Symposium on ‘Quarks to Universe in Computational Science’  
(QUCS2012)

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

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A02: Nuclear Physics

Nara Prefectural New Public Hall  
December 13-16, 2012
Collaborators

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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 initio approaches

- Major challenge of the nuclear physics
  - Understand the nuclear structure from \textit{ab-initio} calculations in non-relativistic quantum many-body system \textit{w/} realistic nuclear forces

  - \textit{ab-initio} approaches: GFMC, NCSM (up to $A \sim 12-14$), CC (closed shell +/- 1,2), SCGF theory, IM-SRG, Lattice EFT, ...

  \rightarrow \text{demand for extensive computational resources}

- \textit{ab-initio}(-like) SM approaches (which attempt to go) beyond standard methods
  - IT-NCSM, IT-CI: R. Roth (TU Darmstadt), P. Navrtil (TRIUMF), ...
  - SA-NCSM: T. Dytrych, K.D. Sviratcheva, J.P. Draayer, C. Bahri, J.P. Vary, ...
  \hspace{2cm} (Louisiana State U, Iowa State U)
  - No-Core Monte Carlo Shell Model (MCSM)
“Ab initio” in nuclear physics

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

\[ H |\Psi\rangle = E |\Psi\rangle \]

\[ H = T + V_{NN} + V_{3N} + \cdots + V_{\text{Coulomb}} \]

- 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)

Cl Conventional Shell model

ab initio No-core shell model

Shell gap
Shell gap

Effective interactions
Talk by Y. Tsunoda

Realistic nuclear interactions
This talk
Nuclear shell model

- Eigenvalue problem of large sparse Hamiltonian matrix

\[ H |\Psi\rangle = E |\Psi\rangle \]

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

~ \mathcal{O}(10^{10})

Large sparse matrix (in m-scheme)
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

Current FCI limit

upper p-shell

lower p-shell

$D_M$ in log scale

$N_{\text{shell}} = e_{\text{max}} + 1$

$^1\text{H}$ (0$^+$) $M=0$

$^3\text{He}$ (0$^+$) $M=0$

$^6\text{Li}$ (1$^+$) $M=1$

$^7\text{Li}$ (3/2$^-$) $M = 3/2$

$^8\text{Be}$ (0$^+$) $M=0$

$^9\text{Be}$ (0$^+$) $M=0$, $^6\text{Li}$ (1$^+$) $M=1$

$^{10}\text{B}$ (3$^+$) $M=3$

$^{12}\text{C}$ (0$^+$) $M=0$

$^{16}\text{O}$ (0$^+$) $M=0$
Power of the MCSM

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

Monte Carlo shell model (MCSM)

- Importance truncation

Standard shell model

\[
\mathbf{H} = \begin{pmatrix}
* & * & * & * & * & \cdots \\
* & * & * & * & & \\
* & * & * & & & \\
* & & & & & \\
& & & & & \\
& & & & & \\
\end{pmatrix}
\]

Diagonalization

\[
\begin{pmatrix}
E_0 \\
E_1 \\
E_2 \\
\vdots
\end{pmatrix}
\]

All Slater determinants

Monte Carlo shell model

\[
\mathbf{H} \sim \begin{pmatrix}
* & * & \cdots \\
* & & \cdots \\
& & \cdots \\
\end{pmatrix}
\]

Diagonalization

\[
\begin{pmatrix}
E_0' \\
E_1' \\
\vdots
\end{pmatrix}
\]

Important bases stochastically selected

\[d_{\text{MCSM}} < O(100)\]
SM Hamiltonian & MCSM many-body w.f.

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

\[ H = \sum_{\alpha \beta}^{N_{sps}} t_{\alpha \beta} c_{\alpha}^{\dagger} c_{\beta} + \frac{1}{4} \sum_{\alpha \beta \gamma \delta}^{N_{sps}} \bar{v}_{\alpha \beta \gamma \delta} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\delta} c_{\gamma} \]

\[ \bar{v}_{ijkl} = v_{ijkl} - v_{ijlk} \]

- Eigenvalue problem

\[ H |\psi(J, M, \pi)\rangle = E |\psi(J, M, \pi)\rangle \]

- MCSM many-body wave function & basis function

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

\[ |\Phi(J, M, \pi)\rangle = \sum_{K} g_K P^J_M K P^\pi |\phi\rangle \]

These coeff. are obtained by the diagonalization.

- Deformed SDs

\[ |\phi\rangle = \prod_{i=1}^{A} a_i^{\dagger} |\rangle \quad a_i^{\dagger} = \sum_{\alpha}^{N_{sps}} c_{\alpha}^{\dagger} D_{\alpha i} \]

This coeff. is obtained by a stochastic sampling.

(\( c^{\dagger}_{\alpha} \) ... spherical HO basis)
Sampling of basis functions in the MCSM

• Deformed Slater determinant basis

\[ |\phi\rangle = \prod_{i}^{A} a_{i}^{\dagger} |-\rangle \quad a_{i}^{\dagger} = \sum_{\alpha}^{\text{N}_{sps}} c_{\alpha}^{\dagger} D_{\alpha i} \quad (c_{\alpha}^{\dagger} \ldots \text{HO basis}) \]

• 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.

\[ |\phi(\sigma)\rangle = \prod_{i}^{N_{AF}} e^{-\Delta}^{\beta} h(\sigma) |\phi\rangle \quad e^{-\beta H} = \int^{+\infty} \prod_{i} d\sigma_{i} \sqrt{\frac{\beta |V_{i}|}{2\pi}} e^{-\beta |V_{i}| \sigma_{i}^{2}} e^{-\beta h(\sigma)} \]

\[ h(\sigma) = \sum_{i} (\epsilon_{i} + s_{i} V_{i} \sigma_{i}) O_{i} \]

\[ H = \sum_{i} \epsilon_{i} O_{i} + \frac{1}{2} \sum_{i} V_{i} O_{i}^{2} \]
Rough image of the search steps

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

\[ |\phi(\sigma)\rangle = \prod_n e^{-\Delta \beta h(\sigma_n)} |\phi\rangle \]
\[ h(\sigma_n) = h_{HF} + \sum_\alpha \sigma_{an} O_\alpha \]
Feasibility study of MCSM for no-core calculations

Recent developments in the MCSM

• Energy minimization by the CG method
  – N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda & T. Otsuka,

• Efficient computation of TBMEs
  – Y. Utsuno, N. Shimizu, T. Otsuka & T. Abe,

• Energy variance extrapolation
  – N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe & M. Honma,

• Summary of recent MCSM techniques
  – N. Shimizu, T. Abe, T. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki,
Energy minimization by Conjugate Gradient method

Stochastic sampling before conjugate gradient to minimize the expectation value energy

Reduction of the number of basis function roughly 30%

$^{64}\text{Ge in pfg9-shell, } 10^{14}\text{dim}$
Efficient computation of the TBMEs

- hot spot: Computation of the TBMEs
  \[
  \frac{\langle \Phi' | V | \Phi \rangle}{\langle \Phi' | \Phi \rangle} = \frac{1}{2} \sum_{ijkl} \tilde{v}_{ijkl} \rho_{ki} \rho_{lj}
  \]  
  (w/o projections, for simplicity)
  c.f.) Indirect-index method
  (list-vector method)

- Utilization of the symmetry

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

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

  \[
  \tilde{v}_{ijkl} \rightarrow \tilde{v}_{ab} \quad \rho_{ki} \rightarrow \tilde{\rho}_a \quad \rho_{lj} \rightarrow \tilde{\rho}_b
  \]

  sparse \quad dense
Schematic illustration of the computation of TBMEs

- Matrix-matrix method

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

where \( \Delta m = -1, 0, +1 \)

\[
\begin{pmatrix}
-1 & 0 & +1 \\
\end{pmatrix}
\times
\begin{pmatrix}
\tilde{\rho}^{(1)} & \tilde{\rho}^{(2)} & \ldots & \tilde{\rho}^{(N_{vec})}
\end{pmatrix}
\]

\[
\begin{pmatrix}
\tilde{v}
\end{pmatrix}
\rightarrow
\text{BLAS Level 3}
\]
Tuning of the density matrix product

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

SPARC64 requires large $N_{\text{bunch}}$ in comparison to Xeon.

Matrix product e.g. $(390 \times 390) \times (390 \times 2N_{\text{bunch}})$

$N_{\text{shell}} = 5$

Standard technique

$N_{\text{vec}}$ 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


  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

• Imported to nuclear physics
  Lanczos diagonalization with particle-hole truncation
  single deformed Slater determinant

Apply to the MCSM (multi deformed SDs)
Energy-variance Extrapolation of $^{12}\text{C}$ 0+ g.s. Energy

- Estimated error ~ 144 keV
- Variational upper bound
- Effective lower bound
- $E = -90.030$ MeV (MCSM) [81 dim]
- $E = -92.18(14)$ MeV (quadratic)
- $E = -92.58$ MeV (linear)
- $D_J = 11,384,214,614 \sim 1.1 \times 10^{10}$
- $D_M \sim 6 \times 10^{11}$
- Nshell = 4 (spsdpf)
- hw = 30 MeV
- w/o Coulomb force
Benchmarks in p-shell nuclei
Helium-4 & carbon-12 gs energies

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

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

Exact result is unknown

w/ optimum hw
w/o Coulomb force
w/o spurious CoM treatment
Energies of the Light Nuclei

Density Profiles from MCSM wave functions
Density Profile from ab initio calc.

- Green’s function Monte Carlo (GFMC)
  “Intrinsic” density is constructed by aligning the moment of inertia among samples


- No-core full configuration (NCFC)
  Translationally-invariant density is obtained by deconvoluting the intrinsic & CM w.f.

Density profile in MCSM

\[ \Phi = C_1 + c_2 + c_3 + \ldots + C_{98} + c_{99} + c_{100} \]

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

\[ \sum_{n=1}^{N_B} c_i |\phi(D^{(n)})\rangle \]

Angular-momentum projection

Alignment by Q-moment

Laboratory frame

“Intrinsic” (body-fixed) frame

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.

"Intrinsic" density

100 bases

before alignment

after alignment

10 bases

8fm

X = 0 fm  X = 1 fm

8fm

X = 0 fm  X = 1 fm

1 basis

Nshell = 4

ρ/2

0.1

0.08

0.06

0.04

0.02

[fm$^{-3}$]
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, ...)

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END