Stochastic generation of low-energy configurations and configuration mixing calculation

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Microscopic structure theories

• Ab-inito-type approaches
  – GFMC, NCSM, CCM, etc.
  – Computationally very demanding for heavier nuclei

• Shell model approaches
  – CI calculation in a truncated space
  – Difficulties in cross-shell excitations

• Microscopic cluster models
  – RGM, GCM, etc.
  – Interaction is tuned for each nucleus

• Energy density functional approaches
  – New configuration-mixing (multi-ref.) calculation
Toward low-energy complete spectroscopy

- Beyond the mean field
  - Correlations, excited states
- Beyond (Q)RPA
  - States very different from the g.s.
- Beyond GCM
  - Lift a priori generator coordinates

Toward the theoretical complete spectroscopy of low-lying states with an effective Hamiltonian and with a very large model space:

“Stochastic” approach to configuration mixing

Shinohara, Ohta, TN, Yabana, PRC 84, 054315 (2006)
Configuration mixing with parity and angular momentum projection

1. Generation and selection of Slater det’s in the 3D Cartesian Coordinate space

\[ \{ \Phi^i \} \quad (i = 1, \ldots, N) \]

2. Projection on good \( J^\pi \) (3D rotation)

\[ \Phi_{MK}^J = P^\pm P_{MK}^J \Phi \]

3. Solution of generalized eigenvalue eq.

\[
\left( H^{J^\pm} - EN^{J^\pm} \right) g = 0
\]

\[
H_{nK,n^{'}K^{'}}^{J^\pm} \quad N_{nK,n^{'}K^{'}}^{J^\pm} = \left\langle \Phi^n \left| \begin{pmatrix} H \\ 1 \end{pmatrix} \right| P^\pm P_{KK'}^J \right\rangle \Phi^{n'}
\]
Variational approach

$^{16}\text{O}$
BKN interaction
Two Parity-projected Slater determinants

$\Psi^{1(+)} = 0.72 \Phi^{1(+)} - 0.24 \Phi^{2(+)}$
$\Psi^{2(+)} = 1.12 \Phi^{1(+)} - 1.40 \Phi^{2(+)}$

<table>
<thead>
<tr>
<th></th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variational</td>
<td>$-142.54$</td>
</tr>
<tr>
<td>PPHF</td>
<td>$-133.35$</td>
</tr>
</tbody>
</table>

“Singular” Slater determinants
Imaginary-time evolution

- Quickly removing high-energy (high-momentum) components
- Slowly moving on low-energy collective surface
- Finding local minima

Efficient method to construct configurations associated with many kinds of low-energy collective motions
Generation of basis states: Imaginary-time method in 3D coordinate space

**Long-range** correlations in terms of the configuration mixing

**Imaginary-time Method**

\[ |\phi_i^{(n+1)}\rangle = e^{-\Delta t \hbar [\rho]} |\phi_i^{(n)}\rangle, \quad i = 1, \cdots A \]

A well-known method in the Skyrme HF calculations

3D space is discretized in lattice

Single-particle orbital:

\[ \phi_i (\mathbf{r}) = \{\phi_i (\mathbf{r}_k)\}_{k=1, \cdots M}, \quad i = 1, \cdots, N \]
Generation of many S-det’s

Initial state

3D real space

Gaussian wave packets (n & p) whose positions are determined by random numbers.

\[ |\phi_{i}^{(n+1)}\rangle = e^{-\Delta t \hbar \rho} |\phi_{i}^{(n)}\rangle, \quad i = 1, \cdots A \]

Imaginary-time evolution

\(12\text{C}\)

\[E \text{ [MeV]} \]

\[\# \text{ of iterations} \]
Screening of Slater determinants

Every one-hundred iterations, we pick up a Slater determinant $|\Phi_i\rangle$.

$|\Phi_i\rangle$ is adopted as the $(M+1)$-th basis configuration, if it satisfies

$$\langle \Phi_i | H | \Phi_i \rangle < E_{HF} + 30 \text{ MeV}$$

$$\langle \Phi_i | \Phi_j \rangle < 0.7 \quad (j = 1, \ldots, M)$$
3D angular momentum projection

Parity and angular momentum projected state

\[
\left| \Psi_{M}^{J \pm} \right\rangle = \frac{2J+1}{8\pi^2} \sum_{K} g_{K} \int d\Omega D_{MK}^{J*}(\Omega) \hat{R}(\Omega) \left| \Phi^{\pm} \right\rangle
\]

\[
\hat{R}(\Omega) = e^{-i\alpha \hat{J}_z} e^{-i\beta \hat{J}_y} e^{-i\gamma \hat{J}_z}
\]

Parity-projected SD

Construct the angular momentum eigenstate by the explicit 3D rotation
Further Selection ...

Eigenvalues of the norm matrix

\[ N_{nK,mK'}^{J^\pm} = \left\langle \Phi^n \left| P_{KK'}^J P^\pm \right| \Phi^m \right\rangle \]

smaller than $10^{-3}$

Garbage box

Small norm only
Numerical detail

• Three-dimensional (3D) Cartesian mesh
  – Mesh size: 0.8 fm
  – All the mesh points inside the sphere of radius of 8 fm

• Euler angles
  – Discretization
    \((\alpha, \beta, \gamma) = (18, 30, 18)\) points

• Numerical difficulties
  – Limiting number of SD
  – 50 Slater determinantns
How complete is the calculation?

- Ten different sets of Slater determinants, generated with different random numbers.
- Low-energy spectra within several hundred keV
- Transition strength within about 10% 

$^{12}\text{C}$
$^{12}\text{C}$ (Sly4)

Exp: M. Chernykh et al., PRL 98, 032501 (2007)
GCM: E. Uegaki, et al., PTP 57, 4 (1977) 1262
RGM: M. Kamimura, NPA 351, 456-480 (1981)

B(E2) in units of e$^2$fm$^4$
Hoyle state: $0^{2+}$

- $41.2\%$
- $36.1\%$
- $31.7\%$
- $28.9\%$

Superposition of many SDs

Correlation energy is 5 MeV

Hoyle state is around 9 MeV

Ground-state rotational band

$0^+_1$
- $89.8\%$
- $86.9\%$
- $86.2\%$

70\% for HF state

Valid points:
- ✓ Correlation energy is 5 MeV
- ✓ Hoyle state is around 9 MeV
- ✓ Ground-state rotational band
Radius, B(E2), B(E3), M(E0)

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>EXP (fm)</th>
<th>present (fm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0_1^+$</td>
<td>2.31(2)</td>
<td>2.52±0.01</td>
</tr>
<tr>
<td>$0_2^+$</td>
<td>2.73±0.02</td>
<td></td>
</tr>
<tr>
<td>$0_3^+$</td>
<td>3.20±0.05</td>
<td></td>
</tr>
<tr>
<td>$2_1^+$</td>
<td>2.60±0.01</td>
<td></td>
</tr>
</tbody>
</table>

Linear-chain state

<table>
<thead>
<tr>
<th>Transitions</th>
<th>Exp (fm)</th>
<th>Cal (fm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B(E2; 2_1^+ \rightarrow 0_1^+)$</td>
<td>7.6±0.4</td>
<td>8.6 ±0.2</td>
</tr>
<tr>
<td>$B(E2; 4_1^+ \rightarrow 2_1^+)$</td>
<td>13.4±0.5</td>
<td></td>
</tr>
<tr>
<td>$B(E2; 0_2^+ \rightarrow 2_1^+)$</td>
<td>13±2</td>
<td>13.6±1.2</td>
</tr>
<tr>
<td>$B(E2; 2_2^+ \rightarrow 0_2^+)$</td>
<td>0.17±0.23</td>
<td></td>
</tr>
<tr>
<td>$B(E2; 2_3^+ \rightarrow 0_2^+)$</td>
<td>5.9±0.7</td>
<td></td>
</tr>
<tr>
<td>$B(E2; 2_4^+ \rightarrow 0_2^+)$</td>
<td>10±1</td>
<td></td>
</tr>
<tr>
<td>$B(E2; 2_4^+ \rightarrow 0_3^+)$</td>
<td>91±13</td>
<td></td>
</tr>
<tr>
<td>$B(E2; 4_2^+ \rightarrow 2_4^+)$</td>
<td>131±22</td>
<td></td>
</tr>
<tr>
<td>$B(E3; 3_1^- \rightarrow 0_1^+)$</td>
<td>107 ±14</td>
<td>77 ± 4</td>
</tr>
<tr>
<td>$M(E0; 0_1^+ \rightarrow 0_2^+)$</td>
<td>5.4±0.2</td>
<td>4.5±0.2</td>
</tr>
</tbody>
</table>
The lowest negative-parity state in each $J$ A few MeV higher than experiment.
Charge form factors

- Elastic (ground)

\[ |F(q)|^2 \sim q^2 (\text{fm}^{-2}) \]

Inelastic (\(0_1^+ \rightarrow 0_2^+\))

Too large diffuseness
Functional dependence

- Robust result
  - G.s. correlation energy varies by about 1 MeV
# Hoyle state

## Radius

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>present</th>
<th>AMD</th>
<th>FMD</th>
<th>$3\alpha$RGM</th>
<th>BEC</th>
<th>$3\alpha$GCM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0_1^+$</td>
<td>2.53 ± 0.03</td>
<td>2.53</td>
<td>2.39</td>
<td>2.40</td>
<td>2.40</td>
<td>2.40</td>
</tr>
<tr>
<td>$0_2^+$</td>
<td>2.72 ± 0.003</td>
<td>3.27</td>
<td>3.38</td>
<td>3.47</td>
<td>3.83</td>
<td>3.40</td>
</tr>
<tr>
<td>$0_3^+$</td>
<td>3.15 ± 0.02</td>
<td>3.98</td>
<td>4.62</td>
<td></td>
<td></td>
<td>3.52</td>
</tr>
<tr>
<td>$2_1^+$</td>
<td>2.61 ± 0.002</td>
<td>2.66</td>
<td>2.50</td>
<td>2.38</td>
<td>2.38</td>
<td>2.36</td>
</tr>
</tbody>
</table>

*Hoyle state*  
*Linear-chain state*

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**Monopole transition**

$$M(E0; 0_1^+ \rightarrow 0_2^+) = 4.5 \pm 0.2 \text{ e fm}^2$$

- 5.4 ± 0.2 \hspace{1cm} \text{Experiment}
- 6.5 – 6.7 \hspace{1cm} \text{Other cal. based on the gaussian anszats}
Shrinkage of the Hoyle state

3-alpha configurations used in the GCM calculation by Uegataki et al.
E. Uegaki, et al., PTP57,4 (1977)1262

<table>
<thead>
<tr>
<th>EXP</th>
<th>IT</th>
<th>IT + 3α</th>
<th>3α</th>
<th>3α(Uegaki)</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius($0^+_1$)</td>
<td>2.31±0.02</td>
<td>2.53</td>
<td>2.54</td>
<td>2.80</td>
</tr>
<tr>
<td>radius($0^+_2$)</td>
<td>2.76</td>
<td>2.73</td>
<td>3.31</td>
<td>3.40</td>
</tr>
<tr>
<td>$M(E0; 0^+_2 \rightarrow 0^+_1)$</td>
<td>5.4±0.2</td>
<td>4.57</td>
<td>4.13</td>
<td>8.72</td>
</tr>
</tbody>
</table>

- 3-alpha configurations keep the radius of Hoyle state large.
- Other configurations generated by the imaginary-time propagation makes it much smaller.
FIG. 10. Density distributions of some SDs out of 31 SDs which are used in Ref. [21]. Unit of vertical and horizontal axes are fm.

Table VII. Radii and $M(E_0)$ in various sets of SD. Results of GCM calculation is also shown [21].

$\Delta E \approx 20$ MeV
Large energy gain mostly associated with the spin-orbit force

$E_{HF} = -90.6$ MeV
Adopting the three-alpha configurations utilized in GCM: E. Uegaki, et al., PTP57,4 (1977)1262
POSITIVE parity

$^{12}\text{C} + \alpha(?)$ like

$0^+_2 : 67.0\%$
$2^+_1 : 66.4\%$
$4^+_2 : 43.1\%$

HF state: 80%

✓ correlation energy is 3.3MeV
NEGATIVE parity

$^{12}$C + $\alpha(\,\,?)$ like

parity doublet partner

particle-hole-like excitation

arrows: $B(E2) (e^2 fm^4)$

$^{16}$O

✓ particle-hole excitation is good agreement with experimental values
$^{20}\text{Ne (Sly4)}$

**POSITIVE parity**

$^{16}\text{O} + \alpha$ (?)

- $0^+_1 : 81.4\%$
- $2^+_1 : 83.1\%$
- $4^+_1 : 66.8\%$

- Correlation energy of about 6 MeV
- B(E2) in good agreement
- Too large moment of inertia
\( ^{20}\text{Ne (Sly4)} \) \( K^\pi = 0^- \)

Overlap

- \( 1^-_2 : 78.7\% \)
- \( 3^-_4 : 75.8\% \)
- \( 5^-_4 : 66.0\% \)

\( K^\pi = 2^- \)

Overlap

- \( 2^-_1 : 90.5\% \)
- \( 3^-_1 : 85.8\% \)
- \( 4^-_4 : 83.1\% \)
- \( 5^-_1 : 74.6\% \)

\((0p)^{-1}(sd)^5\) structure

**NEGATIVE parity**

\[ \begin{align*}
17 & : 83.6 \\
57 & : 57.6 \\
87.7 & : 87.7 \\
\end{align*} \]

\begin{align*}
83.6 & : 117 \\
57.6 & : 164 \pm 26 \\
87.7 & : < 808 \\
\end{align*} \]

**Candidate for parity-doublet partner**

\( K^\pi = 2^- \) band: \( (p)^{-1}(sd)^5 \)

**arrows: B(E2) \( (e^2fm^4) \)**
Computational cost of finite range interaction

**Skyrme interaction**

\[
\langle \Phi | \hat{V}_{t0}^F | \Phi \rangle = -\frac{t_0}{2} x_0 \sum_{i,j} \langle \phi_i \phi_j | \delta(\vec{r}_1 - \vec{r}_2) \hat{P}_r \hat{P}_\sigma \hat{P}_T | \phi_i \phi_j \rangle \\
= -\frac{t_0}{2} x_0 \sum \int d\vec{r} \rho(\vec{r})^2 \quad \rho(\vec{r}) = \sum_{i,\sigma} \phi_i^*(\vec{r}, \sigma) \phi_i(\vec{r}, \sigma)
\]

Computational cost: \( N_x^3 \times N_i \)

**Gogny interaction**

\[
\langle \Phi | \hat{V}_{Wl}^F | \Phi \rangle = -\frac{W_l}{2} \sum \int d\vec{r} \int d\vec{r}' \rho(\vec{r}\sigma, \vec{r}'\sigma') \rho(\vec{r}'\sigma', \vec{r}\sigma) \exp\{- (\vec{r} - \vec{r}')^2 / \mu_l^2 \}
\]

\[
\rho(\vec{r}\sigma, \vec{r}'\sigma') \equiv \sum_{i,\sigma} \phi_i^*(\vec{r}, \sigma) \phi_i(\vec{r}', \sigma') \quad \text{Computational cost: } N_x^6 \times N_i
\]

✓ Same scaling of orbit as the case of Skyrme interaction
✓ scaling of space is power of two
Method 1: finite spherical lattice

\[ W_l \text{ Fock term} \]

\[ V_{W_l}^F = - \frac{W_l}{2} \sum_{\tau} \int d\vec{r} \int d\vec{r}' \rho(\vec{r}, \sigma) \rho(\vec{r}', \sigma') \rho(\vec{r}, \sigma') \exp\left\{-(\vec{r} - \vec{r}')^2 / \mu_l^2\right\} \]

\[ \rho(\vec{r}, \sigma, \vec{r}', \sigma') \equiv \sum_{i,\sigma} \phi_i^*(\vec{r}, \sigma) \phi_i(\vec{r}', \sigma') \]

The range of Gogny interaction is about 4 fm.

it is sufficient to integrate \( r' \) inside 4fm sphere.

Numerical cost: \( N^3_x \times M \times N_i \)

cf. Skyrme interaction

\( N^3_x \times N_i \)

✓ Same scaling as the case of Skyrme interaction, except M
**positive parity**

$^{12}$C

**Computational cost is 7.5 times**

**Energy spectrum is almost same**

Integral points: $(\alpha, \beta, \gamma) = (18, 30, 18)$

512 core x 1.8h
45 SDs

SR16000@YITP
negative parity

$^{12}\text{C}$

Energy spectrum is almost same
Summary

- Complete low-lying spectroscopy with the Skyrme Hamiltonian
- Capable of describing a variety of excited states in a unified way, such as vibrational excitations, cluster excitations, single-particle excitations.

Problems

- $2^{\text{nd}} 0^+$ state in $^{16}\text{O}$
  - Energy too high by about 3 MeV
  - B(E2) Underestimated
  - Center of mass? Weak-coupling phenomena?

- Moment of inertia of $^{20}\text{Ne}$
  - Too large
  - Pairing?

- Hoyle state
  - All properties reasonably agree with experiments, except for its radius.
  - Three-alpha configurations produce a large radius
  - Configuration mixing with other states makes the Hoyle state shrunk

Shinohara et al, PRC 74, 054315 (2006)
Fukuoka et al, in preparation