From Few-Nucleon Forces to Many-Nucleon Structure
ECT*/HIC for FAIR Workshop

Monte Carlo shell model towards ab initio nuclear structure

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THE UNIVERSITY OF TOKYO

ECT*, Italy

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Collaborators

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  - Noritaka Shimizu (CNS)
  - Tooru Yoshida (CNS)
- JAEA
  - Yutaka Utsuno
- Iowa State U
  - James P. Vary
  - Pieter Maris

Outline

- Motivation
- Monte Carlo Shell Model (MCSM)
- Benchmark in the p-shell nuclei
- Density plots from MCSM wave functions
- Summary & perspective

Ab inito approaches

- Major challenge of nuclear physics

  - Understand the nuclear structure from *ab-initio* calculations in non-relativistic quantum many-body system w/ realistic nuclear forces (potentials)

  - *ab-initio* approaches: GFMC, NCSM (A ~ 12-14), CC (sub-shell closure +/- 1,2), Green's Function theory, IM-SRG, Lattice EFT, …

→ demand for extensive computational resources

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

- IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navratil (TRIUMF), …
- SA-NCSM: T. Dytrych, J.P. Draayer (Louisiana State U), …
- No-Core Monte Carlo Shell Model (MCSM) <- this talk

Shell model (Configuration Interaction, CI)

- Eigenvalue problem of large sparse Hamiltonian matirx

$$H|\Psi\rangle = E|\Psi\rangle$$

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} E_1 & & & 0 \\ & E_2 & & \\ & & E_3 & \\ & & & \ddots \\ 0 & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots \end{pmatrix}$$

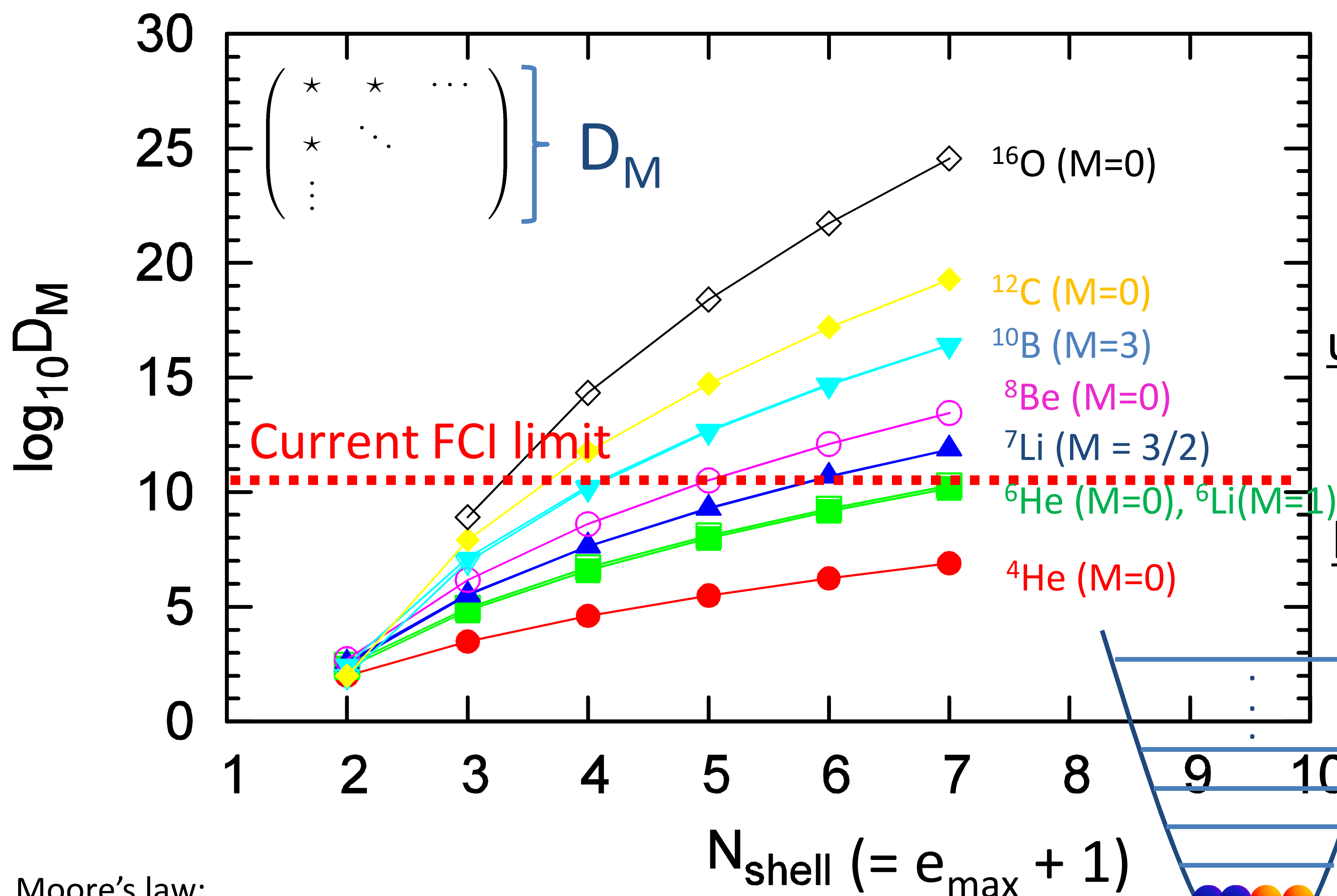
Large sparse matrix (in M-scheme)

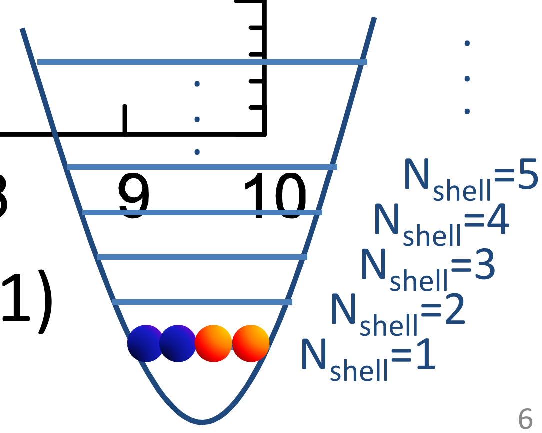
$$\sim \mathcal{O}(10^{10})$$

non-zero MEs $\sim \mathcal{O}(10^{13-14})$

$$\begin{cases} |\Psi_1\rangle = a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle = a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle = \cdots \\ \vdots \end{cases}$$

M-scheme dimension in N_{shell} truncation



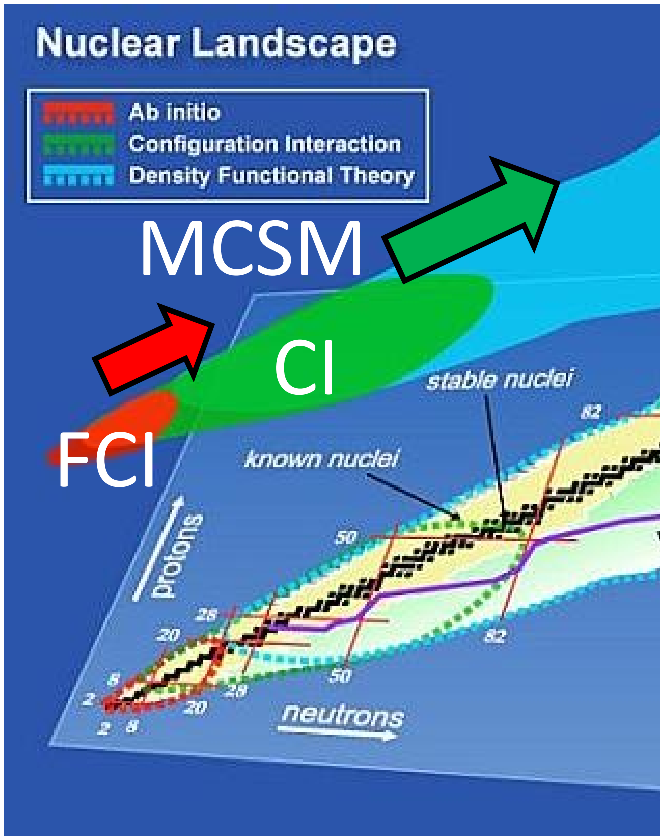


Moore's law:
#transistors doubles every two years. (p = $2^{n/2}$)
x 5.7 after 5 yrs, x 32 after 10 yrs

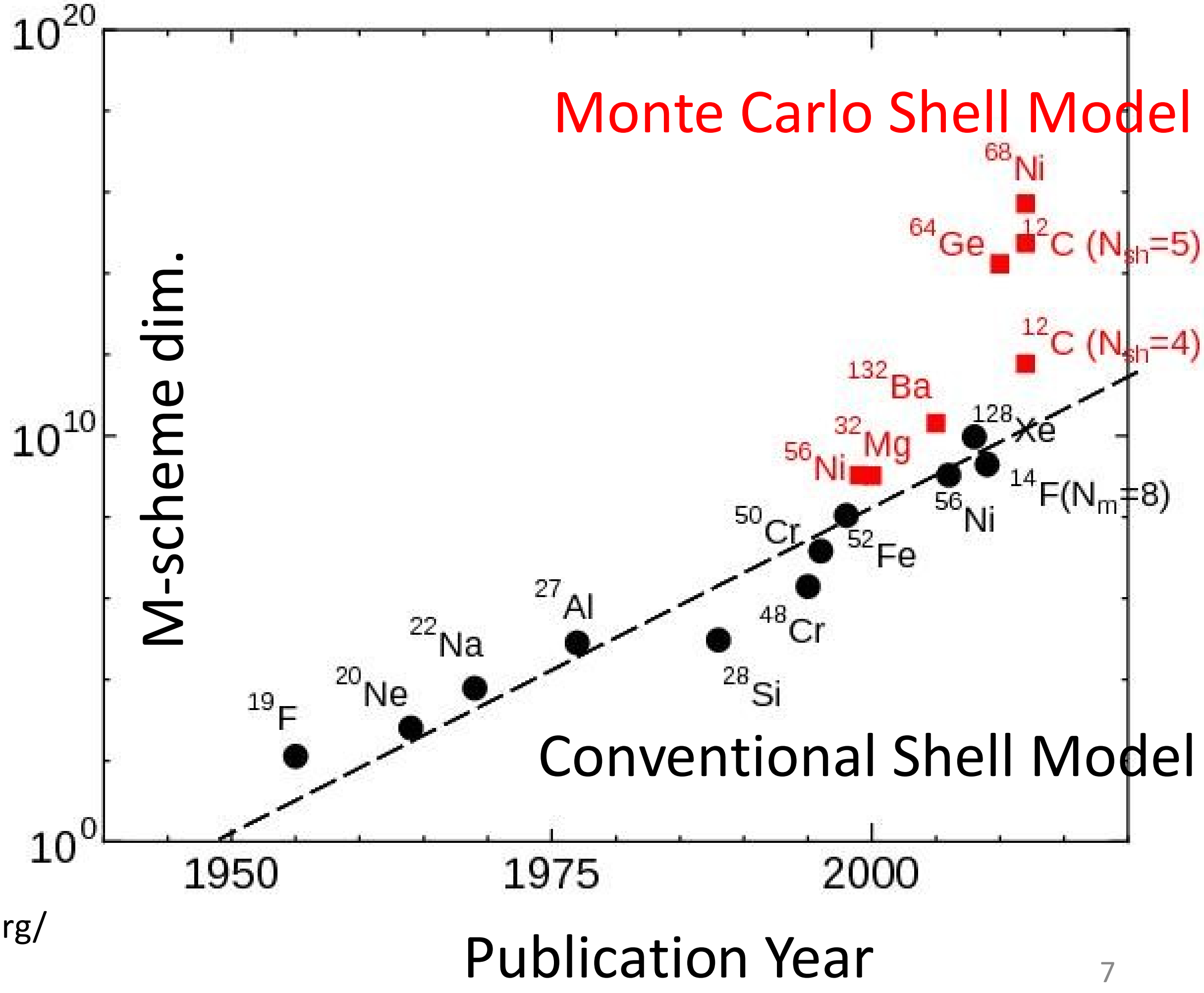
Advantage of the MCSM

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

- MCSM w/ an assumed inert core is one of the powerful shell model algorithms.



UNEDF SciDAC Collaboration: http://unedf.org/



Monte Carlo shell model (MCSM)

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

- Importance truncation

Standard shell model

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

Diagonalization

All Slater determinants

$D_M \sim O(10^{10})$

Monte Carlo shell model

$$H \sim \begin{pmatrix} \star & \star & \cdots \\ \star & \ddots & \\ \vdots & & \end{pmatrix} \Rightarrow \begin{pmatrix} E'_0 & & 0 \\ & E'_1 & \\ 0 & & \ddots \end{pmatrix}$$

Diagonalization

Important bases stochastically selected

$D_{MCSM} \sim O(100)$

$$|\Psi(J,M,\pi)\rangle = \sum_{i=1}^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle$$

$$|\Phi(J,M,\pi)\rangle = \sum_{K=-J}^{J} g_K P^J_{MK} P^\pi |\phi\rangle$$

Diagonalization

$$|\phi\rangle = \prod_i^A a_i^\dagger |-\rangle$$

Energy variation

$$a_i^\dagger = \sum_\alpha^{N_{sps}} c_\alpha^\dagger D_{\alpha i}$$

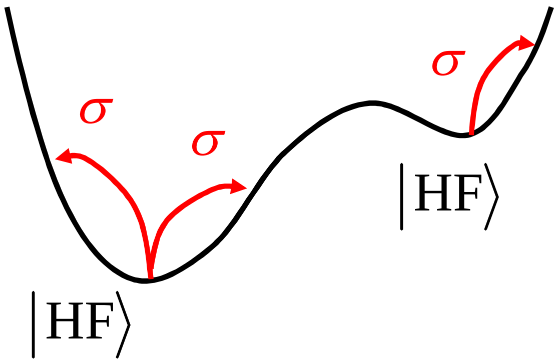
Stochastic sampling of basis functions

- 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)

- Stochastic sampling of deformed SDs



$$|\phi(\sigma)\rangle = e^{-h(\sigma)}|\phi\rangle$$

$$h(\sigma) = h_{HF} + \sum_i^{N_{AF}} s_i V_i \sigma_i O_i$$

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

$$|\phi(\sigma)\rangle = \prod_{N_\tau} e^{-\Delta\beta h(\sigma)}|\phi\rangle$$

$$h(\sigma) = \sum_i^{N_{AF}} (\epsilon_i + s_i V_i \sigma_i) O_i$$

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

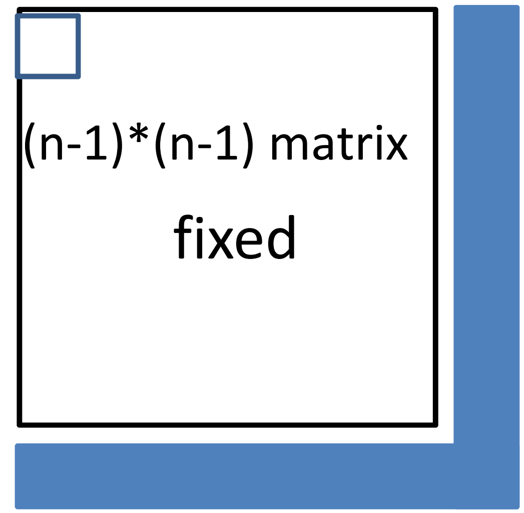
$$H = \sum_i \epsilon_i O_i + \frac{1}{2}\sum_i V_i O_i^2$$

Rough image of search steps

- Basis search
  - HF solution is taken as the 1st basis
  - 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

Hamiltonian kernel

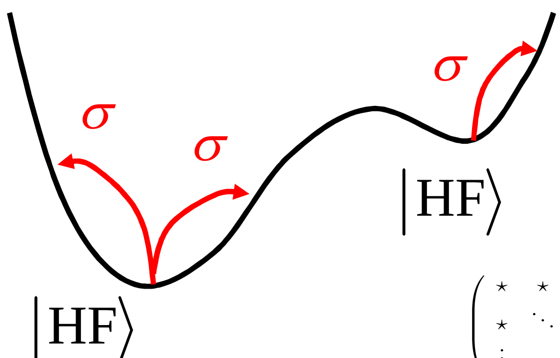
$H(\Phi,\Phi')=$

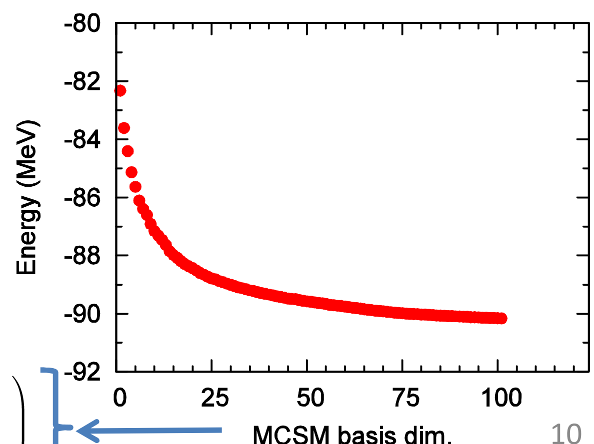


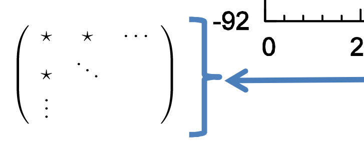
n-th
(to be optimized)

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

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







Feasibility study of MCSM for no-core calculations

PHYSICAL REVIEW C **86**, 014302 (2012)

No-core Monte Carlo shell-model calculation for ^{10}Be and ^{12}Be low-lying spectra

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(Received 24 April 2011; revised manuscript received 1 June 2012; published 3 July 2012)

Recent developments in the MCSM

- Energy minimization by the CG method
  - N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda & T. Otsuka, Phys. Rev. C85, 054301 (2012)

    ~ 30% reduction of # basis
- Efficient computation of TBMEs
  - Y. Utsuno, N. Shimizu, T. Otsuka & T. Abe, Compt. Phys. Comm. 184, 102 (2013)

    ~ 80% of the peack performance

    (~ 10-20% in the old MCSM)
- Energy variance extrapolation
  - N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe & M. Honma, Phys. Rev. C82, 061305 (2010)

    Evaluation of exact eignvalue w/ error estimate
- Summary of recent MCSM developments
  - N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Prog. Theor. Exp. Phys. 01A205 (2012)

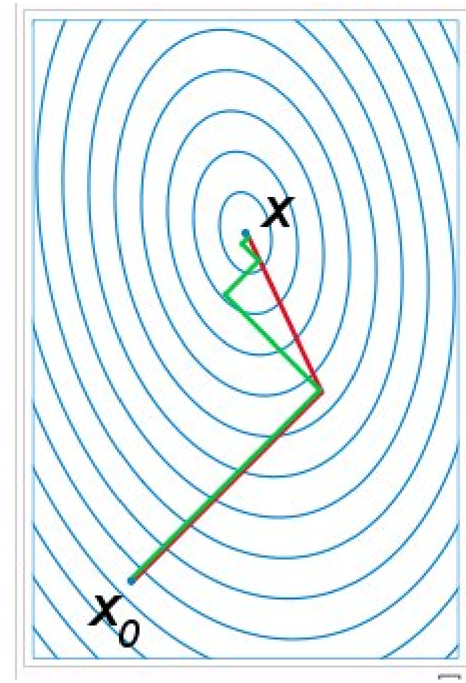
Energy minimization by Conjugate Gradient method

N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y.Tsunoda, T. Otsuka, Phys . Rev. C85, 054301 (2012)

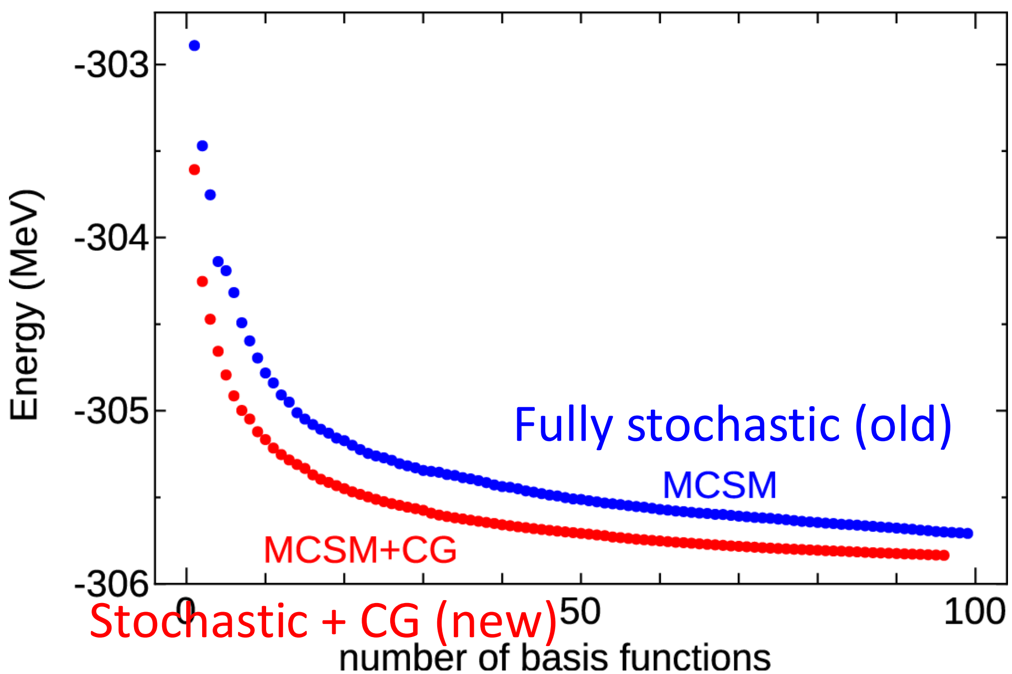
$$\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} f_n \sum_{K=-J}^{J} g_K P_{MK}^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$$

$$E(D) = \left\langle \Psi(D) \middle| H \middle| \Psi(D) \right\rangle$$

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



Minimize E(D) as a function of D by CG method



Few Determinant Approximation
M. Honma, B.A.Brown, T. Mizusaki, and T. Otsuka
Nucl. Phys. A 704, 134c (2002)

Hybrid Multi-Determinant
G. Puddu, Acta Phys. Polon. B42, 1287 (2011)

VAMPIR
K.W. Schmid, F. Glummer, M. Kyotoku, and A. Faessler
Nucl. Phys. A 452, 493 (1986)

Reduction of the # of basis states roughly 30%

Efficient computation of the TBMEs

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Compt. Phys. Comm. 184, 102 (2013)

- 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)

- Utilization of the symmetry

$$j_z(i)+j_z(j) = j_z(k)+j_z(l) \rightarrow j_z(i)-j_z(k) = -(j_z(j)-j_z(l)) \equiv \Delta m$$

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

$\bar{v}_{ijkl} \rightarrow \tilde{v}_{ab}$ $\qquad \rho_{ki} \rightarrow \tilde{\rho}_a \qquad \rho_{lj} \rightarrow \tilde{\rho}_b$

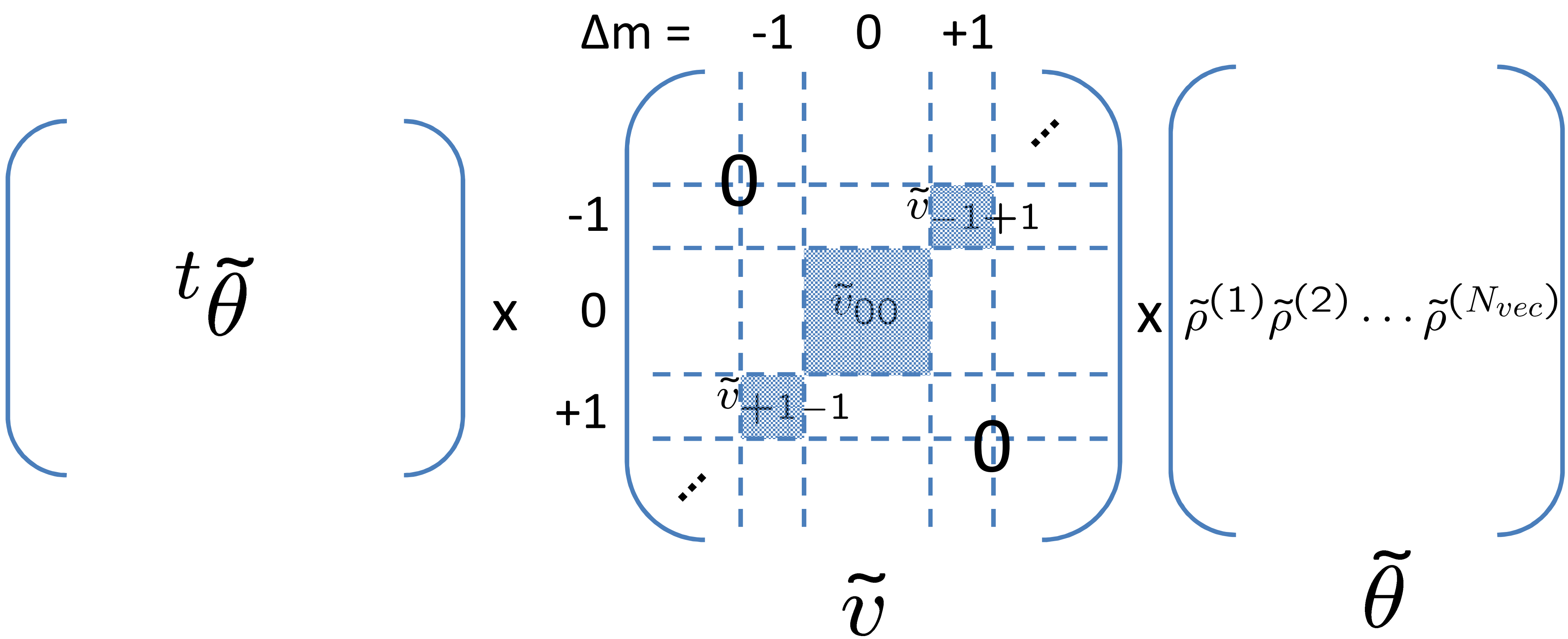
sparse dense

Schematic illustration of the computation of TBMEs

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Compt. Phys. Comm. 184, 102 (2013)

- Matrix-matrix method

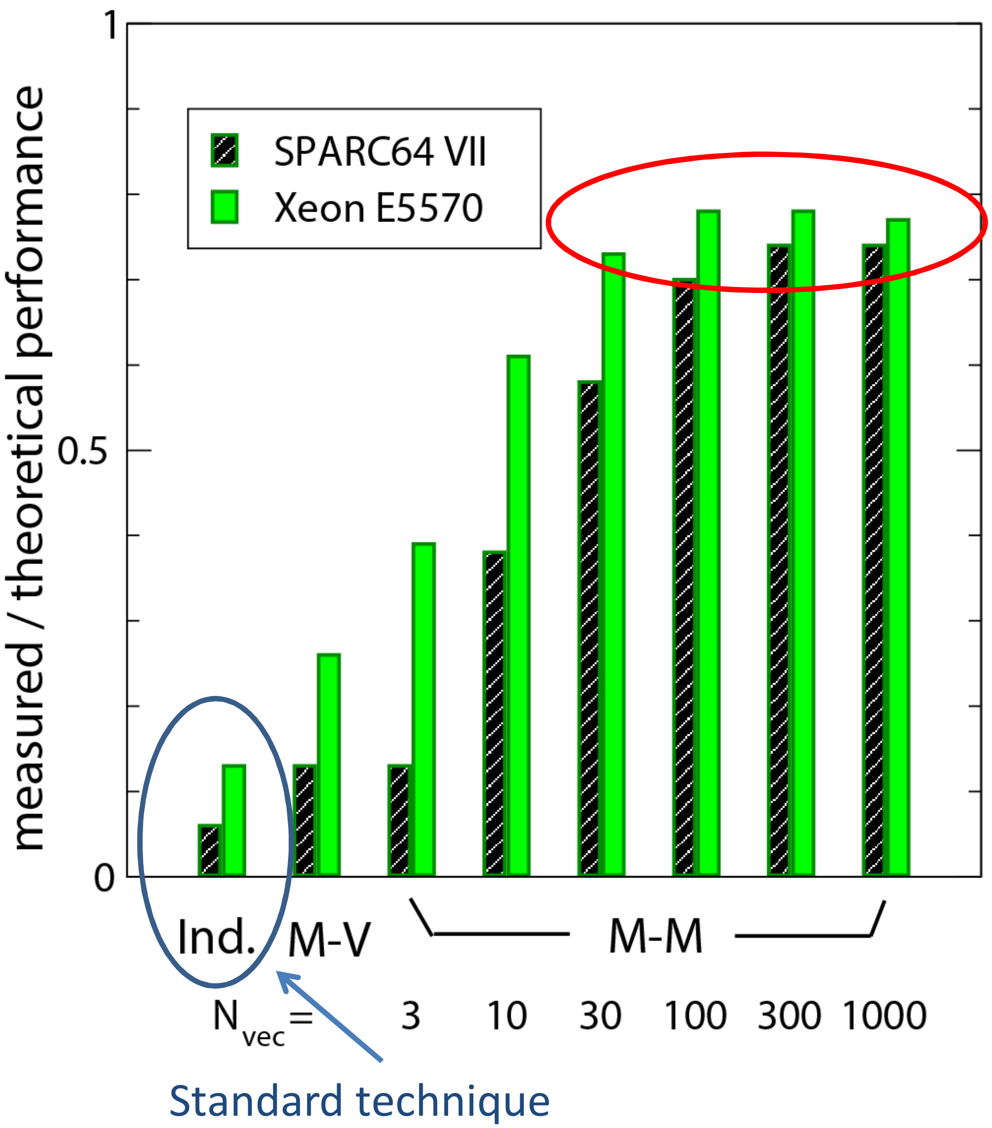
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m} \tilde{\rho}_a \left(\sum_{b\in J_z(b)=\Delta m} \tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



→ BLAS Level 3

Tuning of the density matrix product

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Compt. Phys. Comm. 184, 102 (2013)



Nshell = 5

The performance reaches 80% of the theoretical peak at hot spot.

SPARC64 requires large N_{bunch} in comparison to Xeon

Matrix product e.g.
(390 x 390) x (390 x $2N_{bunch}$)

N_{bunch} controllable tuning parameter
chunk size

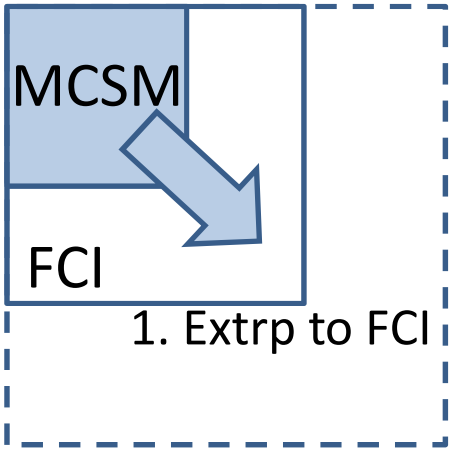
Extrapolations in the MCSM

- Two steps of the extrapolation

1. Extrapolation of our MCSM (approx.) results to the FCI (exact) results in fixed model space

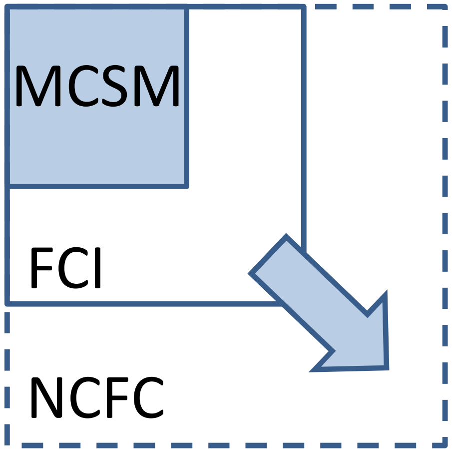
Energy-variance extrapolation

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



2. Extrapolation into the infinite model space
   - Exponential fit w.r.t. Nmax in the NCFC
   - UV/IR cutoff in the NCSM

   Not applied in the MCSM, so far…



2. Extrp to inf. basis dim

Energy-variance extrapolation

- Originally proposed in condensed matter physics

  - Path Integral Renormalization Group method

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

- Imported to nuclear physics

  - Lanczos diagonalization with particle-hole truncation

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

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

  - single deformed Slater determinant

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

→ Apply to the MCSM (multi deformed SDs)

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

Numerical effort

8-folded loop
~O(Nsps^8)

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

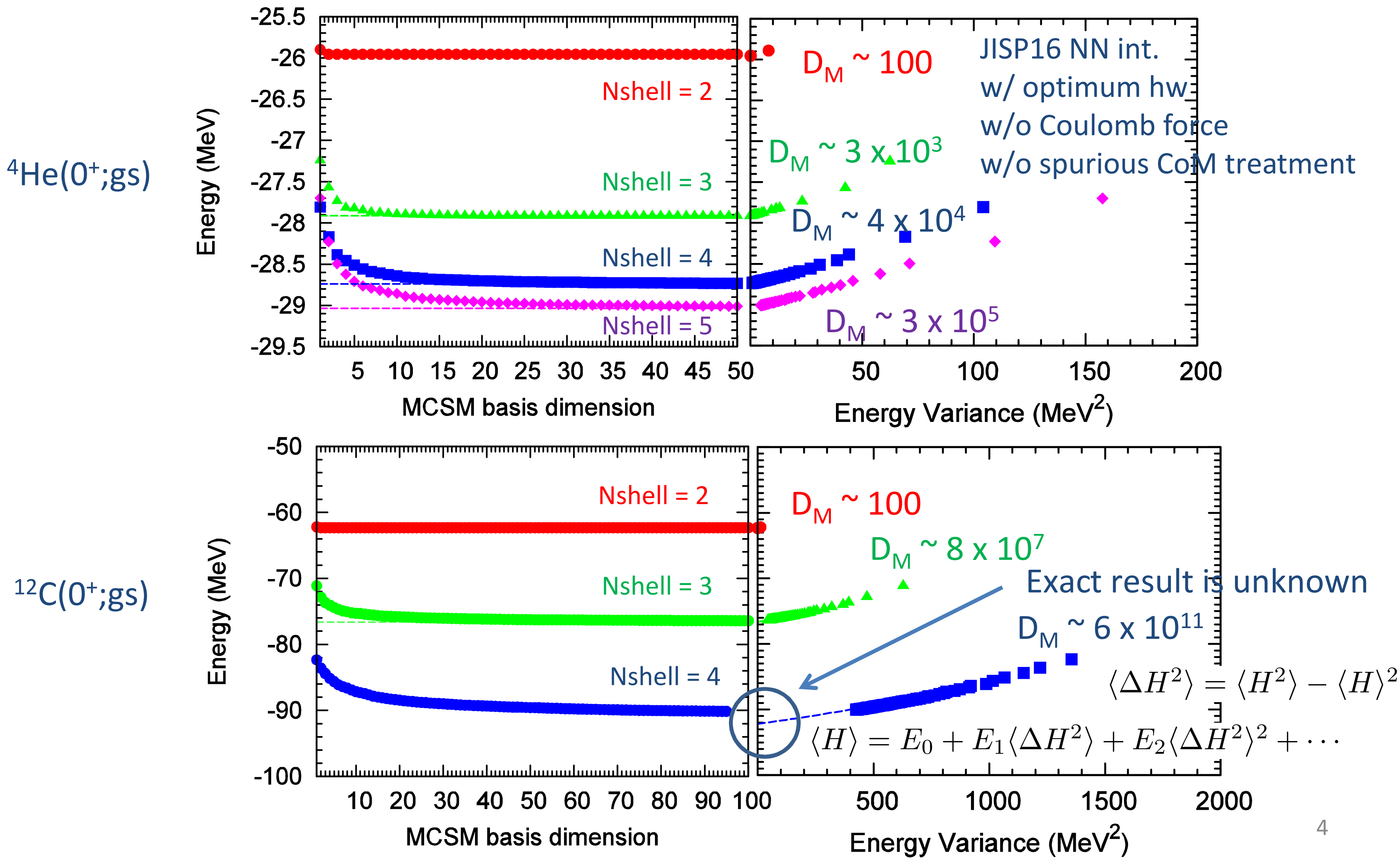
$$= \frac{1}{4}\sum_{ij\alpha\beta}\left(\sum_{kl}\bar{v}_{ijkl}(1-\rho)_{k\alpha}(1-\rho)_{l\beta}\right)\left(\sum_{\gamma\delta}\bar{v}_{\alpha\beta\gamma\delta}\rho_{\gamma i}\rho_{\delta j}\right) + \mathrm{Tr}(\Gamma(1-\rho)\Gamma\rho) + \frac{1}{4}[\mathrm{Tr}(\rho\Gamma)]^2$$

6-folded loop
~O(Nsps^6)

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

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

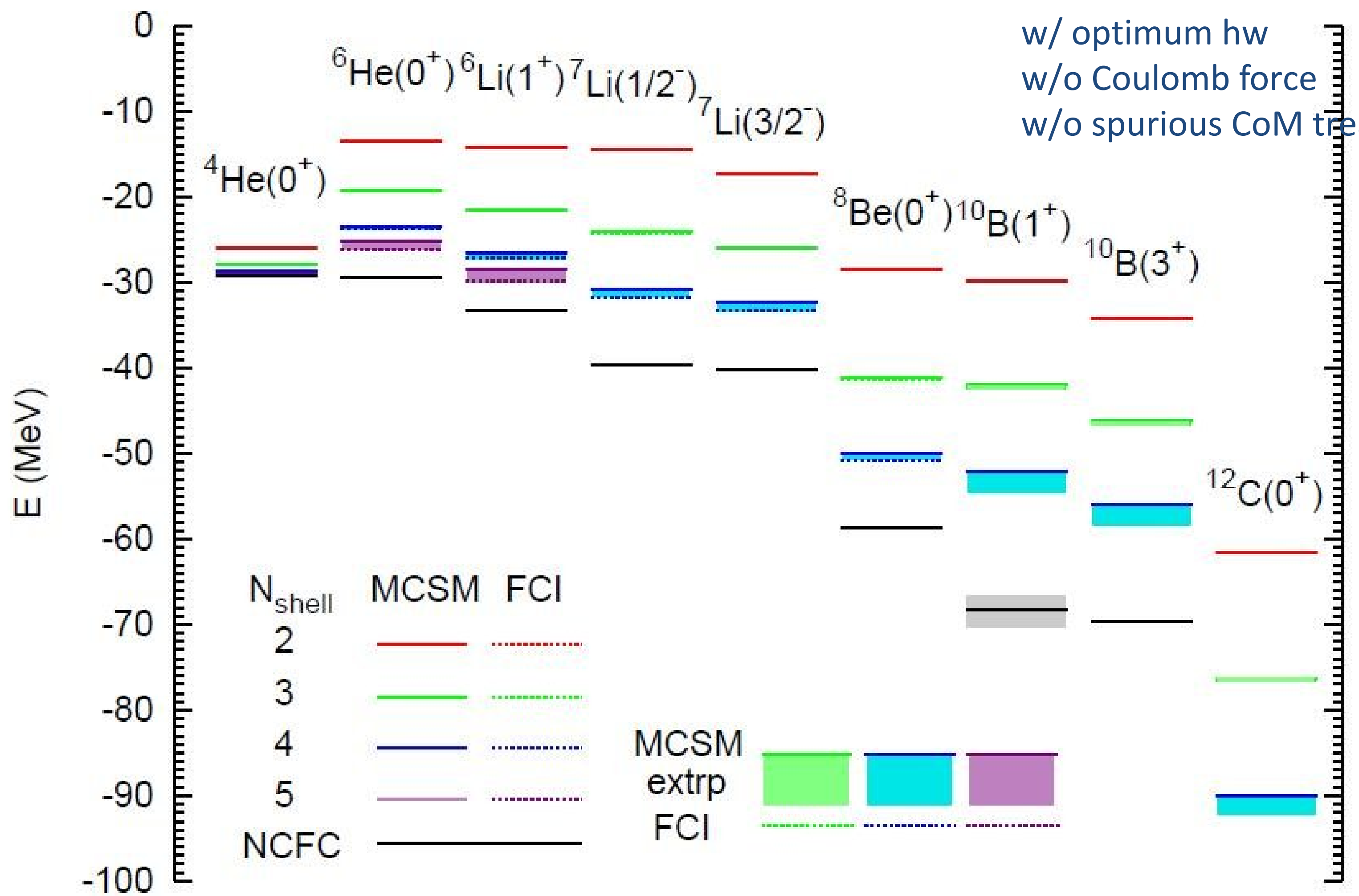
Energies wrt # of basis & energy variance



Energies of the Light Nuclei

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, Phys Rev C86, 054301 (2012)

JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment



MCSM results w/ E-var extrp are consistent w/ FCI results

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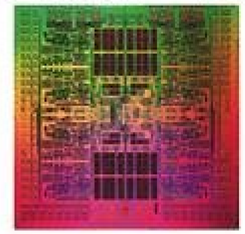
1	TITAN	Cray XK7, Operon 6274 16C 2.2 GHz + Nvidia Kepler GPU, Custom interconnect	DOE/OS/ORNL	USA	560,640	17.6	8.3
2	SEQUOIA	IBM BlueGene/Q, Power BQC 16C 1.60 GHz, Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	16.3	7.9
3	K COMPUTER	Fujitsu SPARC64 VIIIfx 2.0GHz, Custom interconnect	RIKEN AICS	Japan	705,024	10.5	12.7
4	MIRA	IBM BlueGene/Q, Power BQC 16C 1.60 GHz, Custom interconnect	DOE/OS/ANL	USA	786,432	8.16	3.95
5	JuQUEEN	IBM BlueGene/Q, Power BQC 16C 1.60 GHz, Custom interconnect	Forschungszentrum Jülich	Germany	393,216	4.14	1.97

PERFORMANCE DEVELOPMENT

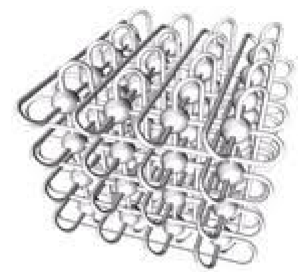
K computer, Japan

SPARC64 TM VIIIfx



128 GFLOPS/CPU
(8 cores/CPU)

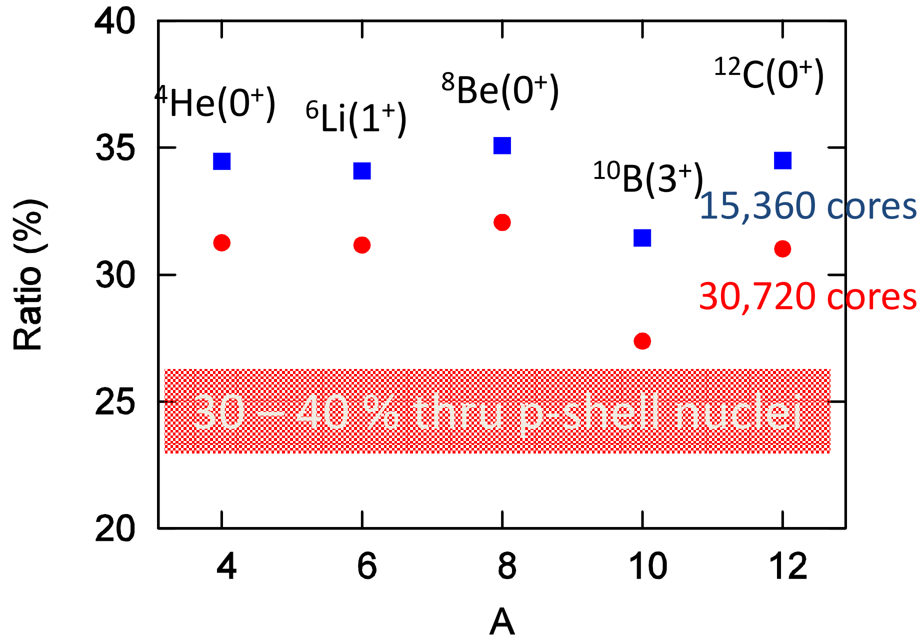
Tofu inter-connection
6D Mesh/Torus



Peak performance & speed-up @ K computer

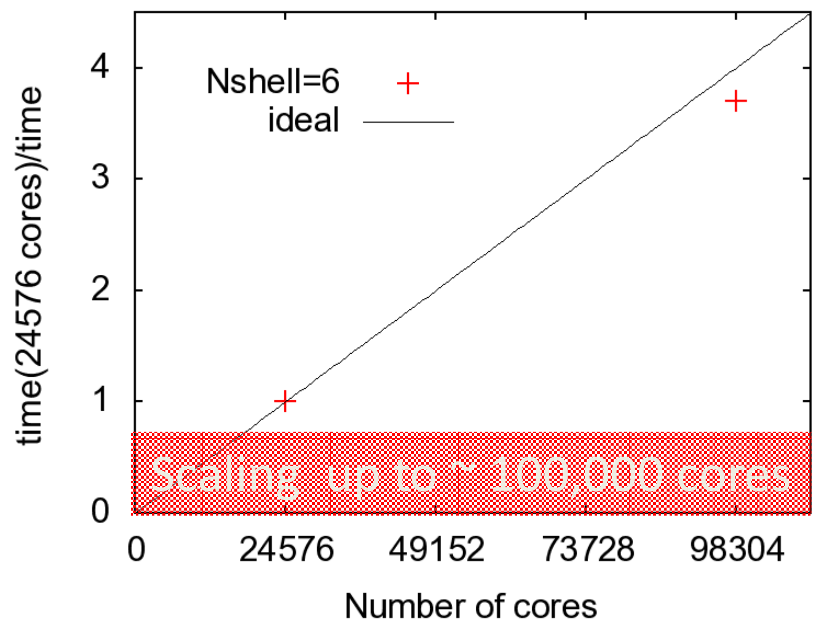
Peak performance

- Optimization of 15th basis dim. of the w.f. in N_{shell}=5 w/ 100 CG iterations (MPI/OpenMP, 8 threads)



Speed-up (strong scaling)

- Optimization of 48th basis dim. of the 4He (0+) w.f. in N_{shell}=6 w/ 100 CG iterations

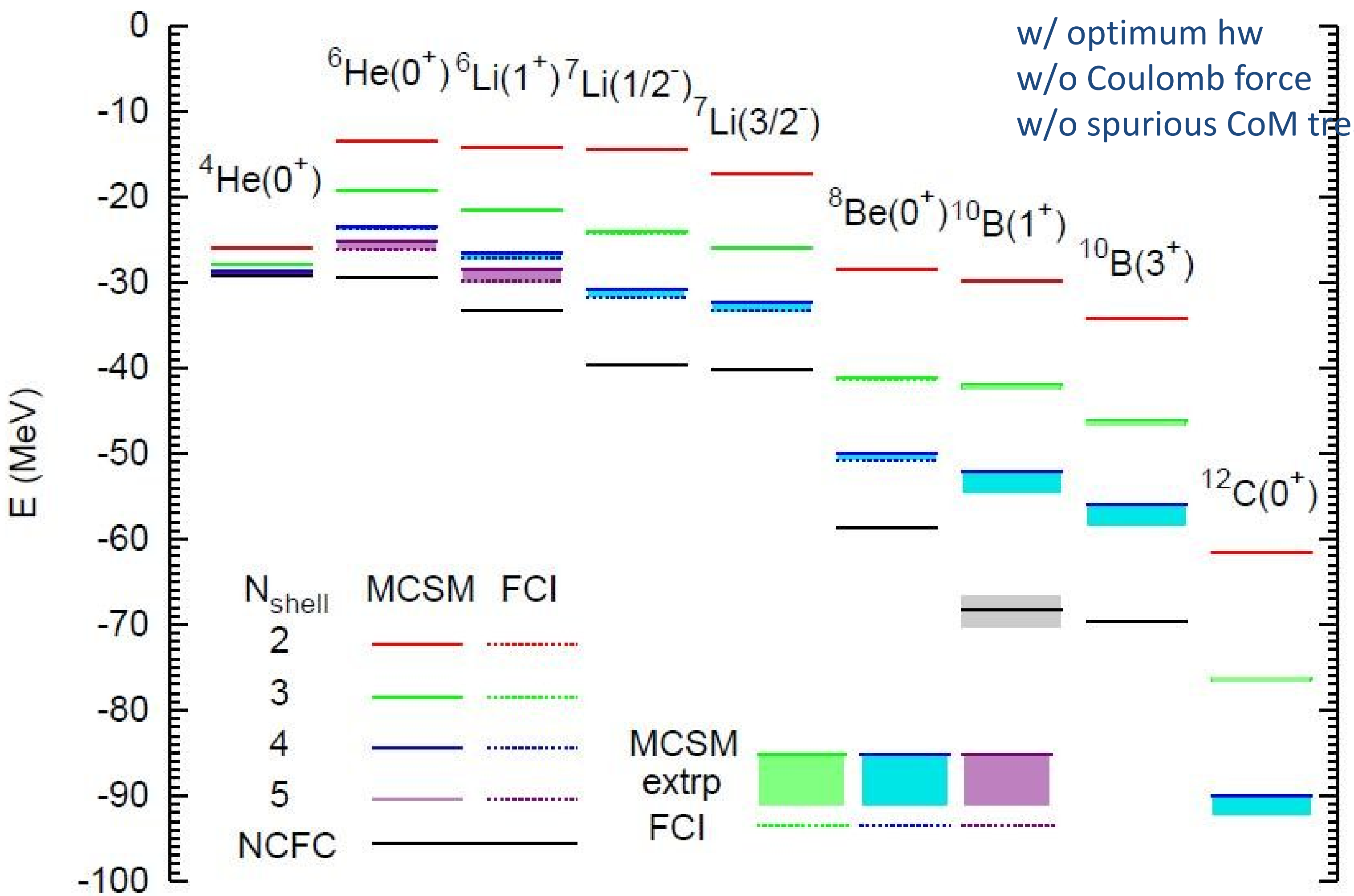


Note: it is a tentative result by early access to the K computer @ AICS, RIKEN.

Energies of the Light Nuclei

T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno, J. P. Vary, Phys Rev C86, 054301 (2012)

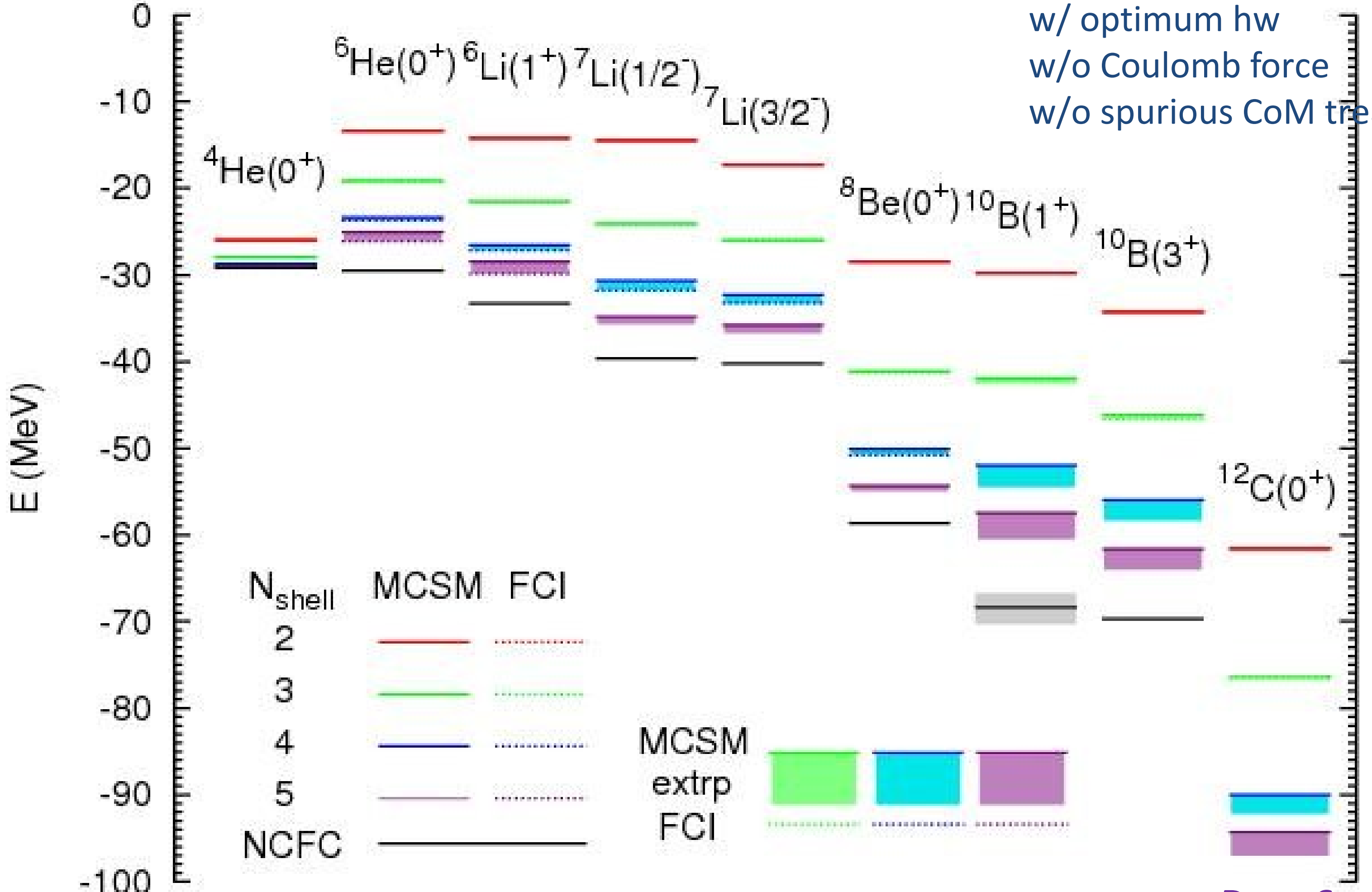
JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment



Energies of the Light Nuclei

Preliminary

JISP16 NN int.
w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment



$D_M \sim 6 \times 10^{14}$

Some MCSM results are not reachable in the current FCI

Density Plots from ab initio calc.

- Green's function Monte Carlo (GFMC)
  - "Intrinsic" density is constructed

    by aligning the moment of inertia among samples

    R. B. Wiringa, S. C. Pieper, J. Carlson, & V. R. Pandharipande, Phys. Rev. C62, 014001 (2000)
- No-core full configuration (NCFC)
  - Translationally-invariant density is obtained

    by deconvoluting the intrinsic & CM w.f.

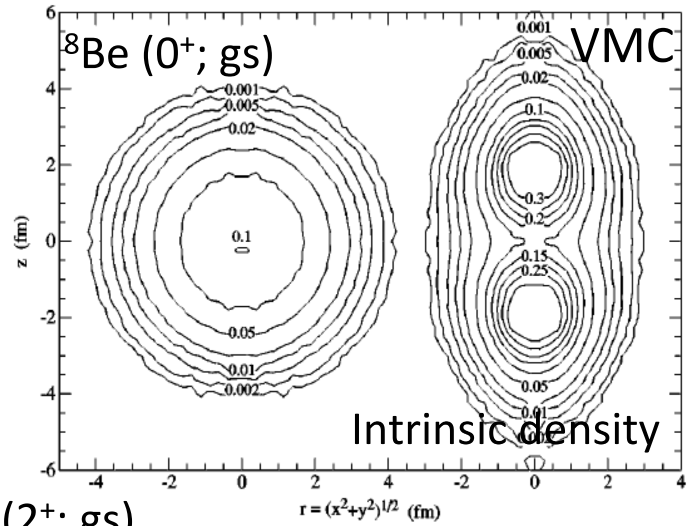
    C. Cockrell J. P. Vary & P. Maris,

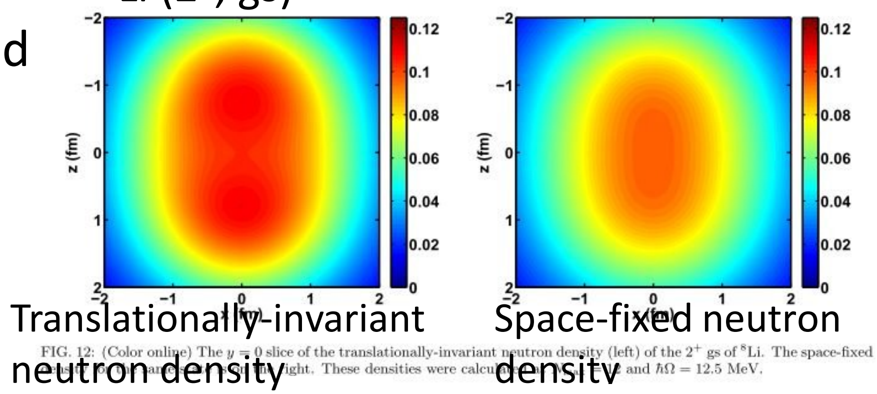
    Phys. Rev. C86, 034325 (2012)
- Lattice EFT
  - Triangle structure in carbon-12

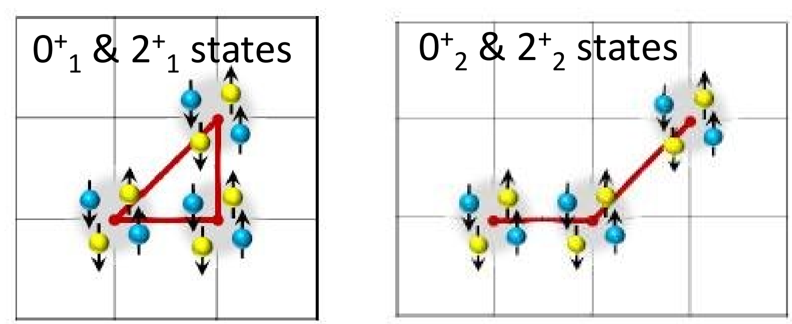
    E. Epelbaum, H. Krebs, T. A. Lahde,

    D. Lee, & U.-G. Meissner,

    Phys. Rev. Lett. 109, 252501 (2012)

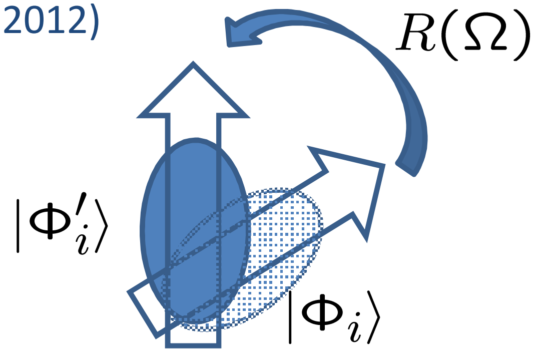






How to construct an “intrinsic” density from MCSM w.f.

N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka,
Progress in Theoretical and Experimental Physics, 01A205 (2012)



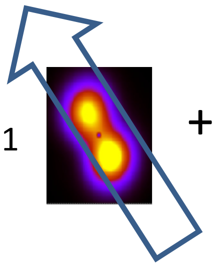
Rotation by diagonalizing Q-moment
(Qzz > Qyy > Qxx)

- MCSM wave function

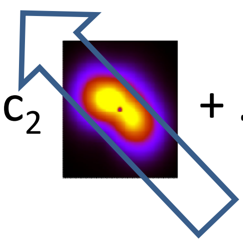
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

- Wave function w/o the projections

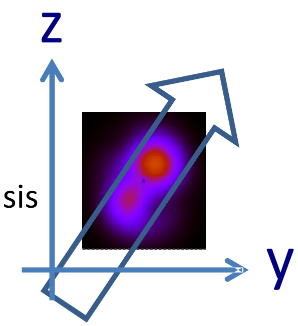
$$\sum_{i=1}^{N_{basis}} c_i |\Phi_i\rangle = c_1$$



$+ c_2$

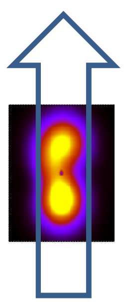


$+ \ldots + c_{Nbasis}$

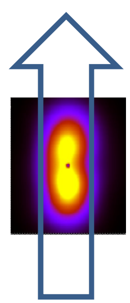


- Wave function w/o the projection w/ the alignment of Q-moment

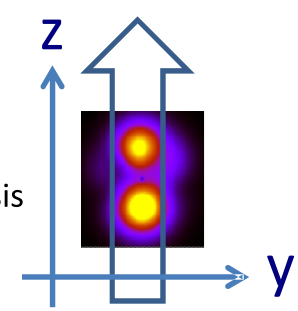
$$\sum_{i=1}^{N_{basis}} c_i |\Phi'_i\rangle = c_1$$



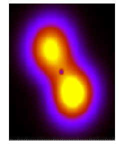
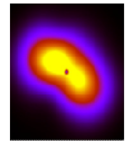
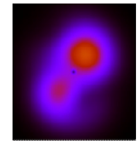
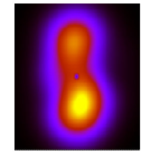
$+ c_2$



$+ \ldots + c_{Nbasis}$



Density plots in MCSM

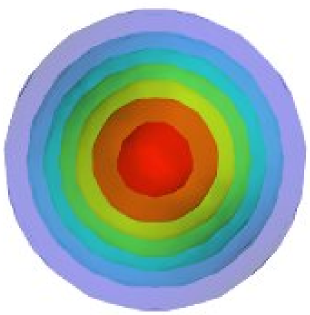
$$|\Phi\rangle = \sum_{i=1}^{N_{basis}} c_i|\Phi_i\rangle = $$ c_1  $+ c_2$  $+ c_3$  $+ c_4$  + …

Angular-momentum projection

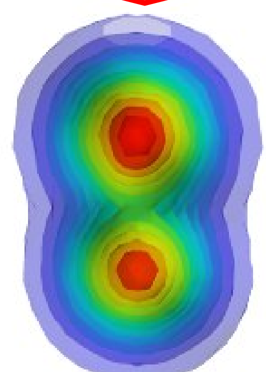
$$|\Psi\rangle = \sum_{i=1}^{N_{basis}} c_i P^J P^\pi |\Phi_i\rangle$$

Rotation of each basis by diagonalizing Q-moment

$$|\Phi'\rangle = \sum_{i=1}^{N_{basis}} c_i R(\Omega_i)|\Phi_i\rangle$$



^{8}Be 0^+ ground state



Laboratory frame

"Intrinsic" (body-fixed) frame

Densities in lab. & body-fixed frames can be constructed by MCSM

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Density plots of ^{8}Be 0^{+} ground state from MCSM w.f.

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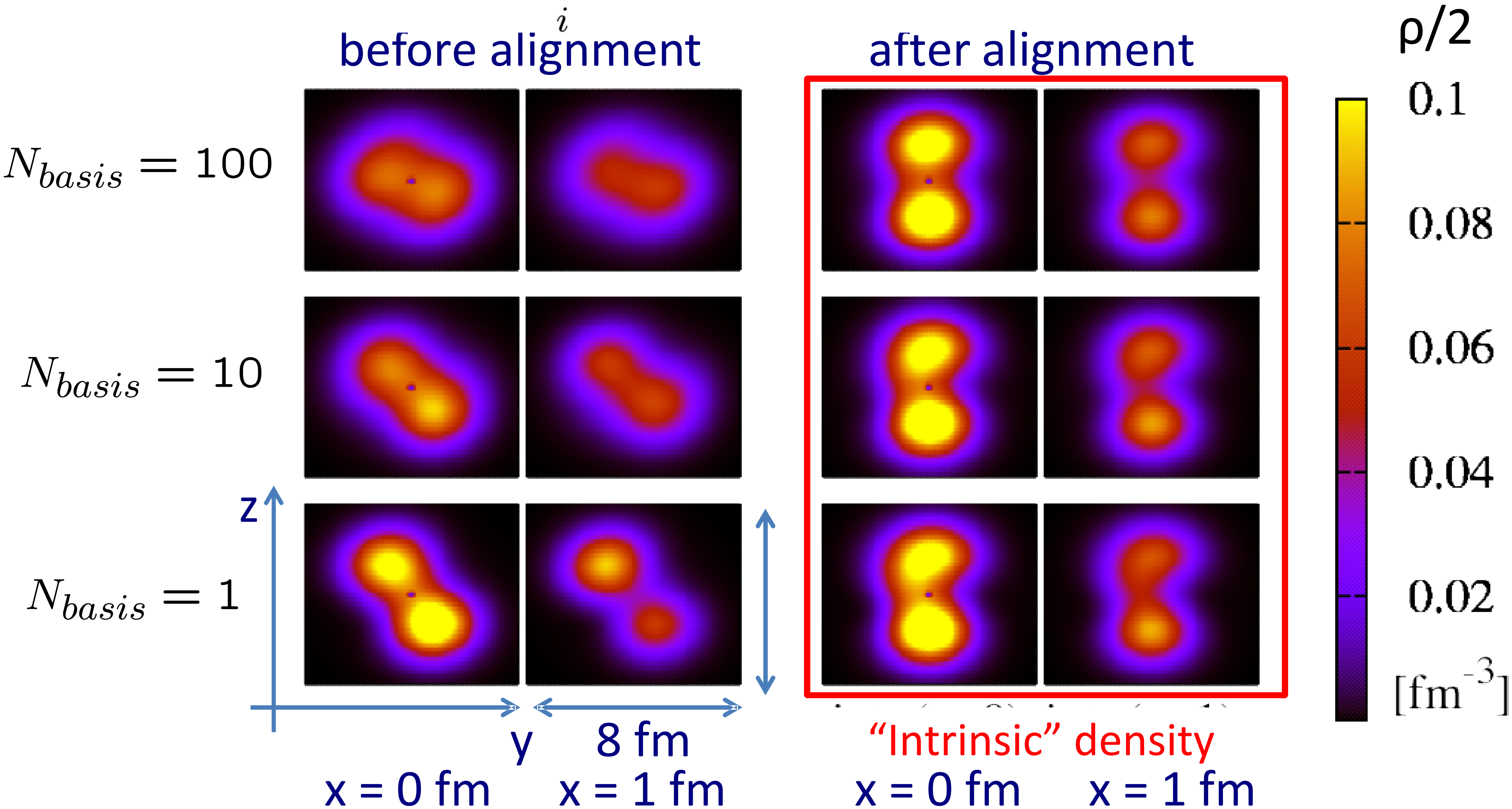
- Test calculation of the density by using the MCSM w.f. in Nshell = 4

$$\rho(\vec{r}) = \langle \Phi(\{\vec{r}_i{}'\}) | \sum_i \delta(\vec{r} - \vec{r}_i{}') | \Phi(\{\vec{r}_i{}'\}) \rangle$$



Summary

- MCSM can be applied to no-core calculations of the p-shell nuclei.

  - Benchmarks for the p-shell nuclei have been performed and gave good agreements w/ FCI results.

  - Density profiles from MCSM many-body w.f. are preliminarily investigated and the cluster-like distributions are reproduced.

Perspective

- MCSM algorithm/computation

  - Extension to larger model spaces (Nshell = 6, 7, …), extrapolation to infinite model space, & comparison with another truncations

  - Inclusion of the 3-body force (thru. effective 2-body force)

  - GPGPU

- Physics

  - Cluster(-like) states (He & Be isotopes, 12C Hoyle state, …)

  - sd-shell nuclei