Introduction to Nuclear Phenomena

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Nuclear properties

- Binding energies and excitation energies
- Mass, radius, spin, magnetic and electric dipole and quadrupole moments
- Decay modes, half-life, reaction modes and cross section

Goal

\[ \gamma \]

\[ ^2 \text{He} (\alpha, \gamma) ^6 \text{Li} \]

Obtain accurate predictions using finite computational resources

Symplectic no-core configuration interaction (SpNCCI)
No-core shell model with continuum (NCSMC)

\[ ^6 \text{Li} \]

Adopted Levels, Gammas 2002Ti10, 1988Aj01 (continued)

6\(^3\)Li Levels (continued)

<table>
<thead>
<tr>
<th>E(level)</th>
<th>J</th>
<th>( \pi )</th>
<th>( \Gamma )</th>
<th>Comments</th>
</tr>
</thead>
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<tr>
<td>24890</td>
<td>55</td>
<td>4</td>
<td>-2</td>
<td>( 5.32 \text{MeV} )</td>
</tr>
<tr>
<td>26590</td>
<td>65</td>
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<td>-8</td>
<td>( 8.68 \text{MeV} )</td>
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<td>31138</td>
<td>16</td>
<td>-1</td>
<td></td>
<td>( 11.58 \text{MeV} )</td>
</tr>
</tbody>
</table>

\( \Gamma: \text{broad.} \) \( \gamma ( ^6 \text{Li}) \)

\( E_i (\text{level}) = J^\pi_{i} \)

\( E(\gamma) = E_f (\text{level}) = J^\pi_{f} \)

\( \text{Mult.} \) \( \text{Comments} \)

\( ^2 \text{He} \) threshold

\( ^6 \text{Li} \) stable
Nuclear binding energy

Difference in mass energy between a nucleus and its constituent protons and neutrons

Usually quoted as binding energy per nucleon $B/A$

$$B = \left\{ Z * m(p) + N * m(n) - \left[ m\left(\frac{AX}{ZX}N\right) - Z * m(e)\right]\right\}$$
Calculating nuclear binding energy

Solve Hamiltonian eigenvalue problem $H = T + V$

$H\psi = E\psi$
Calculating nuclear binding energy

Solve Hamiltonian eigenvalue problem $H = T + V$

\[ H\psi = E\psi \]

\[ V(x) = V(x_0) + \left( \frac{dV}{dx} \right)_{x=x_0} (x-x_0) + \left( \frac{d^2V}{dx^2} \right)_{x=x_0} (x-x_0)^2 + \ldots \]
Calculating nuclear binding energy

Solve Hamiltonian eigenvalue problem \( H = T + V \)

\[
H\psi = E\psi
\]

\[
V(x) = V(x_0) + \left. \frac{dV}{dx} \right|_{x=x_0} (x - x_0) + \left. \frac{d^2V}{dx^2} \right|_{x=x_0} (x - x_0)^2 + \ldots
\]

\[
H \approx T + kx^2
\]
Harmonic oscillator Hamiltonian \( H = T + kx^2 \)

Eigenstates of the Harmonic oscillator Hamiltonian

\[
\phi_{nlm} \propto r^{l+1} L_{n+l}^{l+1/2} (r^2) e^{-r^2/2} Y_{lm}(\hat{r})
\]

- \( n \): radial node number
- \( l, m \): orbital angular momentum and projection

Eigenvalues of Harmonic oscillator Hamiltonian

\[
E_{nl} = \hbar \omega_0 (N + 1/2), \quad N = 2n + l \quad \omega_0 = \sqrt{k/m}
\]

Energy degeneracy! \( d = (N + 1)(N + 2)/2 \)
Harmonic oscillator Hamiltonian \( H = T + kx^2 \)

Major shells labeled by \( N = 2n + l \)

Subshells (orbitals) labeled by \( l = 0, 1, 2, 3, ... \rightarrow s, p, d, f, ... \)
Harmonic oscillator Hamiltonian \( H = T + kx^2 + L \cdot S \)

**Labels: \( N, l \)**

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<th>Energy Level</th>
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<tr>
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<tr>
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**Labels: \( N, l, s, j \)**

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<th>Label</th>
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Shell closures

Figure 5.6: At the left are the energy levels calculated with the potential of Figure 5.5. To the right of each level are shown its capacity and the cumulative number of nucleons up to that level. The right side of the figure shows the effect of the spin-orbit interaction, which splits the levels with $L_p > 0$ into two new levels. The shell effect is quite apparent, and the magic numbers are exactly reproduced.

Spin-Orbit Potential

How can we modify the potential to give the proper magic numbers? We certainly cannot make a radical change in the potential, because we do not want to destroy the physical content of the model—Equation 5.1 is already a very good guess at how the nuclear potential should look. It is therefore necessary to add various terms to Equation 5.1 to try to improve the situation. In the 1940s, many unsuccessful attempts were made at finding the needed correction; success was finally achieved by Mayer, Haxel, Suess, and Jensen who showed in 1949 that the inclusion of a spin-orbit potential could give the proper separation of the subshells. Once again, we are borrowing an idea from our colleagues, the atomic physicists. In atomic physics the spin-orbit interaction, which causes the observed fine structure of spectral lines, comes about because of the electromagnetic interaction of the electron’s magnetic moment with the magnetic field generated by its motion about the nucleus. The effects are typically very small, perhaps one
Solving the nuclear many-body problem

Expand wavefunctions in terms of functions (basis states)

\[ \psi = \sum a_n \phi_n \]

Write Hamiltonian equation as matrix eigenproblem.

\[
\begin{pmatrix}
H_{11} & H_{12} & \cdots \\
H_{21} & H_{22} & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots
\end{pmatrix} = E
\begin{pmatrix}
a_1 \\
a_2 \\
\vdots
\end{pmatrix}
\]

Want basis states \( \phi_n \) for which we can define a hierarchy.
Harmonic oscillator basis

- Basis states are configurations, i.e., distributions of particles over harmonic oscillator shells (\(nlj\) substates)

- States are organized by total number of oscillator quanta above the lowest Pauli allowed number \(N_{\text{ex}}\)

- States with higher \(N_{\text{ex}}\) contribute less to the wavefunction

- Basis must be truncated:
  Restrict \(N_{\text{ex}} \leq N_{\text{max}}\)
Shell model

- Basis space divided into an inert core and a valence space
- Only particles in the valence space allowed to interact and excite
- Effect of states in inert core taken into account in the mean-field shell model interaction
Shell model

- Basis space divided into an inert core and a valence space
- Only particles in the valence space allowed to interact and excite
- Effect of states in inert core taken into account in the mean-field shell model interaction

\[ N = 2n + l \]

\[ N_{\text{ex}} = 0 \]

\[ N_{\text{ex}} = 2 \]

Inert core not physical
Interaction not mean field
Ab initio nuclear physics

- Predict nuclear structure and reactions directly from quantum chromodynamics (QCD)
  
  *Realistic inter-nucleon interactions derived using, e.g., chiral effective field theory (EFT)*
  
- Understanding the origins of simple patterns in complex nuclei
Fundamental forces

There are four fundamental forces between particles:

1. **Gravity**, which obeys this inverse-square law:
   \[ F_{\text{gravity}} = G \frac{m_1 m_2}{d^2} \]

2. **Electromagnetism**, which obeys this inverse-square law:
   \[ F_{\text{static}} = k_e \frac{q_1 q_2}{d^2} \]

And also Maxwell’s equations

Also what?

3. **The strong nuclear force**, which obeys, uh...
   ...well, umm...
   ...it holds protons and neutrons together.

I see.

It’s strong.

4. **The weak force**. It [mumble mumble] radioactive decay [mumble mumble]
   That’s not a sentence. You just said ‘radio—'
   --and those are the four fundamental forces!
Nuclear interactions

Nuclear interaction not given by inverse square law. Interaction obtain by series expansion

Series expansion of interaction
chiral effective field theory

\[ V = (Q/\Lambda^\chi)^0 \left[ \begin{array}{c} \times \end{array} \right] \]
\[ + (Q/\Lambda^\chi)^2 \left[ \begin{array}{c} \times \end{array} \right] \]
\[ + \ldots \]
No-core shell model

- All particles allowed to excite
- Interactions are two-body and three-body

Size of many-body basis grows rapidly with increasing $N_{\text{max}}$ and number of protons and neutrons

How large does $N_{\text{max}}$ need to be?
Convergence Challenge

Results for calculations in a finite space depend upon:
- Many-body truncation $N_{\text{max}}$
- Single-particle basis scale $\hbar \omega$
Convergence Challenge

Results for calculations in a finite space depend upon:

- Many-body truncation $N_{\text{max}}$
- Single-particle basis scale $\hbar\omega$
Why must $N_{\text{max}}$ be so large?

- Mismatch between harmonic oscillator potential and nuclear potential at large $r$.
- Clustering in the wavefunctions
- Kinetic energy

\[ H = V + T \approx T \]
Combating the runaway basis dimension

Obtain accurate predictions using finite computational resources

- Symplectic no-core configuration interaction (SpNCCI)
- No-core shell model with continuum (NCSMC)

\[ ^2\text{He} \ (\alpha, \gamma) \ ^6\text{Li} \]
Outline

– Nuclear symmetries

– Mathematics of symmetries (group theory)

– Symplectic no-core configuration interaction (SpNCCI) framework

– Nuclear rotations in ab initio calculations
Galilean invariance of the nucleus

Newton’s law hold in all frames related to one another by a Galilean transformation

– Time translations $t' = t + b$
– Spacial translations $\mathbf{x}' = \mathbf{x} + \mathbf{a}$
– Rotations $\mathbf{x}' = R(\theta)\mathbf{x}$
– Boosts $\mathbf{x}' = \mathbf{x} + \mathbf{v}t$
Noether’s theorem

Any time you have a continuous symmetry, you have an associated conserved quantity

- Time translations → energy $E$
- Spacial translations → momentum $p$
- Rotations → angular momentum $J$
- Inversion ($x \rightarrow -x$) → parity $\pi$

*Nuclear wavefunctions always have good total angular momentum and parity $J^\pi$. 

\begin{align*}
5.37 &\rightarrow 1^+; 0 \\
5.65 &\rightarrow 2^+; 0 \\
4.31 &\rightarrow 2^+; 1 \\
3.563 &\rightarrow 0^+; 1 \\
2.186 &\rightarrow 3^+; 0 \\
1^+; 0 &\rightarrow 6\text{Li}
\end{align*}
Approximate symmetries

**Isospin:** under the strong force, the proton and neutron are different states of the same particle $|TM_T\rangle$

\[ p : |\frac{1}{2} \frac{1}{2}\rangle \quad n : |\frac{1}{2} -\frac{1}{2}\rangle \]

*Other approximate symmetries include the phase space symmetries SU(3) and Sp(3, \mathbb{R}) which are tied to nuclear collective behavior*
Collective behavior

**Nuclear shape** *Spherical, oblate, prolate*

*Phase space symmetries SU(3) and Sp(3, \( \mathbb{R} \))*
Collective behavior

**Nuclear shape** *Spherical, oblate, prolate*
Phase space symmetries SU(3) and Sp(3, R)

**Nuclear rotation** *Rotational bands*
Rotational, SU(3), and Sp(3, R) symmetries
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*Total angular momentum is intrinsic angular momentum combined with rotational angular momentum*
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**Giant resonances**  *Monopole, dipole, quadrupole*
*Sp(3, R) symmetry*
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**Nuclear rotation**  *Rotational bands*  
*Rotational, SU(3), and Sp(3, R) symmetries*

**Giant resonances**  *Monopole, dipole, quadrupole*  
*Sp(3, R) symmetry*
Mathematics of symmetries

Associated with each symmetry is a Lie group and Lie algebra

A **group** is a set with a binary operation that combines any two elements $a$ and $b$ to form a third element $c$ such that the following axioms are satisfied:

- **Closure**: if $a$ and $b$ are in the set, then $c = a \circ b$ is also in the set
- **Associativity**: $(a \circ b) \circ c = a \circ (b \circ c)$.
- **Identity**: $e \circ a = a \circ e = a$
- **Invertibility**: for every element $a$ there exists another element $d$ such that $a \circ d = e$. 
Symmetry groups

Example: The set of all rotations \( \{ R(\theta) \} \) forms the rotation group SO(3)

**Closure:** \( R(\theta_1) \circ R(\theta_2) = R(\theta_1 + \theta_2) \)

**Associativity:** \( [R(\theta_1) \circ R(\theta_2)] \circ R(\theta_3) = R(\theta_1) \circ [R(\theta_2) \circ R(\theta_3)] = R(\theta_1 + \theta_2 + \theta_3) \)

**Identity:** \( R(0) = I \)

**Invertibility:** \( R(\theta) \circ R(-\theta) = R(0) \)
Generators of a group

You can express a spatial rotation in terms of orbital angular momentum operators

\[ \exp(\theta \cdot \mathbf{L}) = \sum_n \frac{(\theta \cdot \mathbf{L})^n}{n!} \quad \mathbf{L} = (L_1, L_2, L_3) \]

\[ \rightarrow \] \[ \mathbf{L}_1, \mathbf{L}_2 \text{ and } \mathbf{L}_3 \text{ are the generators of the rotations group } \text{SO}(3). \]

In quantum mechanics, there is also a "spin rotation" group SU(2) generated by spin operators

\[ \mathbf{S} = (S_1, S_2, S_3) \]

\[ \text{SO}(3) \sim \text{SU}(2) \]
Angular momentum group SU(2)

The total angular momentum group SU(2) is generated by

\[ J = L + S, \quad J = (J_1, J_2, J_3) \]

Eigenstates of \( J \) are \( |JM\rangle \)
- \( J \): total angular momentum
- \( M \): projection of \( J \) onto the 3rd axis.
  \[ M = -J, -J + 1, ..., J \]

Different eigenstates related by ladder operators

\[ J_\pm = \frac{1}{\sqrt{2}} (J_1 \pm iJ_2) \]

The set of states \( |JM\rangle \) with same \( J \) but different \( M \) form an irreducible representation (irrep) of SU(2).
SU(3)-NCSM

SU(3) generators

\[ Q_{2M} \quad \text{Algebraic quadrupole} \]

\[ L_{1M} \quad \text{Orbital angular momentum} \]

SU(3) ⊃ SO(3)

\((\lambda, \mu) \quad \kappa \quad L \quad \otimes \quad \supseteq \quad \text{SU(2)} \)

SU(2) \quad J

\quad S

(\lambda, \mu) \quad \text{SU(3) irrep label}

\kappa \quad \text{SU(3) to SO(3) branching multiplicity}

L \quad \text{SO(3) orbital angular momentum}

SU(3) symmetry of a configuration

- SU(3) coupling particles within major shells
  
  Each particle has SU(3) symmetry \((N, 0)\),
  \(N = 2n + \ell\).

- SU(3) coupling successive shells

- SU(3) coupling protons and neutrons
Sp(3, ℝ)

Sp(3, ℝ) generators can be grouped into ladder and U(3) operators

Start from a single U(3) irrep at lowest “grade" $N$

$Ladder upward in N using A^{(20)} \quad No limit!$

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Sp(3, \mathbb{R})

Sp(3, \mathbb{R}) generators can be grouped into ladder and U(3) operators.

Start from a single U(3) irrep at lowest "grade" \( N \)

\textit{Lowest grade irrep (LGI)}

Ladder upward in \( N \) using \( A^{(20)} \) \hspace{1cm} \text{No limit!}

\[ B^{(02)} |\sigma\rangle = 0 \]

\[ |\psi^{(\omega)}\rangle \sim [A^{(20)}A^{(20)}\cdots A^{(20)}|\sigma\rangle]^\omega \]

\[ \text{Sp}(3, \mathbb{R}) \supset \text{U}(3) \quad \text{U}(3) \sim \text{U}(1) \otimes \text{SU}(3) \]

\[ \lambda, \mu, \omega, N \omega \quad (\lambda_\omega, \mu_\omega) \]

\[ A^{(20)} \sim b^\dagger b^\dagger \quad \text{Raises } N \]

\[ H^{(00)}, C^{(11)} \sim b^\dagger b \quad \text{U(3) generators} \]

\[ B^{(02)} \sim bb \quad \text{Lowers } N \]
$\text{Sp}(3, \mathbb{R})$

$\text{Sp}(3, \mathbb{R})$ generators can be grouped into ladder and $\text{U}(3)$ operators.

Start from a single $\text{U}(3)$ irrep at lowest "grade" $N$

$\text{Lowest grade irrep (LGI)}$

Ladder upward in $N$ using $A^{(20)}$ \textit{No limit!}

$B^{(02)} |\sigma\rangle = 0$

$|\psi^\omega\rangle \sim [A^{(20)} A^{(20)} \cdots A^{(20)} |\sigma\rangle^\omega$

$\text{Sp}(3, \mathbb{R}) \supset \text{U}(3)$ $\text{U}(3) \sim \text{U}(1) \otimes \text{SU}(3)$

$A^{(20)} \sim b^\dagger b^\dagger$ \textit{Raises} $N$

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$H^{(00)}, C^{(11)} \sim b^\dagger b$ \textit{U(3) generators}$

$B^{(02)} \sim bb$ \textit{Lowers} $N$
Sp(3,R) basis states are highly correlated

States are linear combinations of many different oscillator configurations
Symplectic no-core configuration interaction (SpNCCI)

Expand wavefunction in an $\text{Sp}(3, \mathbb{R})$ basis

Basis states are linear combinations of original harmonic oscillator states which have $\text{Sp}(3, \mathbb{R})$ symmetry
Decompose wavefunctions by $\text{Sp}(3, \mathbb{R})$ symmetry

$N_{\text{ex}} = 0$

$N_{\text{ex}} = 2$

$N_{\text{ex}} = 4$

$N_{\text{ex}} = 6$

$^6\text{Li} \ 1^+_1$

$\text{Sp}(3, \mathbb{R})$

Probability

$\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)$ irrep $\sigma_S$
Allow higher $N_{\text{max}}$ states that are necessary for describing, e.g., radius.
Sp(3, R) decomposition $^7$Be

Families of states emerge with very similar Sp(3, R) decompositions.
Nuclear rotations

Intrinsic state $|\phi_K\rangle$ rotating the the lab frame

$$|\psi_{JKM}\rangle \propto \int d\theta \left( D_{MK}^J(\theta) |\phi_k; \theta\rangle + (-1)^{J+K} D_{M-K}^J(\theta) |\phi_K; \theta\rangle \right)$$

$$E(J) = E_0 + A [J(J+1) + a(-1)^{J+1/2}(J+1/2)]$$

Electric Quadrupole (E2) transitions

$$B(E2; J_f K \rightarrow J_i K) = \frac{|\langle J_f || Q_2 || J_i \rangle|^2}{2J_i + 1}$$

$$\langle J_f || Q_2 || J_i \rangle \propto (2J_i + 1)^{1/2} (J_i K 20 | J_f K)(eQ_0)$$

$$\quad (eQ_0) \equiv (16\pi/5)^{1/2} \langle \phi_K || Q_{2,0} || \phi_K \rangle$$

Yrast $K = 1/2$ rotational band in $^7$Be

\begin{align*}
\text{7Be JISP16} \\
\text{Natural (P=--)}
\end{align*}

\begin{align*}
E (\text{MeV})
\end{align*}

\begin{align*}
1/2 & 3/2 & 5/2 & 7/2 & 9/2 & 11/2 \\
-40 & -30 & -20 & -10 & 0 &
\end{align*}

Sp(3, R) decomposition $^7\text{Be}$

Excited states with same Sp(3, R) content

$E\,\text{(MeV)} \approx \frac{1}{2} J + 2.3, 2.5, 2.7, 2.9, 2.11 J$

$^7\text{Be} \; \text{JISP16 Natural (P=-)}$

$^7\text{Be} \; \text{NNLO}$
Sp(3, \mathbb{R}) decomposition $^7\text{Be}$

Excited states with same Sp(3, \mathbb{R}) content but different SU(3) content
Sp(3, \mathbb{R}) decomposition $^7$Be

Excited states with same Sp(3, \mathbb{R}) content but different SU(3) content

(a) $L=1 \quad K_L=0 \quad K=1/2 \quad 0(3,0)1/2$
(b) $L=5 \quad 9/2$
(c) $L=2 \quad KL=1 \quad 0(1,1)3/2$

\[ E_x \text{ (MeV)} \]

Daejeon16 $N_{\text{max}}=6 \quad \hbar\omega=15 \text{ MeV} \]
Summary

– Exact and approximate symmetries arise in nuclear physics
  \emph{Rotational, isospin, SU(3), Sp(3, \mathbb{R}),...}

– Symmetries can be used to combat the dimension problem in NCSM.
  \emph{Truncation by Sp(3, \mathbb{R}) in SpNCCI}

– Symmetries can also be used to understand collective behavior.
  \emph{SU(3) and Sp(3,R) are tied to nuclear rotations, nuclear deformation and giant resonances}
Thank you!
Merci!

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