Effective Interactions and Large-scale Shell-model Calculations in Sn-Isotopes

"Progress report" and some preliminary results

Eivind Osnes
Department of Physics
University of Oslo
Outline

1. Objectives
2. Effective interactions for the shell model
   - brief reminder
3. Shell-model calculations
   - large-scale (~ 10 ± valence nucleons)
4. Summary and outlooks

T. Engeland, M. Hjorth-Jensen, M. Kartamyshev, E. Osnes
Objectives

- Describe properties of complex nuclei (binding energies, energy spectra, electromagnetic moments and transition rates, etc.) in terms of their constituent particles and the interactions among those particles, focus on general trends rather than details
- Constituent particles = protons and neutrons
- Interaction = effective interaction taking into account the ignored degrees of freedom
- Complex nuclei = medium-heavy and heavy nuclei
- Computation method = shell model wrt inert core
Model-space eigenvalue problem

Instead of solving the full eigenvalue

\[ H \Psi_i(1, \ldots, A) = E_i \Psi_i(1, \ldots, A) \]

we solve a model/valence-space eigenvalue problem with an effective Hamiltonian

\[ PH_{\text{eff}} P \Psi_\mu = P(H_0 + V_{\text{eff}}) P \Psi_\mu = E_\mu P \Psi_\mu \]

with operator \( P \) projecting onto model space, and

\[ H_{\text{eff}} = \tilde{H}_0 + V_{\text{eff}}^{(2)} + V_{\text{eff}}^{(3)} + \ldots \]

\[ \tilde{H}_0 = H_0 + V_{\text{eff}}^{(1)} \]
Q-box formulation of effective interaction

• Construct effective interaction from Q-box formulation of Kuo and collaborators

\[ P \hat{Q} P = P G P + P \left( G \frac{Q}{\omega - H_0} G \right. \]
\[ \left. + G \frac{Q}{\omega - H_0} G \frac{Q}{\omega - H_0} G + \ldots \right) P \]

• Including folded diagrams by differentiation wrt starting energy

\[ V_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \ldots \]

\[ V_{\text{eff}}(n) = \hat{Q} + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{d^m \hat{Q}}{d\omega^m} \{V_{\text{eff}}(n - 1)\}^m \]
# Shell model in Sn isotopes

The light Sn isotopes with $50 < N < 82$

<table>
<thead>
<tr>
<th>PROTONS</th>
<th>NEUTRONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q$-space: $N &gt; 82$</td>
<td></td>
</tr>
<tr>
<td>$h_{11/2}^-$</td>
<td></td>
</tr>
<tr>
<td>3.2 MeV</td>
<td></td>
</tr>
<tr>
<td>$d_{3/2}^+$</td>
<td></td>
</tr>
<tr>
<td>2.55 MeV</td>
<td></td>
</tr>
<tr>
<td>$s_{1/2}^+$</td>
<td></td>
</tr>
<tr>
<td>2.45 MeV</td>
<td></td>
</tr>
</tbody>
</table>

$Q$-space for particles

$Q$-space: $Z > 50$

$Q$-space: $Z \leq 50$

The heavy Sn isotopes with $50 < N < 82$

<table>
<thead>
<tr>
<th>PROTONS</th>
<th>NEUTRONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q$-space: $N &gt; 82$</td>
<td></td>
</tr>
<tr>
<td>$g_{7/2}^+$</td>
<td></td>
</tr>
<tr>
<td>2.43 MeV</td>
<td></td>
</tr>
<tr>
<td>$d_{5/2}^+$</td>
<td></td>
</tr>
<tr>
<td>1.66 MeV</td>
<td></td>
</tr>
</tbody>
</table>

$Q$-space for holes

$Q$-space: $Z > 50$

$Q$-space: $Z \leq 50$

$Q$-space: $N \leq 50$

**Effective interaction:**

Q-box to 3rd order with 2hw excitations + folding

G-mtx evaluated w Bonn B interaction
Calculated $^{101}\text{Sn}$ based on $^{132}\text{Sn}$ core

$\hbar_{11/2}^-$: 3.2 MeV
$\Delta_{3/2}^+$: 2.55 MeV
$\Delta_{1/2}^+$: 2.45 MeV

$\Gamma_{7/2}^+$: 0.08 MeV
$\Delta_{5/2}^+$: 0.00 MeV
 humanities

"Experiment": 31 hole-calculation

Calculated $^{131}\text{Sn}$ based on $^{100}\text{Sn}$ core

$\Gamma_{7/2}^+$: 2.43 MeV
$\Delta_{5/2}^+$: 1.66 MeV
$\Gamma_{1/2}^+$: 0.82 MeV
$\Gamma_{11/2}^-$: 0.24 MeV
$\Gamma_{3/2}^+$: 0.00 MeV

Experiment: 31 particle-calculation

The calculated $^{102}\text{Sn}$ spectrum

2\textsuperscript{+}: 2.31 MeV
4\textsuperscript{+}: 2.10 MeV
0\textsuperscript{+}: 2.05 MeV
6\textsuperscript{+}: 1.96 MeV
2\textsuperscript{+}: 1.73 MeV

0\textsuperscript{+}: 0.00 MeV
4\textsuperscript{+}: 0.00 MeV

2-particle calculation
30-hole calculation

The calculated $^{130}\text{Sn}$ spectrum

4\textsuperscript{+}: 2.39 MeV
0\textsuperscript{+}: 2.38 MeV
2\textsuperscript{+}: 2.61 MeV
0\textsuperscript{+}: 2.11 MeV
2\textsuperscript{+}: 1.46 MeV

0\textsuperscript{+}: 0.00 MeV

2-hole calculation
30-particle calculation
Level systematics and generalized seniority

The near constancy of the position of the first 2+ state throughout the Sn isotopes indicates validity of the generalized seniority (GenSen) scheme.

This is well reproduced by the full shell-model calculation. In fact, the shell-model wave functions have sizeable overlap (80-99%) with the corresponding GenSen wave functions.

However, the GenSen scheme may be too crude to serve as a useful truncation scheme.
Binding energies in Sn isotopes

Effective 2-body interaction gives overbinding, due to a slightly inadequate monopole component (?) Will effective 3-body term help?
Revisit > 10 years after
(taking into account new developments)

• New chiral nucleon-nucleon potentials, such as N3LO
• Compare different potentials
• Note: Previous calculations with Bonn B potential

• Compare different approximations in deriving effective interaction
• Include effective three-body forces (due to truncation of shell-model space)
• Algorithm within Q-box scheme
Experimental (red) 2+, 4+ and 6+ states and calculated 2+ and 4+ states with 2, 2+4, 2+4+6 and 2+4+6+8 hw intermediate states (2-b Q-box to 2nd order + folding)
Experimental (red) 2+, 4+ and 6+ states and calculated 6+ states with 2, 2+4, 2+4+6 and 2+4+6+8 hw intermediate states (2-b Q-box to 2nd order + folding)
Experimental (red) and calculated (with various intermediate state excitations) ground state binding energies (2-b Q-box to 2nd order + folding)
Experimental (red) and calculated (with various intermediate state excitations) 2+ state binding energies (2-b Q-box to 2nd order + folding)
Summary and outlooks

• Capable of handling large shell-model systems
• Present two-body effective interactions reproduce general systematics predicted by generalized seniority, however fail (?) on binding energies (monopole component (?)
• Effective three-body forces due to truncation of valence space may produce desired repulsion, but elimination of disconnected diagrams tricky in practice (although algorithm for doing this exists)
• Need to check dependence on different nucleon-nucleon interactions (and on different many-body schemes)
• With the current and prospective interest in the properties of rare isotopes, aim at deriving an effective interaction with predictive power
"S.p. states" in odd Sn isotopes
(ground states)
Shell model in Ca isotopes

Pure $j^n$ configuration model
- Binding energy wrt closed shell core
  \[ BE(j^n) = n\varepsilon_j + \frac{1}{2}n(n-1)\alpha_j + \left\lfloor \frac{n}{2} \right\rfloor \beta_j \]
- Energy spectra of $j^n$ and $j^{2j+1-n}$ configurations identical, i.e. $^{42}\text{Ca}$ and $^{44}\text{Ca}$ as well as $\nu = 2$ states of $^{44}\text{Ca}$, and similarly $^{43}\text{Ca}$ and $^{45}\text{Ca}$.

Experiment
- Above features well confirmed by experiment
- However, to get detailed agreement with experiment, ought to include entire $1p0f$ shell
$(1p0f)^n$ shell model with 3rd order Q-box and folding to arbitrary order

• Reasonable agreement
  However, fail on two accounts:
  - Overbinding towards the end of the shell
  - Insufficient shell closure in $^{48}$Ca, i.e. first $2^+$ too low
    (inadequate repulsion of the interaction between particles in the $0f_{7/2}$ and $1p_{3/2}$ states)

• Cure by including effective three-body forces??
  - Need evaluate three-body Q-box
    (eliminate unwanted disconnected diagrams by algorithm of Ellis et al., 2005)
Effective three-body interaction

The connected terms are evaluated up to second order in perturbation theory and containing the following diagrams:

Two-body potential used to calculate the diagrams is the G-matrix obtained with CD-Bonn 2000 NN potential and h.o. s.p. basis.
Shell-model calculations of odd $^{40}$Ca isotopes

$^{43}$Ca

MeV

1

0

$-27.67$ $-27.60$ $-27.59$ $-27.78$

$^\frac{11}{2}^-$

$^\frac{3}{2}^-$

$^\frac{5}{2}^-$

$^\frac{7}{2}^-$

$^{45}$Ca

MeV

1

0

$-46.63$ $-46.22$ $-46.24$ $-46.32$

$^\frac{11}{2}^-$

$^\frac{3}{2}^-$

$^\frac{5}{2}^-$

$^\frac{7}{2}^-$

$^{47}$Ca

MeV

2

1

0

$-64.96$ $-64.61$ $-64.36$ $-63.99$

$^\frac{3}{2}^-$

$^\frac{7}{2}^-$

Legend:
- $NN\ V_{eff}$
- $NNN\ V_{eff}$, connected $\hat{Q}$-box terms only
- $NNN\ V_{eff}$
- Experiment
Shell-model calculations of even $^{40}$Ca isotopes

$^{44}$Ca

MeV
3
2
1
0

-38.62
-38.19
-38.24
-38.91

$^{46}$Ca

MeV
3
2
1
0

-57.30
-56.47
-56.53
-56.72

$^{48}$Ca

MeV
4
3
2
1
0

-75.25
-74.75
-74.31
-73.94

$NN\ V_{eff}$

$NNN\ V_{eff}$, connected $\hat{Q}$-box terms only

$NNN\ V_{eff}$

Experiment
Binding energies in Ca isotopes