Shell Model of Nuclei for Stellar Core Collapse: Current Status, Future Prospects

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1. Overview
3. Shell Model Monte Carlo Method
Scientific triple point: nuclear structure, nuclear astrophysics, weak interactions

Nucleosynthesis in the Cosmos

Applications: beyond SM astrophysics

Interplay of weak and strong forces plays a pivotal role in understanding astrophysics.

Astrophysics requires input from nuclear physics.

The three are intertwined.
The big questions

How are heavy elements created, and how do nuclear properties influence stars?
What nuclear properties impact nucleosynthesis?
What is the role of nuclear science in SN explosion mechanisms?

How do complex nuclei derive their properties from their individual constituents?
What is the isospin dependence of the effective interaction?
How to develop theory that will make reliable predictions?

How do complex many-body systems display such astonishing similarities in which new symmetries characterize exotic nuclei?
How does shell structure change as a function of neutron number?
What is the role of the continuum in weakly bound nuclei?

What are the fundamental symmetries of nature?
What nuclear properties can be used to understand e.g., quark mixing, time-reversal symmetry breaking, and other beyond the standard model phenomena?
Nuclear physics input to astrophysical scenarios

Mass trajectory during collapse

e-capture on nuclei dominates e-capture on protons

*See:* Langanke, Kolbe, Dean, PRC63, 032801R (2001)
Langanke et al (PRL, 2003) (rates calculation)
Hix et al (PRL, 2003) (core collapse implications)
Nuclear structure landscapes

The landscape and the models

Density Functional Theory
self-consistent Mean Field

r-process

Large-scale computing

Main theory goals:
- Identify/investigate many-body methods that will extend to RIA
- Generate effective interactions
- Make reliable predictions
- Guide experimental efforts
- Use NN and 3N forces to build nuclei

Various approaches to low-energy nuclear theory:
- Coupled-Cluster theory
- Shell Model Monte Carlo
- DMRG/Factorization
- Shell model diagonalization
- Continuum shell models
- HFB
- QRPA
- TDHF
Shell Model for Nuclear Structure

- When applicable, the shell model is the choice for nuclear structure studies:

Microscopic accounting of the configuration mixing and residual interaction.

Orthogonal basis with a single-particle potential
Solving the quantum many-body problem in a basis

\[ \Phi_\alpha = |1001\cdots\rangle = a_1^+ a_4^+ \cdots - \langle \]

\[ \Phi_0 = |1111\cdots\rangle = a_1^+ a_2^+ \cdots - \langle \]

Many-body basis states

Reference Slater determinant

\[
H = \sum_{pq} \langle p|T_{osc}|q\rangle a_p^+ a_q + \frac{1}{4} \sum_{pqrs} \langle pq|V|rs\rangle a_p^+ a_q^+ a_s a_r
\]

\[
\langle pq|V(\vec{r}_1, \vec{r}_2)|rs\rangle = \int d\vec{r}_1 d\vec{r}_2 \phi_p^*(\vec{r}_1) \phi_q^*(\vec{r}_2) V(\vec{r}_1, \vec{r}_2) \phi_r(\vec{r}_1) \phi_s(\vec{r}_2)
\]

\[
H_{\alpha\beta} = \langle \Phi_\alpha |H|\Phi_\beta \rangle
\]

Methods of solution

1. Diagonalize \( H_{\alpha\beta} \)
2. Determine the optimal (sometimes correlated) basis
3. Reformulate problem as a path-integral (AFMC: SMMC)
4. Resum of quantum many-body perturbation theory diagrams
In the shell model approach

The total number of Slater determinants within a Hilbert space:

\[
\begin{pmatrix}
N_s^p & N_v^n \\
N_s^p & N_v^n
\end{pmatrix}
\]

Number of Z single-particle states

Number of N single-particle states

valence Z

valence N

The conventional shell model with a full major shell has been successful up to A~60 due to large dimensions
Really two problems:

1. Efficient computational methods for large systems.
2. Effective interaction

Exact ab initio treatments for light nuclei:

1. Using tree-body interactions
2. What can these calculations tell us about the shell-model interactions we use in traditional problems?
Begin with a bare NN (+3N) Hamiltonian

\[ H = -\frac{\hbar}{2} \sum_{i=1}^{A} \frac{\nabla_i^2}{m_i} + \frac{1}{2} \sum_{i<j} V_{2N}(\vec{r}_i, \vec{r}_j) + \frac{1}{6} \sum_{i<j<k} V_{3N}(\vec{r}_i, \vec{r}_j, \vec{r}_k) \]

Solve the quantum many-body problem:
- Easier said than done due to combinatorial growth of the problem as a function of particles.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>4 shells</th>
<th>7 shells</th>
</tr>
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<tbody>
<tr>
<td>4He</td>
<td>4E4</td>
<td>9E6</td>
</tr>
<tr>
<td>8B</td>
<td>4E8</td>
<td>5E13</td>
</tr>
<tr>
<td>12C</td>
<td>6E11</td>
<td>4E19</td>
</tr>
<tr>
<td>16O</td>
<td>3E14</td>
<td>9E24</td>
</tr>
</tbody>
</table>

Oscillator single-particle basis states

Many-body basis states
Shell Model Monte Carlo Method for Nuclear Structure - the power and limitations of the approach

- SMMC is well suited to calculate thermal averages of observables in model spaces where the dimensions are prohibitive for direct diagonalization.

- Properties of nuclei at finite temperature are important for various applications.

- We have to deal with the sign problem!
The Hamiltonian:

\[ \hat{H} = \sum_\alpha \epsilon_\alpha \Theta_\alpha + \frac{1}{2} \sum_\alpha V_\alpha \Theta_\alpha^2 \]

- Single-particle energy
- Density operator
- Strength of the TB int.

Dealing with the imaginary-time evolution:

\[ e^{-\beta \hat{H}} |0\rangle \rightarrow |0\rangle \]
Hubbard-Stratonovich Transformation

\[
\int e^{-\frac{\beta V}{2} \Theta^2} = \sqrt{\frac{\beta |V|}{2\pi}} \int_{-\infty}^{\infty} d\sigma e^{-\frac{\beta |V|}{2} \sigma^2} e^{-\beta \sigma SV \Theta}
\]

The strength of the TB interaction phase

We consider thermal averages in the canonical ensemble

\[
\left\langle \hat{A} \right\rangle = \frac{Tr\left( A e^{-\beta H} \right)}{Tr\left( e^{-\beta H} \right)} \approx \int D\sigma W_\sigma \Phi_\sigma A_\sigma
\]

The dimension of the integral \( N_s^2 N_t \)
The sign of the Monte Carlo weight function:

\[ \Phi_\sigma = \frac{Tr(e^{-\beta H})}{|Tr(e^{-\beta H})|} \]

The partition function is not necessarily positive \( \hat{\nu} \) leading to enormous precision problems!

The sign rule:

\[ |\lambda_{K\pi}| = \pi (-1)^{K+1} \]

(Lang at. al, PRC, 1993)
Dealing with the sign problem in SMMC Ö

- Hamiltonians without sign problems
  An important class of interactions are free from the sign problem ſ pairing + quadrupole

- The Extrapolation method ſ the practical solution ſ to the sign problem

- Using schematic interactions

...
How is the extrapolation method Ö

\[ H = H_g + g \, H_b \]

\[ \wedge \quad \wedge \quad \wedge \]

V<0

V>0

E. Caurier at al., PRC 59, 1999
Shifted-Contour Shell Model Monte Carlo Method for Nuclear Structure

Shifting the Hamiltonian with the HF density:

\[ \hat{H} = \sum_{\alpha} \left( \varepsilon_{\alpha} - W_{\alpha} \right) \hat{\Theta}_{\alpha} + \frac{1}{2} \sum_{\alpha} V_{\alpha} \left( \hat{\Theta}_{\alpha} - \tilde{\Theta}_{\alpha} \right)^2 \]

This shift of the Hamiltonian is equivalent to the shift of the contour:

\[ e^{-\frac{\beta V}{2} \Theta^2} = \sqrt{\frac{\beta |V|}{2\pi}} \int_{-\infty}^{\infty} d\sigma e^{-\frac{\beta |V|}{2} (\sigma - S\tilde{\Theta})^2} e^{-\beta (\sigma - S\tilde{\Theta})SV\Theta} \]
Sign

$^{28}\text{Mg}$

$^{26}\text{Si}$

$^{28}\text{Mg, SMMC}$

Sign vs. $\beta [\text{MeV}^{-1}]$
NERSC, Seaborg

POWER 3 Processor

Clock speed 375MHz
Peak Performance 1.5 Gflops

Distributed memory machine with 2,944 compute processors
The processors are distributed among 184 compute nodes
with 16 processors per node.
Each node has between 16 and 64 GBytes of memory.

SMMC Performance: 350 Mflops/processor per up to 1000 processors
Conclusions

We exploit a new method, the shifted-contour Monte Carlo Method (SC-SMMC) for nuclear structure.

Our results show a significant delay of the sign.