The Nuclear Many-Body Problem

Original lecture by Witek Nazarewicz
The Nuclear Many-Body Problem

\[ \hat{H}\Psi = E\Psi \]

\[ \hat{H} = \hat{T} + \hat{V} \]

one-body

\[ \hat{T} = \sum_{i=1}^{A} \frac{\hat{p}_i^2}{2m_i}, \]

Kinetic energy

two-body three-body

\[ \hat{V} = \sum_{i<j} \hat{V}_{2b}(i,j) + \sum_{i<j<k} \hat{V}_{3b}(i,j,k) \]

Potential energy

\[ \Psi = \Psi(\vec{r_1}, \vec{r_2}, \ldots, \vec{r}_A; s_1, s_2, \ldots, s_A; t_1, t_2, \ldots, t_A) \]

3A nucleon nucleon nucleon
coordinates spins: \( \pm \frac{1}{2} \) isospins (p or n): \( \pm \frac{1}{2} \)
in r-space

Eigenstate of angular momentum, parity, and ~isospin

\[ 2^A \times \frac{A!}{N!Z!} \]

coupled integro-differential equations in 3A dimensions
Weinberg’s Laws of Progress in Theoretical Physics
From: “Asymptotic Realms of Physics” (ed. by Guth, Huang, Jaffe, MIT Press, 1983)

First Law: “The conservation of Information” (You will get nowhere by churning equations)

Second Law: “Do not trust arguments based on the lowest order of perturbation theory”

Third Law: “You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you’ll be sorry!”
How are nuclei made?

- Origin of elements, isotopes
- Hot and dense quark-gluon matter
- Hadron structure

Applications of nuclear science

To explain, predict, use…
Interfaces provide crucial clues

number of nuclei < number of processors!
Ab initio theory for light nuclei and nuclear matter

**Ab initio:** QMC, NCSM, CCM,…
(nuclei, neutron droplets, nuclear matter)

**Input:**
- Excellent forces based on the phase shift analysis and few-body data
- EFT based nonlocal chiral NN and NNN potentials
- SRG-softened potentials based on bare NN+NNN interactions

![Diagram]

- **Ab initio input**
  - NN+NNN interactions
  - Renormalization
- **Many body method**
- **Observables**
- • Direct comparison with experiment
  • Pseudo-data to inform theory
Few-nucleon systems

$A=2$: many years ago…

$^3\text{H}$: 1984 (1% accuracy)

$^3\text{He}$: 1987

$^4\text{He}$: 1987

$^5\text{He}$: 1994 (n-$\alpha$ resonance)

$A=6,7,..12$: 1995-2011
In the early decades, the progress was approximately linear in $A$ because the computing power, which increased exponentially according to Moore’s law, was applied to exponentially expensive numerical algorithms. In recent years, new-generation algorithms, which exhibit polynomial scaling in $A$, have greatly increased the reach.
Green’s Function Monte Carlo (imaginary-time method)

\[ |\psi_0\rangle = \lim_{\tau \to \infty} e^{-\left(\hat{H} - E_0\right)\tau} |\psi_V\rangle \]

trial wave function

\[ |\psi(\tau)\rangle = e^{-\left(\hat{H} - E_0\right)\tau} |\psi_V\rangle \]

\[ |\psi(0)\rangle = |\psi_V\rangle, \quad |\psi(\infty)\rangle = |\psi_0\rangle \]

\[ \tau = n\Delta\tau \quad \Rightarrow \quad |\psi(\tau)\rangle = \left[ e^{-\left(\hat{H} - E_0\right)\Delta\tau} \right]^n |\psi_V\rangle \]

- Quantum Monte Carlo (GFMC)
- No-Core Shell Model
- Faddeev-Yakubovsky
- Lattice EFT
- Coupled-Cluster Techniques
- Fermionic Molecular Dynamics
- \(^{12}\text{C}\)
- \(^{14}\text{F}, \ ^{14}\text{C}\)
- \(^{12}\text{C} \text{ (Hoyle)}\)
- \(^{17}\text{F}, \ ^{56}\text{Ni}\)
- …
1-2% calculations of $A = 6 - 12$ nuclear energies are possible excited states with the same quantum numbers computed.
In 1954, Hoyle postulated that a 7.65 MeV carbon state. This state plays a crucial role in the hydrogen burning of stars heavier than our sun and in the production of carbon and other elements necessary for life.
Anthropic Principle

The anthropic principle (from Greek anthropos, meaning "human") is the philosophical consideration that observations of the physical Universe must be compatible with the conscious life that observes it. Some proponents of the anthropic principle reason that it explains why the universe has the age and the fundamental physical constants necessary to accommodate conscious life.


The nucleosynthesis of carbon-12 and Hoyle state
"Varying the light quark mass: impact on the nuclear force and Big Bang nucleosynthesis", Phys. Rev. D 87 (2013) 085018
Ab initio calculation of the neutron-proton mass difference

“...The result of the neutron-proton mass splitting as a function of quark-mass difference and electromagnetic coupling. In combination with astrophysical and cosmological arguments, this figure can be used to determine how different values of these parameters would change the content of the universe. This in turn provides an indication of the extent to which these constants of nature must be fine-tuned to yield a universe that resembles ours.”
ab-initio alpha-alpha scattering

Elhatisari et al., Nature 528, 111 (2015)

http://www.nature.com/nature/journal/v528/n7580/full/nature16067.html
http://www.nature.com/nature/journal/v528/n7580/abs/528042a.html
Anomalous Long Lifetime of $^{14}$C

Determine the microscopic origin of the suppressed $\beta$-decay rate: 3N force

Dimension of matrix solved for 8 lowest states $\sim 10^9$
Solution took $\sim 6$ hours on 215,000 cores on Cray XT5 Jaguar at ORNL

Maris et al., PRL 106, 202502 (2011)
Computational nuclear physics enables us to reach into regimes where experiments and analytic theory are not possible, such as the cores of fission reactors or hot and dense evolving environments such as those found in inertial confinement fusion environment.

Ab initio theory reduces uncertainty due to conflicting data

- The $n^{-3}H$ elastic cross section for 14 MeV neutrons, important for NIF, was not known precisely enough.
- Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility.

Configuration interaction techniques

- light and heavy nuclei
- detailed spectroscopy
- quantum correlations (lab-system description)

Input: configuration space + forces

Method

- NN+NNN interactions
- Renormalization
- Diagonalization
- Truncation+diagonalization
- Monte Carlo

Matrix elements fitted to experiment

Observables

- Direct comparison with experiment
- Pseudo-data to inform reaction theory and DFT
Nuclear shell model

\[ \hat{H} = \sum_i t_i + \frac{1}{2} \sum_{i,j \neq j} v_{ij} = \sum_i (t_i + V_i) + \left[ \frac{1}{2} \sum_{i,j \neq j} v_{ij} - \sum_i V_i \right] \]

One-body Hamiltonian

Residual interactions

- Construct basis states with good \((J_z, T_z)\) or \((J, T)\)
- Compute the Hamiltonian matrix
- Diagonalize Hamiltonian matrix for lowest eigenstates
- Number of states increases dramatically with particle number

Full \(fp\) shell for \(^{60}\text{Zn}\) : \(\approx 2 \times 10^9\) \(J_z\) states

- \(5,053,594\) \(J = 0, T = 0\) states
- \(81,804,784\) \(J = 6, T = 1\) states

- Can we get around this problem? Effective interactions in truncated spaces \((P\)-included, finite; \(Q\)-excluded, infinite\)
- Residual interaction \((G\)-matrix\) depends on the configuration space. Effective charges
- Breaks down around particle drip lines

\[ G = G^p + G^q \]

\(G\)-matrix, obtained from the Bethe-Goldstone equation (scattering within a nuclear medium)
Microscopic valence-space Shell Model Hamiltonian

Coupled Cluster Effective Interaction
(valence cluster expansion)

In-medium SRG Effective Interaction

Energy (MeV)

CCEI  Exp.  USD

22O


Diagonalization Shell Model

(medium-mass nuclei reached; dimensions $10^9$!)

C. Bäumer et al., PRC 68, 031303 (2003)

$^{51}\text{V}(d,^2\text{He})^{51}\text{Ti}$

$E_{\text{lab}} = 171$ MeV

$\Theta_{\text{cm}} < 1^\circ$

Martinez-Pinedo ENAM’04

Honma, Otsuka et al., PRC69, 034335 (2004)
Mean-Field Theory ⇒ Density Functional Theory

Degrees of freedom: nucleonic densities

Nuclear DFT
- two fermi liquids
- self-bound
- superfluid
- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.
Nuclear Energy Density Functional

**Isoscalar (T=0) density**
\[
\rho_0 = \rho_n + \rho_p
\]

**Isovector (T=1) density**
\[
\rho_1 = \rho_n - \rho_p
\]

+ Isoscalar and isovector densities: spin, current, spin-current tensor, kinetic, and kinetic-spin + Pairing densities

\[
E = \int \mathcal{H}(r) d^3r
\]

\[
\mathcal{H}(r) = \frac{\hbar^2}{2m} \tau_0(r) + \sum_{t=0,1} (\chi_t(r) + \tilde{\chi}_t(r))
\]

- Constrained by microscopic theory: ab-initio functionals provide quasi-data!
- Not all terms are equally important. Usually ~12 terms considered
- Some terms probe specific experimental data
- Pairing functional poorly determined. Usually 1-2 terms active.
- Becomes very simple in limiting cases (e.g., unitary limit)
- Can be extended into multi-reference DFT (GCM) and projected DFT

Expansion in densities and their derivatives
Examples: Nuclear Density Functional Theory

Traditional (limited) functionals provide quantitative description

Mass table

$\delta m = 0.581$ MeV

Goriely, Chamel, Pearson: HFB-17
Phys. Rev. Lett. 102, 152503 (2009)

How many protons and neutrons can be bound in a nucleus?

Erler et al.
Nature 486, 509 (2012)

Literature: 5,000-12,000

Skyrme-DFT: 6,900 ± 500_{syst}
Small and Large-Amplitude Collective Motion

- New-generation computational frameworks developed
  - Time-dependent DFT and its extensions
  - Collective Schrödinger Equation
  - Quasi-particle RPA
  - Projection techniques
- Applied to HI fusion, fission, coexistence phenomena

Shape coexistence

Fusion cross section

Hinohara et al. PRC 84, 061302(R) (2011)

also: Tsunoda et al. Phys. Rev. C 89, 031301(R) (2014); HPCI

R. Keser et al., PRC 85, 044606 (2012)
The covariance ellipsoid for the neutron skin $R_{\text{skin}}$ in $^{208}\text{Pb}$ and the radius of a 1.4$M_{\odot}$ neutron star. The mean values are: $R(1.4M_{\odot})$=10 km and $R_{\text{skin}}$ = 0.17 fm.
“High performance computing provides answers to questions that neither experiment nor analytic theory can address; hence, it becomes a third leg supporting the field of nuclear physics.” (NAC Decadal Study Report)

Future: large multi-institutional efforts involving strong coupling between physics, computer science, and applied math