Probing shell evolution with large-scale shell-model calculations

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Mutual communication among microscopic, empirical, and phenomenological approaches becomes important.
Monopole matrix elements: case of $pf$-shell

- Strong $j_j > j'_j$ attraction particularly for the $T=0$ channel: tensor
- Empirical interaction: overall repulsive shift for the $T=1$ monopole

Monopole-based universal interaction $V_{MU}$

(a) central force:
Gaussian
(strongly renormalized)

(b) tensor force:
$\pi + \rho$ meson exchange

$V_{MU} = \quad + \quad$


- Bare tensor
  - Renormalization persistency
- Phenomenological Gaussian central
  - Supported by empirical interactions
Effect of three-nucleon forces

- Contributing to repulsion in $T=1$ two-body forces
- Ab-initio-type calculations give similar effects.
- $V_{\text{MU}}$ includes this effect implicitly.

Outline of this talk

• Shell-model calculations using $V_{MU}$ combined with empirical interactions

1. Shell evolution caused by $T=1$ monopole interactions
   1. Unnatural-parity states of neutron-rich Si isotopes (very briefly)
   2. Unnatural-parity states of neutron-rich Cr-Ni isotopes
   3. Unnatural-parity states of neutron-rich Ca isotopes

2. Application of large-scale shell-model calculation to photonuclear reactions
   – Ca isotopes

3. Analyzing shell-model wave functions in terms of mean-field picture
   – Origin of the exotic isomeric $4^+$ state in $^{44}\text{S}$
Collaborators

- $V_{\text{MU}}$: T. Otsuka, T. Suzuki, M. Honma, K. Tsukiyama, N. Tsunoda, M. Hjorth-Jensen
- sd-pf: T. Otsuka, B. A. Brown, M. Honma, T. Mizusaki, N. Shimizu
- Cr-Ni: T. Togashi, N. Shimizu, T. Otsuka, M. Honma
- Ca: T. Otsuka, N. Shimizu, M. Honma, T. Mizusaki
- E1: N. Shimizu, T. Otsuka, S. Ebata, M. Honma
- $^{44}\text{S}$: N. Shimizu, T. Otsuka, T. Yoshida, Y. Tsunoda
Refined $V_{MU}$ for the shell-model

• tensor: $\pi+\rho$

• spin-orbit: M3Y
  - Works in some cases

• central: to be close to GXPF1
  - Including "density dependence" to better fit empirical interactions

A good guide for a shell-model interaction without direct fitting to experiment

Y. Utsuno et al., EPJ Web of Conferences 66, 02106 (2014).
$T=1$ monopole: case of $sd$-$pf$ shell

- SDPF-MU interaction based on the refined $V_{MU}$
  - USD for the $sd$ shell and GXPF1B for the $pf$ shell
  - Refined $V_{MU}$ for the cross-shell

Cross-shell of SDPF-U: two-body G martix

Evolution of unnatural-parity states in Si

The gap changes with increasing neutrons in $f_{7/2}$ depending on the $T=1$ monopole strength.

Unnatural-parity states are good indicators of the gap.

- A recent experiment at NSCL supports nearly zero value of $T=1$ cross-shell monopole matrix elements.

Sharp drop of the $9/2^+$ level in Cr, Fe and Ni

Experimental $9/2^+$ levels in Cr, Fe, and Ni isotopes

- Does this mean the reduction of the $N=40$ gap due to the $T=1$ monopole interaction?
Shell-model calculation


• Model space
  – Valence shell: full $pf$ shell + $0g_{9/2} + 0d_{5/2}$
  – Allowing up to one neutron excitation from the $pf$ shell to the upper orbits
    • $N \leq 35$ isotopes are $pf$-shell nuclei
    • One can use an empirical $pf$-shell interaction as it is because of no coupling to 2p-2h or 3p-3h configurations.
  – $M$-scheme dimension: up to $1.8 \times 10^{10}$ for $^{59}$Ni (manageable with KSHELL)

• Effective interaction
  – GXPF1Br for the $fp$ shell + the refined $V_{MU}$
  – One modification for $\langle g_{9/2}f_{5/2}|V|g_{9/2}f_{5/2}; J, T = 1 \rangle$
  – SPE of $g_{9/2}$ (one free parameter): determined to fit the overall $9/2^+$ levels
  – SPE of $d_{5/2}$: not sensitive to the results; effective gap from $g_{9/2} \approx 2$ MeV
Good agreement including unfavored-signature states
Evolution of the $9/2^+$ levels

- Positions and spectroscopic strengths are well reproduced.
  - Large single-neutron amplitudes for the $9/2^+$
Evolution of the $g_{9/2}$ orbit

- $g_{9/2}$ and $d_{5/2}$ orbits are kept almost constant with $N$.
  - Due to nearly zero $T=1$ cross-shell monopole matrix elements according to $V_{\text{MU}}$
- Simple estimate of the location of $g_{9/2}$ from measurement
  - Binding energy of the $9/2^+$ level measured from the even-$N$ core $= -S_n + E_x(9/2^+)$
  - Nearly constant with $N$ both from experiment and calculation
Investigating $g_{9/2}$ in $n$-rich Ca isotopes

• $g_{9/2}$ orbit in neutron-rich Ca isotopes
  – Plays a crucial role in determining the drip line and the double magicity in $^{60}$Ca

• What is learned from the study of Cr-Ni isotopes
  – The $g_{9/2}$ orbit does not change sharply at least for $N \leq 35$ isotopes.
  – Similar evolution should occur in Ca isotopes, too.

• How to spot the position of $g_{9/2}$ in Ca isotopes?
  – Unnatural-parity states: similar to Cr-Ni cases
  – One should also take into account excitation from the $sd$ shell to the $pf$ shell:
    not dominant in Cr-Ni region
Shell-model calculation

• Model space
  – Full sd-pf-sdg shell
  – Allowing one nucleon excitation from the sd shell to the pf shell or the pf shell to the sdg shell:
    full $1\hbar\omega$ calculation

• Effective interaction
  – A natural extension of SDPF-MU and the one used for Cr-Ni isotopes:
    SDPF-MU for the sd-pf shell + the refined $V_{\text{MU}}$ for the other
    • SDPF-MU: USD (sd) + GXPF1B (pf) + the refined $V_{\text{MU}}$ for the other
  – SPE of $g_{9/2}$: needed to refit because of activating excitation from sd to pf
    → determined to fit the $9/2^+$ level in $^{50}\text{Ti}$ ($C^2S = 0.37$ or 0.54)
  – SPE of other sdg orbits: to follow schematic Nilsson SPE
Systematics of the $3^-_1$ state in even-$A$ Ca

- Three calculations
  A) excitations from $sd$ to $pf$ only
  B) excitations from $pf$ to $sdg$ only
  C) full $1\hbar\omega$ configurations

- $3^-_1$ levels
  - $sd$-$pf$ calc.
    - good agreement for $N \leq 28$
    - large deviation for $N > 28$
  - full $1\hbar\omega$ calc.
    - Strong mixing with the $sdg$ configuration accounts for the stable positioning of the $3^-_1$ levels.
$3^{-}_1$ configuration probed by direct reaction

- $^{50}\text{Ca}$: strongly populated by the $^{48}\text{Ca}(t, p)$ reaction
  - neutron excitation

- $^{52}\text{Ca}$: strongly populated by the $2p$ knockout from $^{54}\text{Ti}$
  - proton excitation

<table>
<thead>
<tr>
<th>State</th>
<th>Energy (MeV)</th>
<th>$\theta$ (angle in c.m. system)</th>
<th>$\frac{d\sigma(\theta)}{d\Omega}$ (exp)</th>
<th>$\frac{d\sigma(\theta)}{d\Omega}$ (th. $r^4 = 0$)</th>
<th>$\frac{d\sigma(\theta)}{d\Omega}$ (th. $r^4 = 0.02$)</th>
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<td>g.s.</td>
<td>0</td>
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<td>100</td>
<td>100</td>
<td>100</td>
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<tr>
<td>$2^+_1$</td>
<td>1.03</td>
<td>$20^\circ$</td>
<td>42</td>
<td>39</td>
<td>32</td>
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<td>36</td>
<td>40</td>
<td>36</td>
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<td>$0^+_3$</td>
<td>3.53</td>
<td>$5^\circ$</td>
<td>2</td>
<td>5.5</td>
<td>2.4</td>
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<tr>
<td>(3$^-$)</td>
<td>3.99</td>
<td>$28^\circ$</td>
<td>21</td>
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<td>37</td>
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<td>$0^+_3$</td>
<td>4.47</td>
<td>$5^\circ$</td>
<td>2.2</td>
<td>1.0</td>
<td>0.5</td>
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</table>


Without the strong mixing between proton and neutron excitations these properties are hard to explain because larger-$N$ nuclei should be more easily excited to higher orbits.
Energy levels of $^{49}$Ca

- $^{48}$Ca + $n$ system
  - Single-particle structure may appear.
  - Core-coupled states can compete in high excitation energies.

- $9/2^+$ state at 4.017 MeV
  - Firm spin-parity assignment made recently (D. Montanani et al., PLB 697, 288 (2011); PRC 85, 044301 (2012)).
    - Interpreted as core-coupled state.
  - Present calc.: Strong mixing with $g_{9/2}$ is also important.
    - Good B(E3)

<table>
<thead>
<tr>
<th>$3/2^+_1$</th>
<th>$5/2^+_1$</th>
<th>$7/2^+_1$</th>
<th>$9/2^+_1$</th>
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<tbody>
<tr>
<td>% of sdg</td>
<td>6</td>
<td>9</td>
<td>7</td>
</tr>
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Systematics of $g_{9/2}$ strength in $N=29$ isotones

<table>
<thead>
<tr>
<th></th>
<th>dimension</th>
<th>$E_x$ (MeV)</th>
<th>$C^2S$ ($n$ attached)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{49}$Ca</td>
<td>2,515,437</td>
<td>4.02</td>
<td>3.80</td>
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<tr>
<td>$^{51}$Ti</td>
<td>187,386,759</td>
<td>3.77</td>
<td>3.77</td>
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<tr>
<td>$^{53}$Cr</td>
<td>3,411,147,908</td>
<td>3.71</td>
<td>4.04</td>
</tr>
</tbody>
</table>

- $9/2^+$ of $N=29$ isotones
  - Shell-model calc. is possible up to $^{53}$Cr.
  - Strong mixing with $g_{9/2}$ for all the isotones in calc. but small $C^2S$ for $^{49}$Ca in expt.
  - Effect of the doublet? (see right)

Systematics of the $9/2^+_1$ state in odd-A Ca

- $9/2^+_1$ in the *sd-pf* calculation
  - Core-coupled state
  - Located stably at 5-6 MeV
- $9/2^+_1$ in the *pf-sdg* calculation
  - Sharply decreasing due to the shift of the Fermi level
- $9/2^+_1$ in the *full 1$\hbar\omega$* calculation
  - 3-4 MeV up to $N=33$ but drops considerably at $N=35$
    - Different from Cr-Ni
  - The state at $N=55$ is nearly a single-particle character.
    - Interesting to observe at FRIB
Neutron effective single-particle energy

- Global behavior
  - Stable due to very weak $T=1$ monopole matrix elements
- Location of $g_{9/2}$
  - 2-3 MeV higher than $f_{5/2}$
  - Whether $^{60}\text{Ca}$ is a good doubly magic nucleus depends on the evolution of $f_{5/2}$ in going from $N=34$ to 40, which is dominated by the $T=1 f_{5/2}-f_{5/2}$ monopole interaction.
    - Is there experimental data that can constrain this monopole?

Ca isotopes

- Rather stable
- Fermi surface
Application to photonuclear reaction

N. Shimizu et al., in preparation

- A good Hamiltonian for the full $1\hbar \omega$ space is constructed.
- It is expected that photonuclear reaction, dominated by $E1$ excitation, is well described with this shell-model calculation:

$$\sigma_{\text{abs}}(E) = \frac{16\pi^3 E}{9\hbar c} S_{E1}(E)$$

with $S_{E1}(E) = \sum_{\nu} B(E1; \text{g.s.} \rightarrow \nu) \delta(E - E\nu + E_0)$

- Shell-model calculation provides good level density, including non-collective levels, the coupling to which leads to the width of GDR.
- Application of shell model to photonuclear reaction has been very limited due to computational difficulty.

- Sagawa and Suzuki (O isotopes), Brown ($^{208}$Pb)
Lanczos strength function method

• It is almost impossible to calculate all the eigenstates concerned using the exact diagonalization.

  – The shape of the strength function can be obtained with much less Lanczos iterations.
    1. Take an initial vector: $\bar{v}_1 = T(E1)|\text{g. s.}\rangle$
    2. Follow the usual Lanczos procedure
    3. Calculate the strength function $\sum_{\nu} B(E1; \text{g. s.} \rightarrow \nu) \frac{1}{\pi} \frac{\Gamma/2}{(E-E_{\nu}+E_0)^2+(\Gamma/2)^2}$ by summing up all the eigenstates $\nu$ in the Krylov subspace with an appropriate smoothing factor $\Gamma$ until good convergence is achieved.
Convergence of strength distribution

1 iter.

100 iter.

300 iter.

1,000 iter.
Comparison with exact diagonalization

- Smoothing width: $\Gamma = 1$ MeV
- No visible difference between the two methods
Comparison with experiment for $^{48}$Ca

- GDR peak position: good
- GDR peak height: overestimated
- Low-lying states: about 0.7 MeV shifted

Need for $2\hbar\omega$ (g.s.) and $3\hbar\omega$ (1⁻)?
Beyond $1\hbar\omega$ calculation

- $3\hbar\omega$ states in the $sd$-$pf$-$sdg$ shell are included.
  - No single-nucleon excitation to the $3\hbar\omega$ above shell
- Dimension becomes terrible!
KSHELL: MPI + OpenMP hybrid code

- **$M$-scheme code**
  - “On the fly”: Matrix elements are not stored in memory (analogous to ANTOINE and MSHELL64)

- **Good parallel efficiency**
  - Owing to categorizing basis states into “partition”, which stands for a set of basis states with the same sub-shell occupancies


**Parallel performance**

- $^{56}$Ni, pf-shell $10^9$dim.

**Speedup**

- Time/iteration: 25 min. (16 cores) $\Rightarrow$ 30 sec. (1024 cores)
Removal of spurious center-of-mass motion

- Usual prescription of Lawson and Gloeckner
  \[ H' = H + \beta H_{CM} \text{ with } \beta = 10\hbar\omega/A \text{ MeV} \]
  - Confirming that eigenstates are well separated

\[ \langle H_{CM} \rangle - \frac{3}{2} \hbar\omega \approx 0 \]

\[ \langle H_{CM} \rangle - \frac{3}{2} \hbar\omega >> 0 \]
Effect of larger model space

- GDR peak height is improved.
- Low-energy tail is almost unchanged.
Development of pygmy dipole resonance

- PDR develops for $A \geq 50$, but the tail of GDR makes the peak less pronounced.
Analyzing SM w.f. in terms of mean-field


• Motivated by a recent experiment on $^{44}\text{S}$
  – Very hindered $E2$ transition from the $4^+_1$ to the $2^+_1$ state.
  – Shell-model calculation using the SDPF-U interaction “predicts” this property.

• What is the origin of this exotic behavior?
  – Comprehensive description is desired.

Variation after angular-momentum projection

• Optimize the energy $E_{\text{AMVAP}} = \frac{\langle \Psi^I | H | \Psi^I \rangle}{\langle \Psi^I | \Psi^I \rangle}$ within the angular-momentum projected Slater determinant $|\Psi^I\rangle = \sum_K g_K \hat{P}_{MK} |\Phi\rangle$ with $|\Phi\rangle = a_1^\dagger \cdots a_n^\dagger |0\rangle$ and $a_k^\dagger = \sum_l D_{lk} c_l^\dagger$.
  
  – One-basis limit of MCSM

• Model space and effective interaction
  
  – SDPF-MU in the $\pi(sd)\nu(pf)$ shell

• Intrinsic properties of the variation after angular-momentum projected (AM-VAP) wave function
  
  – Deformation ($\beta, \gamma$): from $Q_0$ and $Q_2$ of $|\Phi\rangle$
  
  – Distribution of $K$ numbers: from $g_K$
An isometric $4^+_1$ state is obtained both in the SM and the AM-VAP.
Overlap probability between SM and AM-VAP

- $|\langle \Psi(SM)^{IM} | \Psi(AMVAP)^{IM} \rangle|^2$ is a good measure for the quality of AM-VAP states.

$$\langle \Psi(SM)^{IM} | \Psi(AMVAP)^{IM} \rangle = \langle \Psi(SM)^{IM} | \sum g_K \hat{P}^I_{MK} | \Phi \rangle = \sum g_K^* \langle \Phi | \hat{P}^I_{KM} | \Psi(SM)^{IM} \rangle^* = \sum g_K^* \langle \Phi | \Psi(SM)^{IK} \rangle^*$$

<table>
<thead>
<tr>
<th>AM-VAP</th>
<th>SM</th>
<th>Overlap probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1$</td>
<td>$0^+_1$</td>
<td>0.915</td>
</tr>
<tr>
<td>$2^+_1$</td>
<td>$2^+_1$</td>
<td>0.808</td>
</tr>
<tr>
<td>$3^+_1$</td>
<td>$3^+_1$</td>
<td>0.755</td>
</tr>
<tr>
<td>$4^+_1$</td>
<td>$4^+_1$</td>
<td>0.859</td>
</tr>
<tr>
<td>$4^+_2$</td>
<td>$4^+_2$</td>
<td>0.881</td>
</tr>
<tr>
<td>$5^+_1$</td>
<td>$5^+_1$</td>
<td>0.895</td>
</tr>
<tr>
<td>$6^+_1$</td>
<td>$6^+_1$</td>
<td>0.545</td>
</tr>
<tr>
<td></td>
<td>$6^+_2$</td>
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</tr>
<tr>
<td>$6^+_2$</td>
<td>$6^+_2$</td>
<td>0.538</td>
</tr>
<tr>
<td></td>
<td>$6^+_1$</td>
<td>0.392</td>
</tr>
</tbody>
</table>

AM-VAP w.f.’s are good approximations to the shell model including $4^+_1$. 
Intrinsic properties in $^{44}\text{S}$

| $I^\pi_\sigma$ | $|K|$ | $\beta$ | $\gamma$ |
|---------------|------|--------|--------|
|               | 0    | 1      | 2      | 3      | 4      | 5      | 6      |
| $0^+_1$       | 1.00 |        |        |        |        |        |        |
| $2^+_1$       | 0.98 | 0.00   | 0.01   |        |        |        |        |
| $4^+_2$       | 0.92 | 0.08   | 0.00   | 0.00   | 0.00   |        |        |
| $6^+_1$       | 0.76 | 0.23   | 0.01   | 0.00   | 0.00   | 0.00   | 0.00   |
| $4^+_1$       | 0.00 | 0.00   | 0.00   | 0.07   | 0.93   |        |        |
| $5^+_1$       | 0.00 | 0.00   | 0.01   | 0.08   | 0.85   | 0.07   |        |
| $6^+_2$       | 0.00 | 0.01   | 0.01   | 0.14   | 0.80   | 0.04   | 0.00   |

- $K=0$ and $K=4$ bands
  - $K=0$: usual yrast property; growing $K=1$ with spin due to the Coriolis coupling
  - $K=4$: Concentration of $K$ in spite of significant triaxiality
    - Diagonalization in $K$ space works.
Why yrast $K=4$ state?: a hint from $^{43}\text{S}$

- Isomeric $7/2^-\_1$ state in $^{43}\text{S}$
  - Reproduced by full calc. and AM-VAP
  - $K$ forbiddeness between $K=1/2$ and $K=7/2$ bands
- Consistent with AMD calc. (Kimura et al., 2013)
- The band-head energies are very close
Unified understanding of isomerism in sulfur

- Two quasiparticle orbits $\Omega=1/2$ and $\Omega=7/2$
  - Located close in energy
- $K=4$: dominated by the two-quasiparticle state $\Omega=1/2 \times \Omega=7/2$
  - $K=0$ vs. $K=4$ $4^+$: competition between pairing and rotational energies
    - $2\Delta \approx 2.5$ MeV $< \text{rotational energy} \approx 3$ MeV
- Two $K=0$ states: origin of the very low $0^+_2$
Summary

• Shell evolution caused by $T=1$ cross-shell monopole matrix elements is investigated with large-scale shell-model calculations.

  1. Evolution of the unnatural-parity states of neutron-rich Si
  2. Evolution of the $9/2^+$ states of neutron-rich Cr-Ni isotopes

Comparison with experiment indicates nearly zero monopole matrix elements, which is consistent with the $V_{\text{MU}}$ interaction.

• The evolution of the $g_{9/2}$ orbit in Ca isotopes is discussed.
  — Competition and mixing with core-coupled states

• $E1$ strength functions in Ca isotopes are calculated.
  — Correlation due to coupling to $p-h$ states decreases the total $B(E1)$ values.

• Intrinsic properties of SM w.f. are discussed using variation after angular-momentum projection.
  — Demonstrating a $K=4$ isomer in $^{44}\text{S}$