The No-Core Shell Model

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Nuclear structure at the dawn of the 21\textsuperscript{st} century

- P-shell nuclei have been studied for a long time
- But there are still many mysteries
  - But they are a rich laboratory to test a basic understand of nuclear physics
  - Vast array of physics: deformation, clustering, super-allowed beta decay, three-body forces, parity inversion, halos, etc.
- Newer methods and faster computers are making a comprehensive study from first principles possible
  - GFMC
  - No-core shell model
  - Coupled cluster methods

Exactly how nuclei are put together is one of the most fundamental questions in nuclear physics
Goal: Exact calculation of Nuclear Structure for light nuclei

- Two nucleons $\Rightarrow$ A-nucleons
  - Properties: binding energies, decay mechanisms, etc.
  - Do we need three-body forces? (Yes)
  - How about four-body?

- Hasn’t the Shell Model already solved this problem?
  - Yes and NO!
    - The Shell Model as practiced is an empirical tool that often requires arbitrary and unsatisfying approximations to make it work

If we work hard enough, we can use effective interaction theory to apply the shell model correctly
We start with the many-body Hamiltonian

\[ H = \sum_i \frac{\vec{p}_i^2}{2m} + \sum_{i < j} V_{NN}(\vec{r}_i - \vec{r}_j) \]

- **Add the center-of-mass oscillator potential**

\[ H_{CM} = \frac{1}{2} Am\Omega^2 \vec{R}^2 = \sum_i \frac{1}{2} m\Omega \vec{r}_i^2 - \sum_{i < j} \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2 \]

- **The Good:**
  - Provides a convenient basis to build the many-body Slater determinants
  - Does not affect the intrinsic motion
  - Exact separation between intrinsic and center-of-mass motion

- **The Bad:**
  - Radial behavior is not right for large \( r \)
  - Provides a confining potential, so all states are effectively bound
  - Some dependence on oscillator parameter \( \hbar \Omega \) (goes away with larger model space)
Many-body solutions

• Typical eigenvalue problem

\[ H \Psi_i = E_i \Psi_i \]

• Construct many-body states \(|\phi_i\rangle\) so that

\[ \Psi_i = \sum_n C_n \phi_n \]

• Calculate Hamiltonian matrix \(H_{ij} = \langle \phi_j | H | \phi_i \rangle\)
  
  - Diagonalize to obtain eigenvalues

\[
\begin{pmatrix}
H_{11} & H_{12} & \cdots & H_{1N} \\
H_{21} & H_{22} & \cdots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
H_{N1} & \cdots & \cdots & H_{NN}
\end{pmatrix}
\]

\[ \phi = \frac{1}{\sqrt{A!}} \begin{pmatrix}
\phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \cdots & \phi_i(\mathbf{r}_A) \\
\phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & \cdots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
\phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \cdots & \phi_l(\mathbf{r}_A)
\end{pmatrix}
\]

\[ = a_i^+ a_j^+ a_k^+ 0 \]

Problem: Short-range repulsion requires an infinite space
Can we get around this problem?
Effective interactions

- Choose subspace of $\phi_n$ for a calculation ($P$-space)
  - Include most of the relevant physics
  - $Q$-space (excluded - infinite)

- Effective interaction:

$$H_{\text{eff}} \hat{P} \Psi_i = E_i \hat{P} \Psi_i$$

- Lee-Suzuki:

$$H_{\text{eff}} = P X H X^{-1} P$$

$$Q X H X^{-1} P = 0$$
The general idea behind effective interactions

$P$-space defined by $N_{\text{max}} \hbar \Omega$

$H_{\text{eff}}$ has one-, two, three-, … A-body terms

Exact reproduction of $N$ eigenvalues
Choose P-space for \( A \)-body calculation, with dimension \( d_p \)

- P-space basis states: \( |\alpha_P\rangle \) and Q-space basis states: \( |\alpha_Q\rangle \)
- Need \( d_p \) solutions, \( |k\rangle \), in the “infinite” space, i.e., \( H|k\rangle = E_k|k\rangle \)
- Write \( X=e^{-\omega} \)

\[
Qe^{-\omega}He^{\omega}P = 0; \quad \omega = Q\omega P
\]

\[
\langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{k}^{d_p} \langle \alpha_Q | k \rangle \langle \tilde{k} | \alpha_P \rangle; \quad \sum_{\alpha_p}^{d_p} \langle \tilde{k} | \alpha_P \rangle \langle \alpha_P | k' \rangle = \delta_{kk'}
\]

\[
\langle \beta_P | H_{\text{eff}} | \alpha_P \rangle = \sum_{k}^{d_p} \sum_{\alpha'}^{d_p} \sum_{\alpha''}^{d_p} \langle \beta_P | (1 + \omega^+ \omega)^{-1/2} | \alpha' \rangle \langle \alpha' | \tilde{k} \rangle E_k \langle \tilde{k} | \alpha'' \rangle \langle \alpha'' | (1 + \omega^+ \omega)^{-1/2} | \alpha_P \rangle
\]

\[
\langle \beta_P | (1 + \omega^+ \omega) | \alpha_P \rangle = \sum_{k}^{d_p} \langle \beta_P | \tilde{k} \rangle \langle \tilde{k} | \alpha_P \rangle
\]

\( \langle \beta_P | H_{\text{eff}} | \alpha_P \rangle \) exactly reproduces \( d_p \) solutions of the full problem

• Essentially the same procedure is used for \( n \)-body clusters
The NCSM uses a variety of realistic interactions

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<table>
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<tr>
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<tbody>
<tr>
<td>Argonne potentials</td>
<td>Potential model, v18, v8’</td>
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<tr>
<td>Bonn potentials</td>
<td>Local</td>
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<td>Fit to Nijmegan scattering data</td>
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<td>Based on meson exchange</td>
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<td>Non-local, off shell behavior</td>
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<td>Charge-dependence, CD-Bonn</td>
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<tr>
<td>Effective field theory EFT</td>
<td>Guided by QCD</td>
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<tr>
<td>Three-body</td>
<td>Idaho-A, N³LO, etc</td>
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<tr>
<td>INOY</td>
<td>Softer, → faster convergence</td>
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$n=3$ clusters in $H_{\text{eff}}$

Tucson-Melbourne Urbana and EFT-based

Two-body

Inside non-local, outside Yukawa

Fit to NN data and $^3\text{H}$ and $^3\text{He}$
Computational aspects of the NCSM

- Two-body interactions
  - Model-space limitation $\sim 10^8$ states
    - $A=3$, $N_{\text{max}} = 36$, Jacobi coordinates
    - $A=4$, $N_{\text{max}} = 20$, Jacobi coordinates
    - $A=6$, $N_{\text{max}} = 14$, M-scheme
    - $7 \leq A \leq 11$, $N_{\text{max}} \sim 10$, M-scheme
    - $A \geq 12$, $N_{\text{max}} = 6$, M-scheme

- Three-body interactions
  - Limited by number of three-body matrix elements
    - For $N_{\text{max}}=4$, 39,523,066
    - For $N_{\text{max}}=6$ over 600,000,000
    - Practical limit is $N_{\text{max}} = 6$ for all the p-shell
    - Four-body - $N_{\text{max}} = 4$
Application to A=3 and convergence

- $^3\text{H}$ with CD-Bonn and N$^3$LO

<table>
<thead>
<tr>
<th>Potential</th>
<th>$E_{gs}$ (MeV)</th>
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<tr>
<td>AV18</td>
<td>-7.62</td>
</tr>
<tr>
<td>N$^3$LO</td>
<td>-7.86</td>
</tr>
<tr>
<td>CD-Bonn</td>
<td>-8.00</td>
</tr>
<tr>
<td>INOY</td>
<td>-8.48</td>
</tr>
<tr>
<td>Exp</td>
<td>-8.48</td>
</tr>
</tbody>
</table>
Application to A=3 and convergence

- $^3$H with CD-Bonn and N$^3$LO
Effective interactions really work

- $^4\text{He}$ with the effective-field theory Idaho-A potential

![Graph showing energy levels for $^4\text{He}$ with different potentials](image)

- Effective interactions improve convergence!
- Are EFT potentials useful for nuclear-structure studies?
Results with two-body - frequency dependence

- $^9\text{Be}$ with CD-Bonn

- NCSM result taken in region with least dependence on frequency
- Note NCSM is not variational
Results with three-body effective interactions

Three-body effective interactions represent a significant improvement and give results within 400 keV of the GFMC.
Excitation spectra with NN-interactions

So far, things are looking pretty good!
The NN-interaction clearly has problems

• The NN-interaction by itself does not describe nuclear structure
• Also true for A=11

Note inversion of spins!
How about the three-body interaction?

- Tucson-Melbourne
Three-body interaction in a nucleus

The three-nucleon interaction plays a critical role in determining the structure of nuclei.
Can we explain the parity inversion in p-shell nuclei?

$^9$Be
Can we explain the parity inversion in p-shell nuclei?

$^9$Be - Extrapolation

Exponential fits:

$$E_{\text{exc}} = E_0 + a \cdot \exp(b \cdot N_{\text{max}})$$

Legend:
- CD-Bonn 2000 ($h\Omega = 12$ MeV)
- Argonne V8* ($h\Omega = 12$ MeV)
- $N^3$LO ($h\Omega = 11$ MeV)
- INOY ($h\Omega = 16$ MeV)
- Exp.
Can we explain the parity inversion in p-shell nuclei?

$^{11}\text{Be}$
Can we explain the parity inversion in p-shell nuclei?

$^{11}\text{Be}$ - Extrapolation

Exponential fits:

$$E_{\text{exc}} = E_0 + a \cdot \text{Exp}(b \cdot N_{\text{max}})$$
A new formalism for nuclear reactions

- Nuclear reactions from scratch - Petr Navratil
- Ingredients:
  - Exact intrinsic wave functions for entrance and exit channels - ab initio shell model
  - Wave function for composite
  - Radial-cluster form factor
  - Solve couple integro-differential equation for relative wave function
  - Extract cross section from asymptotic normalization

\[
\left[ -\frac{\hbar^2}{2M} \left( \frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} \right) + V_{Coul} + E^{7\text{Be}} + E^{8\text{Be}} - E \right] u_\Gamma(r) + \sum_{\Gamma''n'0}^\infty \int dr \mathcal{R}_{nL}(r) \mathcal{H}_{\Gamma n, \Gamma' n'} \mathcal{R}_{n'L'}(r') u_{\Gamma'}(r') = 0
\]

Entrance-channel wave function
\[
\left[ \left\langle 3\text{He} \right| \times \left\langle 4\text{He} \right\rangle \right] \times Y_L(\hat{r}) g_J(r) \right]^{JM}
\]

Relative wave function

Orbital angular momentum \( L \)

Radial-cluster overlap enters in these matrix elements of \( H \)

Harmonic oscillator functions

Sum over all channels

Physics and Advanced Technologies
Example: $^4\text{He} + t \rightarrow ^7\text{Li}$ and $^6\text{Li} + n \rightarrow ^7\text{Li} \rightarrow ^4\text{He} + t$

- Formalism is in place for computing radial-cluster overlaps
- Resonances for $^4\text{He} + t$ and $^6\text{Li} + n$ are in accordance with experiment
- Model-space renormalization in FY05
<table>
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<th>Summary</th>
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<tr>
<td>• Significant progress towards an exact understanding of nuclear structure is being made!</td>
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<td>• These are exciting times!!</td>
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<td>– Determine the form of the NNN-interaction</td>
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<td>– Implementation of effective operators for transitions</td>
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<tr>
<td>– Four-body effective interactions</td>
</tr>
<tr>
<td>– Effective field-theory potentials; are they any good for structure?</td>
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<tr>
<td>– Integrate the structure into some reaction models (underway)</td>
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<th>Questions and open problems to be addressed:</th>
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<td>– Is it possible to improve the mean field?</td>
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<td>– Can we improve the convergence of the higher $\hbar\Omega$ states?</td>
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<tr>
<td>– Unbound states. Can we use a continuum shell model?</td>
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<tr>
<td>– How high in A can we go?</td>
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<tr>
<td>– Can we use this method to derive effective interactions for conventional nuclear structure studies?</td>
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