Effective Shell-Model Hamiltonians from Realistic NN Potentials

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Elba XII Workshop - Electron-Nucleus Scattering XII
What is a realistic effective shell-model hamiltonian?
An example: $^{19}\text{F}$

- 9 protons & 10 neutrons interacting
- Spherically symmetric mean field (e.g. harmonic oscillator)
- 1 valence proton & 2 valence neutrons interacting in a truncated model space

The degrees of freedom of the core nucleons and the excitations of the valence ones above the model space are not considered explicitly.
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Effective shell-model hamiltonian

The shell-model hamiltonian has to take into account in an effective way all the degrees of freedom not explicitly considered.

Two alternative approaches
- phenomenological
- microscopic

\[ V_{NN} ( + V_{NNN} ) \Rightarrow \text{many-body theory} \Rightarrow H_{\text{eff}} \]

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Workflow for a realistic shell-model calculation

1. Choose a realistic $NN$ potential ($NNN$)
2. Determine the model space better tailored to study the system under investigation
3. Derive the effective shell-model hamiltonian by way of a many-body theory
4. Calculate the physical observables (energies, e.m. transition probabilities, ...)

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At present several realistic $V_{NN}$s are available: CD-Bonn, Argonne V18, Nijmegen, ...

Strong short-range repulsion

How to handle the short-range repulsion?

Old way: Brueckner $G$-matrix vertices instead of the $V_{NN}$ ones in the perturbative expansion of $H_{eff}$
Realistic nucleon-nucleon potential: $V_{NN}$

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- $V_{\text{low-}k}$
- chiral potentials rooted in EFT: e.g. $N^3$LO by Entem & Machleidt (smooth cutoff $\approx 2.5 \text{ fm}^{-1}$) or $N^3$LOW (sharp cutoff $= 2.1 \text{ fm}^{-1}$)
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The shell-model effective hamiltonian

A-nucleon system Schrödinger equation

\[ H |\psi_\nu\rangle = E_\nu |\psi_\nu\rangle \]

with

\[ H = H_0 + H_1 = \sum_{i=1}^{A} (T_i + U_i) + \sum_{i<j} (V_{ij}^{NN} - U_i) \]

Model space

\[ |\Phi_i\rangle = [a_1^\dagger a_2^\dagger ... a_n^\dagger]_i |c\rangle \Rightarrow P = \sum_{i=1}^{d} |\Phi_i\rangle \langle \Phi_i| \]

Model-space eigenvalue problem

\[ H_{\text{eff}} P |\psi_\alpha\rangle = E_\alpha P |\psi_\alpha\rangle \]
The shell-model effective hamiltonian

$\begin{pmatrix} PHP & PHQ \\ QHP & QHQ \end{pmatrix}$

$H = X^{-1} H X$

$\Rightarrow$

$Q H P = 0$

$H_{\text{eff}} = P H P$

Suzuki & Lee $\Rightarrow X = e^{\omega}$ with $
\omega = \begin{pmatrix} 0 \\ Q \omega P \\ 0 \end{pmatrix}$
The shell-model effective hamiltonian

\[
\begin{pmatrix}
    \text{PHP} & \text{PHQ} \\
    \text{QHP} & \text{QHQ}
\end{pmatrix}
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\[\mathcal{H} = X^{-1}HX \Rightarrow Q\mathcal{H}P = 0\]

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\[
\begin{pmatrix}
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\[H_{\text{eff}} = P\mathcal{H}P\]

Suzuki & Lee \Rightarrow \quad X = e^\omega \quad \text{with} \quad \omega = \begin{pmatrix}
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The shell-model effective Hamiltonian

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\[ H_{\text{eff}} = P\mathcal{H}P \]

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**The shell-model effective hamiltonian**

**Folded-diagram expansion**

\[ \hat{Q}(\epsilon) = PH_1 P + PH_1 Q \frac{1}{\epsilon - QHQ} QH_1 P \]

\[ \Rightarrow \text{Recursive equation for } H_{\text{eff}} \Rightarrow \text{iterative techniques} \]

(Krenciglowa-Kuo, Lee-Suzuki, ...)

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

generalized folding
The perturbative approach to the shell-model $H^\text{eff}$

\[ \hat{Q}(\epsilon) = PH_1 P + PH_1 Q \frac{1}{\epsilon - QHQ} QH_1 P \]

The $\hat{Q}$-box can be calculated perturbatively

\[ \frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty} \frac{(QH_1 Q)^n}{(\epsilon - QH_0 Q)^{n+1}} \]

The diagrammatic expansion of the $\hat{Q}$-box
The perturbative approach to the shell-model $H_{\text{eff}}$

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The diagrammatic expansion of the $\hat{Q}$-box
The perturbative approach to the shell-model $H_{\text{eff}}$

- $H_{\text{eff}}$ for systems with one and two valence nucleons
- $\hat{Q}$-box $\Rightarrow$ Goldstone diagrams up to third order in $V_{NN}$ (up to 2p-2h core excitations)
- Padè approximant $[2|1]$ of the $\hat{Q}$-box

$$[2|1] = V_{Qbox}^0 + V_{Qbox}^1 + V_{Qbox}^2 (1 - (V_{Qbox}^2)^{-1} V_{Qbox}^3)^{-1}$$
Test case: \( p \)-shell nuclei

- \( V_{NN} \Rightarrow \) chiral N\(^3\)LO potential by Entem & Machleidt
- \( H_{\text{eff}} \) for two valence nucleons outside \(^4\text{He}\)
- Single-particle energies and residual two-body interaction are derived from the theory. No empirical input

First, some convergence checks!
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First, some convergence checks!
Convergence checks

The intermediate-state space $Q$

$Q$-space is truncated: intermediate states whose unperturbed excitation energy is greater than a fixed value $E_{max}$ are disregarded

$$|\epsilon_0 - QH_0 Q| \leq E_{max} = N_{max}\hbar\omega$$

$^6$Li yrast states

results quite stable for $N_{max} \geq 20$
Convergence checks

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Order-by-order convergence

Compare results from $H_{\text{eff}}^{1\text{st}}$, $H_{\text{eff}}^{2\text{nd}}$, $H_{\text{eff}}^{3\text{rd}}$ and $H_{\text{Padè}}^{\text{eff}}$. 
Convergence checks

Order-by-order convergence

Compare results from $H_{1\text{st}}^{\text{eff}}$, $H_{2\text{nd}}^{\text{eff}}$, $H_{3\text{rd}}^{\text{eff}}$, and $H_{\text{Pade'}}^{\text{eff}}$.

- $2_{1}^{+}$
- $3_{1}^{+}$
- $0_{1}^{+}$
- $1_{1}^{+}$
Convergence checks

Dependence on $\hbar \omega$

Auxiliary potential $U \Rightarrow$ harmonic oscillator potential

HF-insertions

zero in a self-consistent basis

neglected in most applications

neglect introduces relevant dependence on $\hbar \omega$
Convergence checks

Dependence on $\hbar \omega$

Auxiliary potential $U \Rightarrow$ harmonic oscillator potential

![Graph showing dependence on $\hbar \omega$]

- $2_{\frac{1}{2}}^+$
- $3_{\frac{3}{2}}^+$
- $0_{\frac{1}{2}}^+$
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- zero in a self-consistent basis
- neglected in most applications
- neglect introduces relevant dependence on $\hbar \omega$
Approximations are under control ... and what about the accuracy of the results?

Compare the results with the “exact” ones

*ab initio* no-core shell model (NCSM)

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Benchmark calculation

To compare our results with NCSM we need to start from a translationally invariant Hamiltonian

\[ H_{int} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} \left( V_{ij}^{NN} - \frac{p_i \cdot p_j}{mA} \right) = \]

\[ = \left[ \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + U_i \right) \right] + \left[ \sum_{i<j=1}^{A} \left( V_{ij}^{NN} - U_i - \frac{p_i^2}{2mA} - \frac{p_i \cdot p_j}{mA} \right) \right] \]
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(a) not translationally invariant Hamiltonian
(b) purely intrinsic Hamiltonian
Benchmark calculation

Remark

$H^{\text{eff}}$ derived for 2 valence nucleon systems $\Rightarrow$ 3-, 4-, .. $n$-body components are neglected
Benchmark calculation

Remark

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- ground-state energies for $N = Z$ nuclei
- discrepancy grows with the number of valence nucleons
Benchmark calculation

$^{10}$B relative spectrum

Discrepancy $\leq 1$ MeV

Minor role of many-body correlations

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Benchmark calculation

$^{10}\text{B}$ relative spectrum

- discrepancy $\leq 1$ MeV
- minor role of many-body correlations

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Neutron-rich Carbon isotopes

... At long last some physics ...
Observation of a Large Reaction Cross Section in the Drip-Line Nucleus $^{22}\text{C}$


$^{19,20,22}\text{C} + p$

10 $^{22}\text{C}$ counts per hour

**TABLE I. Reaction cross sections ($\sigma_R$) in millibarns.**

<table>
<thead>
<tr>
<th>A</th>
<th>$\sigma_R$</th>
</tr>
</thead>
<tbody>
<tr>
<td>19</td>
<td>754(22)</td>
</tr>
<tr>
<td>20</td>
<td>791(34)</td>
</tr>
<tr>
<td>22</td>
<td>1338(274)</td>
</tr>
</tbody>
</table>

RIKEN Radioactive Isotope Beam Factory (RIBF)
\( ^{22}\text{C} \) is the heaviest Borromean nucleus ever observed

Borromean nucleus \( \Rightarrow \) weakly bound nucleus that has, considered as a three-body system, no bound states in the binary subsystems.

\( ^{22}\text{C} \) is weakly bound \( S_{2n}^{\text{est}} = 420\text{keV} \)

\( ^{21}\text{C} \) is unstable for one-neutron emission

\(^{22}\)C structure

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Shell-model calculation

Realistic potential $V_{NN} \Rightarrow N^3\text{LOW}$

$\Rightarrow H_{\text{eff}}$

Single-particle energies & effective interaction from the theory. No empirical input
Shell-model calculation

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Shell-model calculation

- Realistic potential $V_{NN} \Rightarrow N^3$LOW
- $\Rightarrow H_{\text{eff}}$
- Single-particle energies & effective interaction from the theory. No empirical input
Model space

$^{22}\text{C}$

$^{14}\text{C}$ inert core

**Neutrons:**
shell $sd \Rightarrow 1s_{1/2}, 0d_{5/2}, 0d_{3/2}$

**Protons:**
$0p_{1/2}$

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Results

- $^{22}$C & drip line
- N=14 shell closure

<table>
<thead>
<tr>
<th>$nlj$</th>
<th>$\epsilon$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s1/2</td>
<td>0.0 (-0.793)</td>
</tr>
<tr>
<td>0d5/2</td>
<td>5.914</td>
</tr>
<tr>
<td>0d3/2</td>
<td>1.394</td>
</tr>
</tbody>
</table>
Results: $^{22}$C & drip line

g.s. energies of even mass
Carbon isotopes

$S_n(^{21}C) = -1.6$ MeV

$S_{2n}(^{22}C) = 456$ keV
Results: $^{22}\text{C} \& \text{drip line}$

g.s energies of even mass Carbon isotopes

\[
\begin{array}{c|c|c|c}
\text{N} & \text{Expt.} & \text{Calc.} & \text{shifted s.p.e.} \\
10 & 12 & 14 & 16 & 18 \\
\end{array}
\]

\[S_n(^{21}\text{C}) = -1.6 \text{ MeV}\]

\[S_{2n}(^{22}\text{C}) = 456 \text{ keV}\]
Results: N=14 shell closure

Experimentally the N=14 shell closure in oxygen isotopes disappears in carbon isotopes
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Excitation energies of $2^+_1$ states in heavy carbon isotopes

<table>
<thead>
<tr>
<th>N</th>
<th>Expt.</th>
<th>Calc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.6</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>2.4</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>5.6</td>
<td></td>
</tr>
</tbody>
</table>

Expt. = Experimental, Calc. = Calculated
Results: N=14 shell closure

The pn monopole component of $V_{\text{eff}}$ reproduces correctly the g.s. inversion in $^{15}\text{C}$ and $^{17}\text{O}$

$$\epsilon_j(^{17}\text{O}) = \epsilon_j(^{15}\text{C}) + V_{p_1}^{\text{mon}} \times 2$$
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$$\epsilon_j(^{17}\text{O}) = \epsilon_j(^{15}\text{C}) + V_{\text{mon}}^{^{15}\text{C};j} \times 2$$
Concluding remarks

- Approximations involved may be kept under control
- Effective shell-model hamiltonians derived from realistic NN potentials are reliable
- Realistic shell-model calculations $\Rightarrow$ fully microscopic description of nuclear structure
  - no parameters modified *ad hoc*
  - enhanced predictive power
- Effective realistic shell-model hamiltonians may be employed successfully to describe the properties of nuclei close to the drip lines
  - drip-lines position
  - properties of loosely bound nuclei
  - evolution of nuclear properties when varying $N/Z$
  - shell-quenching
  - new magic numbers
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Results: $B(E2; 2^+_1 \rightarrow 0^+_1)$ transition probabilities

Reduced Experimental $B(E2; 2^+_1 \rightarrow 0^+_1) \Rightarrow$ effective charges quenching

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Reduced Experimental $B(E2; 2^+_1 \rightarrow 0^+_1) \Rightarrow$ effective charges quenching

![Graph showing $B(E2)$ values for different isotopes]

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Calc.</th>
<th>Expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{16}\text{C}$</td>
<td>1.8</td>
<td>$2.6 \pm 0.2 \pm 0.7$</td>
</tr>
<tr>
<td>$^{18}\text{C}$</td>
<td>3.0</td>
<td>$4.15 \pm 0.73$</td>
</tr>
<tr>
<td>$^{20}\text{C}$</td>
<td>3.7</td>
<td>$4.3 \pm 0.2 \pm 1.0$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$&lt; 3.7$</td>
</tr>
</tbody>
</table>