Simplicity and complexity in the study of nuclei

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I. The big question:
"Given a lump of nuclear material, what are its properties, where did it come from, and how does it react?"

How are we going to describe nuclei that we cannot measure?
We need robust and predictive nuclear theory.
We need nuclear data to constrain that theory.
Goal: build a unified theory of nuclei

II. Ab initio treatments of nuclei
(building a nucleus from the ground up)

III. Emergent nuclear phenomena
(deformation, pairing, ‘magic’ numbers…)

IV. Whither RIA? How does physics of exotic nuclei fit into the global U.S. science strategy??
RIA Theory Group: 160 theorists
RIA Theory Roadmap: www.orau.org/ria/RIATG
The challenge of neutron rich nuclei

Enhanced 'Normal' Scattering Cross section

New magic numbers

Normal magic numbers

Continuum

Halos

Compact

Size

Important

Unimportant

Shell closures

New magic numbers

Normal magic numbers

Half-life

Long/stable

Short

'Scattering Cross section'

'Normal'

Enhanced

'Size'

Compact

Halos

'Continuum'

Important

Unimportant

208\(^\text{Pb}\): Well Bound Heavy Nucleus
“If you want more accuracy, you have to use more theory (more orders)"

Effective Lagrangian $\to$ obeys QCD symmetries (spin, isospin, chiral symmetry breaking)

Lagrangian $\to$ infinite sum of Feynman diagrams

Expand in $O(Q/\Lambda_{QCD})$

Weinberg, Ordonez, Ray, van Kolck

NN amplitude uniquely determined by two classes of contributions: contact terms and pion exchange diagrams.

24 parameters (rather than 40 from meson theory) to describe 2400 data points with $\chi^2_{dof} \approx 1$
Nuclear interactions: Cornerstone of the entire theoretical edifice

\[ H = \sum_{i=1, A M_i} \frac{\hbar^2}{2 M_i} \nabla_i^2 + \sum_{i<j} V(r_i, r_j) + V_{NNN} \]

Bare (GFMC)
Basis expansion

Many-body problems

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Choice of model space and the G-matrix

\[ G(\tilde{\omega}) = V + V \frac{Q}{\tilde{\omega} - QtQ} G(\tilde{\omega}) \]

Use BBP to eliminate \( \omega \)-dependence below fermi surface.

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

\[ \hbar \]

Q-Space

P-Space

ph intermediate states
Similarity transformed H

\[
H | k \rangle = E_k | k \rangle; \quad P + Q = 1
\]

\[
Q e^{-\omega} H e^{\omega} P = 0 \quad \Rightarrow \quad \langle \alpha_Q | k \rangle = \sum_{\alpha_P} \langle \alpha_Q | \omega | \alpha_P \rangle \langle \alpha_P | k \rangle
\]

\[
\overline{H}_{\text{eff}} = \left[ P \left( 1 + \omega^+ \omega \right) P \right]^{1/2} P H \left( P + Q \omega P \right) \left[ P \left( 1 + \omega^+ \omega \right) P \right]^{-1/2}
\]

**Advantage:** less parameter dependence in the interaction

**Current status**
- Exact deuteron energy obtained in P space
- Working on full implementation in CC theory.
- G-matrix + all folded-diagrams + ...
- Implemented, very new results follow....
Another approach: $V_{\text{lowk}}$

\[
T(k', k; k^2) = V_{\text{NN}}(k', k) + \frac{2}{\pi} \mathcal{P} \int_0^\infty \frac{V_{\text{NN}}(k', p) T(p, k; k^2)}{k^2 - p^2} p^2 dp,
\]

\[
T(k', k; k^2) = V_{\text{lowk}}^{\Lambda}(k', k) + \frac{2}{\pi} \mathcal{P} \int_0^\Lambda \frac{V_{\text{lowk}}^{\Lambda}(k', p) T(p, k; k^2)}{k^2 - p^2} p^2 dp.
\]

\[
\frac{d}{d\Lambda} V_{\text{lowk}}^{\Lambda}(k', k) = \frac{2}{\pi} \frac{V_{\text{lowk}}^{\Lambda}(k', \Lambda) T^{\Lambda}(\Lambda, k; \Lambda^2)}{1 - (k/\Lambda)^2}
\]

Method due to Schwenk, Bogner, Brown, Kuo

Produces a phase-equivalent potential that may then be used in many-body calculations.

The potential over binds.

Must be augmented by a 3-body force.

This approach does engender controversy, but it is an interesting one to investigate.
Interactions within the P-space

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

Q-space (integrated out of the problem)

P-Space

Mean-field level (Hartree Fock)

\[ | \Phi_0 \rangle \]
Coupled Cluster Theory: ab initio in medium mass nuclei

\[ |\Psi\rangle = \exp(T)|\Phi\rangle \]

Correlated Ground-State wave function

Correlation operator

Reference Slater determinant

Energy

Amplitude equations

\[ E = \langle \Phi | \exp(-T)H \exp(T)|\Phi\rangle \]

\[ \langle \Phi_{ij...} | \exp(-T)H \exp(T)\Phi \rangle = \langle \Phi_{ij...} | H | \Phi \rangle = 0 \]

- **Nomenclature**
  - Coupled-clusters in singles and doubles (CCSD)
  - …with triples corrections CCSD(T);
Comparisons with other many-body techniques

Quantum chemistry example (Bartlett et al)

Nuclear Example (Kowalski et al PRL 2004)
Inclusion of three-body forces:

Results with three-body forces included coming soon.....
Using the similarity transform: $H = T - T_{cm} + V$
\[ \rho_{\alpha\beta} = \left\langle \Phi \left| L^{(\mu)} \left[ e^{-T} a_\alpha^+ a_\beta e^T \right] R^{(\mu)} \right| \Phi \right\rangle \]

Also includes second-order corrections from the two-body density.

**Nuclear Properties**

- 5 shells, CM corrected
- 6 shells, CM corrected
- 7 shells, 5 shells, CM corrected
- 6 shells, \( r_{\text{rms}} = 2.45 \text{ fm} \)
- 7 shells, \( r_{\text{rms}} = 2.50 \text{ fm} \)
- 7 shells, \( r_{\text{rms}} = 2.51 \text{ fm} \)

\( 16^\text{O} \) matter density

\[ V = \text{Idaho-A} \]
### N=8 results for $^{15}$O, $^{17}$O (G-matrix)

Diagonalize $\bar{H}$ (T's solved for $n$ nucleons) in the $n \pm 1$ Fock space. $H \leftarrow T + V - \langle T_{cm} \rangle$

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>Expt.</th>
<th>N$^3$LO</th>
<th>CD-Bonn</th>
<th>AV18</th>
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</thead>
<tbody>
<tr>
<td>$^{15}$O</td>
<td>7.46</td>
<td>6.64</td>
<td>7.58</td>
<td>5.25</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>7.98</td>
<td>7.4</td>
<td>8.33</td>
<td>5.90</td>
</tr>
<tr>
<td>$^{17}$O</td>
<td>7.75</td>
<td>7.17</td>
<td>8.03</td>
<td>5.62</td>
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</table>

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</tr>
</thead>
<tbody>
<tr>
<td>$3/2^+$</td>
<td>5.085</td>
<td>5.68</td>
<td>6.41</td>
<td>3.946</td>
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<tr>
<td>$1/2^+$</td>
<td>0.870</td>
<td>-0.088</td>
<td>0.31</td>
<td>-0.390</td>
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<tr>
<td>$5/2^+$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
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</thead>
<tbody>
<tr>
<td>$3/2^-$</td>
<td>6.176</td>
<td>6.26</td>
<td>7.35</td>
<td>4.452</td>
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<tr>
<td>$1/2^-$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

$^{17}$O, all MeV

$^{15}$O, all MeV
What about the first excited 3-?

From CCSD

\[ \Delta \varepsilon_\pi = 15.846 \text{ MeV} \]

\[ \Delta \varepsilon_\nu = 15.789 \text{ MeV} \]

Interactions among nucleons lowers by about 15.8 - 11.5 = 4.3 MeV

From experiment

\[ \Delta \varepsilon_\pi = \varepsilon_\pi(0d_{5/2}) - \varepsilon_\pi(0p_{1/2}) = \left[ \text{BE}(^{16}\text{O}) - \text{BE}(^{17}\text{F}) \right] + \left[ \text{BE}(^{16}\text{O}) - \text{BE}(^{15}\text{N}) \right] = 11.526 \text{ MeV} \]

\[ \Delta \varepsilon_\nu = \varepsilon_\nu(0d_{5/2}) - \varepsilon_\nu(0p_{1/2}) = \left[ \text{BE}(^{16}\text{O}) - \text{BE}(^{17}\text{O}) \right] + \left[ \text{BE}(^{16}\text{O}) - \text{BE}(^{15}\text{O}) \right] = 11.521 \text{ MeV} \]

Interactions among nucleons lowers by about 11.5 - 6.1 = 5.4 MeV

Much of the discrepancy comes from where the interaction places the 0p shell relative to the 0d1s shell.
$V_{\text{lowk}}\, ^{16}\text{O}$ results using N3LO and CD-Bonn
Some studies of $V_{\text{low}k}$ in nuclear matter

Bozek, Dean, Muether, PRC submitted
Emergent phenomena

Nanoscale

~10 nm

2-d quantum dot in strong magnetic field. The field drives localization.

Molecules

Molecular scale: conductance through molecules. Delocalized conduction orbitals

Nuclei

~7 fm

Quantum mechanics plays a role when the size of the object is of the same order as the interaction length.

Common properties

- Shell structure
- Excitation modes
- Correlations (superfluidity)
- Phase transitions
- Interactions with external probes

• Studies of the interaction
• Degrees of freedom
• Astrophysical implications
What happens to pairing in a (hot) rotating nucleus?

Y-rast states (states of lowest spin at a given energy)

All nucleons paired

Spin-aligned quasi-particle state

Energy

Spin

$H \leftarrow H + \hbar \omega J_z$
Thermal effects on pairing and deformation in nuclear systems

Pairing+Quadrupole Hamiltonian: solve using Auxiliary Field Monte Carlo techniques.

fp-gds model space (\(^{40}\text{Ca}\) is the core)

\(68\text{Ni} \rightarrow\) Spherical ground state; weak N=40 shell closure
\(70\text{Zn} \rightarrow\) stronger proton pairing correlations; some quadrupole collectivity; erosion of N=40 shell gap
\(72\text{Ge} \rightarrow\) shape coexistence phenomena; static proton and neutron pairing
\(80\text{Zr} \rightarrow\) very deformed; large N=40 shell effects, weakened pairing

\(10^{20}\) many-body basis states
Simple AFMC

Single-particle energy

\[ \hat{H} = \varepsilon \hat{\Omega} + \frac{V}{2} \hat{\Omega}^2 \]

two-body interaction

We want:

\[ Z = \text{Tr}[\exp(-\beta \hat{H})] \rightarrow \langle \hat{H} \rangle = \frac{\text{Tr}[\exp(-\beta \hat{H}) \hat{H}]}{Z} \]

use the Hubbard-Stratonovich transformation

\[ \exp(-\beta \hat{H}) = \sqrt{\frac{\beta |V|}{2\pi}} \int_{-\infty}^{\infty} d\sigma \exp(-\beta |V| \sigma^2 / 2) \exp(-\beta \hat{h}) \]

\[ \hat{h} = \varepsilon \hat{\Omega} + s V \sigma \hat{\Omega} \]

\( s = 1 \) for \( V < 0 \)

\( s = i \) for \( V > 0 \)
Pairing, deformation, and the specific heat

\[ E(\beta) = \frac{Tr[\exp(-\beta H)H]}{Tr[\exp(-\beta H)]} \]

\[ C_v = -\beta^2 \frac{dE}{d\beta} \]

Langanke, Dean, Nazarewicz (NPA, 2005)
Low temperature and rotation

Dean, Nazarewicz, Langanke (in prep)
Interplay between rotation and temperature
What questions does your research pose that only “RIA” can answer?

I prefer to take the long view on this question.....
Marburger …the American Competitive Initiative is keyed to research that will promote competitiveness…. Concerning DOE Office of Science programs, he commented that high energy physics and nuclear physics research are important and cited societal contributions they have made….But DOE's Basic Energy Sciences program is key, Marburger said, as its research is closely aligned with competitiveness.

Bodman's remarks reinforced these comments…”The ACI is the significant investment needed to produce transformational technologies to help us achieve the President's goals.”

After discussing DOE's proposed work in ethanol production and the Global Nuclear Energy Partnership, Bodman reiterated…: "The American people, the taxpayers, expect more from basic science research than new knowledge alone. We expect and I believe that the investments being made today will one day result in countless additional benefits -- benefits to our health, our national defense, our productivity and economic expansion, and our energy security."
The Advanced Burn Reactor recycles used nuclear fuel

The ABR would **destroy transuranics** in used fuel from nuclear power plants, avoiding the need to accommodate this radioactive, radiotoxic, and heat-producing material in a geological repository for hundreds of thousands of years while it decays.

To “burn” this material, an ABR takes advantage of high-energy or **fast neutrons to fission** … transuranics. Here, “burn” means to **transmute or convert transuranics into shorter-lived isotopes**. As transuranics are consumed, significant energy is released and converted into electricity, hereby producing useful energy from material that would otherwise be waste.
Theoretical challenges must be met during the next decade in order to facilitate the success of an experimental program focused on short-lived isotopes and to enhance the national effort in nuclear science.

These efforts include:

• Development of ab initio approaches to medium-mass nuclei


• Development of reaction theory that incorporates relevant degrees of freedom for weakly bound nuclei.

• Exploration of isospin degrees of freedom of the density-dependence of the effective interaction in nuclei.

• Development and synthesis of nuclear theory, and its consequent predictions, into various astrophysical models to determine the nucleosynthesis in stars.

• Development of robust theory and error analysis for nuclear reactions relevant to NNSA and GNEP.
FY 2007-2011 Nuclear Physics Program
Impacts / Implications

Facility Operations
- Operate and implement the capabilities of the user facilities (RHIC, CEBAF, HRIBF and ALTAS) to achieve their scientific goals.
  - Proceed with the 12 GeV CEBAF Upgrade project.
  - RHIC accelerator/detector upgrades implemented and RHIC II construction starts midway in period
  - ATLAS and HRIBF research capabilities are developed to mount forefront programs.
- R&D is supported to provide the basis for a decision to initiate preliminary engineering design at the end of this planning period for construction of a U.S. world-class exotic beam facility.

Research
- Research efforts and investments are supported to achieve the scientific goals and address highest priority new scientific opportunities
  - CEBAF 6-GeV program will be completed with several key experiments
  - RHIC program will characterize the newly discovered new states of matter with heavy ion beams and establish the contributions of gluons to the spin of the proton using a polarized beams
  - U.S. researchers at LHC will search for new states of matter at conditions different than RHIC
  - Studies of new nuclear structures and nuclear behaviors start with GRETINA
  - Measurements of fundamental neutron properties will begin at the FNPB at SNS
  - A neutrinoless Double Beta Decay experiment is fabricated
  - Investments in LQCD (with HEP) will provide the opportunity for unprecedented advances.
  - Accelerator R&D for next-generation nuclear physics research capabilities are supported.
  - Nuclear data measurements and code development will contribute to improved designs of next generation nuclear reactors
  - Support of graduate students will result in over 400 PhD degrees over this period

• RIA is no longer in the President’s budget
• Reaccelerated Exotic Beam R&D is in the budget
• RISAC (NAS) is evaluating the scientific case for Rare Isotope Physics
• That scientific case has been formulated many times. It will need retuning for the future without RIA.

Exotic Beam physics remains a key capability of the future DOE scientific portfolio.