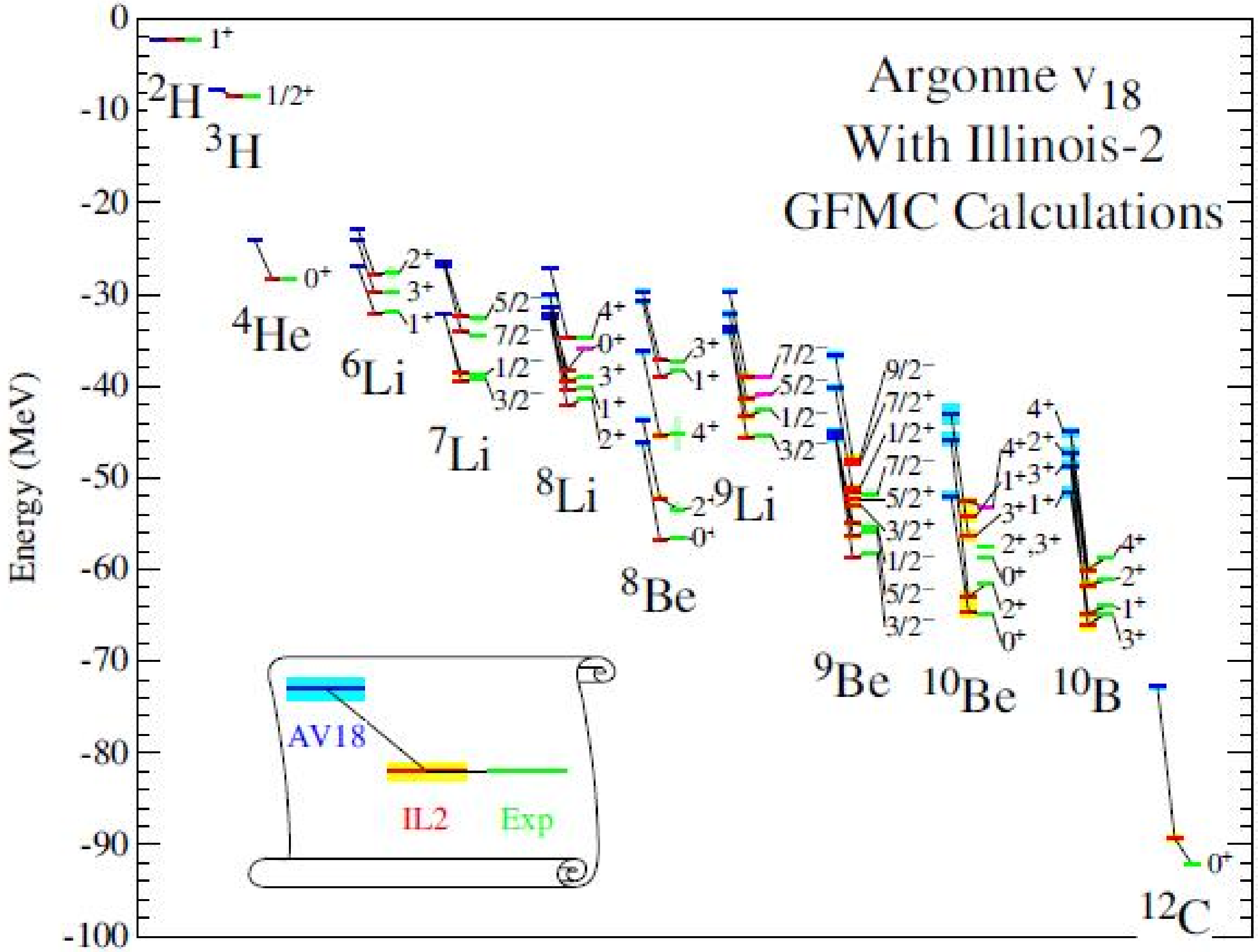


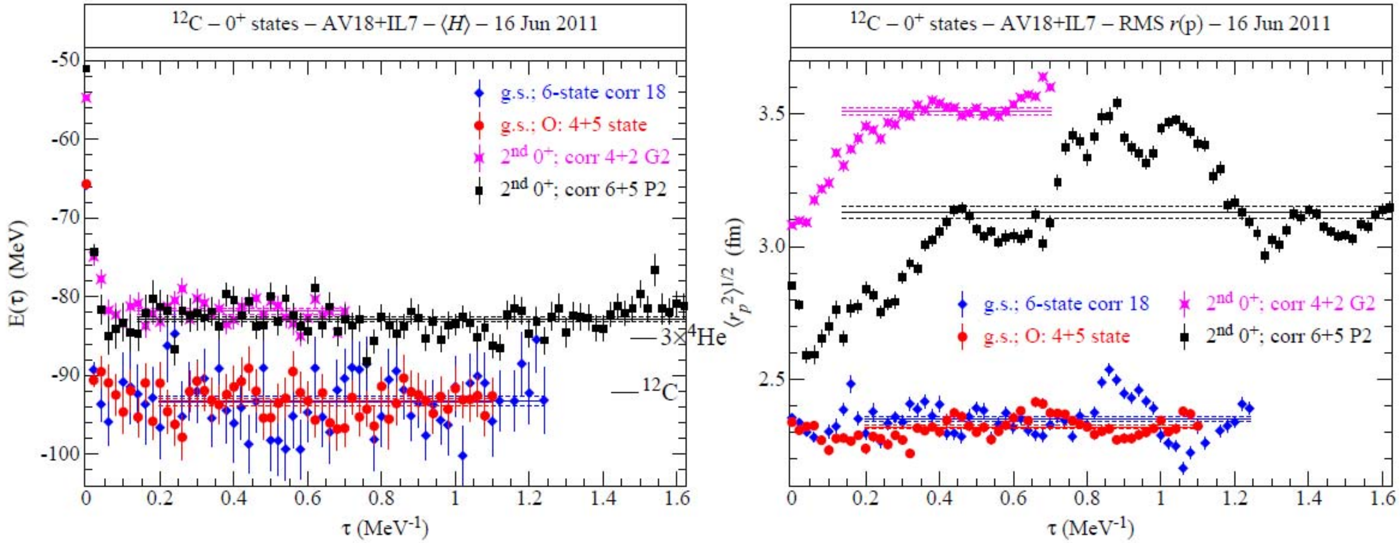
Fig. 3. – GFMC computations of energies for the AV18 and AV18+IL2 Hamiltonians compared with experiment.

S.C. Pieper, Enrico Fermi Lecture (2007)

Current Status of Green's Function Monte Carlo (GFMC)

SECOND 0^+ (HOYLE) STATE OF ^{12}C – PRELIMINARY

Convergence as a function of imaginary time (τ)



	g.s. energy			$2^{nd}\ 0^+\ E^*$		
	VMC	GFMC	Expt.	VMC	GFMC	Expt.
AV18	–44.9(2)	–73.2(5)		10.0(3)	7.9(6)	
AV18+IL7	–65.7(2)	–93.3(4)	–92.16	14.7(2)	10.4(5)	7.65

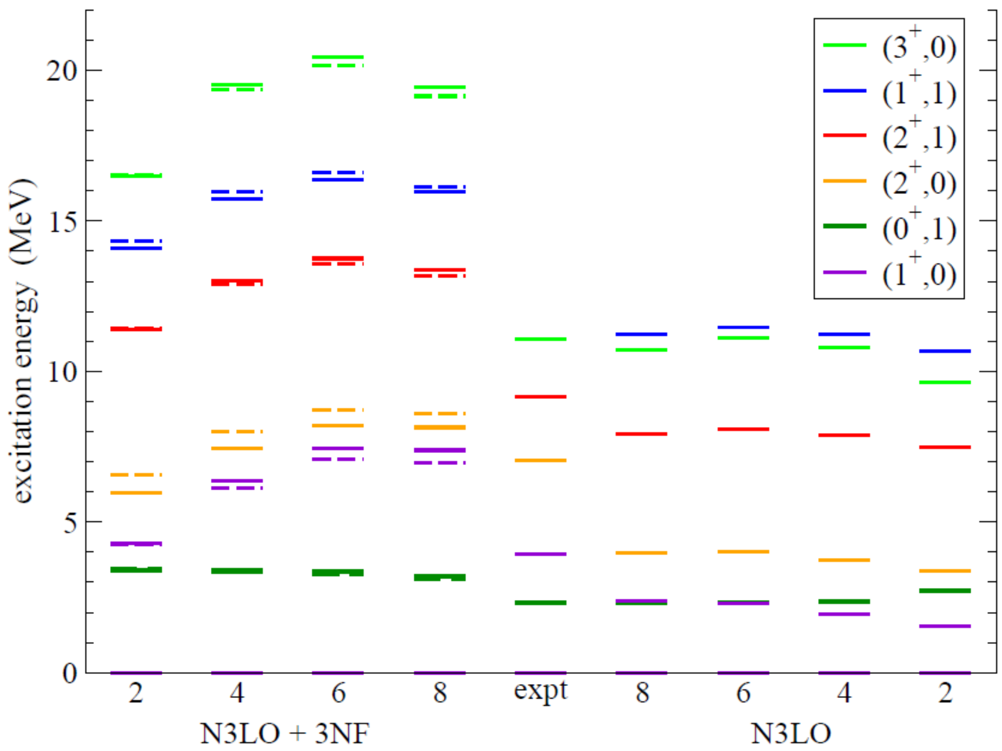
S.C. Pieper, Annual UNEDF Collaboration Meetings (2011)
http://unedf.org/content/annual_mtg.php

Current Status of No-Core Shell Model (NCSM)

Ab initio structure of Carbon-14 and Nitrogen-14

Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)

14N



chiral 2-body plus 3-body forces (left) and 2-body forces only (right)

P. Maris, Annual UNEDF Collaboration Meetings (2011)
http://unedf.org/content/annual_mtg.php

Current Status of Importance-Truncated No-Core Shell Model (IT-NCSM)

- First ab initio NCSM calculations w/ SRG-evolved chiral NN+3N interaction throughout p-shell nuclei
  - Surpass all previous NCSM calc. incl. 3N int. regarding A & Nmax

    Previous study: Nmax = 8 for ^{14}C w/ NN + 3N (NCSM) [P. Maris, et al., PRL 106, 202502 (2011)]

    This study: Nmax = 12 for ^{12}C & ^{16}O w/ NN + 3N (IT-NCSM)

R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navratil, arXiv:1105.3173 [nucl-th]

R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navratil, arXiv:1105.3173 [nucl-th]

Ground-state energy for lower p-shell nuclei

<u>NN only</u>
alpha dependent
-> SRG-induced 3N contrib.
originating initial NN int.

α : flow parameter
c.f.) $\Lambda = \alpha^{-1/4}$ =

α = 0.04 fm^4	2.24 fm^{-1}
0.05 fm^4	2.11 fm^{-1}
0.0625 fm^4	2 fm^{-1}
0.08 fm^4	1.88 fm^{-1}
0.16 fm^4	1.58 fm^{-1}

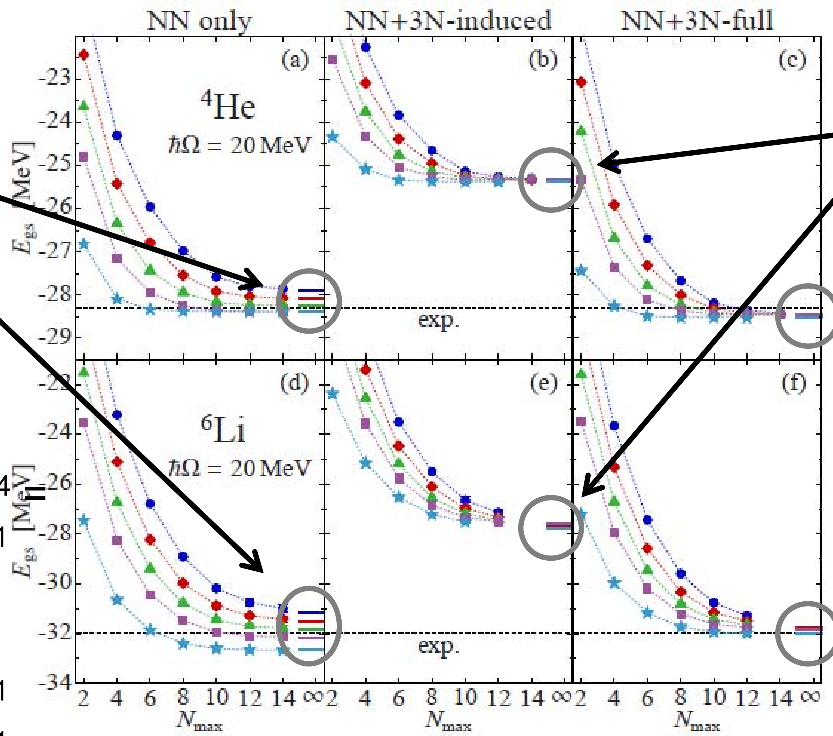


FIG. 1: (color online) IT-NCSM ground-state energies for ^{4}He and ^{6}Li as function of N_{max} for the three types of Hamiltonians (see column headings) for a range of flow parameters: α = 0.04 fm^4 (●), 0.05 fm^4 (◆), 0.0625 fm^4 (▲), 0.08 fm^4 (■), and 0.16 fm^4 (★). Error bars indicate the uncertainties of the threshold extrapolations. The bars at the right-hand-side of each panel indicate the results of exponential extrapolations of the individual N_{max}-sequences (see text).

<u>NN+3N-induced</u>
alpha independent
-> negligible SRG-induced
higher many-body contrib.
originating initial NN int.

induced 4N (4He)
ind. 4N, 5N, & 6N (6Li)
originating initial NN int.

<u>NN+3N-full</u>
alpha independent
reproduce exp data

For lower p-shell nuclei, induced 3N terms originating from the initial NN interaction are important, but induced 4N (and higher) terms are not important

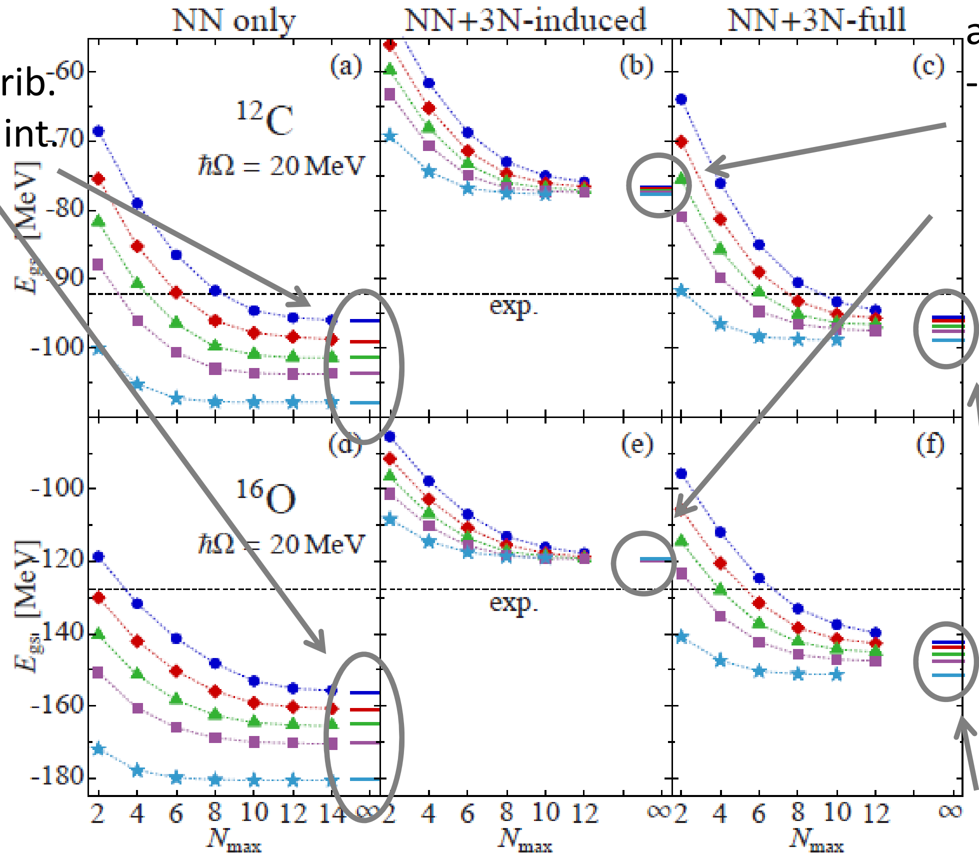
R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navratil, arXiv:1105.3173 [nucl-th]

Ground-state energy for upper p-shell nuclei

<u>NN only</u>
alpha dependent
-> SRG-induced 3N contrib.
originating initial NN int.

<u>NN+3N-induced</u>
alpha independent
-> negligible SRG-induced
higher many-body contrib.
originating initial NN int.

induced 4N-12N (12C)
ind. 4N-16N (16O)
originating initial NN int.



<u>NN+3N-full</u>
alpha dependent
-> SRG-induced 4N contrib.
originating initial 3N int.

FIG. 2: (color online) IT-NCSM ground-state energies for ^{12}C and ^{16}O as function of N_{max} for the three types of Hamiltonians and a range of flow parameters (for details see Fig. 1).

For upper p-shell nuclei, induced 4N terms originating from the initial 3N interaction are sizable

R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navratil, arXiv:1105.3173 [nucl-th]

Excitation spectra of carbon-12

First six excited states of positive parity for fixed alpha = 0.08 fm^4

Induced 3N terms
-> over-all compression of the spectrum

Initial (genuine) 3N terms
-> different behavior among the different states

2^+ & 4^+ states: improved
1^+ & 0^+_2 (Hoyle) states: not well described

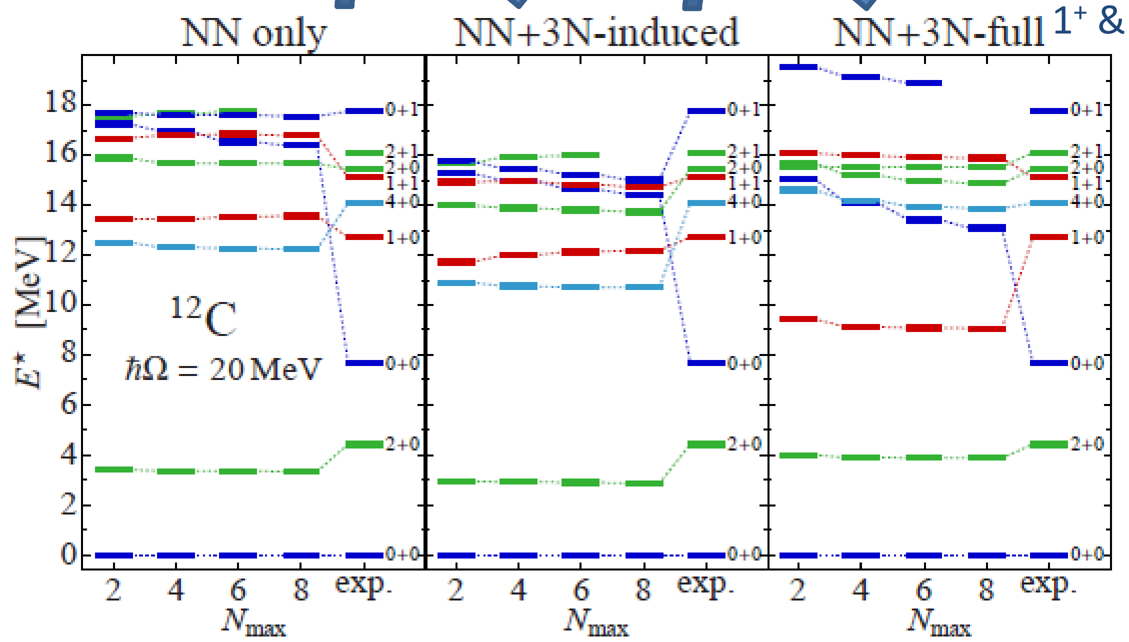
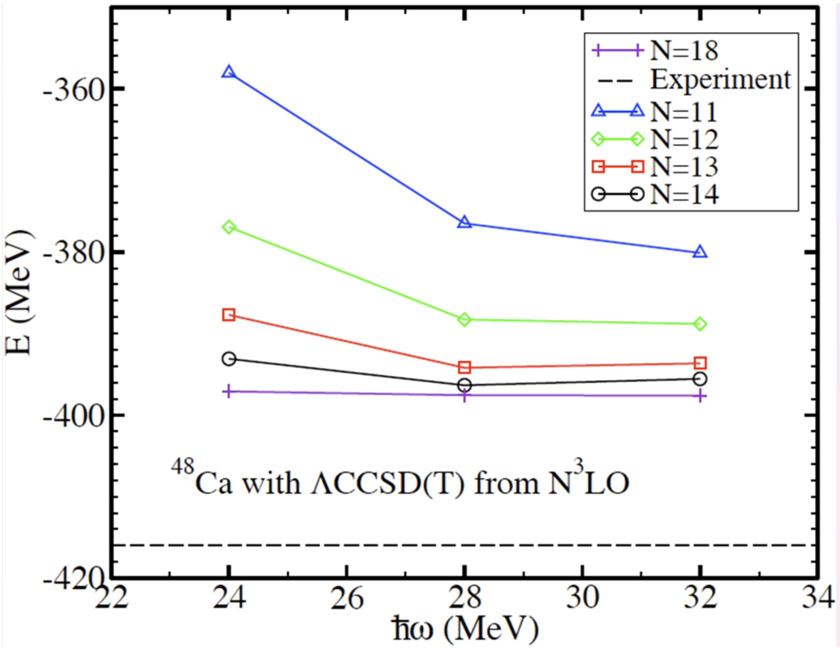


FIG. 4: (color online) Excitation spectrum for the lowest positive-parity states (labelled $J\pi T$) in ^{12}C for the NN-only, the NN+3N-induced, and the NN+3N-full Hamiltonian with $\alpha = 0.08$ fm^4.

Excited states: alpha dependence is much weaker than that in ground states (not shown in Fig.4, though)
~ a few 100 keV for $E^*(0^+_2)$ w/ NN+3N-full -> negligible induced 4N contrib.

Current Status of Coupled Cluster (CC) Theory

Saturation of N^{3}LO (NN only) in medium mass nuclei



	CCSD		Λ-CCSD(T)	
Nucleus	E/A	$\Delta E/A$	E/A	$\Delta E/A$
^{16}O	-6.72	1.25	-7.56	0.41
^{40}Ca	-7.72	0.84	-8.63	-0.08
^{48}Ca	-7.40	1.27	-8.26	0.40

Benchmarks in light nuclei:

Coupled-cluster meets few-body benchmarks for ^{4}He. Recent IT-NCSM and UMOA calculations of ^{16}O agree with CCM.
R. Roth *et al,* arXiv:1105.3173 (2011)
Fujii *et al,* PRL 103, 182501(2009)

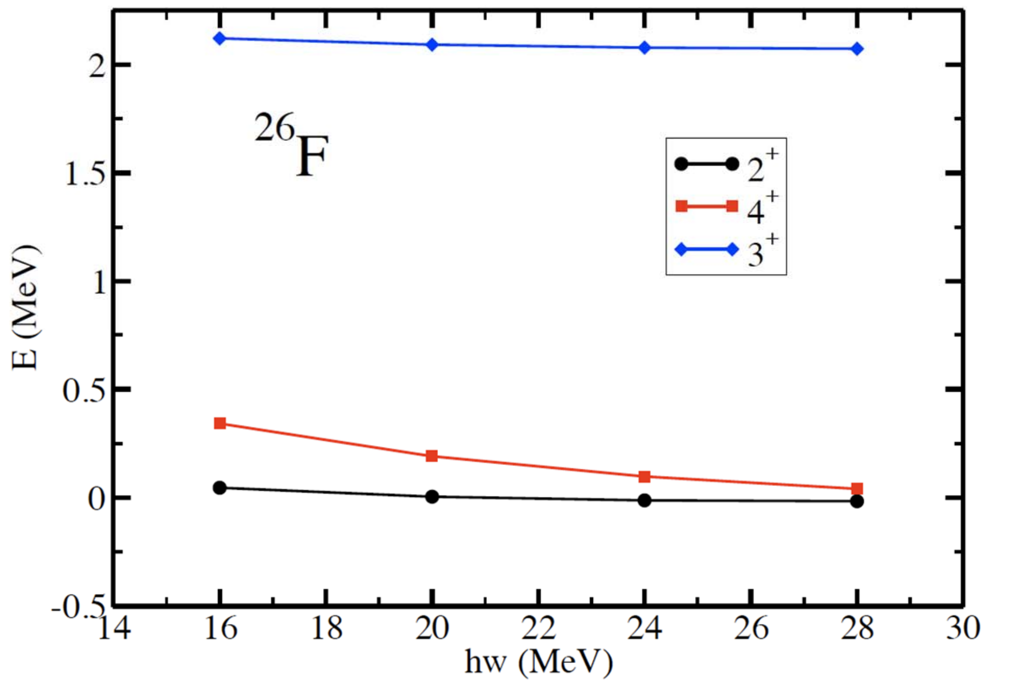
	CCM	(IT-)NCSM	UMOA
	E/A	E/A	E/A
^{4}He	-6.39(5)	-6.35	
^{16}O	-7.56(8)	-7.48(4)	7.47

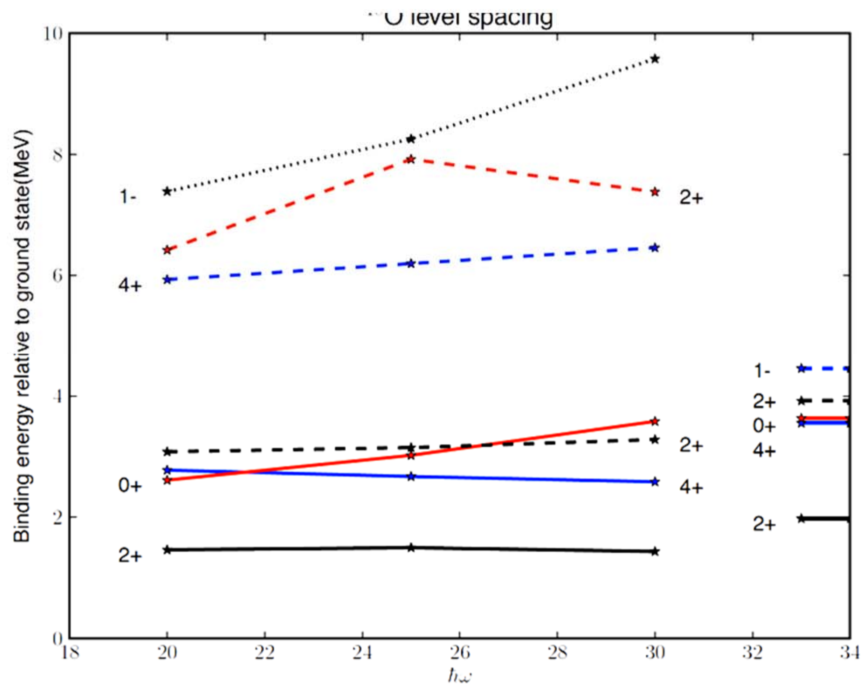
G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. C 82, 034330 (2010).

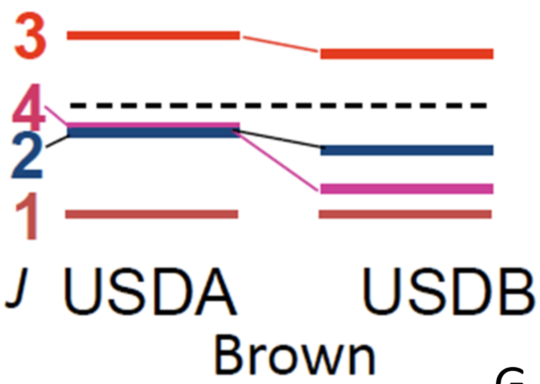
G. Hagen, Annual UNEDF Collaboration Meetings (2011)

Current Status of Coupled Cluster (CC) Theory

Going beyond closed-shell nuclei. Low-lying states in ^{18}O and ^{26}F (Preliminary)







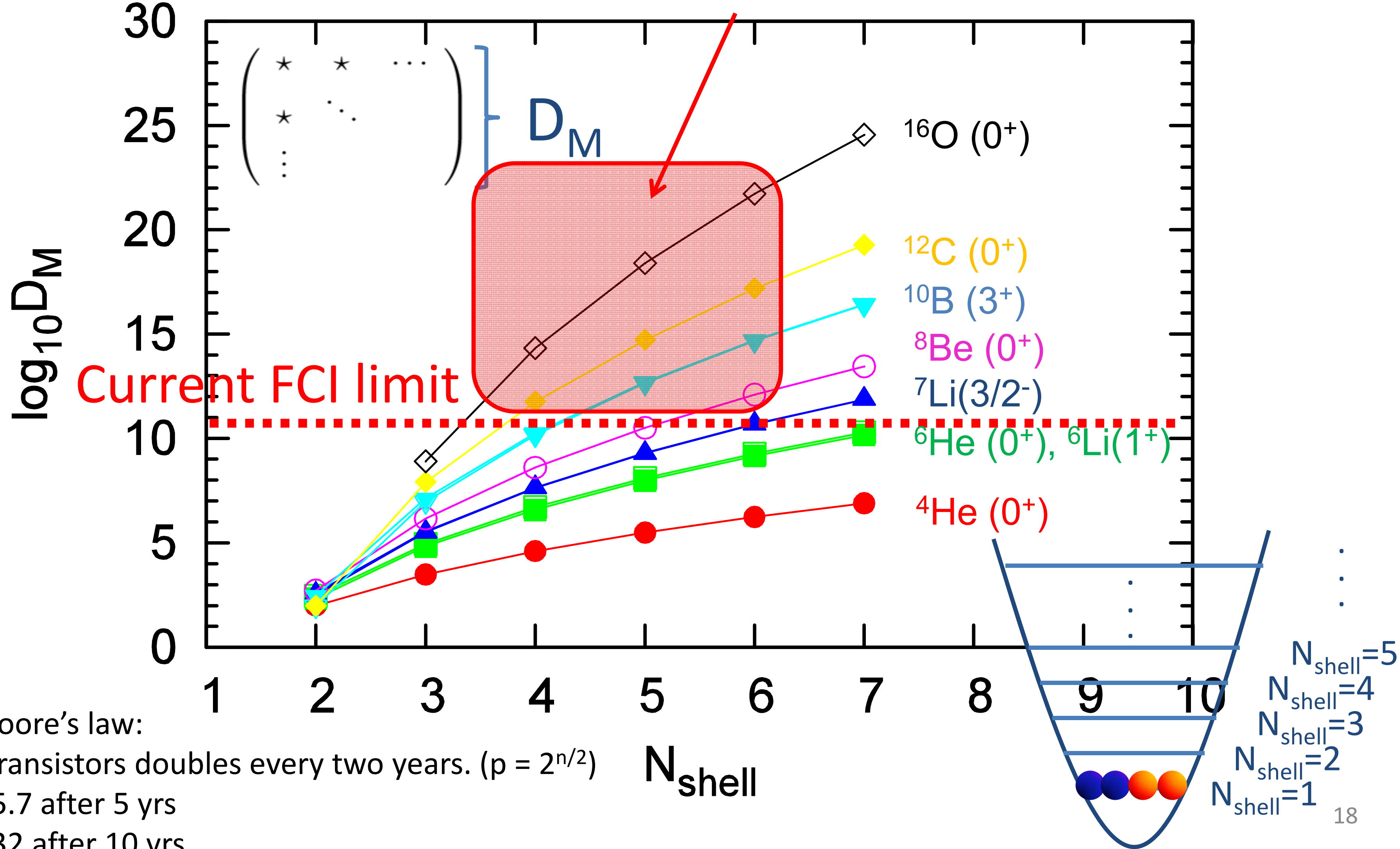
Two-particle attached coupled-cluster works very well for low-lying states in open-shell nuclei like ^{18}O and ^{26}F.
Our results for ^{26}F seem to suggest a more compressed spectrum as compared to USDA/USDB calculations.
G. Jansen, M. Hjorth-Jensen, G. Hagen, T. Papenbrock, Phys. Rev. C 83, 054306 (2011).

G. Hagen, Annual UNEDF Collaboration Meetings (2011)

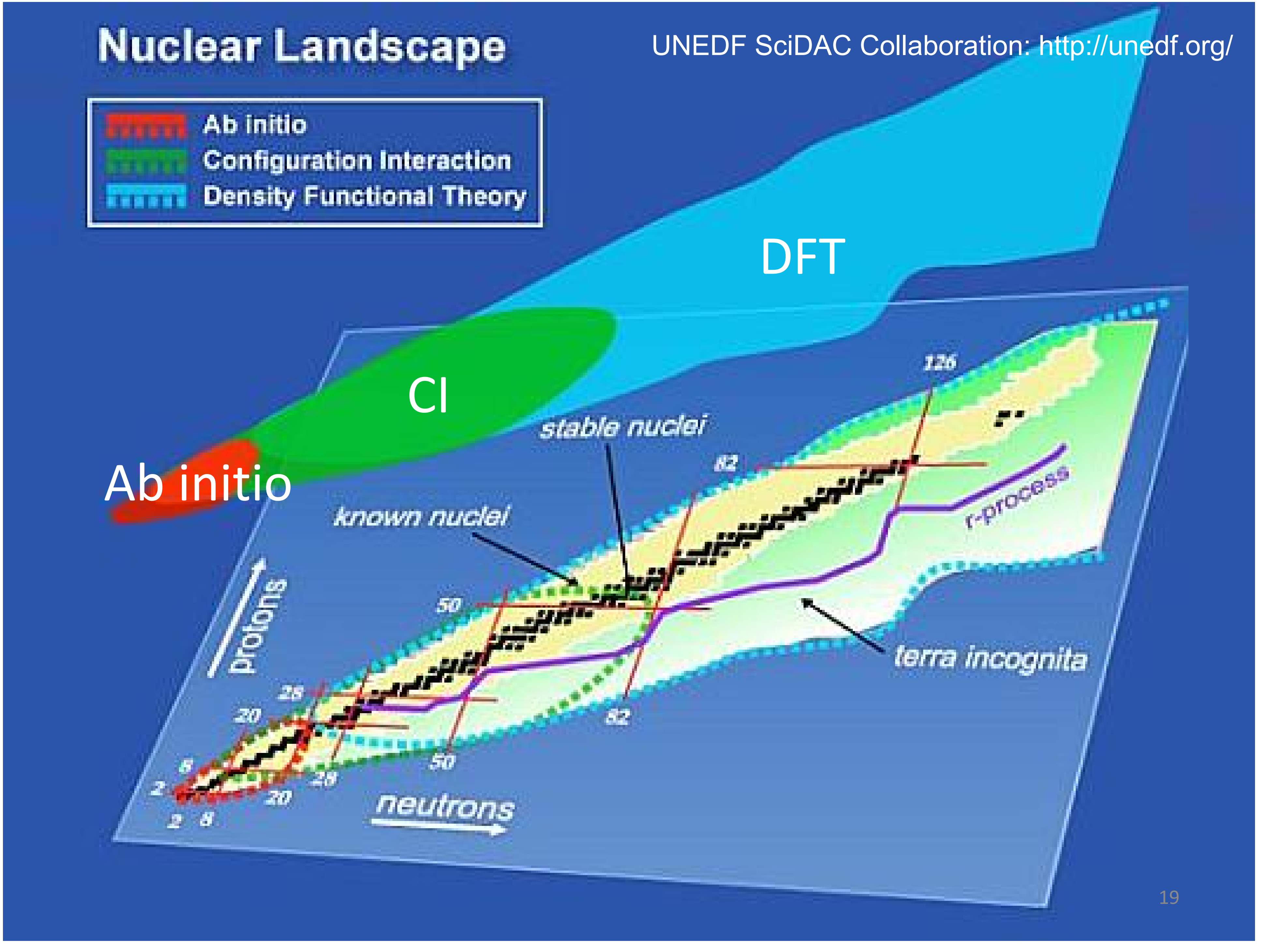
Current status of some ab initio calc

- GFMC: A = 12 w/ NN + NNN
- NCSM: A = 14 w/ NN + NNN @ Nmax = 8
- IT-NCSM: A = 16 w/ NN + NNN @ Nmax = 12
- CC: Closed core +/- A = 2 w/ NN (+NNN)

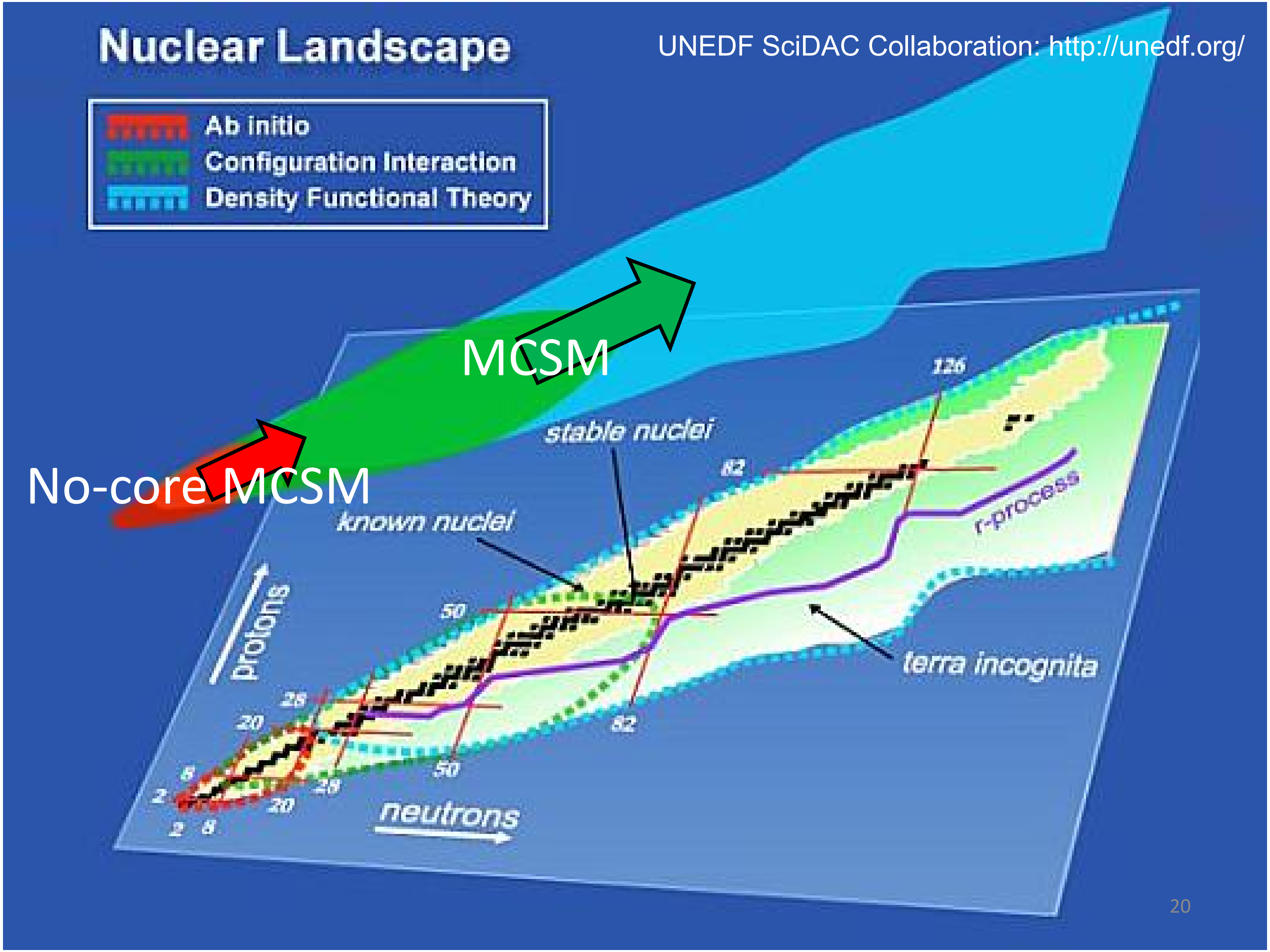
M-scheme dimension



Moore's law:
#transistors doubles every two years. ($p = 2^{n/2}$)
x 5.7 after 5 yrs
x 32 after 10 yrs



Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
DFT
CI
Ab initio
stable nuclei
known nuclei
terra incognita
r-process
protons
neutrons
126
82
50
28
20
8
2


Nuclear Landscape
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No-core MCSM
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126
82
50
28
20
8
2

NCSM, FCI, NCFC, MCSM

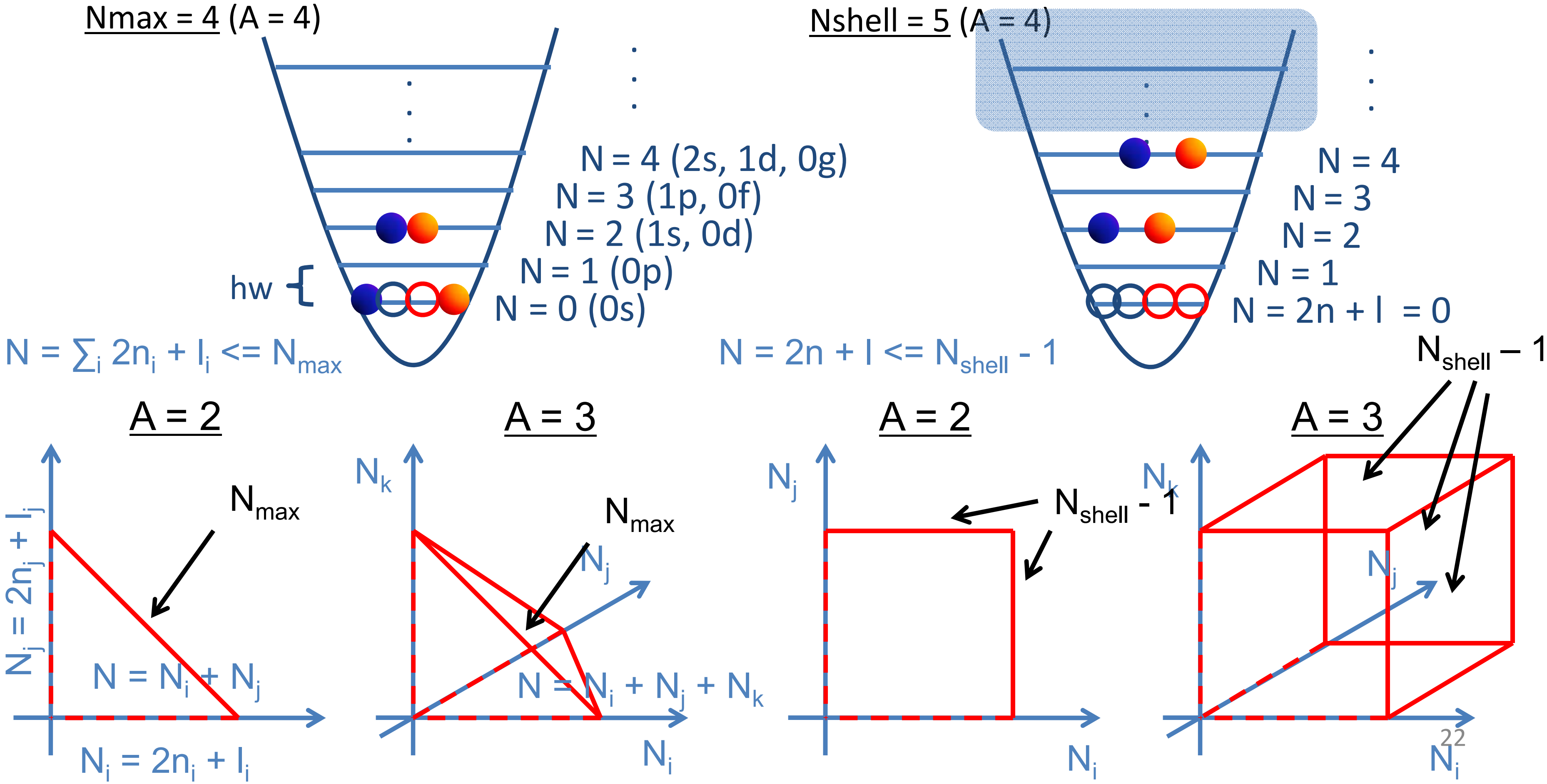
	Truncation	Interaction
NCSM	Nmax	Bare/Effective
FCI	Nshell	Bare
NCFC	Nmax	Bare
MCSM	Nshell	Bare/Effective

- ✓ 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).

Truncations of the Model Space in NCSM & FCI

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

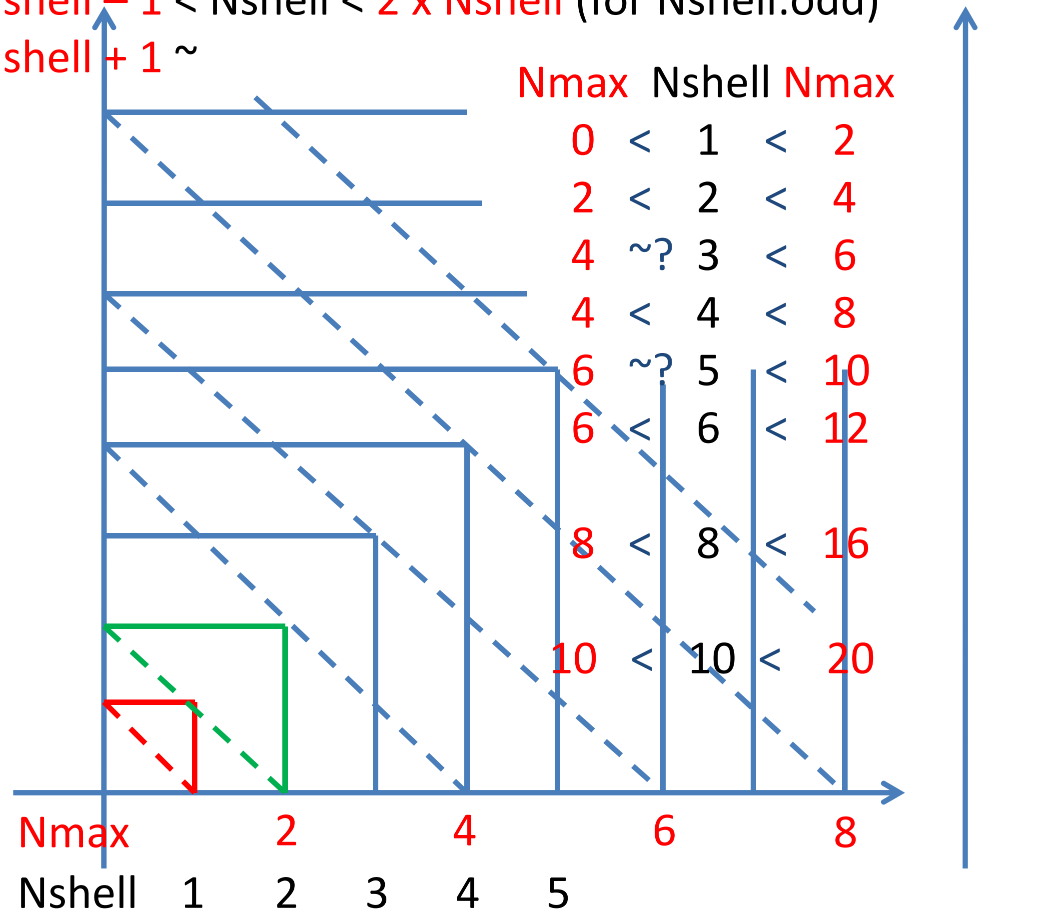
- Nshell (FCI, MCSM, IT-CI, …)
  - Max. # of HO quanta of single-particle basis



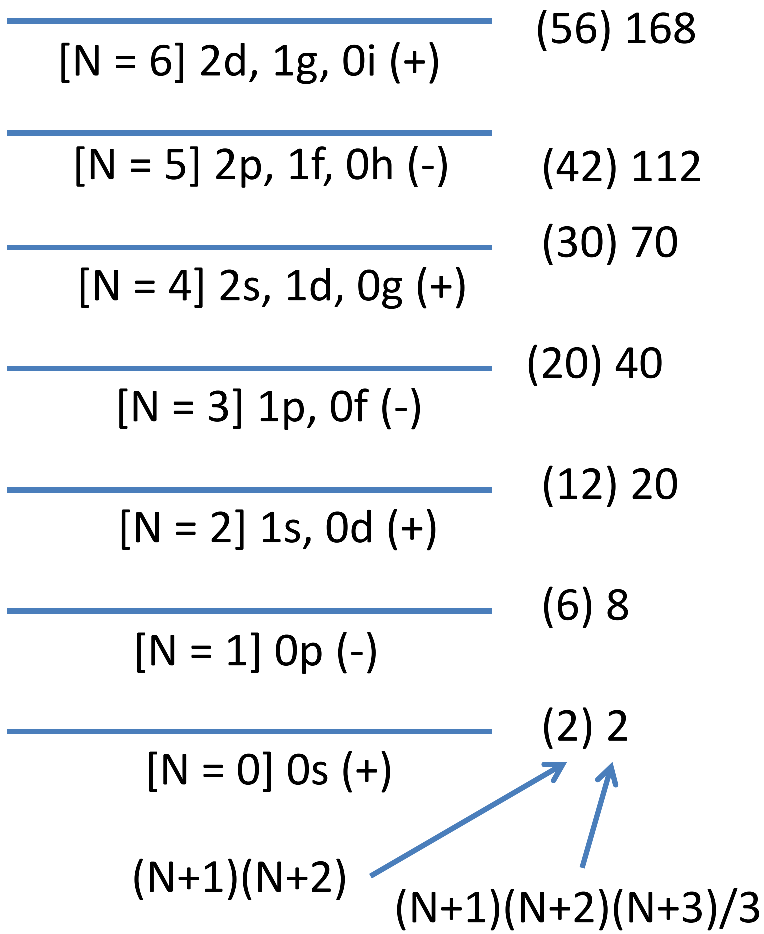
Truncations of Model Space: Nshell & Nmax

Nmax :	Nshell:	Nmax
Nshell	< Nshell <	2 x Nshell (for Nshell:even)
Nshell – 1	< Nshell <	2 x Nshell (for Nshell:odd)
Nshell + 1 ~		

N = 2n + l

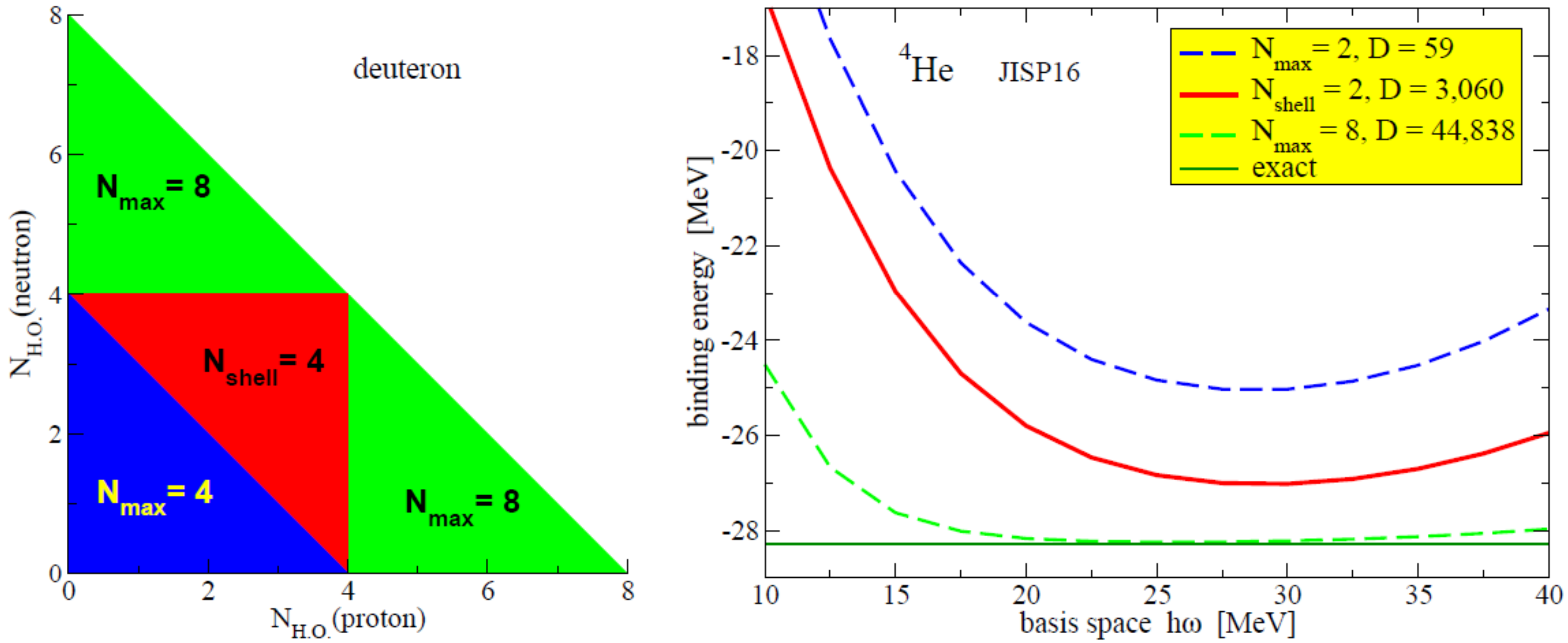


Nshell = N + 1



FCI versus $N_{\max}$ truncation – dimensionality

- $N_{\max}$ truncation on number of H.O. quanta of Many-Body basis
- N_{shell} truncation on number of H.O. quanta of Single-Particle basis



- deuteron: $N_{\max} = 4$ is subset of $N_{\text{shell}} = 4$ is subset of $N_{\max} = 8$
- ^{4}He: $N_{\max} = 2$ is subset of $N_{\text{shell}} = 2$ is subset of $N_{\max} = 8$

P. Maris, EFES-Iowa workshop (2010)

Monte Carlo Shell Model (MCSM)

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

Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

$$H = \begin{pmatrix} \star & \star & \star & \star & \star & \cdots \\ \star & \star & \star & \star & & \\ \star & \star & \star & & & \\ \star & \star & & \ddots & & \\ \star & & & & & \\ \vdots & & & & & \end{pmatrix} \quad \xrightarrow{\text{Diagonalization}} \quad \begin{pmatrix} E_0 & & & 0 \\ & E_1 & & \\ & & E_2 & \\ & & & \ddots \\ 0 & & & \end{pmatrix}$$

All Slater determinants

Monte Carlo shell model

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \quad \xrightarrow{\text{Diagonalization}} \quad \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Important bases stochastically selected

d_{MCSM} ~ O(10-100)

Hamiltonian & wave function

- Second-quantized Hamiltonian (up to two-body int.)

$$H = \sum_{\alpha\beta}^{N_{sps}} t_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta}^{N_{sps}} \bar{v}_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \quad \bar{v}_{ijkl} = v_{ijkl} - v_{ijlk}$$

- Many-body wave function: superposition of non-orthogonal SDs

$$|\Psi(I, M, \pi)\rangle = \sum_i^{N_{basis}} f_i |\Phi_i(I, M, \pi)\rangle$$

- Angular-momentum & parity projected MCSM basis

$$|\Phi(I, M, \pi)\rangle = \sum_K g_K P^I_{MK} P^\pi |\phi\rangle$$

- Deformed SDs

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle \qquad a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

($c_\alpha{}^\dagger$ … HO basis)

Monte Carlo Shell Model

- Deformed Slater determinant basis

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle \qquad a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

($c_\alpha{}^\dagger$ … HO basis)

- MCSM basis

$$|\phi(\sigma)\rangle = e^{-h(\sigma)}|\phi\rangle \qquad h(\sigma) = h_{HF} + \sum_i^{N_{AF}} s_i V_i \sigma_i O_i$$

c.f.) Imaginary-time evolution & Hubbard-Stratonovich transf.

$$|\phi(\sigma)\rangle = \prod_{N_\tau} e^{-\Delta\beta h(\sigma)}|\phi\rangle \qquad h(\sigma) = \sum_i^{N_{AF}} (\epsilon_i + s_i V_i \sigma_i) O_i$$

$$H = \sum_i \epsilon_i O_i + \frac{1}{2}\sum_i V_i O_i^2$$

$$e^{-\beta H} = \int_{-\infty}^{+\infty} \prod_i d\sigma_i \sqrt{\frac{\beta|V_i|}{2\pi}} e^{-\frac{\beta}{2}|V_i|\sigma_i^2} e^{-\beta h(\vec{\sigma})}$$

P. Ring, P. Schuck, The Nuclear Many-Body Problem, Springer

Monte Carlo Shell Model

Euler angles

$$\Omega = (\alpha, \beta, \gamma)$$

Wigner function

$$D^{I*}_{MK}(\Omega)$$

- Symmetry restoration by projection method
  - Angular momentum projection operator (same as the parity)

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2} \int D^{I*}_{MK}(\Omega) \hat{R}(\Omega) d\Omega$$

Unitary rotational operator

$$R(\Omega) = e^{i\alpha J_z} e^{i\beta J_y} e^{i\gamma J_z}$$

  - General (GCM) ansatz

$$|\Psi^{IM}\rangle = \sum_K g^I_K \hat{P}^I_{MK} |\Phi\rangle = \sum_K \frac{2I+1}{8\pi^2} \int d\Omega D^{I*}_{MK}(\Omega) R(\Omega) |\Phi\rangle$$

  - Projected energy

$$E^I_{proj} = \frac{\langle \Psi^{IM} | H | \Psi^{IM} \rangle}{\langle \Psi^{IM} | \Psi^{IM} \rangle} = \frac{\sum_{KK'} g^*_K g_{K'} h^I_{KK'}}{\sum_{KK'} g^*_K g_{K'} n^I_{KK'}}$$

Kernels

$$h^I_{KK'} = \langle \Phi | H \hat{P}^I_{KK'} | \Phi \rangle$$
$$n^I_{KK'} = \langle \Phi | \hat{P}^I_{KK'} | \Phi \rangle$$

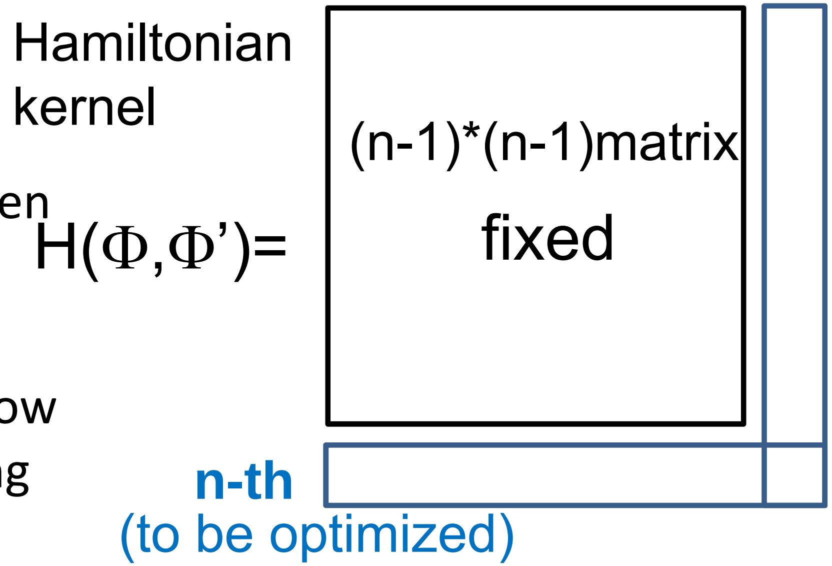
Hot spot in MCSM:

$$\langle \Phi' | H \hat{P}^I_{MK} | \Phi \rangle \rightarrow \sum_{\Omega} W^I_{MK}(\Omega) \langle \Phi' | H R(\Omega) | \Phi \rangle$$
$$= \sum_{\alpha,\beta,\gamma} W^I_{MK}(\alpha,\beta,\gamma) \langle \Phi' | H e^{i\alpha J_z} e^{i\beta J_y} e^{i\gamma J_z} | \Phi \rangle$$

~ 30 x 30 x 30 mesh points

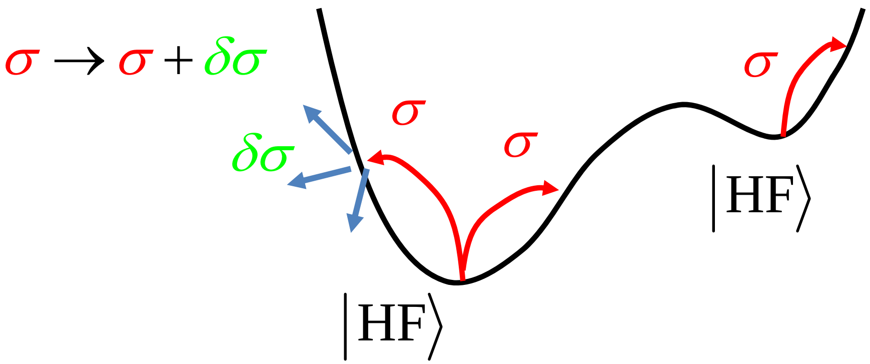
Monte Carlo Shell Model

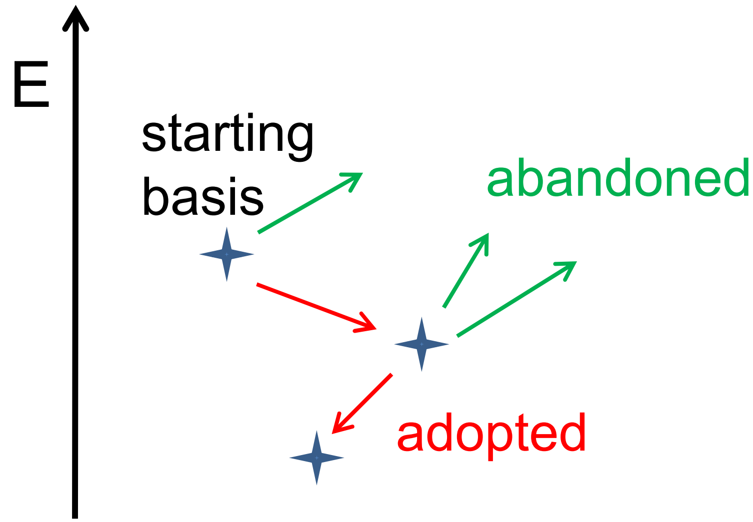
- Basis search
  - Fix the n-1 basis states already taken
  - Requirement for the new basis: atopt the basis which makes the energy (of a many-body state) as low as possible by a stochastic sampling



$$\left|\phi(\sigma)\right\rangle = \prod_n e^{-\Delta\beta h(\vec{\sigma}_n)} \left|\phi\right\rangle$$

$$h(\vec{\sigma}_n) = h_{HF} + \sum_\alpha \sigma_{\alpha n} O_\alpha$$





Recent developments in MCSM

- Acceleration of the computation of two-body matrix elements

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

Matrix product is performed w/ bundled density matrices by DGEMM subroutine in BLAS library

<u>800 % performance improvement from the original MCSM code</u>

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, in preparation.

- Extrapolation method by the energy variance

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

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

$$+\mathrm{Tr}((t+\Gamma)(1-\rho)(t+\Gamma)\rho) + \left(\mathrm{Tr}(\rho(t+\frac{1}{2}\Gamma))\right)^2 \qquad \Gamma_{ik} = \sum_{jl} v_{ijkl}\rho_{lj}$$

(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)

Computation of the TBMEs

- hot spot: Computation of the TBMEs

(w/o projections, for simplicity)

$$\frac{\langle \Phi' | V | \Phi \rangle}{\langle \Phi' | \Phi \rangle} = \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl} \rho_{ki} \rho_{lj}$$

c.f.) Indirect-index method (list-vector method)

- non-zero ME: jz(i) + jz(j) = jz(k) + jz(l) -> jz(i) - jz(k) = - (jz(j) – jz(l))

$$\sum_{ijkl} \bar{v}_{ijkl} \rho_{ki} \rho_{lj} = \sum_{\Delta m} \left[\sum_{a \in J_z(a) = -\Delta m} \tilde{\rho}_a \left(\sum_{b \in J_z(b) = \Delta m} \tilde{v}_{ab} \tilde{\rho}_b \right) \right]$$

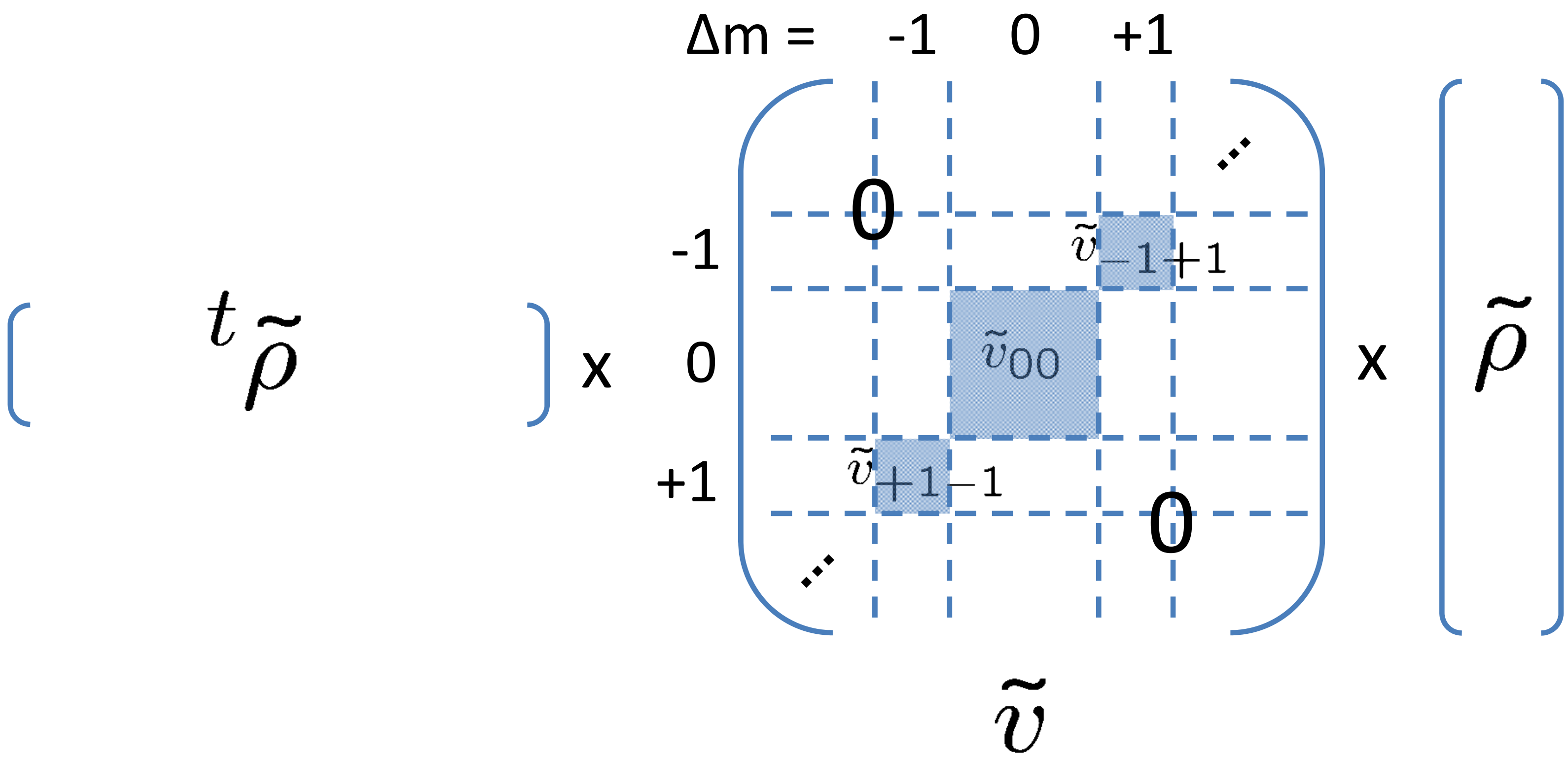
Operations: sparse matrix -> dense matrix

$\bar{v}_{ijkl} \to \tilde{v}_{ab}$ (sparse → dense) $\qquad \rho_{ki} \to \tilde{\rho}_a \qquad \rho_{lj} \to \tilde{\rho}_b$

Schematic illustration of the computation of TBMEs

- Matrix-vector method

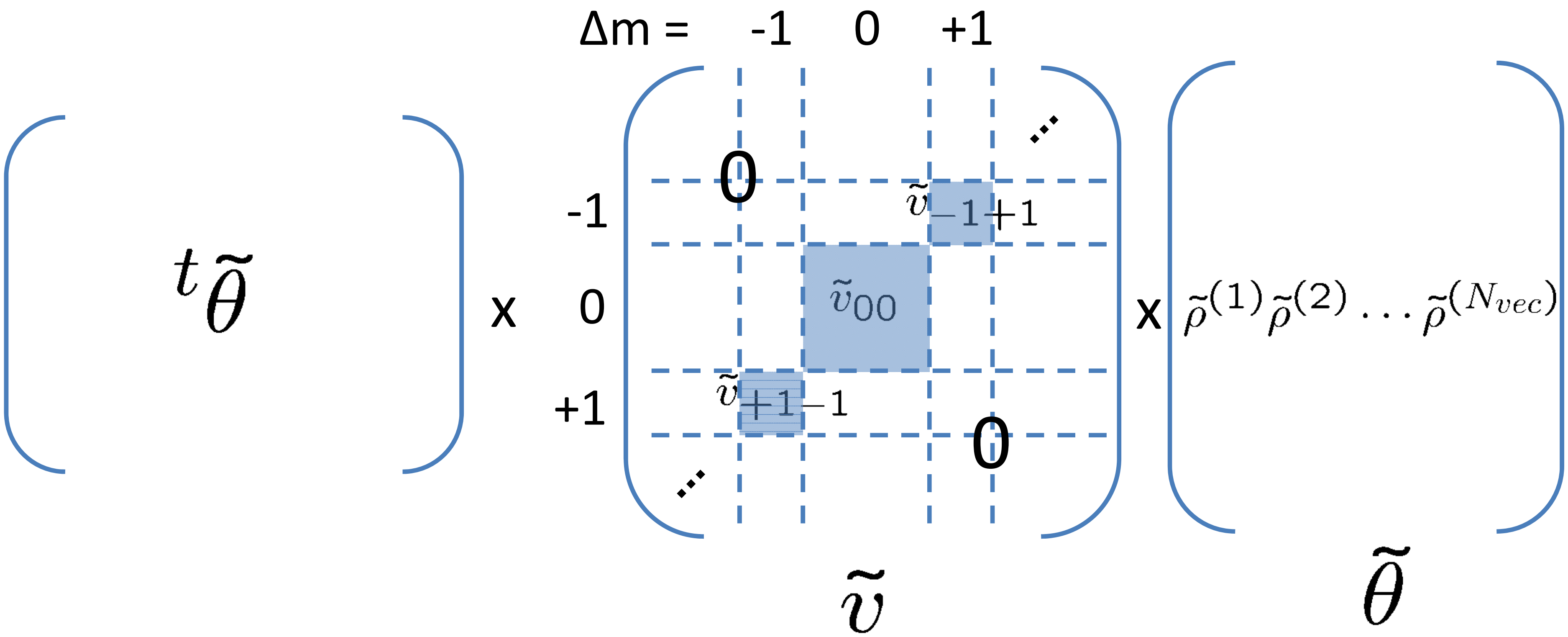
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



Schematic illustration of the computation of TBMEs

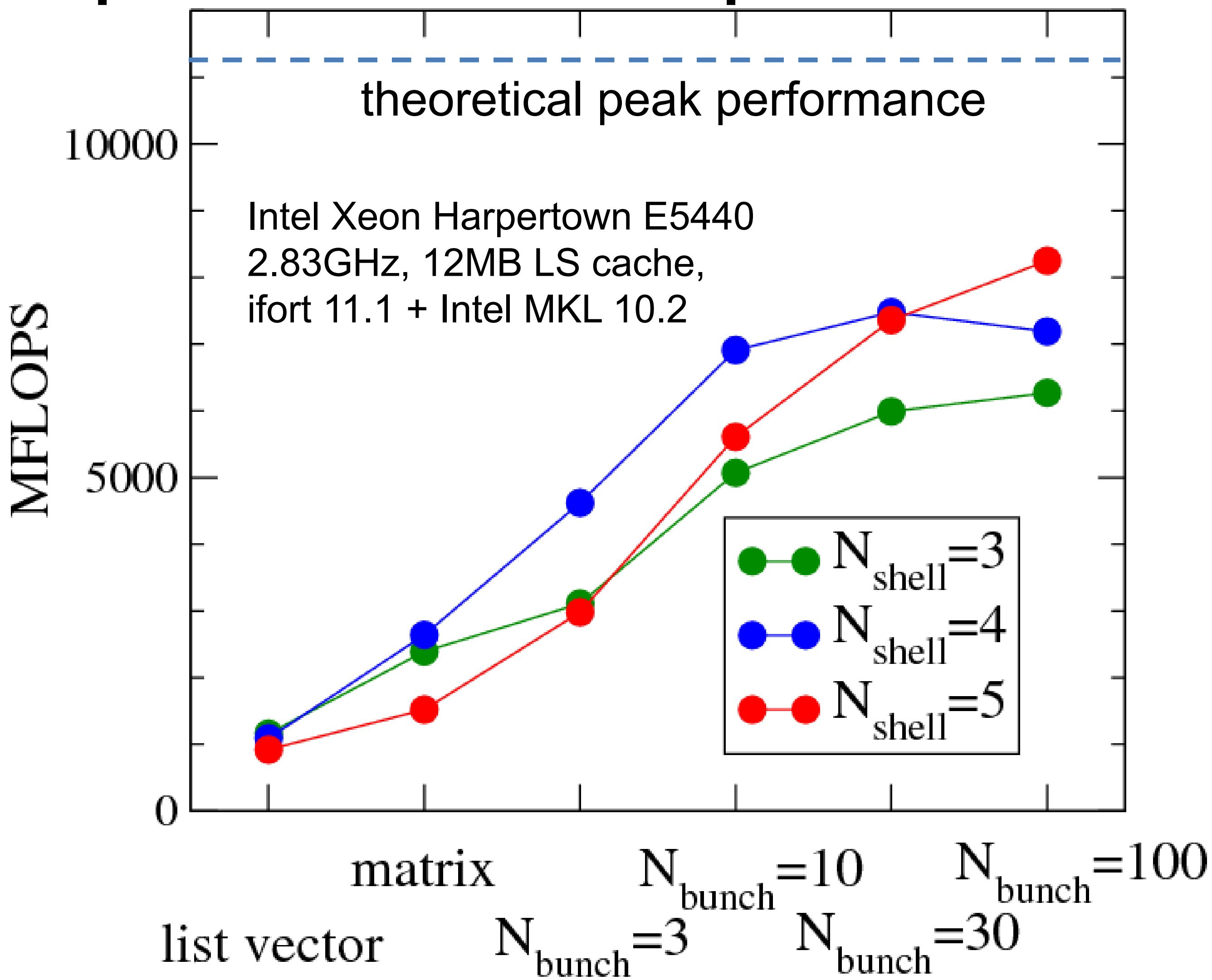
- Matrix-matrix method

$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



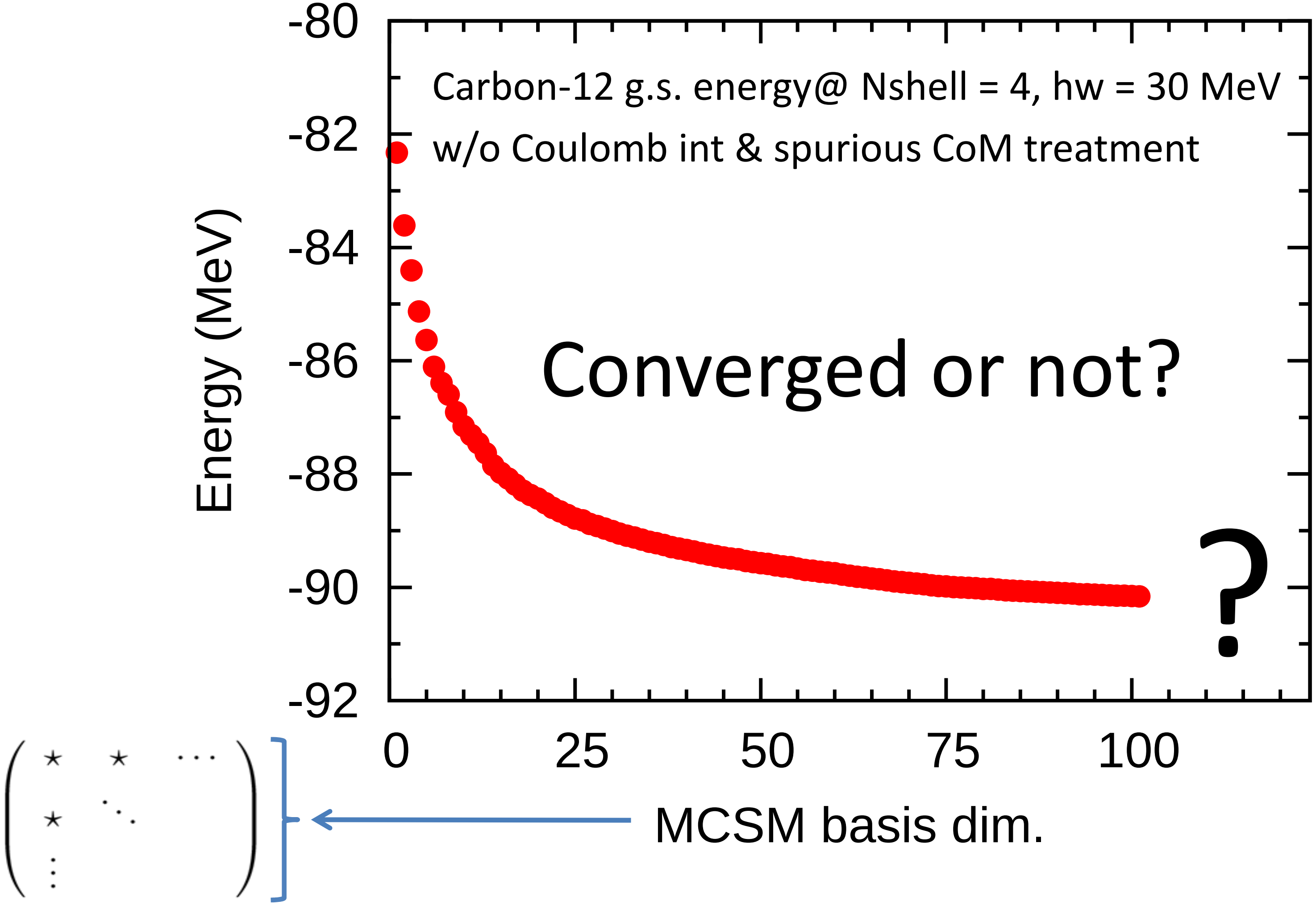
→ BLAS Level 3

Comparison of the performance



Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, in preparation.

Energy-variance extrapolation



$D_M \sim 6 \times 10^{11}$

Energy variance extrapolation

- Originally proposed in condensed matter physics

  Path Integral Renormalization Group method

  M. Imada and T. Kashima, J. Phys. Soc. Jpn 69, 2723 (2000)

- Imported to nuclear physics

  Lanczos diagonalization with particle-hole truncation

  T. Mizusaki and M. Imada Phys. Rev. C65 064319 (2002)

  T. Mizusaki and M. Imada Phys. Rev. C68 041301 (2003)

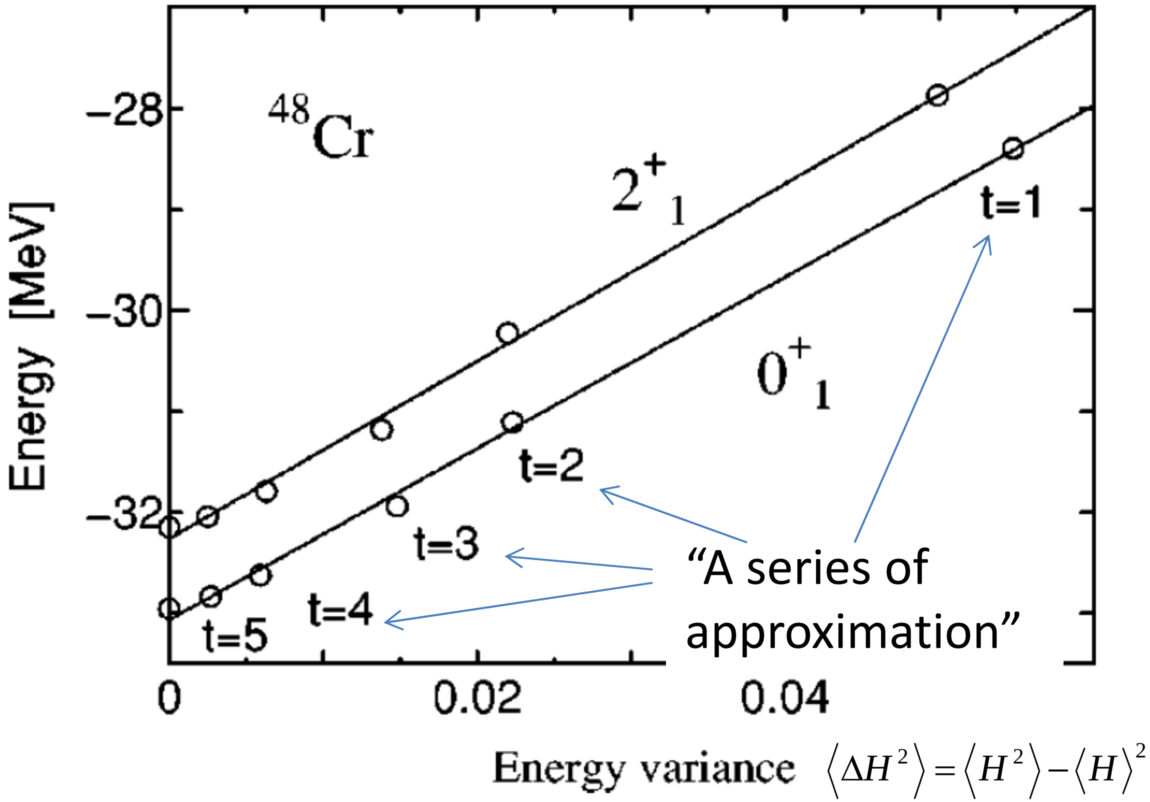
  single deformed Slater determinant

  T. Mizusaki, Phys. Rev. C70 044316 (2004)

→ Apply to the MCSM

What is the energy-variance extrapolation?

Demonstrated by Mizusaki in the framework of conventional shell model



Energy variance is defined as

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

If the wave function is an exact eigenstate of the Hamiltonian, energy variance is exactly zero

$$\langle \Delta H^2 \rangle = 0$$

A series of approximated wave functions:

$$\langle H \rangle = E_0 + a\langle \Delta H^2 \rangle + b\langle \Delta H^2 \rangle^2 + \ldots$$

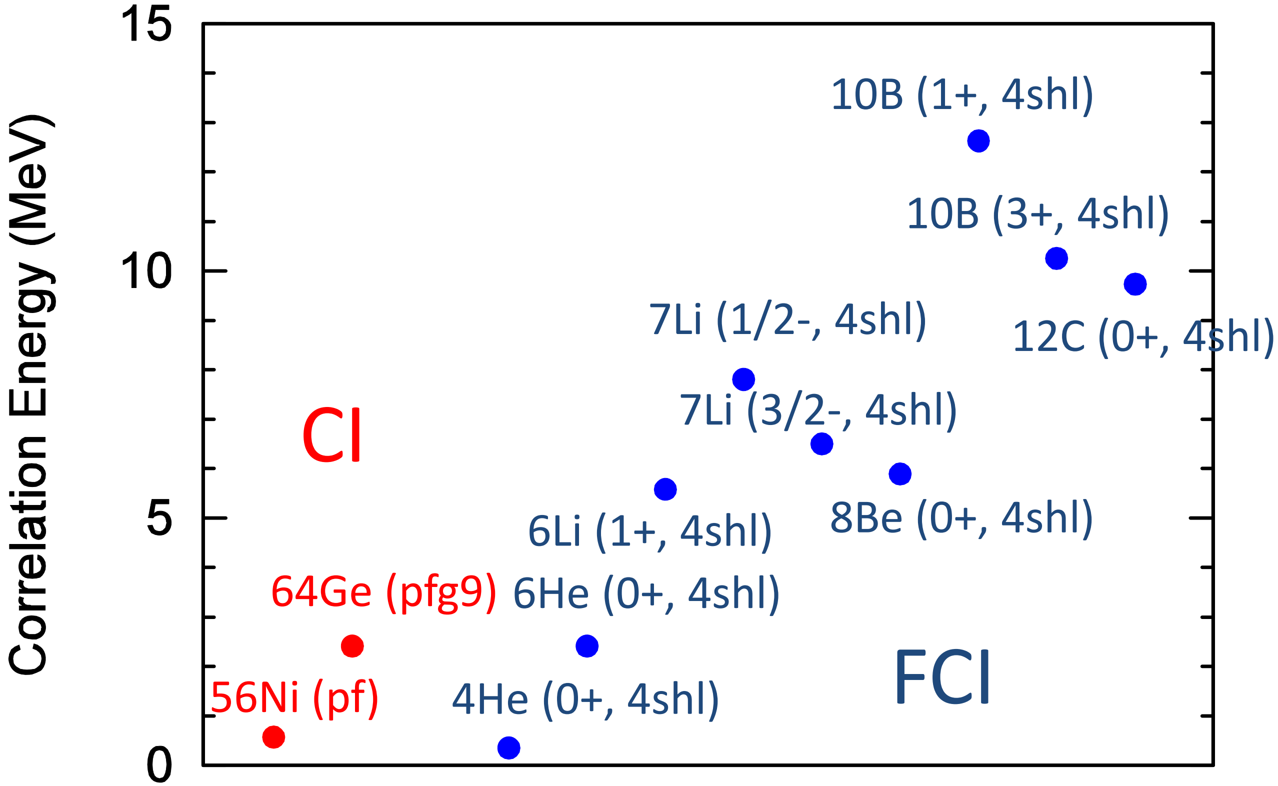
With a sequence of approximate energies,

extrapolate $\langle \Delta H^2 \rangle \to 0$ so that $\langle H \rangle$ becomes E_0, true energy.

Ref. T. Mizusaki and M. Imada, Phys. Rev. **C65** 064319 (2002)

Why we need to extrapolate the energies

- Definition: (Correlation Energy) $\equiv \langle\Psi|H|\Psi\rangle_{\rm JHF} - \langle\Psi|H|\Psi\rangle_{\rm Exact}$



NCSM wf w/ realistic NN int is more correlated (complicated) than SSM wf w/ effective int

<u>Need energy-variance extrapolation for No-Core MCSM calc</u>

Numerical effort

8-folded loop
~O(Nsps^8)

$$\frac{\langle\Phi'|\hat{V}^2|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \sum_{ijkl\alpha\beta\gamma\delta}\bar{v}_{ijkl}\bar{v}_{\alpha\beta\gamma\delta}\Big[\frac{1}{4}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\rho_{\gamma i}\rho_{\delta j} + \rho_{\gamma\alpha}(1-\rho)_{l\beta}\rho_{ki}\rho_{\delta j} + \frac{1}{4}\rho_{ki}\rho_{lj}\rho_{\gamma\alpha}\rho_{\delta\beta}\Big]$$

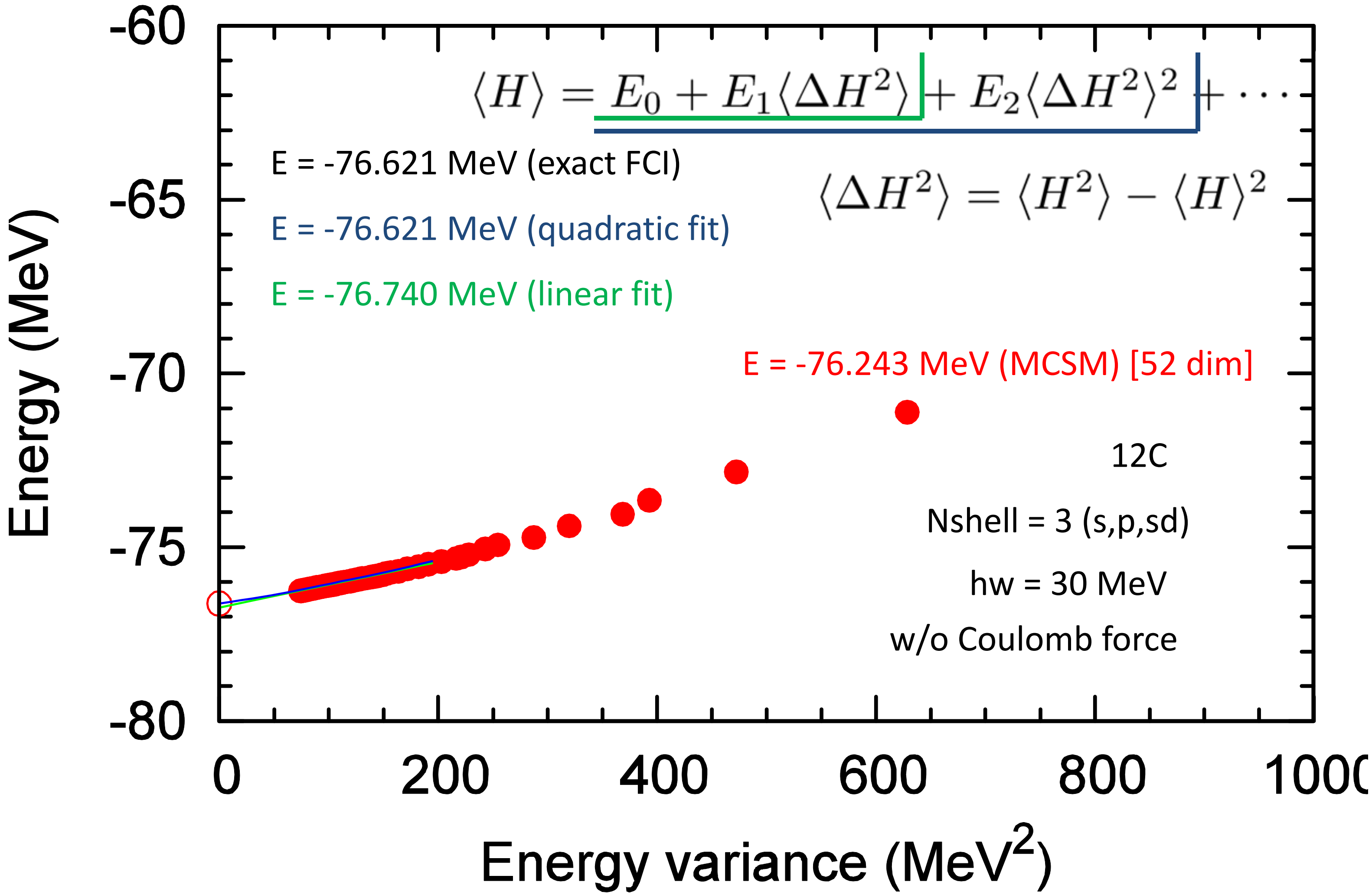
$$= \frac{1}{4}\sum_{ij\alpha\beta}\left(\sum_{kl}\bar{v}_{ijkl}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\right)\left(\sum_{\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma i}\rho_{\delta j}\right) + \mathrm{Tr}(\Gamma(1-\rho)\Gamma\rho) + \frac{1}{4}[\mathrm{Tr}(\rho\Gamma)]^2$$

6-folded loop
~O(Nsps^6)

$$\rho_{\beta\alpha} = \frac{\langle\Phi'|c^\dagger_\alpha c_\beta|\Phi\rangle}{\langle\Phi'|\Phi\rangle} \quad \Gamma_{ik} = \sum_{jl}\bar{v}_{ijkl}\rho_{lj} \quad \frac{\langle\Phi'|V|\Phi\rangle}{\langle\Phi'|\Phi\rangle} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma\alpha}\rho_{\delta\beta}$$

Extrapolation of 12C Energy

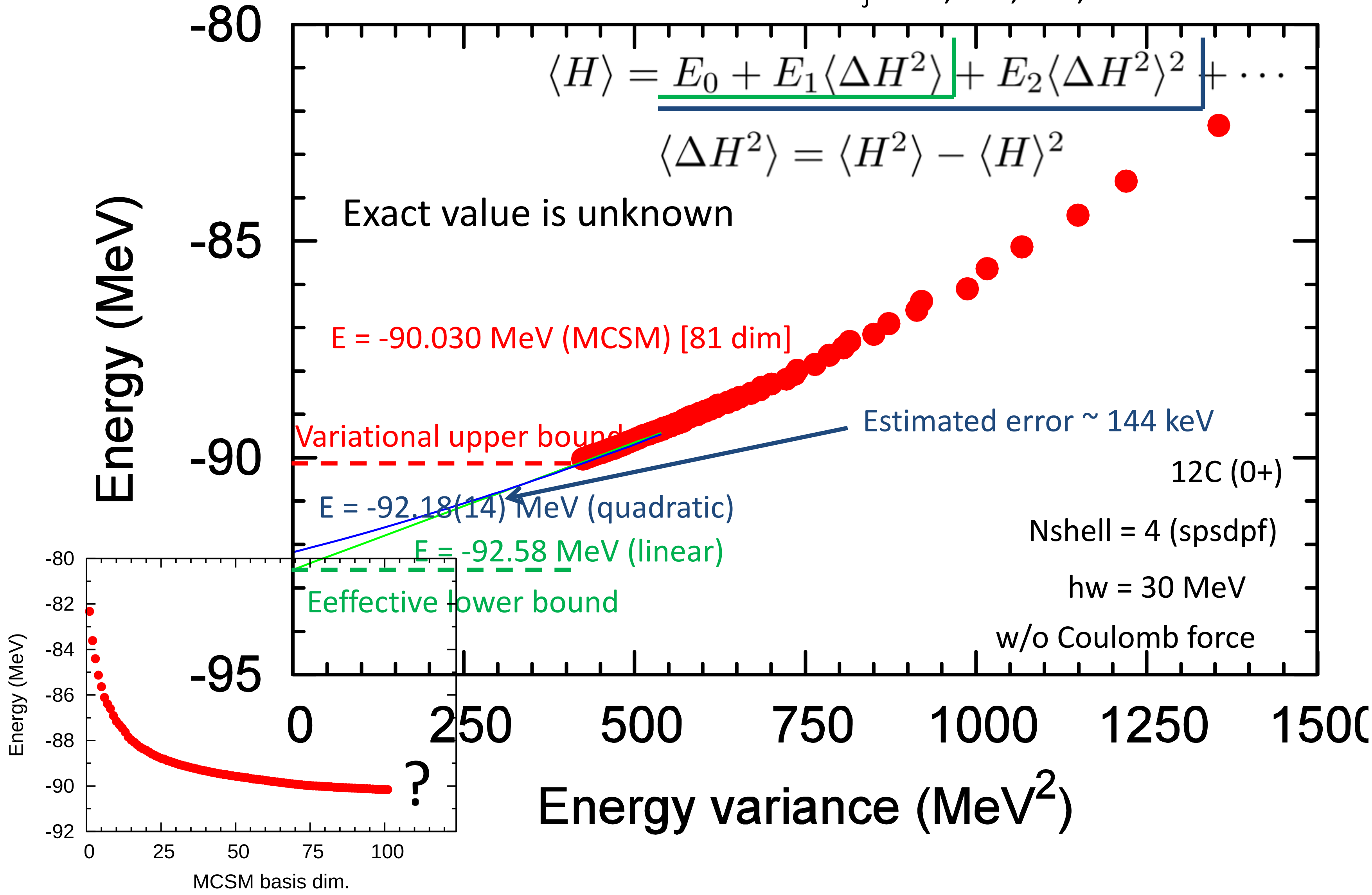
D_J =2,936,582 = 2.9 x 10^6



$D_M \sim 6 \times 10^{11}$

Extrapolation of 12C Energy

D_J = 11,384,214,614 ~ 1.1×10^{10}



Benchmark results

- Energy
- RMS
- Q-moment
- μ-moment

What we have calculated as Benchmark

- Comparison btw MCSM & FCI (exact diag.) calc
- 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 (matter)
  - Electromagnetic moments (Q, μ)

Our test set up:

- NN interaction: JISP16
- model space: Nshell = 2, 3, 4
- optimal hw selected for states & Nshell's
- w/o Coulomb
- w/o Gloeckner-Lawson prescription

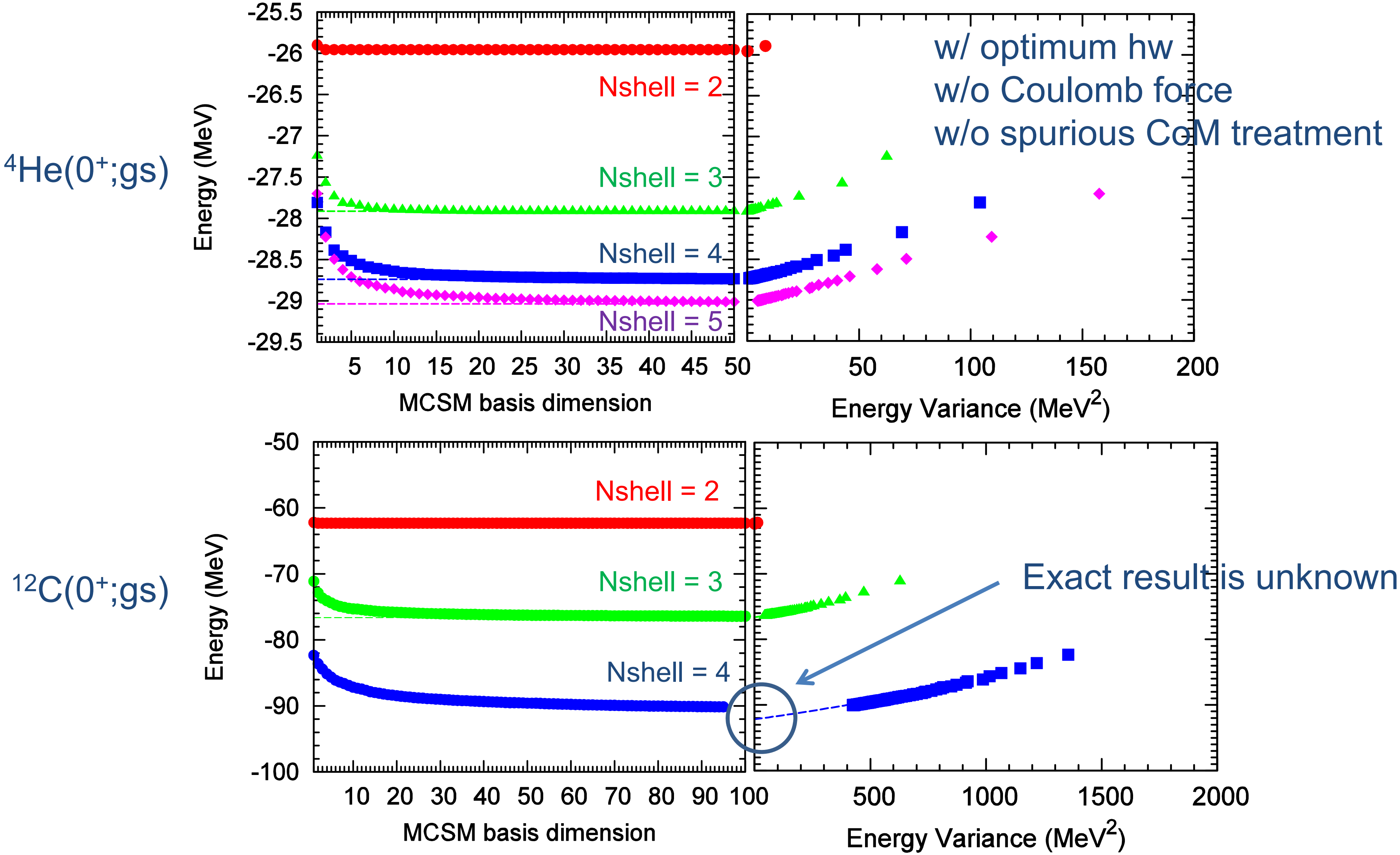
MCSM: Abe, Otsuka, Shimizu, Utsuno (Tokyo)
T2K (Tokyo, Tsukuba), BX900 (JAEA)

FCI: Maris, Vary (Iowa)
Jaguar, Franklin (NERSC, DOE)

JISP16:
A.M. Shirokov, J.P. Vary, A. I. Mazur, T.A. Weber, Phys. Lett. B644, 33 (2007)

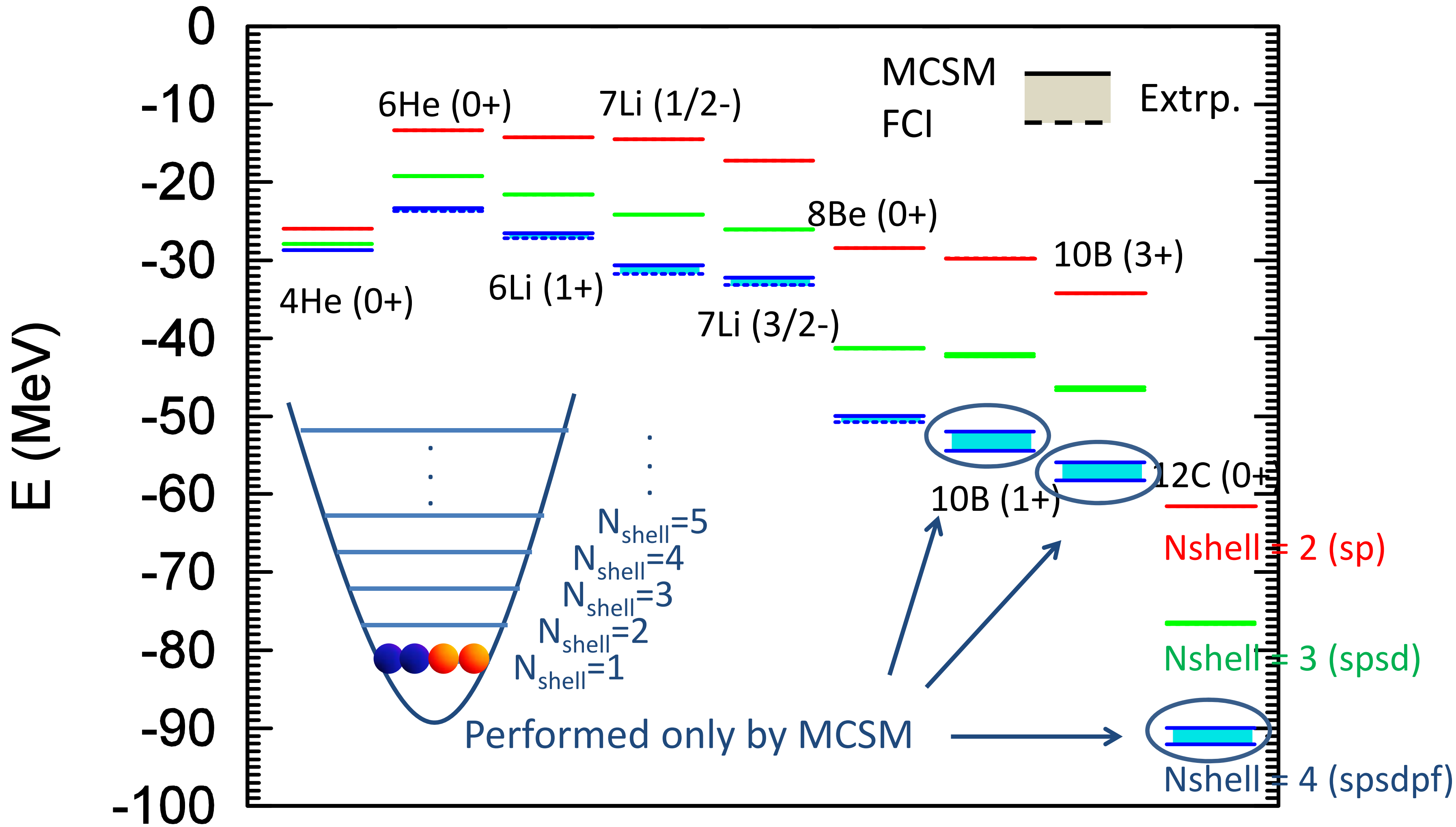
NCFC calc of light nuclei w/ JISP16:
P. Maris, J.P. Vary, A.M. Shirokov, Phys. Rev. C 79, 014308 (2009)

Helium-4 & carbon-12 gs energies



T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary

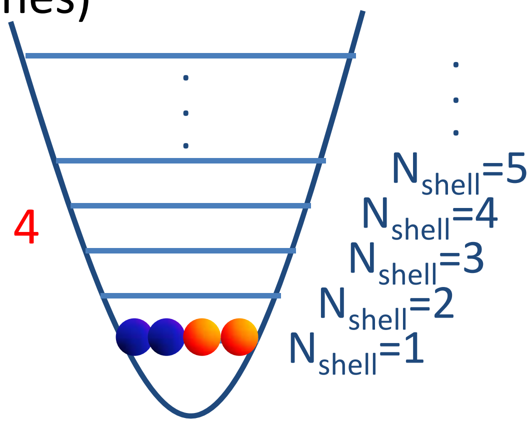
Energies of Light Nuclei



MCSM & FCI results are consistent within the size of lines

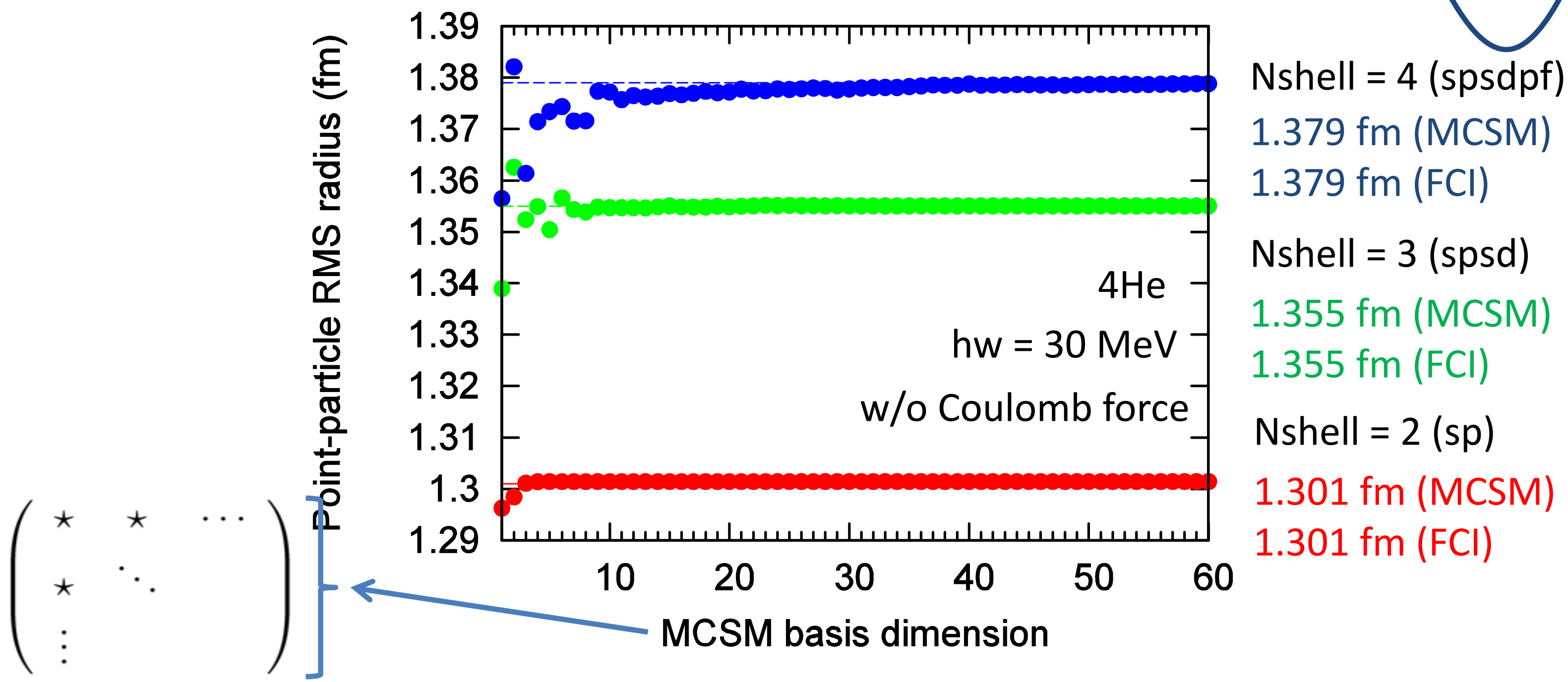
Convergence pattern of the 4He point-particle RMS radius w.r.t. MCSM basis dimension

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



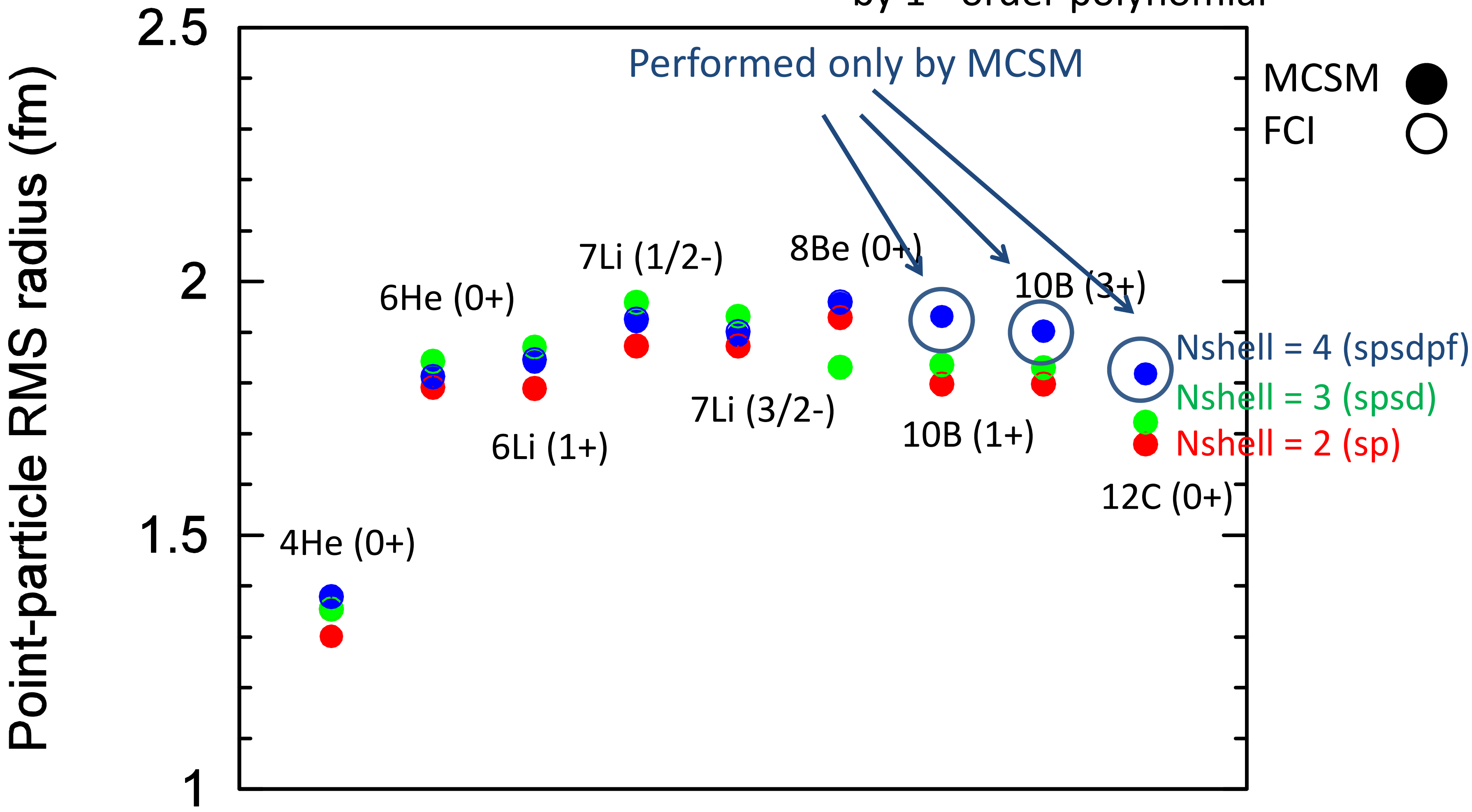
Good agreement w/ FCI within 0.001 fm up to Nshell = 4

H = Hint + β Hcm, (β = 0)



Point-particle RMS matter Radius

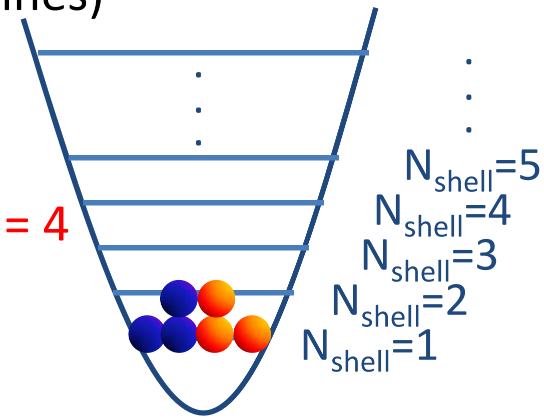
w/ energy-variance extrapolation by 1st-order polynomial



MCSM & FCI results are consistent within the size of symbols

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

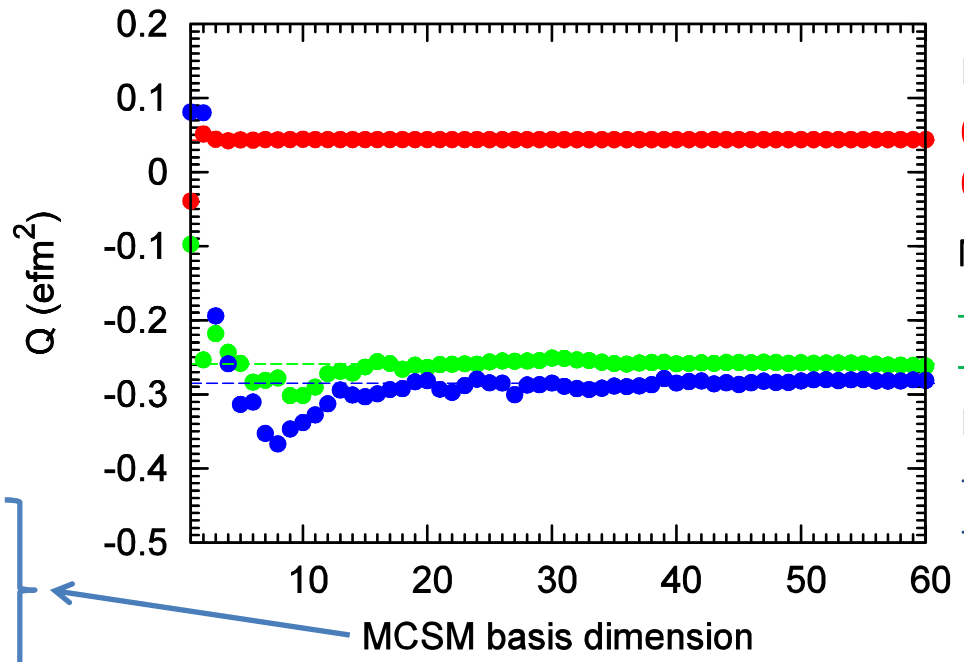
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines) @ Nshell = 2 (sp), 3 (spsd), & 4 (spsdpf)



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

H = Hint + β Hcm, (β = 0)

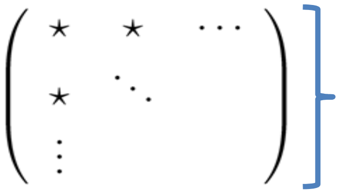
w/o Coulomb force



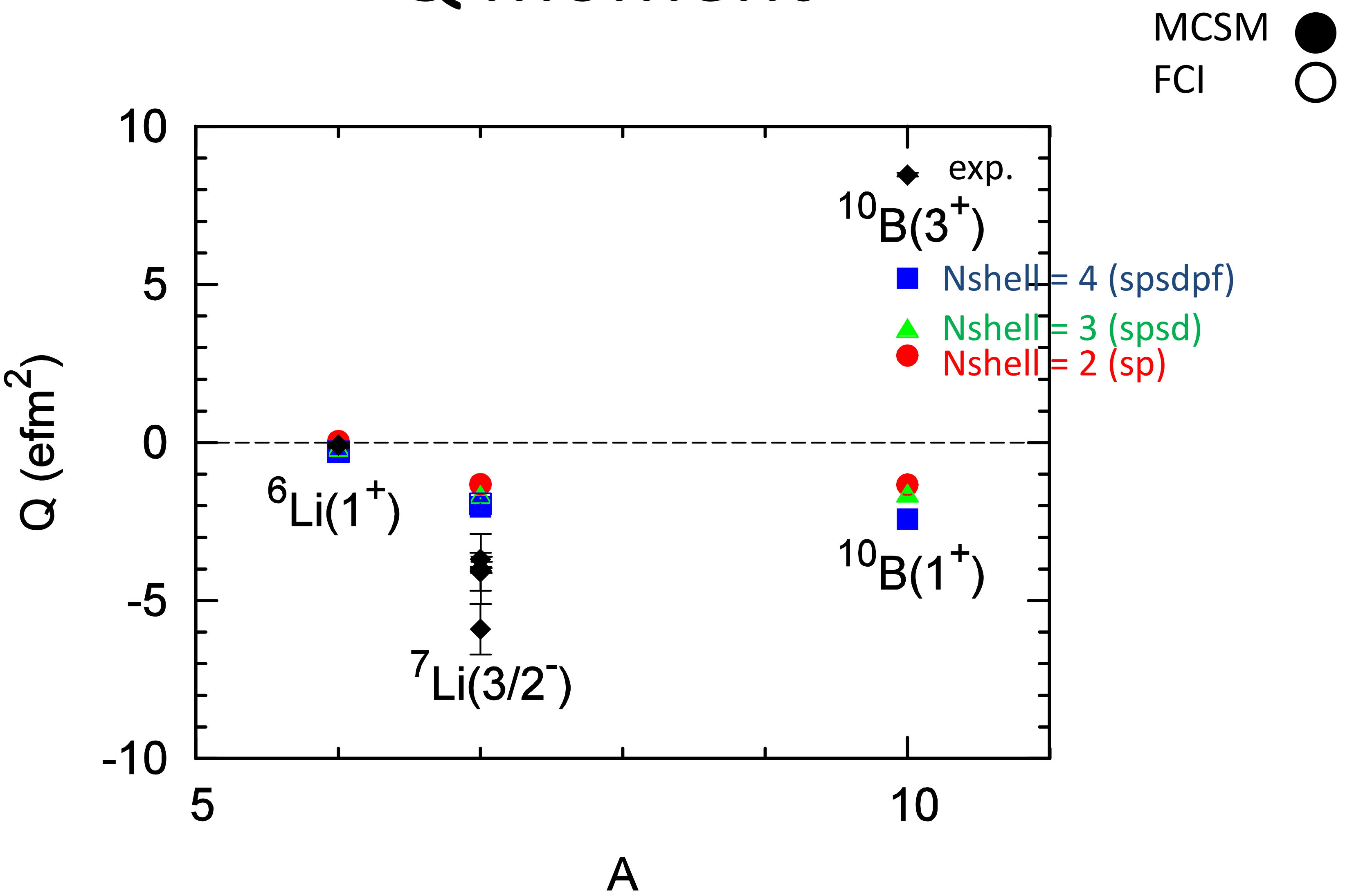
N_{shell} = 2 (s,p)
0.044 efm^2 (MCSM)
0.043 efm^2 (FCI)

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)



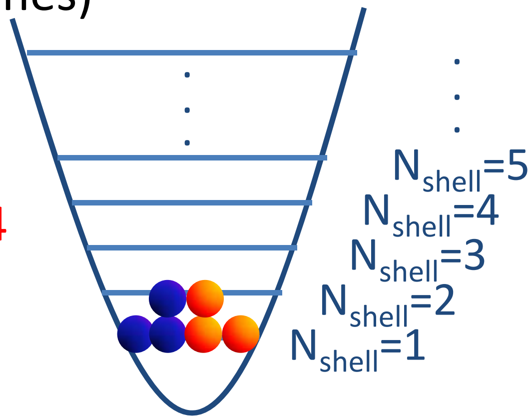
Q moment



MCSM & FCI results are consistent within the size of symbols

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

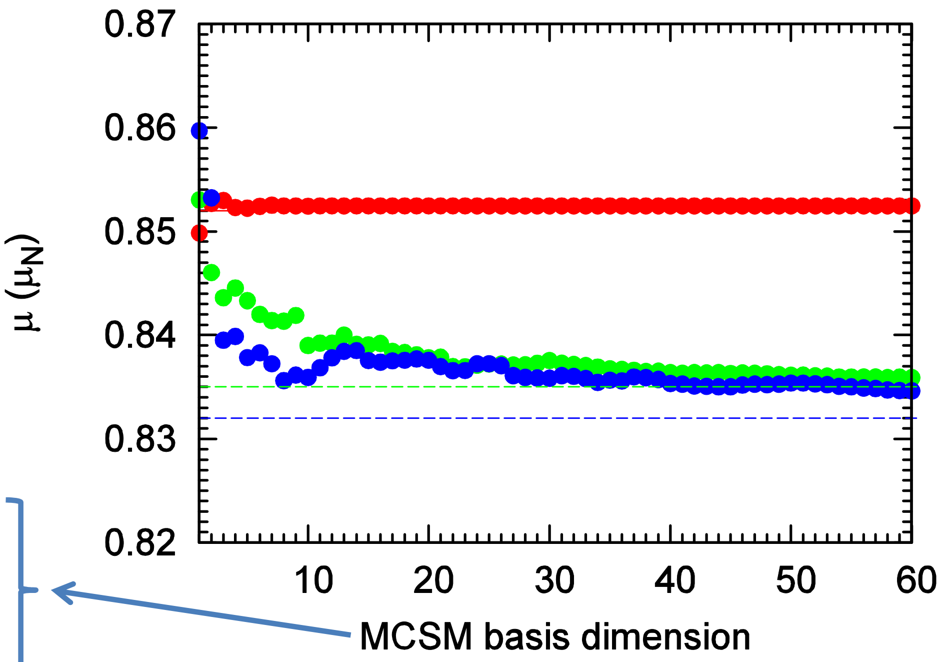
- Comparison of MCSM (solid symbols) w/ FCI (dashed lines)
  @ Nshell = 2 (s,p), 3 (s,p,sd), & 4 (s,p,sd,pf)

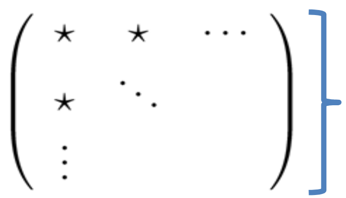


Good agreement w/ FCI within 0.01 μ_N up to Nshell = 4

H = Hint + β Hcm, (β = 0)

w/o Coulomb force



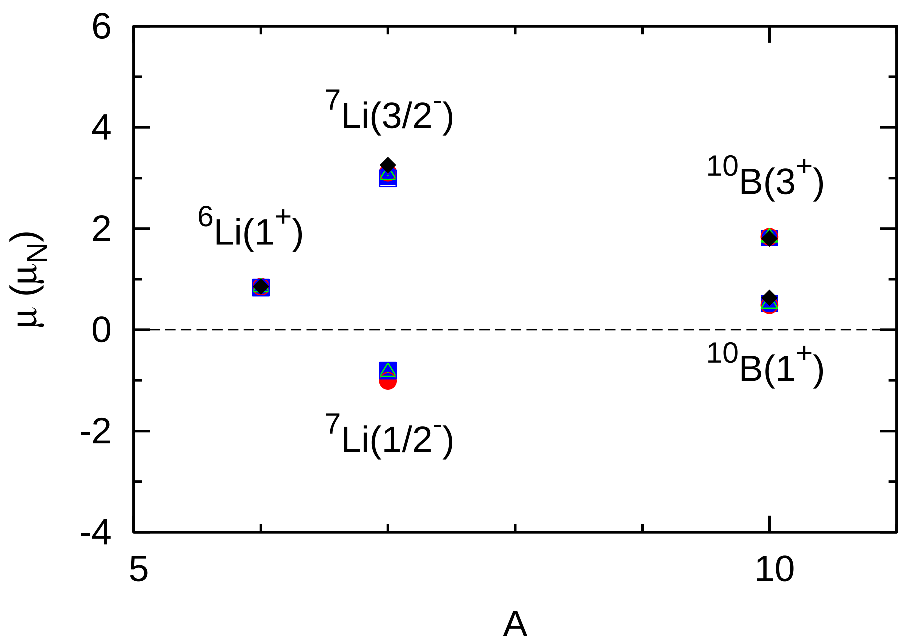


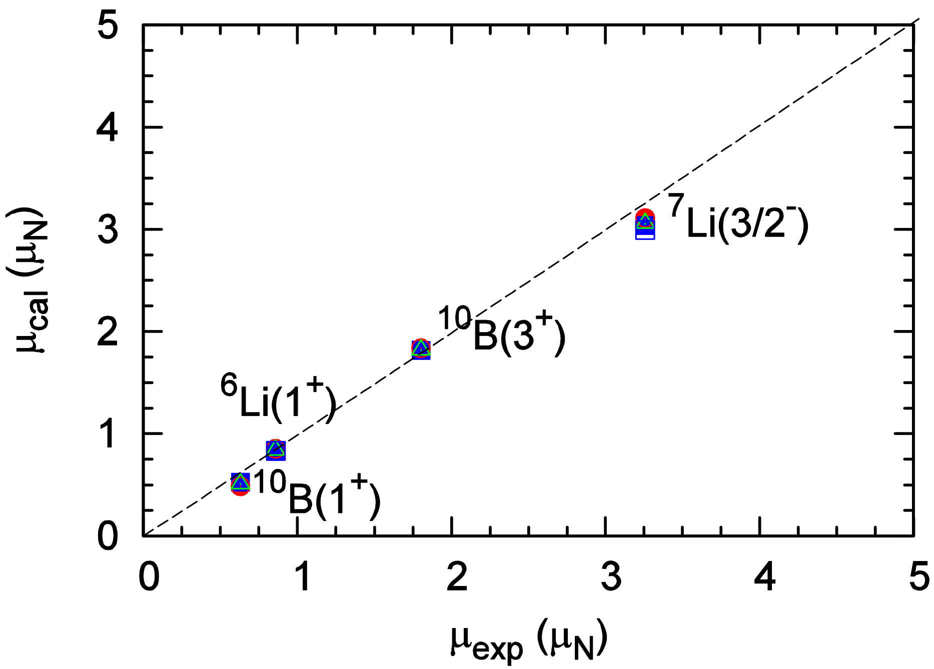
Nshell = 2 (sp)
0.852 μN (MCSM)
0.852 μN (FCI)

Nshell = 3 (spsd)
-0.836 μN (MCSM)
-0.833 μN (FCI)

Nshell = 4 (spsdpf)
-0.835 μN (MCSM)
-0.832 μN (FCI)

μ moment





MCSM & FCI results are consistent with each other, and μ moments are well-reproduced even at small Nshell.

Summary

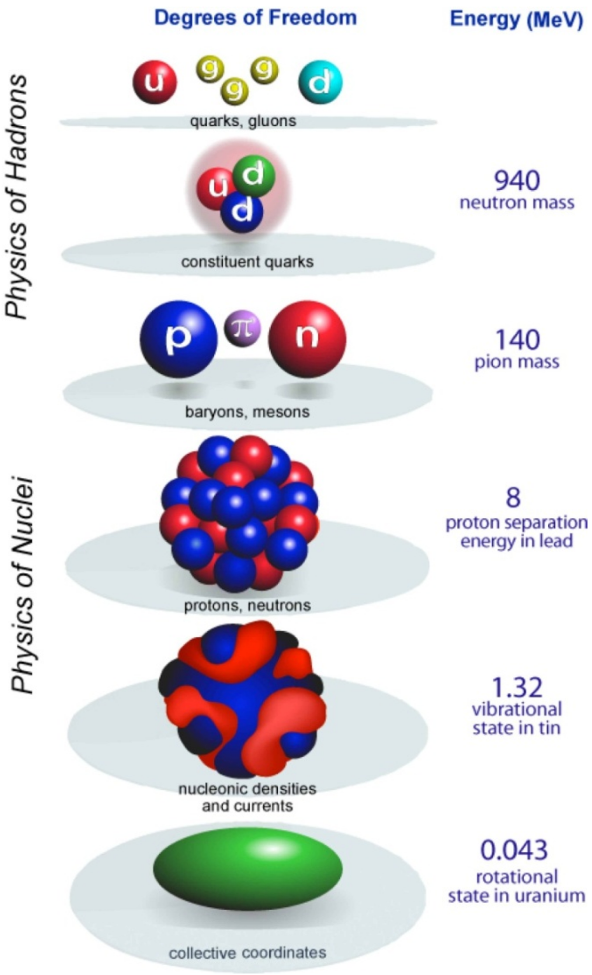
- MCSM can be applied to the no-core calculations & the benchmarks for the p-shell nuclei have been performed.
  - MCSM & FCI results are consistent with each other.

Outlook

- Larger model spaces
- Inclusion of the 3-body force in the MCSM algorithm
- Coupling to the continuum states
- Search for the cluster states

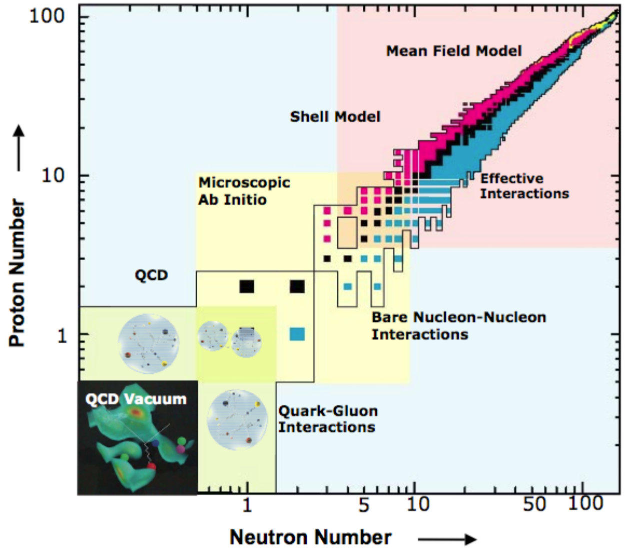
- Tuning of the MCSM code on the K Computer

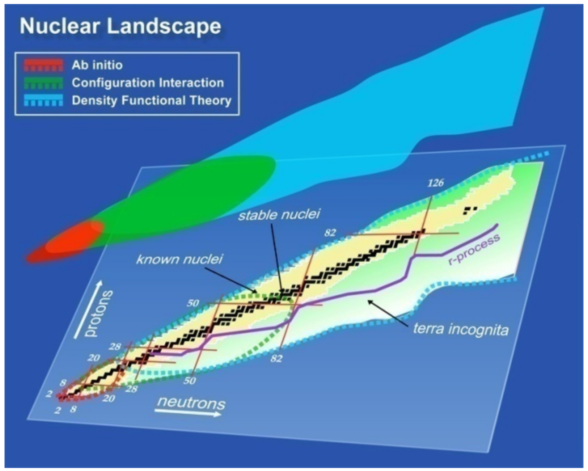
Bridging the nuclear physics scales



QCD

Nuclear Structure

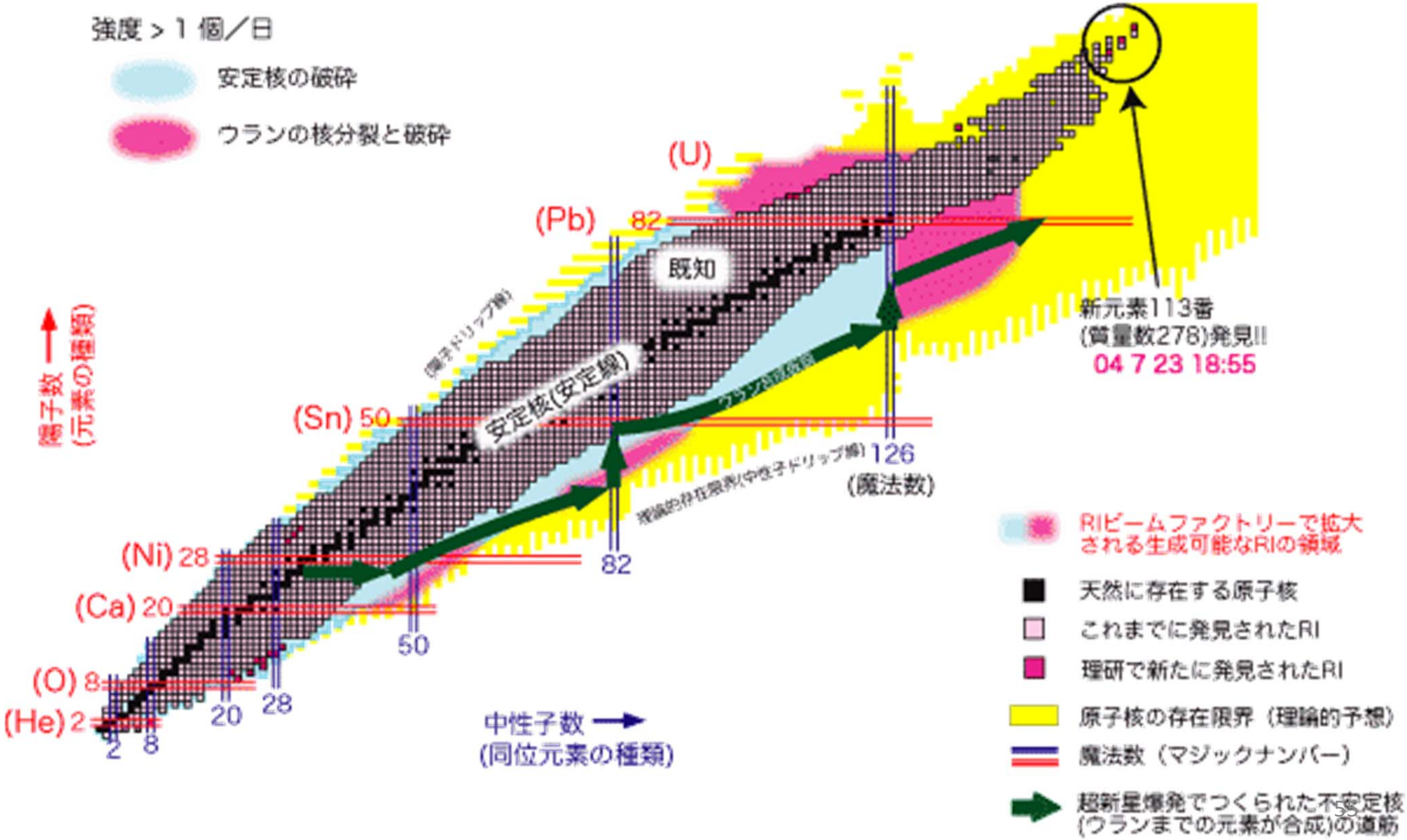




Applications in astrophysics, defense, energy, and medicine

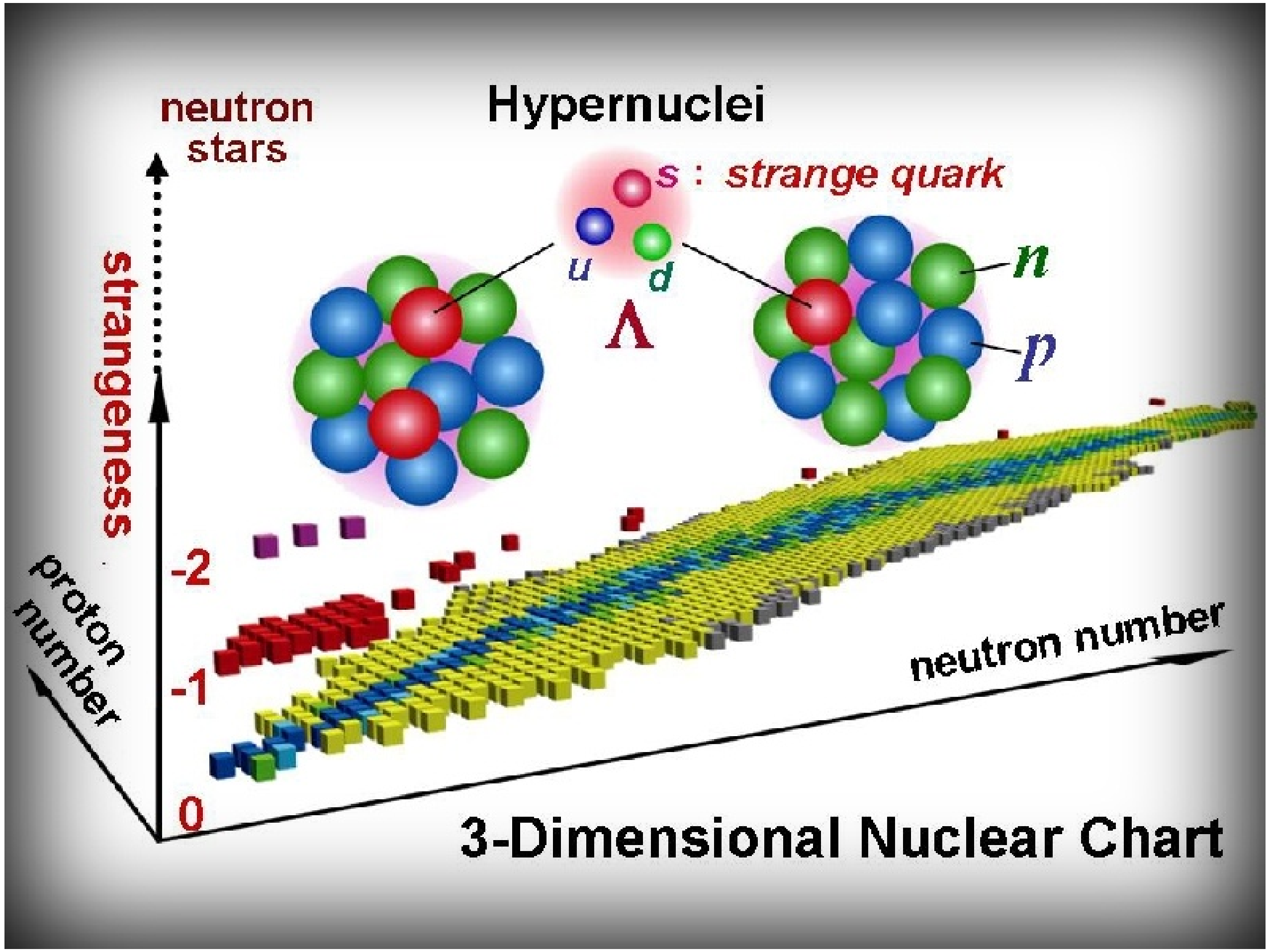
Adapted from D. Dean, JUSTIPEN Meeting, 2009 http://www.rarf.riken.go.jp/pub/newcontents/contents/sisetu/RIBF.html

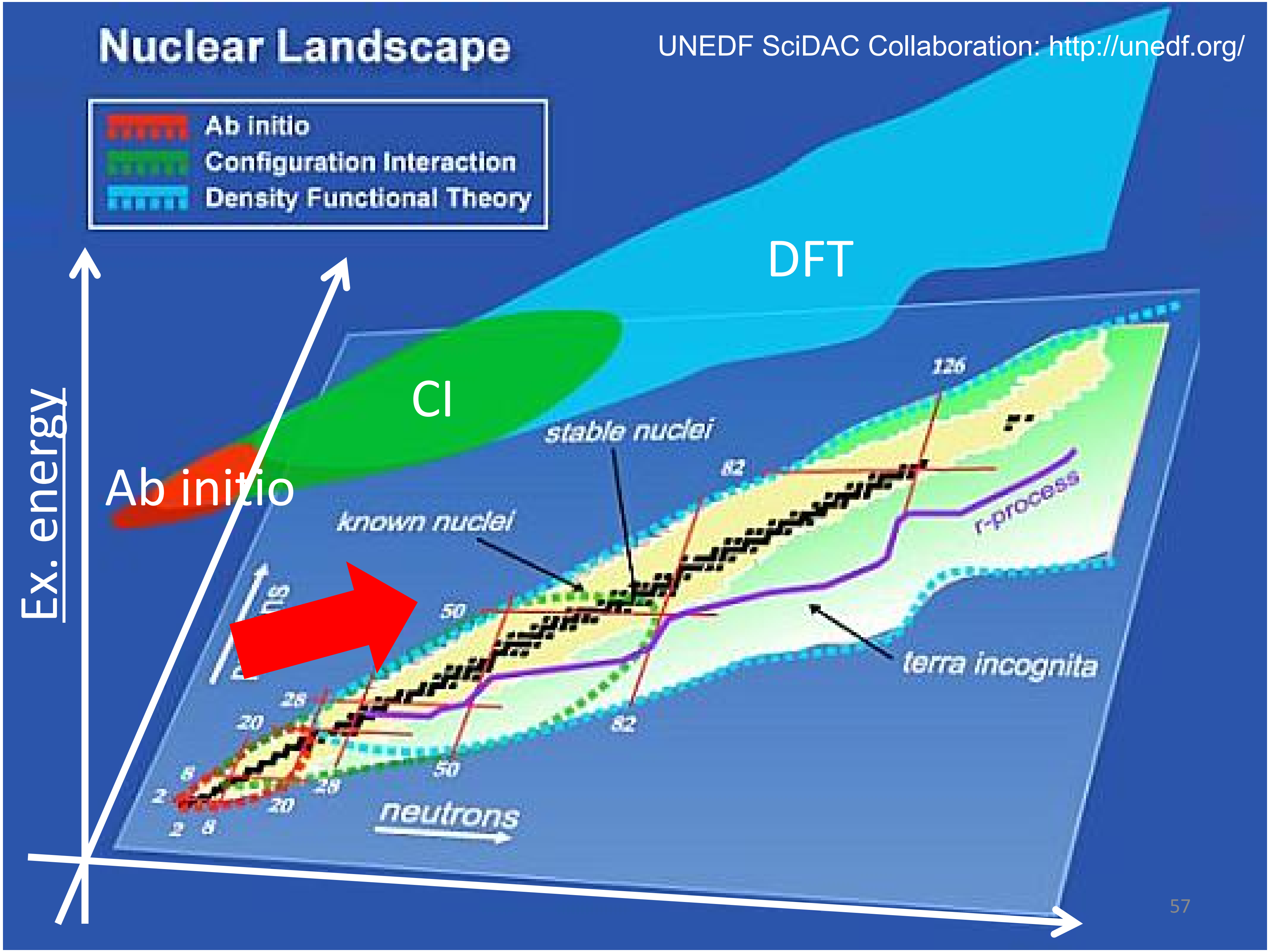
Table of Nuclides (Nuclear Chart)



http://www.sci.tohoku.ac.jp/mediaoffce_s/_src/sc911/3Dchart.jpg

3D Nuclear Chart




Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
DFT
CI
Ab initio
Ex. energy
stable nuclei
known nuclei
r-process
terra incognita
126
82
50
28
20
8
2
82
50
28
20
8
2
neutrons

END