Nuclei as Bound States

Lecture 1: Hamiltonian

Robert Roth
Overview

- **Lecture 1: Hamiltonian**
  - Prelude
  - Nuclear Hamiltonian
  - Matrix Elements
  - Two-Body Problem
  - Correlations & Unitary Transformations

- **Lecture 2: Light Nuclei**
  - Similarity Renormalization Group
  - Many-Body Problem
  - Configuration Interaction
  - No-Core Shell Model
  - Hypernuclei

- **Lecture 3: Beyond Light Nuclei**
  - Normal Ordering
  - Coupled-Cluster Theory
  - In-Medium Similarity Renormalization Group
Prelude
Playground

Why Should We Care?

Properties of stable and exotic nuclei impact the world at large.

**Nuclear structure meets astrophysics**

- Life and burning cycles of stars
- Nucleosynthesis
- Death of stars: supernova explosions
- Mass, size and structure of neutron stars
- Transients: kilonovae, gamma-ray bursts,...
LIGO: Gravitational Waves

Abbott et al., PRL 116, 061102 (2016)
Neutron Star Mergers

Inspiral Phase
- Maximum mass and size of neutron stars determined by the equation of state of neutron-rich matter

Merger Phase
- Neutron-rich material is ejected; rapid neutron-capture process; synthesis of heavy elements

Ringdown Phase
- Equation of state of neutron-rich matter determines ringdown dynamics

LIGO Collaboration, Bernuzzi, Sathyaprakash
Neutron Star Mergers

structure of nuclei and nuclear matter at the extremes, often beyond the reach of laboratory experiments
Theoretical Context

- finite nuclei
- few-nucleon systems
- nuclear interaction
- hadron structure
- quarks & gluons
- deconfinement
New Era of Nuclear Structure Theory

- **QCD at low energies**
  improved understanding through lattice simulations & effective field theories
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  advances in ab initio treatment of the nuclear many-body problem
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  increase of computational resources and developments of algorithms
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- **experimental facilities**
  amazing perspectives for the exploration of nuclei far-off stability
$H \left| \psi_n \right\rangle = E_n \left| \psi_n \right\rangle$

**Assumptions**

- use nucleons as effective degrees of freedom
- use non-relativistic framework, relativistic corrections are absorbed in Hamiltonian
- use Hamiltonian formulation, i.e., conventional many-body quantum mechanics
- focus on bound states, though continuum aspects are very interesting
The Problem

\[ H |\psi_n\rangle = E_n |\psi_n\rangle \]

What is this many-body Hamiltonian?
- nuclear forces, chiral effective field theory, three-body interactions, consistency, convergence, ...

What about these many-body states?
- many-body quantum mechanics, antisymmetry, second quantisation, many-body basis, truncations, ...

How to solve this equation?
- ab initio methods, correlations, similarity transformations, large-scale diagonalization, coupled-cluster theory, ...
Nuclear Hamiltonian
Nuclear Hamiltonian

- general form of **many-body Hamiltonian** can be split into a center-of-mass and an intrinsic part

\[ H = T + V_{NN} + V_{3N} + \cdots = T_{\text{cm}} + T_{\text{int}} + V_{NN} + V_{3N} + \cdots \]
\[ = T_{\text{cm}} + H_{\text{int}} \]

- **intrinsic Hamiltonian** is invariant under translation, rotation, Galilei boost, parity, time evolution, time reversal, ...

\[ H_{\text{int}} = T_{\text{int}} + V_{NN} + V_{3N} + \cdots \]
\[ = \sum_{i<j} \frac{1}{2mA} (\vec{p}_i - \vec{p}_j)^2 + \sum_{i<j} V_{NN,ij} + \sum_{i<j<k} V_{3N,ijk} + \cdots \]

- these symmetries constrain the possible operator structures that can appear in the interaction terms...

... but how can we really **determine the nuclear interaction**?
The nuclear interaction is **not fundamental**

- residual force analogous to van der Waals interaction between neutral atoms

- **based on QCD** and induced via polarization of quark and gluon distributions of nucleons

- **encapsulates all the complications** of the QCD dynamics and the structure of nucleons

- acts only if the nucleons overlap, i.e. at **short ranges**

- irreducible **three-nucleon interactions** are important
until 2005: **high-precision phenomenological NN interactions** were state-of-the-art in ab initio nuclear structure theory

- **Argonne V18**: long-range one-pion exchange plus phenomenological parametrization of medium- and short-range terms, local operator form
- **CD Bonn 2000**: more systematic one meson-exchange parametrization including pseudo-scalar, scalar and vector mesons, inherently nonlocal

parameters of the NN potential supplemented by **phenomenological 3N interactions** consisting of a Fujita-Miyazawa-type term plus various hand-picked contributions

fit to ground states and spectra of light nuclei, sometimes up to $A \leq 8$
\[
\nu_{NN} = \sum_{S,T} \nu^c_{ST}(r) \Pi_{ST} + \sum_{S,T} \nu^{l2}_{ST}(r) \vec{L}^2 \Pi_{ST} \\
+ \sum_{T} \nu^t_{T}(r) S_{12} \Pi_{1T} + \sum_{T} \nu^{ls}_{T}(r) (\vec{L} \cdot \vec{S}) \Pi_{1T} \\
+ \sum_{T} \nu^{ls2}_{T}(r) (\vec{L} \cdot \vec{S})^2 \Pi_{1T} + \ldots
\]

(\(S, T\))
- (1, 0)
- (1, 1)
- (0, 0)
- (0, 1)
first attempts towards construction of nuclear interactions directly from lattice QCD simulations

compute relative two-nucleon wave function on the lattice

invert Schrödinger equation to extract effective two-nucleon potential

only schematic results so far (unphysical masses and mass dependence, model dependence,...)

alternatives: phase-shifts or low-energy constants from lattice QCD
Today... from Chiral EFT

- low-energy **effective field theory** for relevant degrees of freedom ($\pi, N$) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- systematic expansion in a small parameter with power counting enable **controlled improvements** and **error quantification**
- hierarchy of **consistent** NN, 3N, 4N,... interactions
- consistent **electromagnetic and weak operators** can be constructed in the same framework

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Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...
Many Options

- **standard chiral NN+3N**
  - NN: N3LO, Entem&Machleidt, nonlocal, cutoff 500 MeV
  - 3N: N2LO, Navratil, local, cutoff 500 (400) MeV

- **nonlocal LO...N3LO**
  - NN: LO...N3LO, Epelbaum, nonlocal, cutoff 450...600 MeV
  - 3N: N2LO, Nogga, nonlocal, cutoff 450...600 MeV

- **N2LO-opt, N2LO-sat, ...**
  - NN: N2LO, Ekström et al., nonlocal, cutoff 500 MeV
  - 3N: N2LO, Ekström et al., nonlocal, cutoff 500 MeV

- **local N2LO**
  - NN: N2LO, Gezerlis et al., local, cutoff 1.0...1.2 fm
  - 3N: N2LO, Gezerlis et al., local, cutoff 1.0...1.2 fm

- **semilocal LO...N4LO**
  - NN: LO...N4LO, Epelbaum, semilocal, cutoff 0.8...1.2 fm
  - 3N: N2LO...N3LO, LENPIC, semilocal, cutoff 0.8...1.2 fm

- first generation, most widely used up to now
- also first generation, but scarcely used
- improved fitting, also many-body inputs
- designed specifically for QMC applications
- the future...
Momentum-Space Matrix Elements

\[ \langle q(LS)JM; TM_T|v_{NN}|q'(L'S)JM; TM_T \rangle \]

**Argonne V18**
- \( J=1 \)
- \( L=0 \)
- \( L'=0 \)
- \( S=1 \)
- \( T=0 \)

**chiral NN**
- \( J=1 \)
- \( L=0 \)
- \( L'=2 \)
- \( S=1 \)
- \( T=0 \)

(N3LO, E&M, 500 MeV)
Matrix Elements
Single-Particle Basis

- effective constituents are nucleons characterized by **position, spin and isospin** degrees of freedom

\[ |\alpha\rangle = |\text{position}\rangle \otimes |\text{spin}\rangle \otimes |\text{isospin}\rangle \]

- **typical basis choice** for configuration-type bound-state methods

\[ |\text{position}\rangle = |nlm_l\rangle \quad \text{spherical harmonic oscillator or other spherical single-particle potential} \]

\[ |\text{spin}\rangle = |s = \frac{1}{2}, m_s\rangle \quad \text{eigenstates of } s^2 \text{ and } s_z \text{ with } s=1/2 \]

\[ |\text{isospin}\rangle = |t = \frac{1}{2}, m_t\rangle \quad \text{eigenstates of } t^2 \text{ and } t_3 \text{ with } t=1/2 \]

- use **spin-orbit coupling** at the single-particle level

\[ |n(l^{\frac{1}{2}})jm; \frac{1}{2}m_t\rangle = \sum_{m_l,m_s} \, c\left( \begin{array}{c} l \\ m_l \\ \frac{1}{2} \\ m_s \\ j \\ m \end{array} \right) \ |nlm_l\rangle \otimes |\frac{1}{2}m_s\rangle \otimes |\frac{1}{2}m_t\rangle \]
Many-Body Basis

- **Slater determinants**: antisymmetrized A-body product states
  \[
  |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = \frac{1}{\sqrt{A!}} \sum_{\pi} \text{sgn}(\pi) P_\pi (|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_A\rangle)
  \]

- convenient to work with **second quantization**: string of creation operators acting on vacuum state
  \[
  |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = a_\alpha^1 a_\alpha^2 \ldots a_\alpha^A |0\rangle
  \]

- given a complete single-particle basis \{ |\alpha\rangle \} then the set of Slater determinants formed by all possible combinations of A different single-particle states is a **complete basis of the antisymmetric A-body Hilbert space**

- **expansion of general antisymmetric state** in Slater determinant basis
  \[
  |\psi\rangle = \sum_{\alpha_1<\alpha_2<\ldots<\alpha_A} C_{\alpha_1\alpha_2\ldots\alpha_A} |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = \sum_i C_i |\{\alpha_1 \alpha_2 \ldots \alpha_A\}_i\rangle
  \]
Partial-Wave Matrix Elements

- **relative partial-wave matrix elements** of NN and 3N interaction are **universal input** for many-body calculations.

- selection of **relevant partial-wave bases** in two and three-body space with all \( M \) quantum numbers suppressed:
  
  - two-body relative momentum: \(|q (LS)JT\rangle\)
  - two-body relative HO: \(|N (LS)JT\rangle\)
  - three-body Jacobi momentum: \(|\pi_1 \pi_2; [(L_1 S_1)J_1, (L_2 \frac{1}{2}) J_2] J_{12}; (T_1 \frac{1}{2}) T_{12}\rangle\)
  - three-body Jacobi HO: \(|N_1 N_2; [(L_1 S_1)J_1, (L_2 \frac{1}{2}) J_2] J_{12}; (T_1 \frac{1}{2}) T_{12}\rangle\)
  - antisym. three-body Jacobi HO: \(|E_{12} i J_{12}^{\pi} T_{12}\rangle\)

- lots of **transformations** between the different bases are needed in practice.

- **exception**: Quantum Monte-Carlo methods working in coordinate representation need local operator form.
Symmetries and Matrix Elements

- relative partial-wave matrix elements make **maximum use of the symmetries** of the nuclear interaction

- consider, e.g., the relative two-body matrix elements in HO basis

\[
\langle N (LS)JM; TM_T|v_{NN}|N' (L'S')J'M'; T'M'_T\rangle
\]

- the matrix elements of the NN interaction
  
  ... do not connect different \(J\)
  
  ... do not connect different \(M\) and are independent of \(M\)
  
  ... do not connect different parities
  
  ... do not connect different \(S\)
  
  ... do not connect different \(T\)
  
  ... do not connect different \(M_T\)

\[
\Rightarrow \langle N (LS)J; TM_T|v_{NN}|N' (L'S)J; TM_T\rangle
\]

- relative matrix elements are **efficient and simple to compute**
Transformation to Single-Particle Basis

- most many-body calculations need **matrix elements with single-particle quantum numbers** (cf. second quantization)
  
  \[ \langle \alpha_1 \alpha_2 | v_{NN} | \alpha'_1 \alpha'_2 \rangle = \]
  
  \[ = \langle n_1 l_1 j_1 m_1 m_{t1}, n_2 l_2 j_2 m_2 m_{t2} | v_{NN} | n'_1 l'_1 j'_1 m'_1 m'_{t1}, n'_2 l'_2 j'_2 m'_2 m'_{t2} \rangle \]

- obtained from relative HO matrix elements via **Moshinsky-transformation**

  \[ \langle n_1 l_1 j_1, n_2 l_2 j_2 ; JT | v_{NN} | n'_1 l'_1 j'_1, n'_2 l'_2 j'_2 ; JT \rangle = \]
  
  \[ = \sqrt{(2j_1 + 1)(2j_2 + 1)(2j'_1 + 1)(2j'_2 + 1)} \sum \sum \sum \sum \sum \sum \sum \sum \sum \sum \]
  
  \[ \times \frac{1}{\sqrt{(2l_1 + 1)(2l_2 + 1)}} \]
  
  \[ \times \frac{(2j_1 + 1)(2S + 1)(2L + 1)(2L' + 1)(-1)^{L+L'} \{1 - (-1)^{\lambda+S+T}\}}{(2j'_1 + 1)(2S' + 1)(2L' + 1)(2L + 1)(-1)^{L'+L} \{1 - (-1)^{\lambda'+S+T}\}} \]
  
  \[ \times \langle v (\lambda S) jT | v_{NN} | v'(\lambda' S) jT \rangle \]

**This analytic transformation from relative to single-particle matrix elements only exists for the harmonic oscillator basis.**
beneath any ab initio many-body method there is a **machinery for computing, transforming and storing matrix elements** of all operators entering the calculation.

- compute and store relative two-body HO matrix elements of NN interaction
- compute and store Jacobi three-body HO matrix elements of 3N interaction
- perform unitary transformations of the two- and three-body relative matrix elements (e.g. Similarity Renormalization Group)
- transform to single-particle JT-coupled two-body HO matrix elements and store
- transform to single-particle JT-coupled three-body HO matrix elements and store

same for 4N with four-body matrix elements
Two-Body Problem
Solving the Two-Body Problem

- **simplest ab initio problem**: the only two-nucleon bound state, the deuteron

- start from **Hamiltonian in two-body space**, change to center of mass and intrinsic coordinates

\[ H = H_{\text{cm}} + H_{\text{int}} = T_{\text{cm}} + T_{\text{int}} + V_{\text{NN}} \]

\[ = \frac{1}{2M} \bar{p}_{\text{cm}}^2 + \frac{1}{2\mu} \bar{q}^2 + V_{\text{NN}} \]

- separate two-body state into center of mass and intrinsic part

\[ |\psi\rangle = |\Phi_{\text{cm}}\rangle \otimes |\phi_{\text{int}}\rangle \]

- solve **eigenvalue problem for intrinsic part** (effective one-body problem)

\[ H_{\text{int}} |\phi_{\text{int}}\rangle = E |\phi_{\text{int}}\rangle \]
Solving the Two-Body Problem

- expand eigenstates in a **relative partial-wave HO basis**

\[ |\phi_{\text{int}}\rangle = \sum_{NLSJMTM_T} C_{NLSJMTM_T} |N(LS)JM; TM_T\rangle \]

\[ |N(LS)JM; TM_T\rangle = \sum_{M_LM_S} c \left( \frac{L}{M_L} \frac{S}{M_S} \right) |NLM_L\rangle \otimes |SM_S\rangle \otimes |TM_T\rangle \]

- **symmetries** simplify the problem dramatically:
  - \( H_{\text{int}} \) does not connect/mix different \( J, M, S, T, M_T \) and parity \( \pi \)
  - angular mom. coupling only allows \( J=L+1, L, L-1 \) for \( S=1 \) or \( J=L \) for \( S=0 \)
  - total antisymmetry requires \( L+S+T=\text{odd} \)

- for given \( J^n \) at most two sets of angular-spin-isospin quantum numbers contribute to the expansion
Deuteron Problem

- assume $J^n = 1^+$ for the **deuteron ground state**, then the basis expansion reduces to

\[ |\phi_{\text{int}, J^{\pi} = 1^+} \rangle = \sum_N C_N^{(0)} |N(01) \, 1M; 00 \rangle + \sum_N C_N^{(2)} |N(21) \, 1M; 00 \rangle \]

- inserting into Schrödinger equation and multiplying with basis bra leads to **matrix eigenvalue problem**

\[
\begin{pmatrix}
\langle N'(01) \ldots | H_{\text{int}} | N(01) \ldots \rangle & \langle N'(01) \ldots | H_{\text{int}} | N(21) \ldots \rangle \\
\langle N'(21) \ldots | H_{\text{int}} | N(01) \ldots \rangle & \langle N'(21) \ldots | H_{\text{int}} | N(21) \ldots \rangle
\end{pmatrix}
\begin{pmatrix}
C_N^{(0)} \\
C_N^{(2)}
\end{pmatrix}
= 
\begin{pmatrix}
C_{N'}^{(0)} \\
C_{N'}^{(2)}
\end{pmatrix}
\]

- eigenvectors yield expansions coefficients and eigenvalues the energies

- truncate matrices to $N \leq N_{\text{max}}$ and choose $N_{\text{max}}$ large enough so that observables are converged, i.e., do not depend on $N_{\text{max}}$ anymore
Deuteron Solution

- Deuteron wave function show two characteristics that are **signatures of correlations** in the two-body system:
  - suppression at small distances due to short-range repulsion
  - \( L=2 \) admixture generated by tensor part of the NN interaction
Correlations &
Unitary Transformations
Correlations

- many-body eigenstates of independent-particle models described by one-body Hamiltonians are **Slater determinants**
- thus, a single Slater determinant **does not describe correlations**
- but Slater determinants are a basis of the antisym. A-body Hilbert space, so any state can be expanded in Slater determinants
- to describe **short-range correlations**, a superposition of many Slater determinants is necessary
Why Unitary Transformations?

Realistic nuclear interactions generate strong short-range correlations in many-body states.

**Unitary Transformations**
- Adapt Hamiltonian to truncated low-energy model space
- Improve convergence of many-body calculations
- Preserve the physics of the initial Hamiltonian and all observables

Many-body methods rely on truncated Hilbert spaces not capable of describing these correlations.
unitary transformations **conserve the spectrum** of the Hamiltonian, with a unitary operator $U$ we get

$$H |\psi\rangle = E |\psi\rangle$$
$$U^\dagger H U |\psi\rangle = E U^\dagger |\psi\rangle$$

with

$$\tilde{H} |\tilde{\psi}\rangle = E |\tilde{\psi}\rangle$$

for **other observables** defined via matrix elements of an operator $A$ with the eigenstates we obtain

$$\langle \psi | A |\psi'\rangle = \langle \psi | U U^\dagger A U U^\dagger |\psi'\rangle = \langle \tilde{\psi} | \tilde{A} |\tilde{\psi}'\rangle$$

**unitary transformations conserve all observables as long as the Hamiltonian and all other operators are transformed consistently**
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