Symposium on
`Quarks to Universe in Computational Science'
(QUCS2012)

No-core Monte Carlo shell model towards ab initio nuclear structure

A02: Nuclear Physics

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THE UNIVERSITY OF TOKYO

Nara Prefectural New Public Hall

December 13-16, 2012

Collaborators

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- JAEA
  - Yutaka Utsuno
- Iowa State U
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  - Pieter Maris

Outline

- Motivation
- No-Core Monte Carlo Shell Model (MCSM)
- Benchmark in p-shell nuclei
- Density profile from MCSM wave functions
- Summary & perspective

Current status of ab inito approaches

- Major challenge of the nuclear physics

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

  - *ab-initio* approaches: GFMC, NCSM (up to A ~ 12-14), CC (closed shell +/- 1,2), SCGF 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, K.D. Sviratcheva, J.P. Draayer, C. Bahri, J.P. Vary, … (Louisiana State U, Iowa State U)
- No-Core Monte Carlo Shell Model (MCSM)

“Ab initio” in nuclear physics

- Solve non-relativistic Schroeding eq. and obtain the eigenvalues and eigenvectors.

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

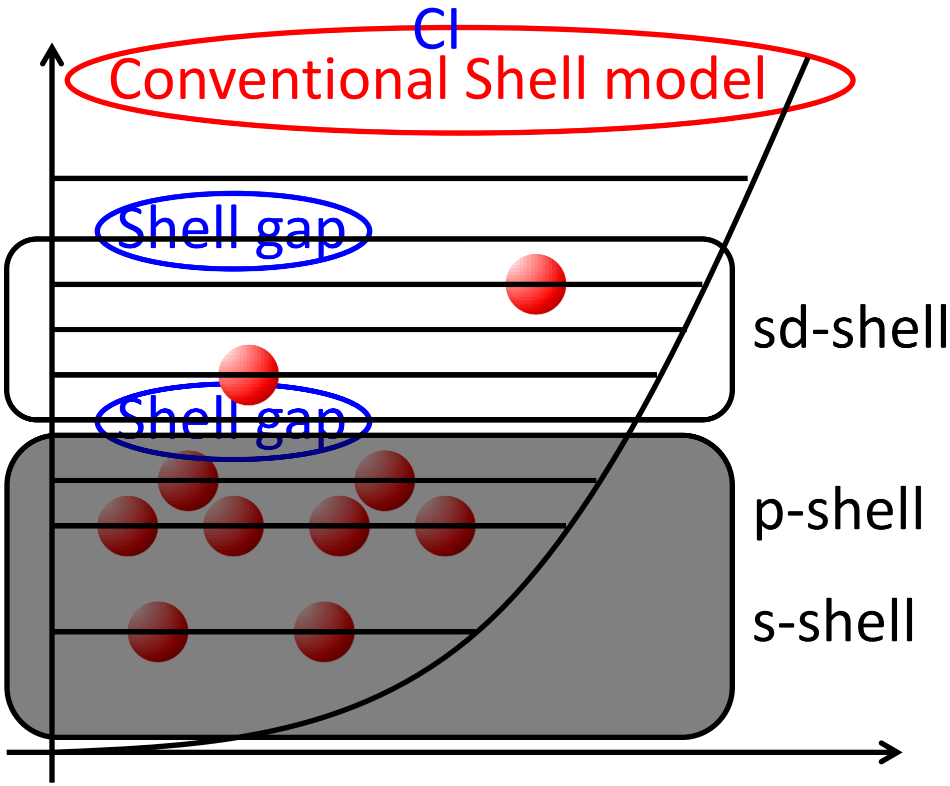
$$H = T + V_{\mathrm{NN}} + V_{\mathrm{3N}} + \cdots + V_{\mathrm{Coulomb}}$$

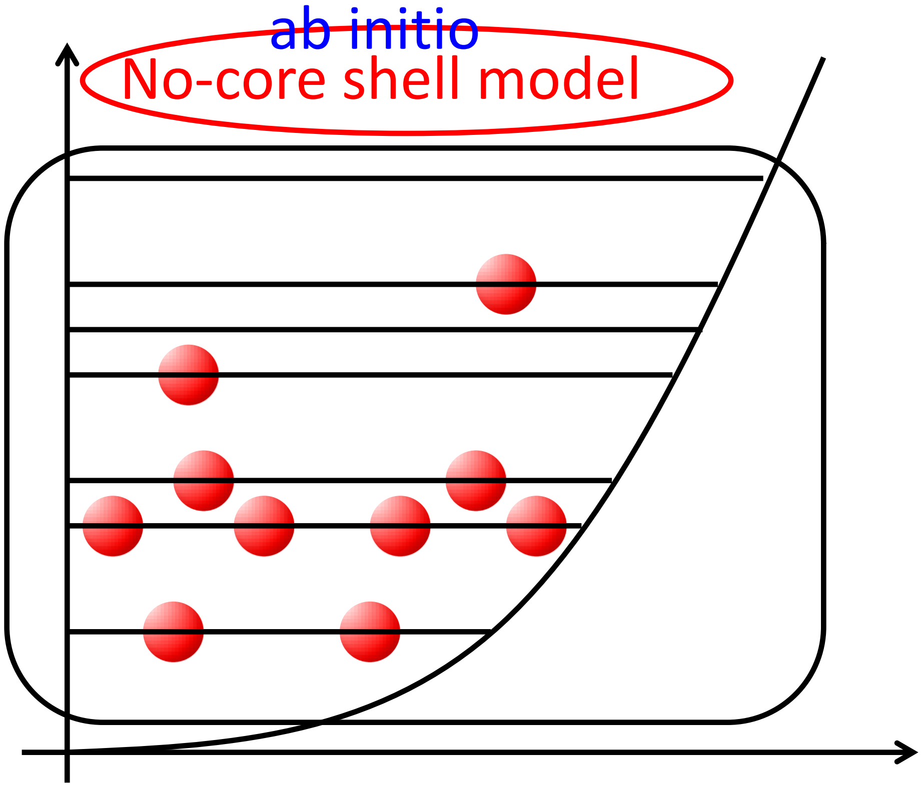
  – Ab initio: All nucleons are active, and use realistic NN (+ 3N) interactions.

- Two sources of errors:
  – Nuclear forces (interactions btw/among nucleons), in principle, they should be obtained by QCD.
  – Finite # of basis space, we have to extrapolate to infinite basis dimensions

Core & no-core shell models

- Conventional (core) shell model vs. No-core shell model (NCSM)





Effective interactions

Talk by Y. Tsunoda

Realistic nuclear interactions

This talk

Nuclear shell model

- Eigenvalue problem of large sparse Hamiltonian matirx

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

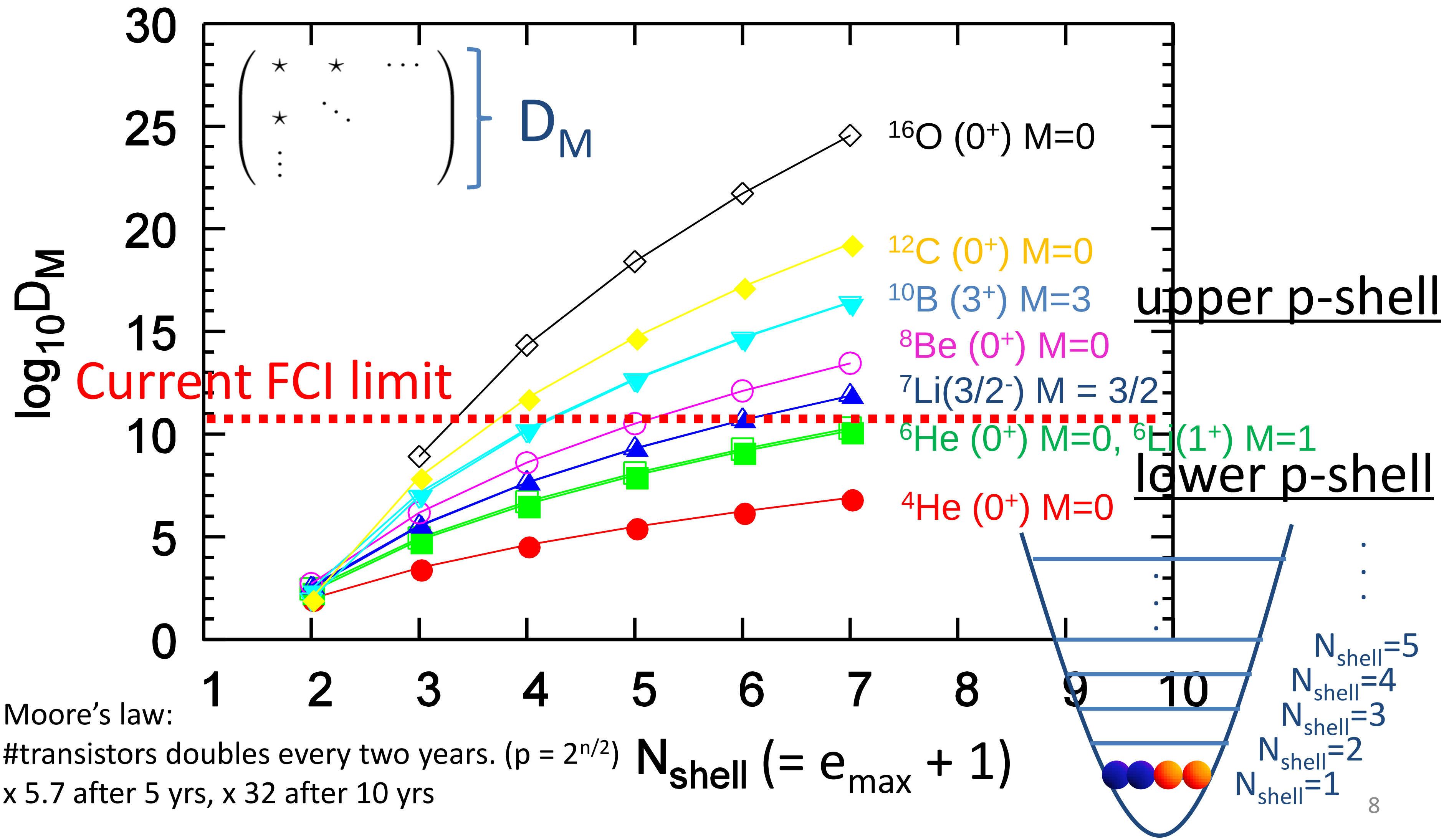
$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & \cdots \\ H_{21} & H_{22} & H_{23} & H_{24} & & \\ H_{31} & H_{32} & H_{33} & & & \\ H_{41} & H_{33} & & \ddots & & \\ H_{51} & & & & & \\ \vdots & & & & & \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_5 \\ \vdots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

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

Large sparse matrix (in m-scheme)

$$\left\{ \begin{array}{lcl} |\Psi_1\rangle & = & a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma \cdots |-\rangle \\ |\Psi_2\rangle & = & a^\dagger_{\alpha'} a^\dagger_{\beta'} a^\dagger_{\gamma'} \cdots |-\rangle \\ |\Psi_3\rangle & = & \cdots \\ & \vdots & \end{array} \right.$$

M-scheme dimension of p-shell nuclei

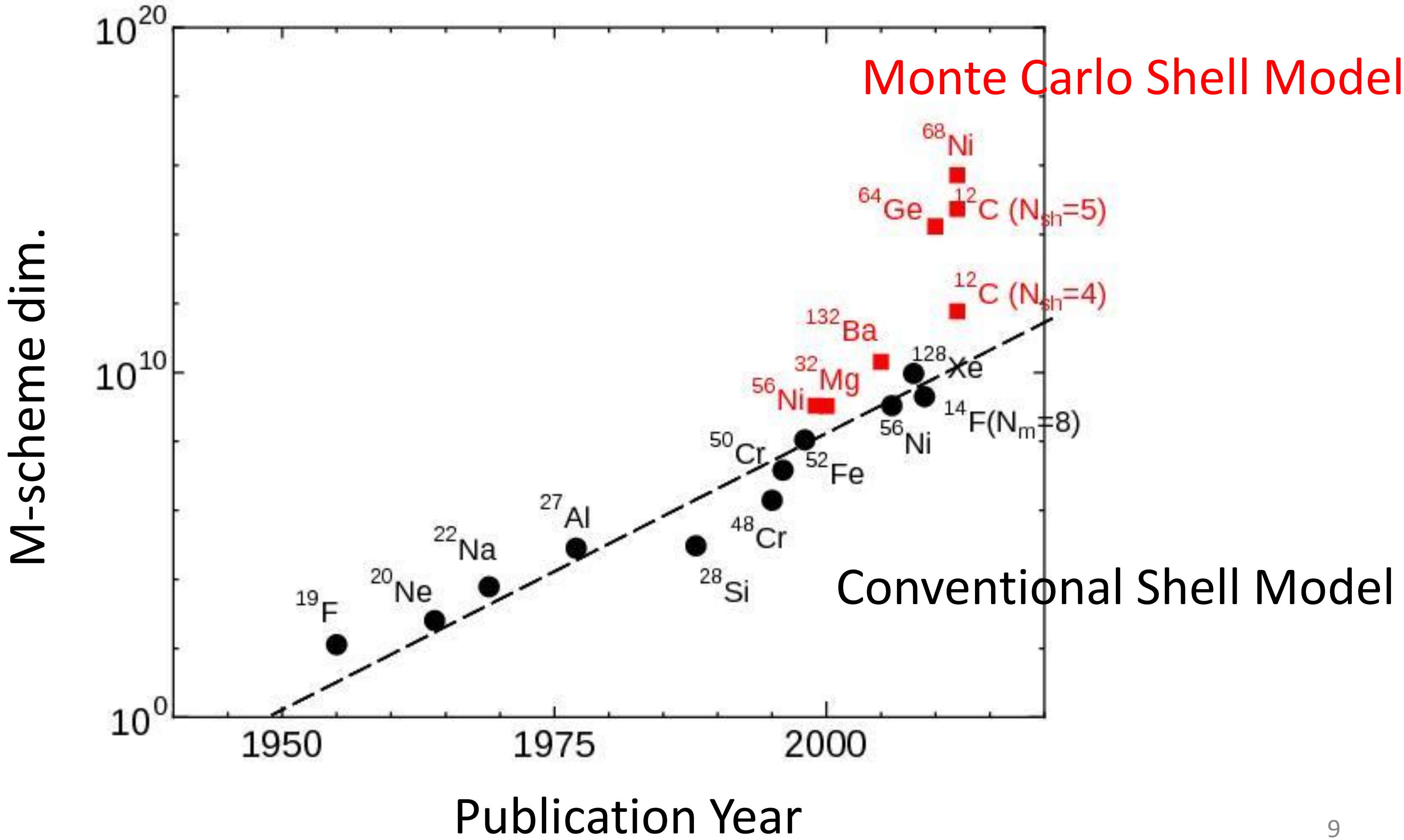


Moore's law:
#transistors doubles every two years. (p = $2^{n/2}$)
x 5.7 after 5 yrs, x 32 after 10 yrs

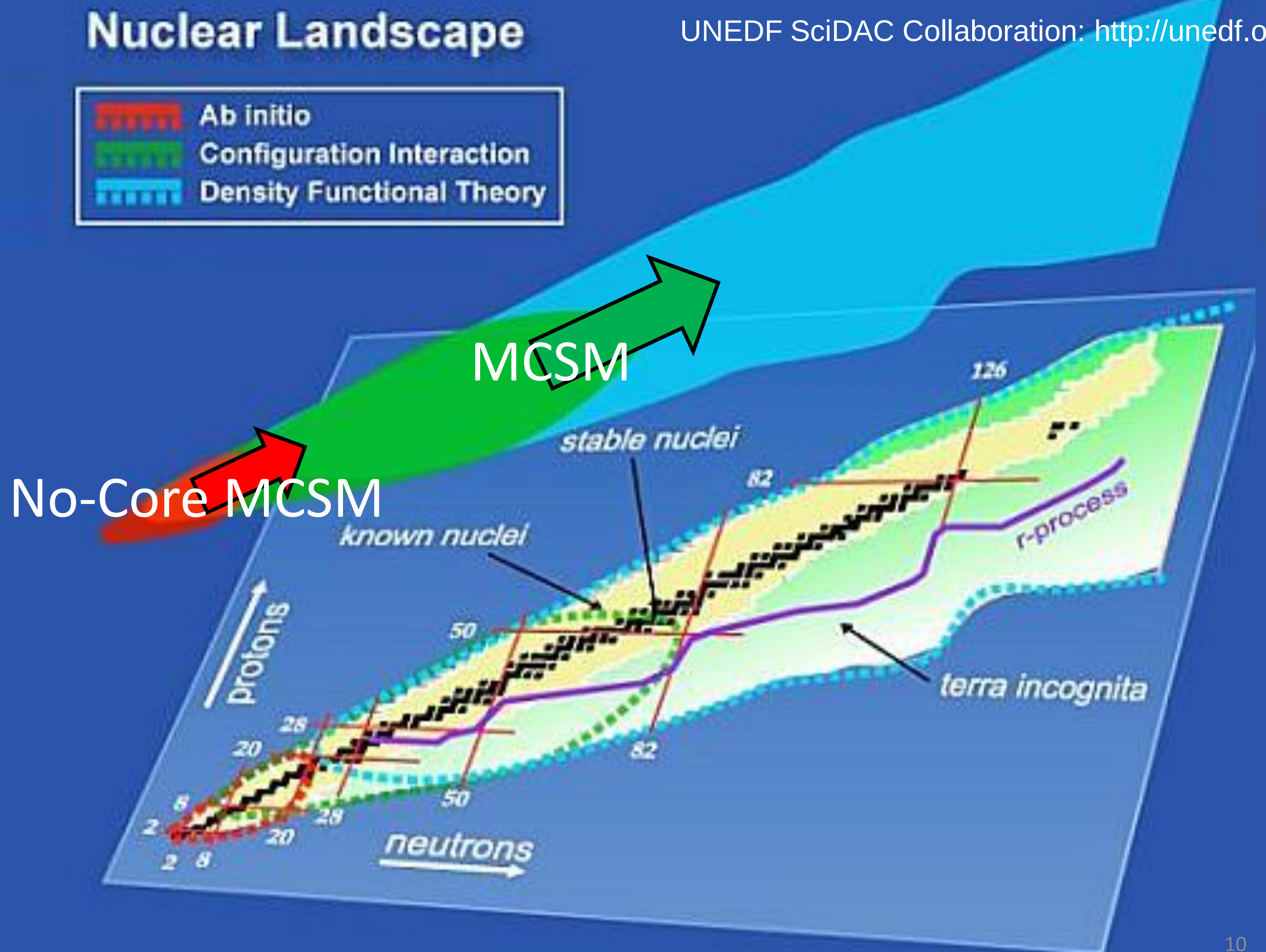
Review: T. Otsuka , M. Honma, T. Mizusaki, N. Shimizu, Y. Utsuno, Prog. Part. Nucl. Phys. 47, 319 (2001)

Power of the MCSM

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



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



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

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

All Slater determinants

$d > O(10^{10})$

Monte Carlo shell model

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

Important bases stochastically selected

$d_{MCSM} < O(100)$

SM Hamiltonian & MCSM many-body w.f.

- 2nd-quantized non-rel. Hamiltonian (up to 2-body term, so far)

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

- Eigenvalue problem

$$H|\Psi(J,M,\pi)\rangle = E|\Psi(J,M,\pi)\rangle$$

- MCSM many-body wave function & basis function

$$|\Psi(J,M,\pi)\rangle = \sum_i^{N_{basis}} f_i |\Phi_i(J,M,\pi)\rangle \qquad |\Phi(J,M,\pi)\rangle = \sum_K g_K P^J_{MK} P^\pi |\phi\rangle$$

These coeff. are obtained by the diagonalization.

- Deformed SDs

This coeff. is obtained by a stochastic sampling.

$$|\phi\rangle = \prod_i^A a^\dagger_i |-\rangle \qquad a^\dagger_i = \sum_\alpha^{N_{sps}} c^\dagger_\alpha D_{\alpha i}$$

($c_\alpha^\dagger$ ... spherical HO basis)

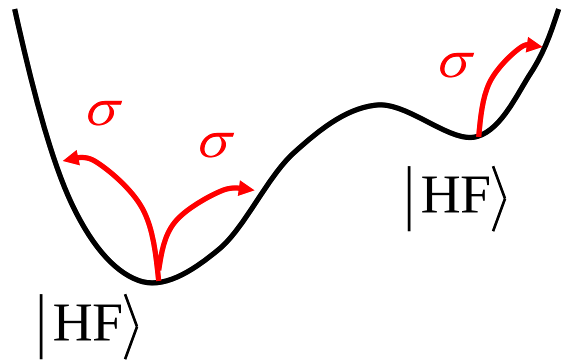
Sampling of basis functions in the MCSM

- 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.

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

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

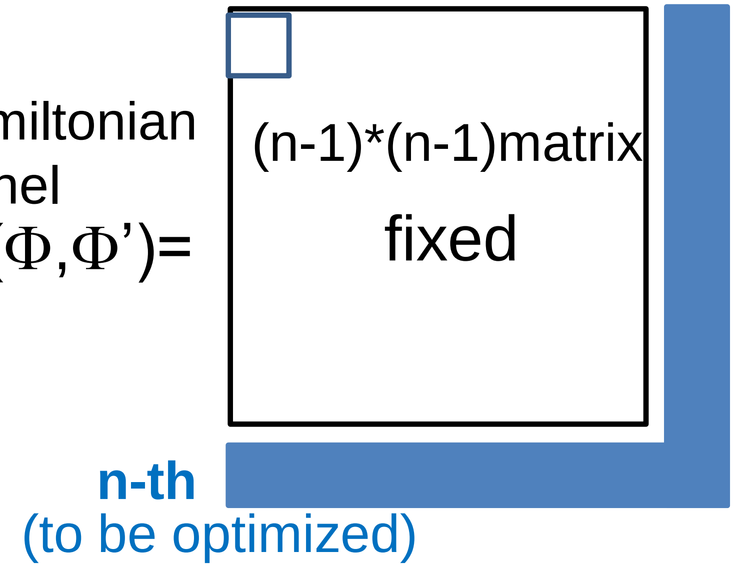
$$e^{-\beta H} = \int_{-\infty}^{+\infty} \prod_i d\sigma_i \sqrt{\frac{\beta|V_i|}{2\pi}} e^{-\frac{\beta}{2}|V_i|\sigma_i^2} e^{-\beta h(\vec{\sigma})}$$

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

Rough image of the search steps

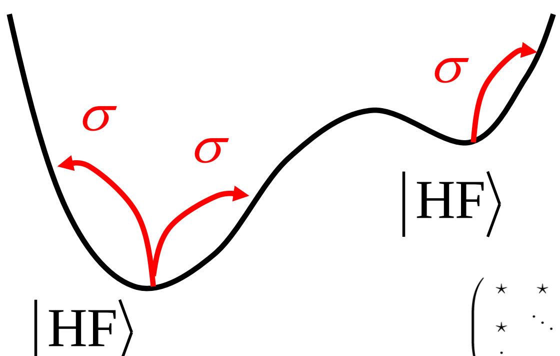
- Basis search
  - HF solution is taken as the 1st basis
  - Fix the n-1 basis states already taken
  - Requirement for the new basis: atopt the basis which makes the energy (of a many-body state) as low as possible by a stochastic sampling

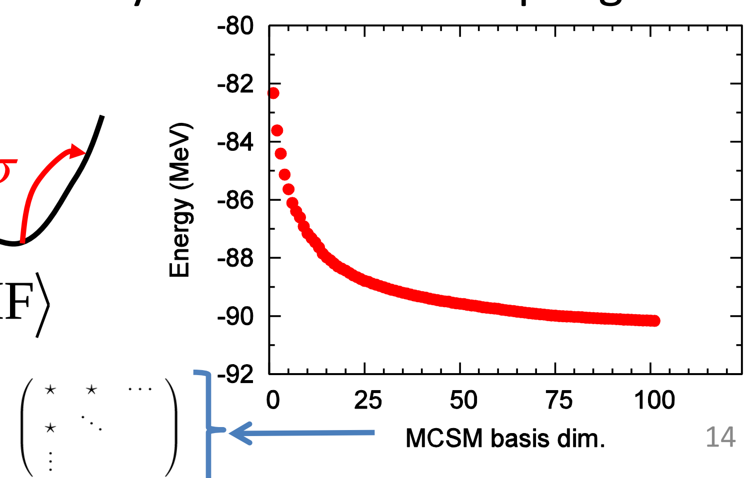
Hamiltonian kernel
$H(\Phi,\Phi')=$



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

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





L. Liu, T. Otsuka, N. Shimizu, Y. Utsuno, R. Roth, Phys. Rev C86, 014302 (2012)

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)

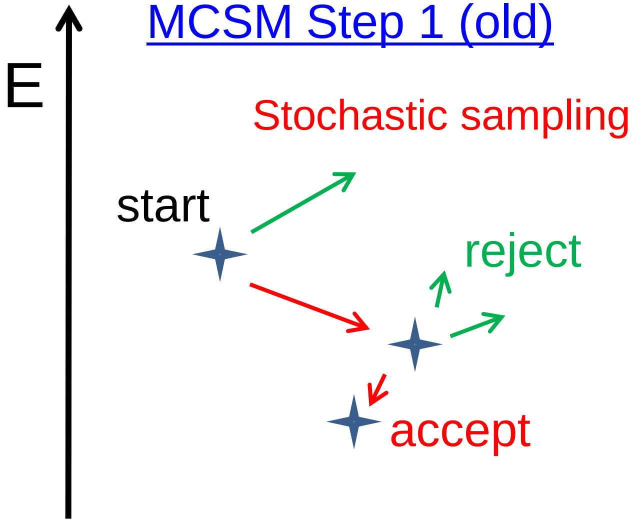
Recent developments in the MCSM

- Energy minimization by the CG method
  - N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda & T. Otsuka, Phys. Rev. C85, 054301 (2012)
- Efficient computation of TBMEs
  - Y. Utsuno, N. Shimizu, T. Otsuka & T. Abe, Compt. Phys. Comm. 184, 102 (2013)
- Energy variance extrapolation
  - N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe & M. Honma, Phys. Rev. C82, 061305 (2010)

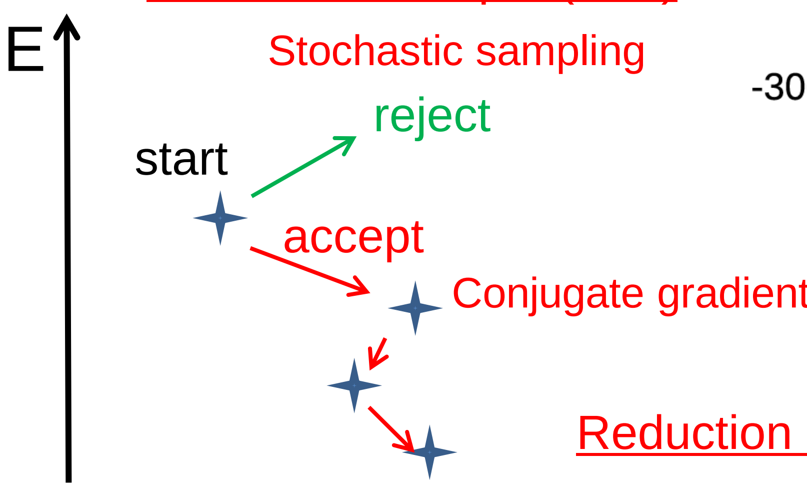
- Summary of recent MCSM techniques
  - N. Shimizu, T. Abe, T. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma, T. Otsuka, Prog. Theor. Exp. Phys. (2012)

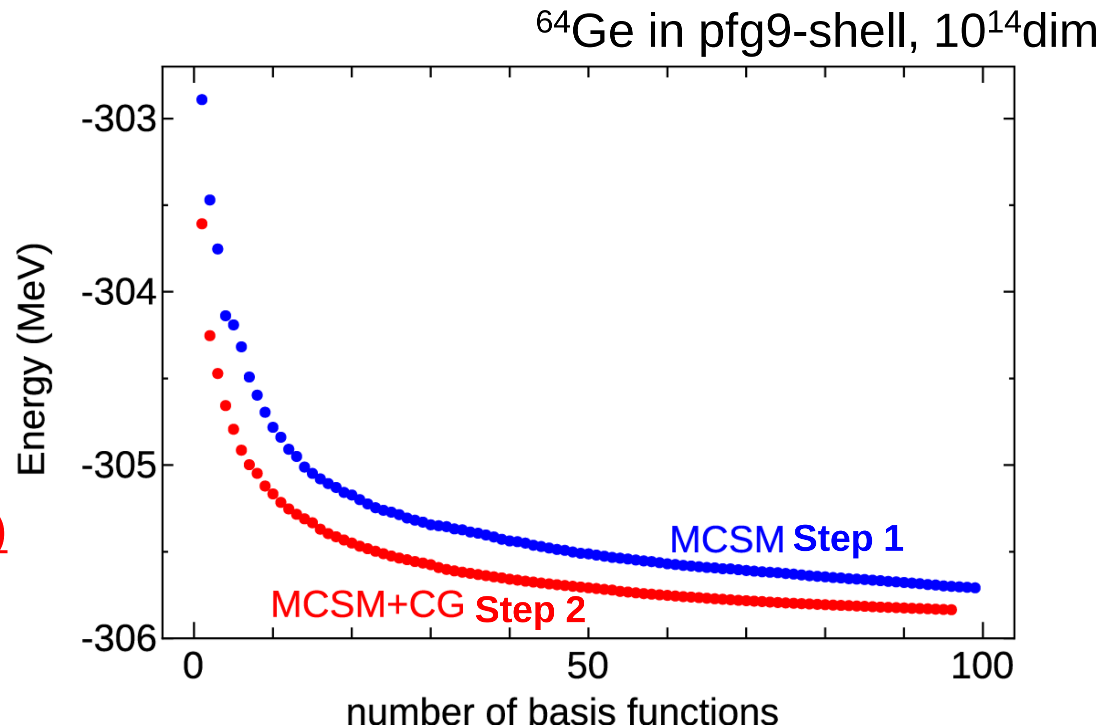
Energy minimization by Conjugate Gradient method

MCSM Step 1 (old)



MCSM+CG Step 2 (new)





Stochastic sampling before conjugate gradient to minimize the expectation value energy

Reduction of the number of basis function roughly 30%

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Comp. Phys. Comm., in press, arXiv:1202.2957 [nucl-th]

Efficient 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)

- Utilization of the symmetry

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

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

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

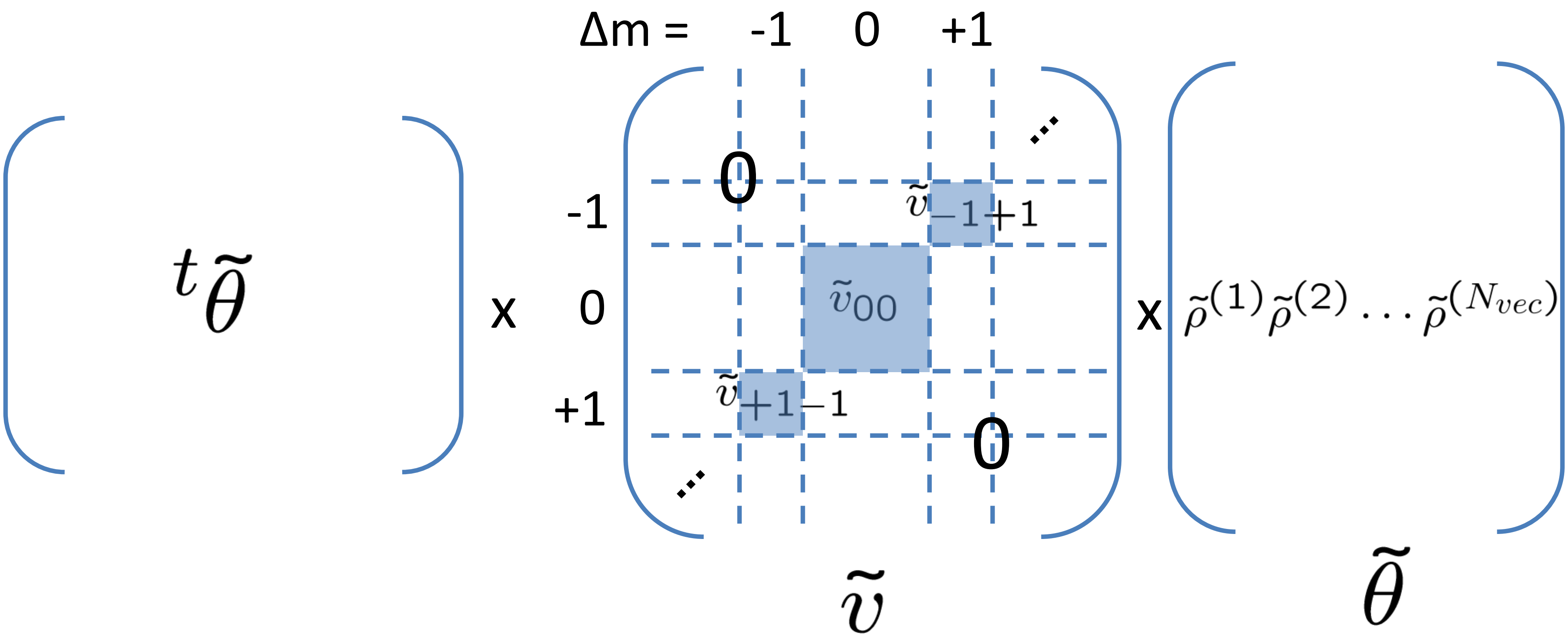
sparse $\qquad$ dense

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, arXiv:1202.2957 [nucl-th] (Comp. Phys. Comm. In press)

Schematic illustration of the computation of TBMEs

- Matrix-matrix method

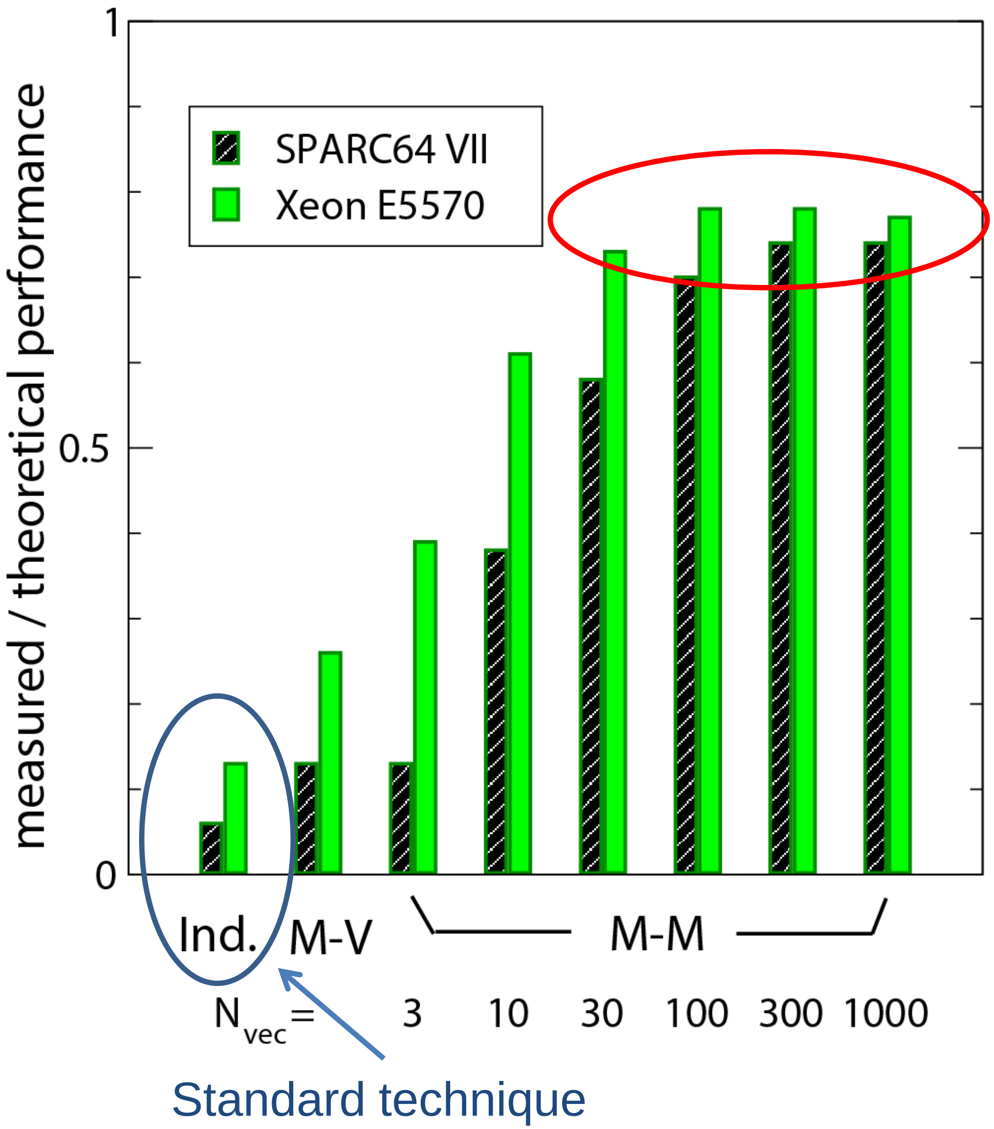
$$\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}\rho_{lj} = \sum_{\Delta m}\left[\sum_{a\in J_z(a)=-\Delta m}\tilde{\rho}_a\left(\sum_{b\in J_z(b)=\Delta m}\tilde{v}_{ab}\tilde{\rho}_b\right)\right]$$



→ BLAS Level 3

Y. Utsuno, N. Shimizu, T. Otsuka, and T. Abe, Comp. Phys. Comm., in press, arXiv:1202.2957 [nucl-th]

Tuning of the density matrix product



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

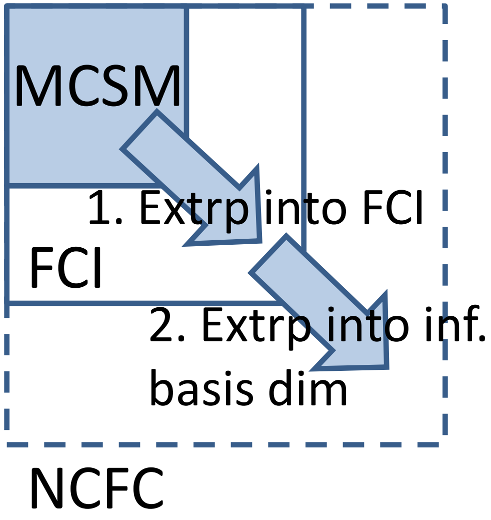
     Energy-variance extrapolation

  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

     Not applied in the MCSM, so far…



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)

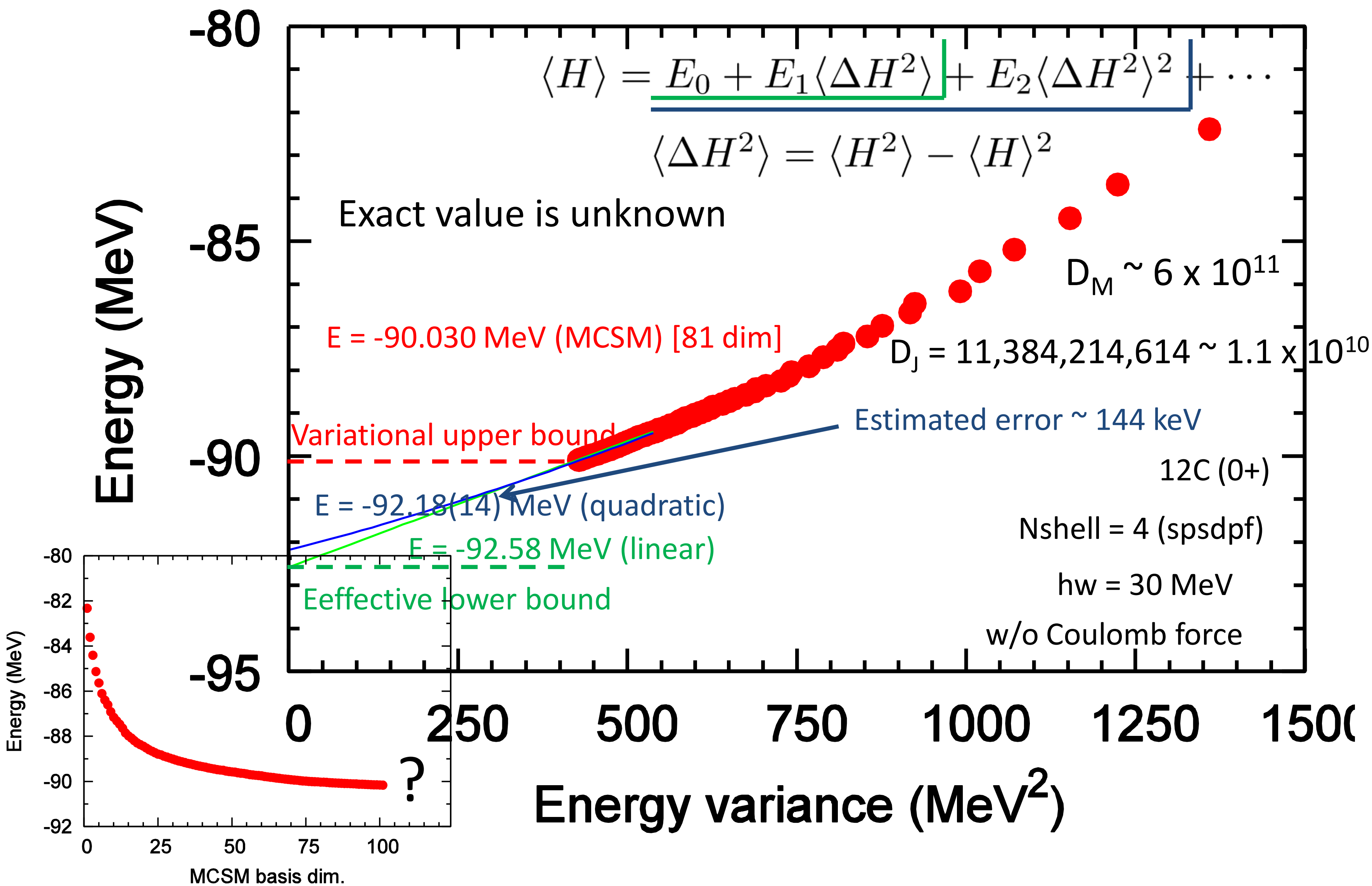
single deformed Slater determinant

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

→ Apply to the MCSM (multi deformed SDs)

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

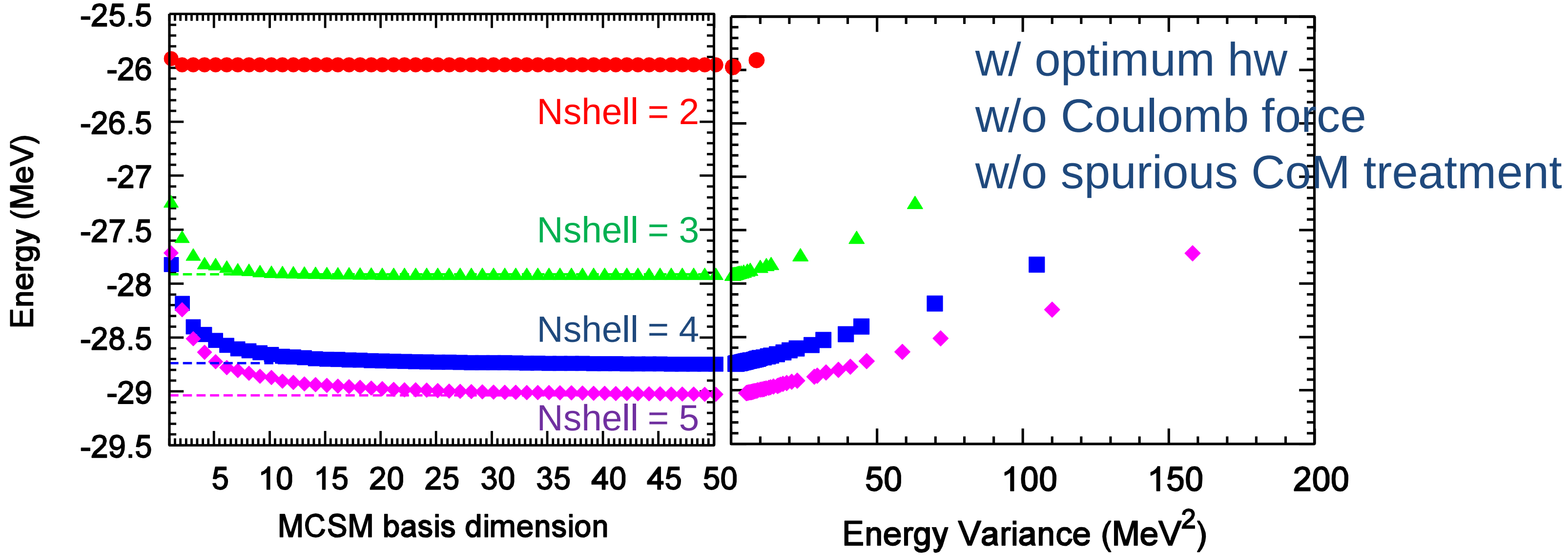
Energy-variance Extrapolation of 12C 0+ g.s. Energy



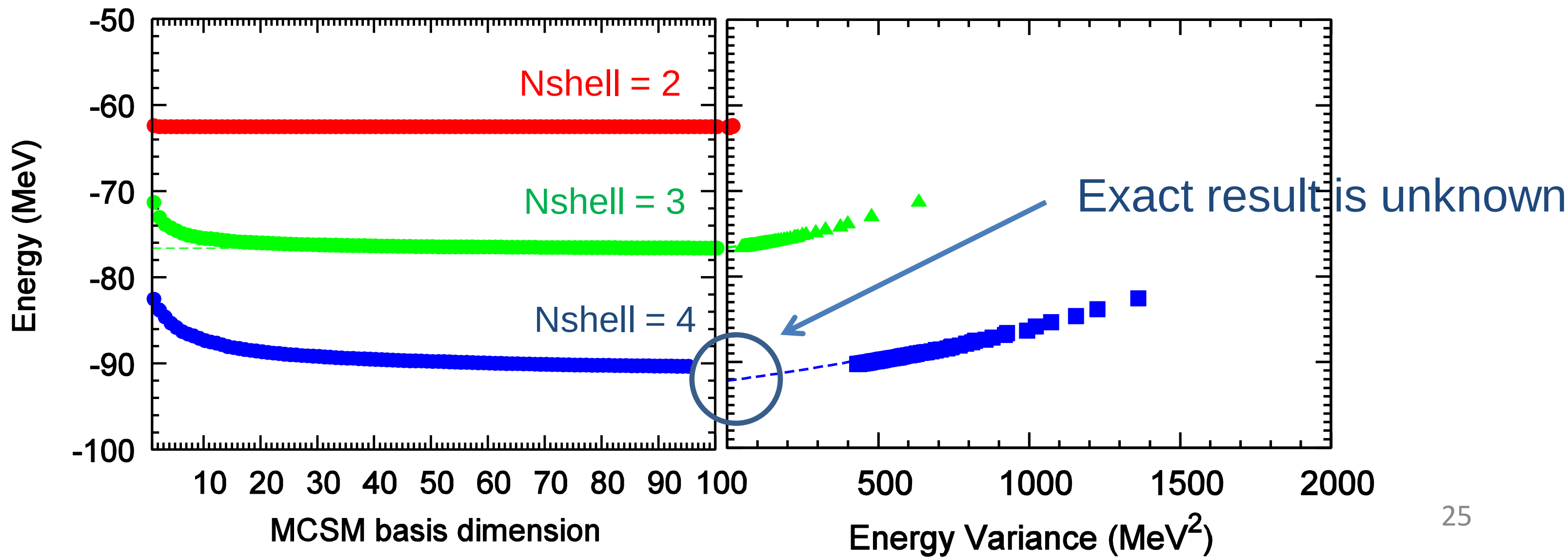
Benchmarks in p-shell nuclei

Helium-4 & carbon-12 gs energies

$^{4}He(0^{+};gs)$

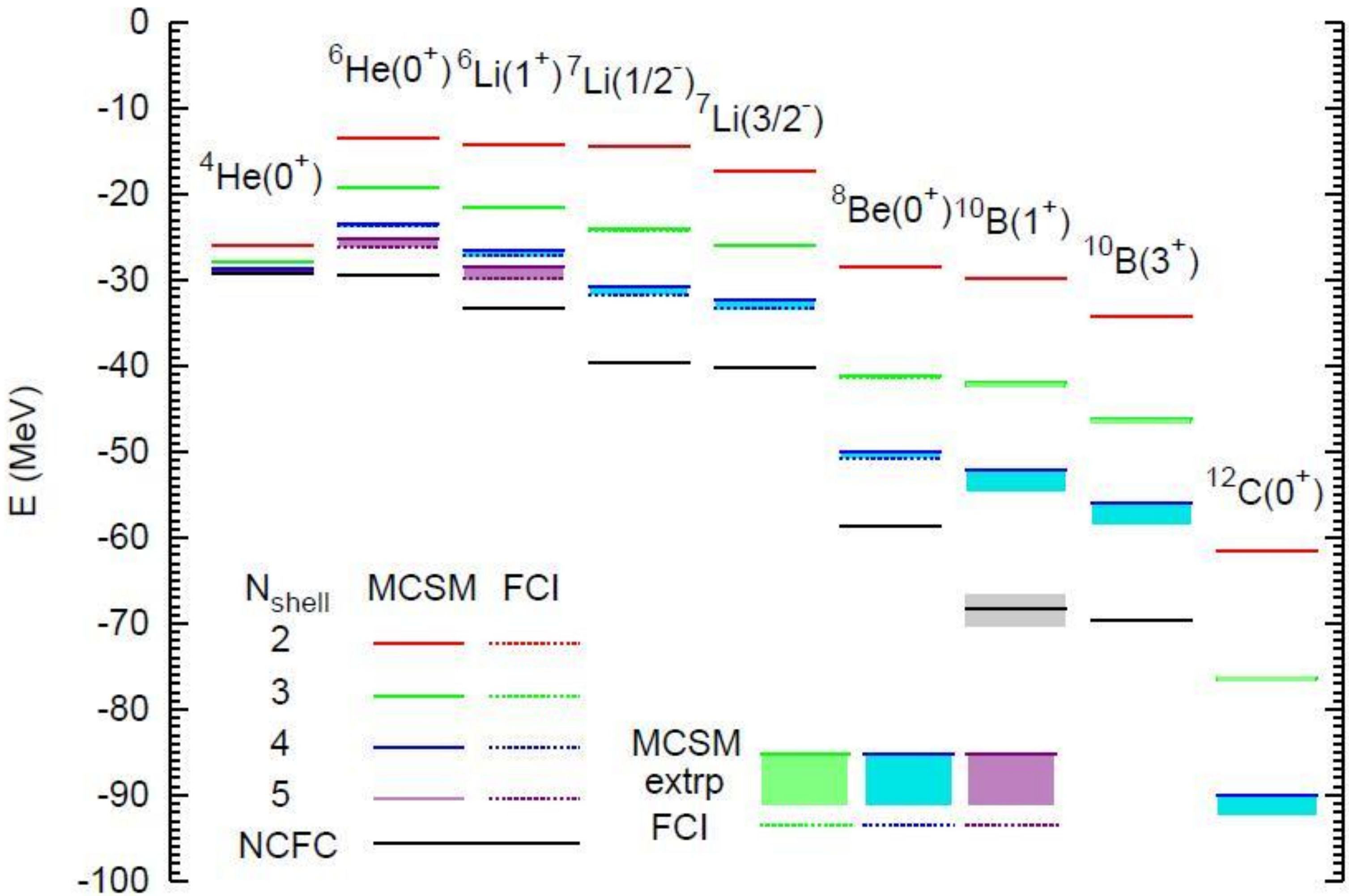


$^{12}C(0^{+};gs)$



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

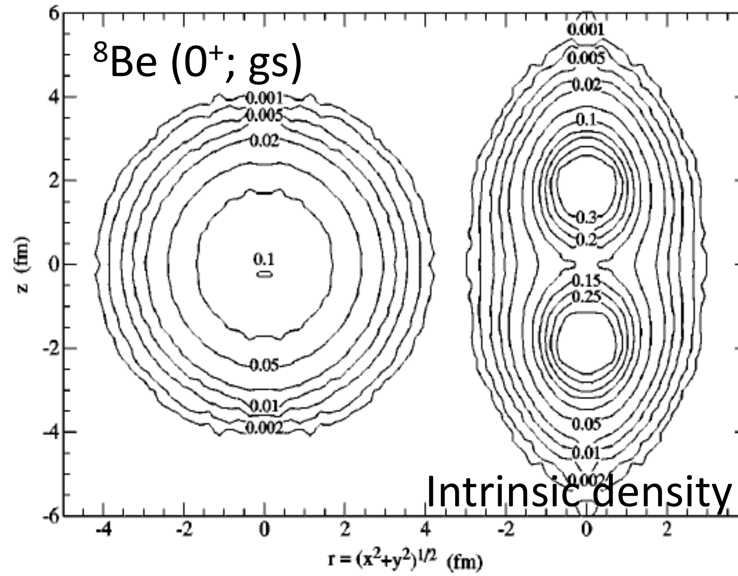
Energies of the Light Nuclei



Density Profiles from MCSM wave functions

Density Profile from ab initio calc.

VMC



- 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)

^{8}Li (2^{+}; gs)

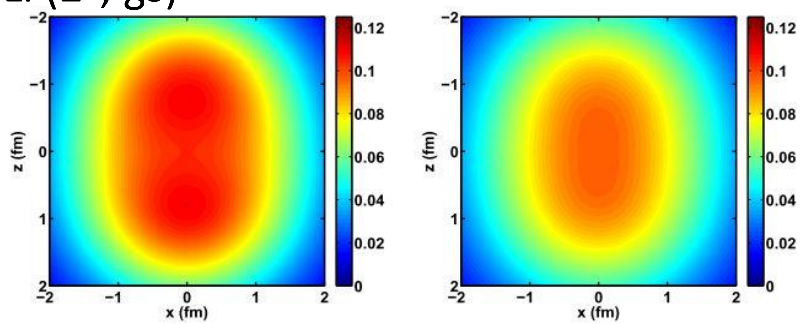


FIG. 12: (Color online) The $y = 0$ slice of the translationally-invariant neutron density (left) of the 2^+ gs of ^{8}Li. The space-fixed density for the same state is on the right. These densities were calculated at $N_{max} = 12$ and $\hbar\Omega = 12.5$ MeV.

Translationally-invariant neutron density

Space-fixed neutron density

- No-core full configuration (NCFC)

  Translationally-invariant density is obtained

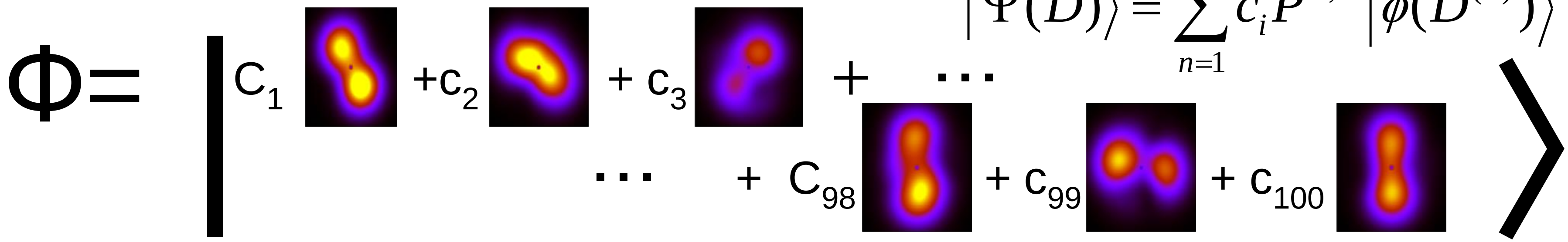
  by deconvoluting the intrinsic & CM w.f.

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

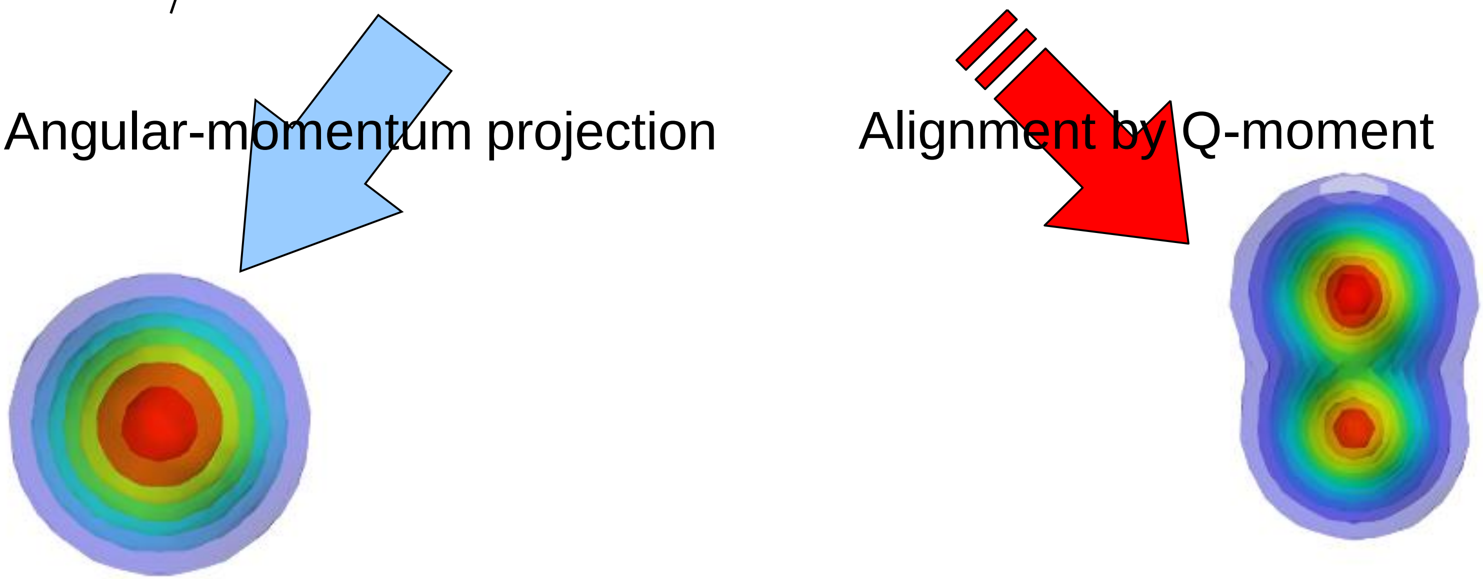
  Phys. Rev. C86, 034325 (2012)

Density profile in MCSM

$$\left|\Psi(D)\right\rangle = \sum_{n=1}^{N_B} c_i P^{J,\Pi} \left|\phi(D^{(n)})\right\rangle$$



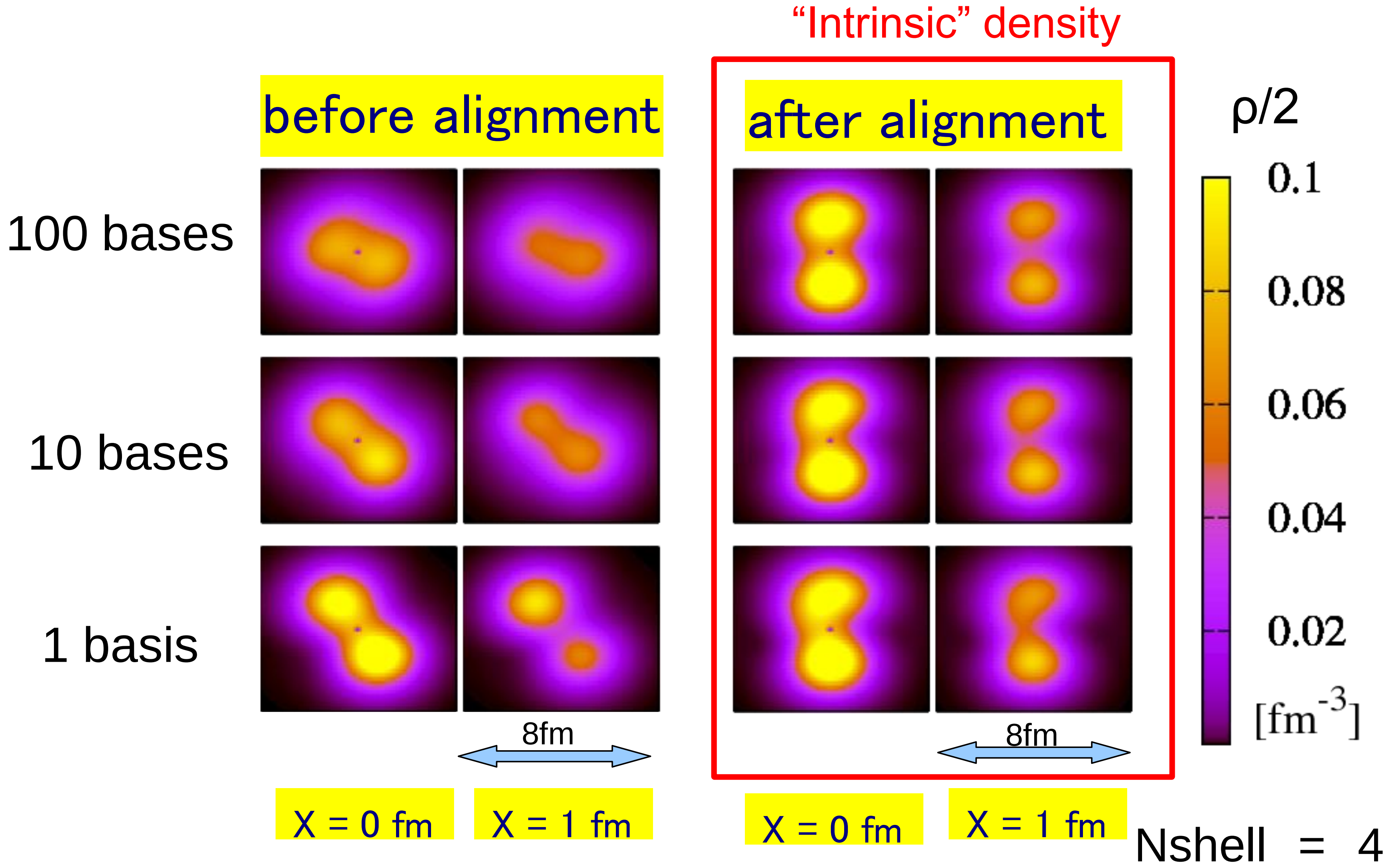
$$\sum_{n=1}^{N_B} c_i \left|\phi(D^{(n)})\right\rangle$$



<u>Laboratory frame</u> <u>"Intrinsic" (body-fixed) frame</u>

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

Density profile of ^{8}Be 0^{+} g.s. state from MCSM w.f.



Summary

- MCSM can be applied to the no-core calculations of 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 investigated and the cluster-like distributions are reproduced.

Perspective

- MCSM algorithm

  - Access to larger model spaces (Nshell = 5, 6, …)

  - Inclusion of the 3-body force by effective 2-body force.

- Physics

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

END