Perspectives in Low-Energy Nuclear Physics

Robert Roth
Dear Robert,

David and I would like to ask you if you are willing to give a colloquium at TRIUMF on February 19th 2016.

This is the week before the Nuclear Theory workshop, during which we will have another colloquium by Thomas Papenbrock on "Recent Advances in Nuclear Theory".

In the light of this, we thought that having a preparatory talk where the big questions in nuclear physics are introduced in a very simple manner would be useful...

We feel this will help to communicate the importance of nuclear physics and nuclear theory to the general laboratory...

Please let us know if you are interested in this.

Thanks a lot,
Sonia
The Big Picture
Low-Energy Nuclear Physics

Diversity
- structure emerging from microscopic dynamics
- thousands of isotopes, many very special
- zoo of phenomena: shell structure, clustering, deformation, stability, excitations, resonances, transitions, decays, reactions,…

Complexity
- multi-physics: strong, weak and el.mag. interactions
- multi-scale: from keV to GeV
- multi-process: structure, decays and reactions
- multi-observable: energies, el.mag.,…

Impact
- key input for understanding the evolution of the universe
- tiny things have huge implications: deuteron, Hoyle state,…
- foundation for atomic and molecular physics, chemistry, solid state,…
- direct applications

...a multi-faceted lab connecting fundamental physics with daily life
Low-Energy Nuclear Theory

the most challenging quantum many-body problem...

- systems of 2 - 300 nucleons
- nucleons are composite themselves
- dominated by correlations
- self-bound system
- translational & rotational symmetry
- competition of large energy contributions
- interaction inherits complexity of QCD
- residual van der Waals interaction
- significant three-body forces
- bound and continuum states
- range of different observables
- weak binding and threshold physics

...try a non-relativistic quantum description with nucleons as relevant degrees of freedom
The Problem

\[ H \left| \psi \right\rangle = E \left| \psi \right\rangle \]

- We do not know the interaction...
  - ...we need additional models to construct a nuclear interaction to start with

- We do not know how to solve the equation...
  - ...we need truncations or approximations to make the problem tractable
Strategy I: Phenomenology

- pick a **simple approximation scheme** for the Schrödinger equation tailored for the observables of interest
- construct a computationally convenient **model for the nuclear interaction** compatible with this approximation
- **fit the parameters** of the interaction model **to observables** within the chosen approximation scheme

\[ H |\psi\rangle = E |\psi\rangle \]

**Skyrme-Hartree-Fock**
- approximate many-body state by single Slater determinant and parameterize interaction with contact terms

**Valence-Space Shell Model**
- freeze core nucleons and treat a few valence nucleons in small valence space with fitted interaction matrix elements
Strategy II: Ab Initio

- construct **realistic nuclear interactions** based on as much QCD input as possible and fit to few-nucleon properties in exact calculations

- **solve the Schrödinger equation** using systematic truncations with **controlled uncertainties**

\[ H |\psi\rangle = E |\psi\rangle \]

- interactions are independent of many-body framework
- different many-body methods can employ the same interaction
- different interactions can be tested in one many-body approach
Interactions
Nature of the Nuclear Interaction

- 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

\[
\rho_0^{-1/3} = 1.8\text{fm}
\]

\[\sim 1.6\text{fm}\]
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
Tomorrow... from Lattice QCD

Beane et al., PRD87, 034506 (2013), PRC88, 024003 (2013)

\[
\begin{align*}
\text{Extensive study of s-shell nuclei and hypernuclei, and} \\
\text{baryon-baryon interactions at SU(3) symmetric point}
\end{align*}
\]

\[m_\pi \sim 800 \text{ MeV}\]
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
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. NN+3N**
  - NN: N2LO, Ekström et al., nonlocal, cutoff 500 MeV
  - 3N: N2LO, Ekström et al., nonlocal, cutoff 500 MeV

- **local NN+3N**
  - 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

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- 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
- order-by-order uncertainty estimates

All these interactions are equally valid, use them all to study uncertainties.
Many-Body Solution
- Eigenvalue Problem -
Eigenvalue Problem

- Start from **many-body Schrödinger equation**

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

- Define an **many-body basis** and expand eigenstates in this basis

\[ |\psi_n\rangle = \sum_i C_i^{(n)} |\phi_i\rangle \]

- Convert Schrödinger equation into a **matrix eigenvalue problem**

\[
\begin{pmatrix}
\ddots \\
C_{i'}^{(n)} \\
\ddots \\
\end{pmatrix}
= E_n
\begin{pmatrix}
\ddots \\
C_i^{(n)} \\
\ddots \\
\end{pmatrix}
\]

Numerically solve large-scale matrix eigenvalue problem for few low-lying eigenvalues
Configuration Interaction

- have to **introduce truncations** of the basis to make the Hamilton matrix finite and numerically tractable

  - **single-particle truncation (full CI):**
    truncate the underlying single-particle basis, e.g., at a maximum single-particle energy $e_{\text{max}}$, and construct all possible Slater determinants

  - **many-body truncation (NCSM):**
    truncate the many-body Slater-determinant basis at a maximum number of harmonic-oscillator excitation quanta $N_{\text{max}}$

---

- one has to **demonstrate convergence** with respect to the model-space truncation for accurate results
- incomplete convergence as **only source of uncertainties** in the many-body treatment
- model space dimension **grows dramatically** with truncation parameter $e_{\text{max}}$ or $N_{\text{max}}$ and particle number
Convergence

\[ E \text{ [MeV]} \]

\[ N_{\text{max}} \]

\[ \exp. \]

\[ 6^\text{Li} \]

\[ 12^\text{C} \]

IT-NCSM

chiral NN+3N

EM, 500 MeV

\( \alpha = 0.08 \text{ fm}^4 \)

\( \hbar \Omega = 20 \text{ MeV} \)

convergence depends very much on observable

convergence defines range of applicability of CI methods

extrapolation techniques and softening of Hamiltonian help
of course, spectra depend on choice of initial chiral NN+3N interaction, but the dependence is not dramatic

important contribution to the total theory uncertainty
individual states show systematic disagreement with experiment:
- second $0^+$: Hoyle state, cluster structure not captured in HO basis
- first $1^+$: systematic problem with N2LO-3N interaction?
Electric quadrupole (E2) observables involving $0^+$ ground state & first excited $2^+$

Model-space convergence is terrible, E2 operator sensitive to long-range wave functions

$B(E2, 2^+ \rightarrow 0^+) [e^2 fm^4]$ vs $Q(2^+) [e fm^2]$ for $^{12}\text{C}$

$\hbar\Omega = 16 \text{ MeV}$

$N_{\text{max}}$ vs $NN/3N$

- 2
- 4
- 6
- 8
p-Shell Spectroscopy: Correlations

- **electric quadrupole (E2)** observables involving $0^+$ ground state & first excited $2^+$

- model-space convergence is terrible, E2 operator sensitive to long-range wave functions

- **extremely robust correlation** predicted by NCSM for all interactions and model spaces
**p-Shell Spectroscopy: Correlations**

- **electric quadrupole (E2)** observables involving $0^+$ ground state & first excited $2^+$
- model-space convergence is terrible, E2 operator sensitive to long-range wave functions
- **extremely robust correlation** predicted by NCSM for all interactions and model spaces
- predict $Q(2^+)$ with very high accuracy based on experimental datum for $B(E2)$

**New way to exploit ab initio calculations and to bridge to effective models**

Calci, Roth; arXiv:1601.07209
p-Shell Spectroscopy: Precision

- **magnetic dipole (M1)** observables involving $1^+$ ground state & $0^+$ excited state

- dipole moment and $B(M1)$ are **very robust** (few % changes)

- mild systematic model-space dependence of $B(M1)$

- dipole moment affected by 3N interaction and in slight disagreement with experiment

■ ready for precision studies, e.g., on electromagnetic two-body currents
Many-Body Solution
- Unitary Transformation -
Unitary Transformations

- partially **diagonalize Hamilton matrix** through a unitary transformation and read-off eigenvalues from the diagonal

\[
\begin{pmatrix}
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\end{pmatrix}

\textbf{continuous unitary transformation} of many-body Hamiltonian

\[ H_\alpha = U_\alpha^\dagger H U_\alpha \]

morphs the initial Hamilton matrix \((\alpha = 0)\) to diagonal form \((\alpha \rightarrow \infty)\)
Similarity Renormalization Group

**Continuous unitary transformation** to pre-diagonalize the Hamiltonian with respect to a given basis

- **Consistent unitary transformation** of Hamiltonian and observables
  \[ H_\alpha = U_\alpha^\dagger H U_\alpha \quad \text{and} \quad O_\alpha = U_\alpha^\dagger O U_\alpha \]

- **Flow equations** for \( H_\alpha \) and \( U_\alpha \) with continuous parameter \( \alpha \)
  \[ \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \quad \text{and} \quad \frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha \]

- The physics of the transformation is governed by the **dynamic generator** \( \eta_\alpha \)

- Design generator for desired **diagonalization or decoupling pattern**

*Free-Space SRG* well established for softening the Hamiltonian in two- and three-body space
In-Medium SRG

- flow equation for Hamiltonian and Wegner-type generator
  \[ \frac{d}{ds} H(s) = \left[ \eta(s), H(s) \right] \]
  \[ \eta(s) = \left[ H(s), H^{\text{off-diag}}(s) \right] \]

- write everything in normal ordered form with respect to a single- or multi-determinantal reference state

\[ H(s) = E(s) + \sum_{ij} f_j^i(s) \tilde{A}_j^i + \frac{1}{4} \sum_{ijkl} \Gamma_{kl}^{ij}(s) \tilde{A}_{kl}^{ij} + \frac{1}{36} \sum_{ijklmn} W_{klmn}^{ijkl}(s) \tilde{A}_{lmn}^{jk} \]

use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations

discard normal-ordered three-body terms

additional truncation that causes uncertainties
Flowing Energy

16\(^{16}\)O

chiral NN+3N
\[ \Lambda_{3N}=400 \text{ MeV} \]
\[ \alpha=0.08 \text{ fm}^4 \]
\[ \hbar\Omega=20 \text{ MeV} \]
\[ e_{\text{max}}=12 \]
\[ N_{\text{max}}=0 \]
reference state

Hamilton matrix in \( N_{\text{max}}=2 \) space
Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

\[
\Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\text{max}} = 14, \quad \text{optimal } h\Omega
\]
Ground States of Oxygen Isotopes

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Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

\[ \text{NN+3N} \]

\[ \text{full} \]

\[ \text{chiral NN+3N} \]

\[ A \]

\[ \text{E} \]

\[ \text{MeV} \]

\[ \text{AO} \]

\[ \text{experiment} \]

\[ \text{IT-NCSM} \]

\[ \text{MR-IM-SRG} \]

\[ \text{CCSD} \]

\[ \Lambda-\text{CCSD(T)} \]

\[ \Lambda \]

\[ 3N = 400 \text{ MeV}, \alpha = 0.08 \text{ fm}, E_{3N}^x = 14 \text{, optimal} \]

\[ \tilde{h} \]

\[ \Omega \]

\[ \text{different many-body approaches using the same chiral NN+3N interaction give consistent results} \]

\[ \text{minor differences are understood in terms of uncertainties due to truncations} \]
Merging CI and IM-SRG

- combine CI/NCSM with IM-SRG to get the **best aspects of both methods**

- solve NCSM problem in small $N_{\text{max}}$
- extract reference state

- solve MR-IM-SRG flow equations
- decoupling of particle-hole excitations in many-body space

- solve CI problem with IM-SRG evolved Hamiltonian
- extract ground and excitation energies and other observables
instead of using the zero-body piece of the normal-ordered Hamiltonian, we can use the complete flowing Hamiltonian in a CI calculation.
instead of using the zero-body piece of the normal-ordered Hamiltonian, we can use the complete **flowing Hamiltonian in a CI calculation**

• decoupling though the IM-SRG transformation causes **ridiculously fast convergence** of CI calculation

\[ \Lambda_{3N}=400 \text{ MeV} \]
\[ \alpha=0.08 \text{ fm}^4 \]
\[ \hbar \Omega=20 \text{ MeV} \]
\[ e_{\text{max}}=12 \]
\[ N_{\text{max}}=0 \]

reference state
CI-IM-SRG: Ground State

\begin{align*}
\Lambda_{3N} &= 400 \text{ MeV} \\
\alpha &= 0.08 \text{ fm}^4 \\
h\Omega &= 20 \text{ MeV} \\
e_{\text{max}} &= 12 \\
N_{\text{max}} &= 0
\end{align*}

reference state

Gebrerufael et al.; in prep.

\textbf{12C}

chiral NN+3N

Hamilton matrix in \(N_{\text{max}}=2\) space
CI-IM-SRG: Ground State

\[ \Lambda_{3N} = 400 \text{ MeV} \]
\[ \alpha = 0.08 \text{ fm}^4 \]
\[ \hbar \Omega = 20 \text{ MeV} \]
\[ e_{\text{max}} = 12 \]
\[ N_{\text{max}} = 0 \]

reference state

effects of IM-SRG truncation at the normal-ordered two-body level
CI-IM-SRG: Excited States

- from the same CI calculation we get the *excited states*

\[ \Lambda_{3N}=400 \text{ MeV} \]
\[ \alpha=0.08 \text{ fm}^4 \]
\[ \hbar\Omega=20 \text{ MeV} \]
\[ e_{\text{max}}=12 \]
\[ N_{\text{max}}=0 \]
reference state

Gebrerufael et al.; in prep.
CI-IM-SRG: Excited States

- from the same CI calculation we get the excited states
- excitation energies only show subtle changes with IM-SRG flow...

Gebrerufael et al.; in prep.

\[ \Lambda_{3N} = 400 \text{ MeV} \]
\[ \alpha = 0.08 \text{ fm}^4 \]
\[ \hbar \Omega = 20 \text{ MeV} \]
\[ e_{\text{max}} = 12 \]
\[ N_{\text{max}} = 0 \]

Reference state

\[ ^{12}\text{C} \]
CI-IM-SRG: Excited States

- from the same CI calculation we get the **excited states**
- excitation energies only show subtle changes with IM-SRG flow...
  ...but there are notable exceptions... **Hoyle state?**

### $^{12}$C

- **chiral NN+3N**
  - $\Lambda_{3N}=400$ MeV
  - $\alpha=0.08$ fm$^4$
  - $\hbar\Omega=20$ MeV
  - $e_{\text{max}}=12$
  - $N_{\text{max}}=0$

reference state
CI-IM-SRG: Spectrum

- **promising starting point** for ab initio studies of arbitrary open-shell nuclei

Gebrerufael et al.; in prep.

```
12C
chiral NN+3N
Λ_3N=400 MeV
α=0.08 fm^4
ħΩ=20 MeV
e_max=12
N_max=0
reference state
s=0.2 MeV^{-1}
```
- the decoupling concept can also be used to **connect ab initio methods to traditional phenomenological approaches**

- **valence-space shell model**: construct a valence-space interaction by decoupling core and excluded space from valence space though IM-SRG or Lee-Suzuki transformation

- **unification** of nuclear structure approaches and their interpretation
nuclear structure physics has evolved rapidly over the past few years

many new ideas have emerged for nuclear interactions and many-body approaches... and more is coming

moving towards a comprehensive theory of nuclear structure and reactions with quantified theory uncertainties

it’s fun to be part of it...
Epilogue

- **thanks to my group and my collaborators**

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