Building Nuclei From the Ground Up

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Aims in Nuclear Structure

Wish to solve to $A$-body nuclear Hamiltonian

\[ H = T - T_{CoM} + V = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{k_i^2}{2m} + \sum_{i<j}^{A} \left(V(i,j) - \frac{k_i \cdot k_j}{mA}\right). \]
From realistic to effective interactions: $V_{\text{low}-k}$

The free N-N interaction generates strongly repulsive and/or diverging matrix elements at short internucleonic distances. Need a **Renormalized Interaction**!

Different high-precision potentials

Universal low-momentum potential

Low-momentum nucleon-nucleon interaction.

\( V_{\text{low-}k} \) may be constructed by either Renormalization Group Theories (where high momentum modes are integrated out) or Similarity Transformation techniques.

\[
P = \{ |\vec{k}_p\rangle, \ |k| \leq \Lambda \}, \quad Q = \{ |\vec{k}_q\rangle, \ \Lambda < |k| < \infty \}.
\]

\[
\tilde{H} = X^{-1}HX, \quad |\Phi_k\rangle = X^{-1}|\Psi_k\rangle.
\]

\[
\begin{pmatrix}
P\tilde{H}P & P\tilde{H}Q \\
Q\tilde{H}P & Q\tilde{H}Q
\end{pmatrix}
\begin{pmatrix}
P\Phi_k \\
Q\Phi_k
\end{pmatrix}
= E_k
\begin{pmatrix}
P\Phi_k \\
Q\Phi_k
\end{pmatrix},
\]

Decoupling equation \( Q\tilde{H}P = Q(X^{-1}HX)P = 0 \), Lee-Suzuki gives \( X = \exp(\omega) = 1 + \omega \) where the wave operator \( \omega \) satisfies the decoupling condition

\[
\omega = Q\omega P.
\]

The Lee-Suzuki effective interaction in the \( P \)-space is then derived

\[
P V_{\text{LS}} P = PH(P + \omega) - PH_0 P = PVP + PV\omega = PVP + PVQ\omega.
\]
$V_{\text{low}-k}$: Pros and Cons

1. Energy and nucleus independent interaction.
2. Soft core, suitable for Many-Body perturbation calculations.
3. Means to probe importance of missing Many-Body forces.
4. Generates a cutoff ($\lambda$) dependence, which can only be removed by including corresponding Many-Body forces.

Question: Is 3-N force sufficient to remove $\lambda$ dependence and if so can the 3-N force be treated perturbatively?
Answer: Coupled Cluster approach to medium mass nuclei

1. Coupled Cluster Theory is fully microscopic.
2. Coupled Cluster is size consistent. The energy of two non-interacting fragments computed separately is the same as that computed for both fragments simultaneously.
3. Low computational cost (CCSD scales as $n_o^2 n_u^4$).
4. Capable of systematic improvements.
5. Amenable to parallel computing.

Computational Chemistry: 100’s of publications in any year (Science Citation Index) for applications and developments.
**Motivation**

- Renormalized Interactions
- CCSD
- CCSD at the dripline

**Conclusion**

- **Coupled Cluster Expansion**

**Coupled-Cluster:** An “Exponential Ansatz” for the wave function

\[
\Psi_{CC} = \exp(T) \Phi_0 = \exp(T_1 + T_2 + T_3 + ...) \Phi_0
\]

Truncation of the Coupled Cluster operator \( T \) leads to:

- \( T = T_1 + T_2 \rightarrow \text{CCSD} \)
- \( T = T_1 + T_2 + T_3 \rightarrow \text{CCSDT} \)

\[
T_1 = \sum_{ia} t_i^a a_i a_i^\dagger, \quad T_2 = \sum_{ijab} t_{ij}^{ab} a_i a_i^\dagger a_j a_j^\dagger
\]

**CCSD energy equation**

\[
E = \langle \Phi_0 | H(1 + T + \frac{T^2}{2!} + \frac{T^3}{3!} + ...) | \Phi_0 \rangle
\]

\[
= \langle \Phi_0 | H | \Phi_0 \rangle + \langle \Phi_0 | HT | \Phi_0 \rangle + \langle \Phi_0 H | \frac{T^2}{2!} | \Phi_0 \rangle.
\]

The single \( t_i^a \) and double excitation amplitudes \( t_{ij}^{ab} \) may be determined from

\[
0 = \langle \Phi_i^a | H | \Phi_0 \rangle, \quad 0 = \langle \Phi_{ij}^{ab} | H | \Phi_0 \rangle;
\]
Coupled Cluster Results for $^{16}\text{O}$

$V_{\text{lowk}}^{16}\text{O}$ results using N3LO and CD-Bonn

$E_{\text{CCSD}}$ (MeV) vs $h\omega$ (MeV)

N3LO
-143.5 +/- 0.4 MeV

CD-Bonn
-153.4 +/- 0.4 MeV
Coupled Cluster Results for $^{16}$O with three-body force

$V_2: V_{\text{low} - k}$ with cutoff $\lambda = 1.9 \text{ fm}^{-1}$ generated from the Argonne V18 N-N interaction model

- (1): $V_2$ only
- (2): (1) + $V_3$ normal ordered contribution to vacuum energy
- (3): (1) + (2) + $V_3$ normal ordered contribution to CCSD energy
- (4): (1) + (2) + (3) + $V_3$ normal ordered contribution to one-body operator
- (5): (1) + (2) + (3) + (4) + $V_3$ normal ordered contribution to two-body operator
- (6): (1) + (2) + (3) + (4) + (5) + t1 and t2 amplitudes calculated with $V_3$

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<td>-134.710</td>
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<td>-135.930</td>
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Hagen, Papenbrock, Dean, et. al., to be published.
Berggren Single-Particle Basis

\[ 1 = \sum_{n=a,b,c,d} |\psi_{i}(k_n)\rangle \langle \tilde{\psi}_{i}(k_n)| + \int_{L^+} dk \ k^2 |\psi_{i}(k)\rangle \langle \tilde{\psi}_{i}(k)|. \]
Gamow-Hartree-Fock basis for the He-isotopes.

Gamow Shell Model calculations with $V_{\text{low-k}}$ ($\Lambda = 1.9 \text{fm}^{-1}$) generated from the N$^3$LO interaction model (Hagen, Hjorth-Jensen, Michel, Phys. Rev. C, in press).

Hole and particle states in $^4\text{He}$ calculated at Hartree-Fock level

<table>
<thead>
<tr>
<th>$lj$</th>
<th>$\Lambda = 1.8 \text{fm}^{-1}$</th>
<th>$\Lambda = 1.9 \text{fm}^{-1}$</th>
<th>$\Lambda = 2.0 \text{fm}^{-1}$</th>
<th>Expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s_{1/2}$</td>
<td>-25.731</td>
<td>0.000</td>
<td>-24.541</td>
<td>0.000</td>
</tr>
<tr>
<td>$p_{3/2}$</td>
<td>0.819</td>
<td>-0.325</td>
<td>1.041</td>
<td>-0.479</td>
</tr>
<tr>
<td>$p_{1/2}$</td>
<td>2.497</td>
<td>-3.697</td>
<td>2.514</td>
<td>-3.777</td>
</tr>
</tbody>
</table>

Gamow Shell Model calculation of the $0^+$ ground and $2^+$ excited states in $^6\text{He}$.

<table>
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<tr>
<th>$J^\pi$</th>
<th>$0^+_1$</th>
<th>$2^+_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_{\text{max}}$</td>
<td>Re[E]</td>
<td>Im[E]</td>
</tr>
<tr>
<td>4</td>
<td>-0.4760</td>
<td>0.0000</td>
</tr>
<tr>
<td>10</td>
<td>-0.4721</td>
<td>0.0000</td>
</tr>
<tr>
<td>16</td>
<td>-0.4721</td>
<td>0.0000</td>
</tr>
<tr>
<td>20</td>
<td>-0.4721</td>
<td>0.0000</td>
</tr>
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**Motivation**

- Renormalized Interactions
  - CCSD
  - CCSD at the dripline

**Conclusion**

- **CCSD**: How deal with explosion of basis states?

- Very low neutron separation energy. \( p \)–orbits are the main decay channel and build up the main part of halo-densities.

- Protons have large separation energies (20-30 MeV), mainly occupying deeply bound \( s \)-orbits.

**Neutrons**

- 15s\( \frac{1}{2} \)
- 15p\( \frac{3}{2} \)
- 15p\( \frac{1}{2} \)
- 4d\( \frac{5}{2} \)
- 4d\( \frac{3}{2} \)

**Protons**

- 5s\( \frac{1}{2} \)
- 4p\( \frac{3}{2} \)
- 4p\( \frac{1}{2} \)
- 4d\( \frac{5}{2} \)
- 4d\( \frac{3}{2} \)

**Neutron orbitals**

- Neutron orbitals are Gamow states for s-p partial waves and Oscillators for higher partial waves (d-g)

**Proton orbitals**

- Proton orbitals are Oscillators restricted by \( N = 10 \) major shells and \( l_{\text{max}} \).

**Building Nuclei From the Ground Up**
CCSD calculation of the $^4_{-10}\text{He}$ ground states with the low-momentum N$^3$LO nucleon-nucleon interaction ($\Lambda = 1.9\text{fm}^{-1}$) for increasing number partial waves. The energies $E$ are given in MeV for both real and imaginary parts. (Hagen et. al. in preparation)

| $lj$ | $^4\text{He}$ | | $^5\text{He}$ | | $^6\text{He}$ | | $^7\text{He}$ | | $^8\text{He}$ | | $^9\text{He}$ | | $^{10}\text{He}$ |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| $s - p$ | -24.92 | 0.00 | -20.08 | -0.54 | -18.02 | -0.44 | -28.30 | 0.00 | -27.41 | -0.33 | -29.27 | 0.00 |
| $s - d$ | -26.58 | 0.00 | -23.45 | -0.23 |         |        | -17.02 | -0.24 | -16.97 | -0.00 | -15.28 | -0.40 |
| $s - f$ | -27.57 | 0.00 |         |        | -28.98 | 0.00 | -28.98 | 0.00 | -28.98 | 0.00 | -13.82 | -0.12 |

Expt. | -28.82 | -0.15 | -31.41 | 0.00 | -30.26 | -0.1 | -30.34 | ? | ? | ? | ? | ? |
CCSD has been implemented for two and three body forces, and we have extensive calculations of $^{16}$O.

Preliminary results with $V_{\text{low}-k}$ and corresponding three-body force for $^{16}$O. Larger model-space, more channels in $V3 \rightarrow$ more repulsion?

Two and three-body effective interactions generated via similarity transformation techniques are underway. No $\Lambda$ dependence, convergence with respect to size of $P$.

CCSD has been applied with a Gamow basis suitable for description of loosely bound and unbound nuclear states along the dripline.
Coupled Cluster in pictures

\[ T_1 = \sum_{i} t_i^a |\Phi_i^a\rangle, \quad T_2 = \sum_{i>j} t_{ij}^{ab} |\Phi_{ij}^{ab}\rangle, \quad T_3 = \sum_{i>j>k} t_{ijk}^{abc} |\Phi_{ijk}^{abc}\rangle \]

- \( m_A = N \), exact theory;
- \( m_A < N \), approximate theory

\[ m_A = 2 \quad T = T_1 + T_2 \quad CCSD \quad n_o^2 n_u^4 \left( n_o^2 n_u^2 \right) \]

\[ m_A = 3 \quad T = T_1 + T_2 + T_3 \quad CCSDT \quad n_o^3 n_u^5 \left( n_o^3 n_u^3 \right) \]
Coupled Cluster Amplitude Equations

In CCSD the single $t_i^a$ and double excitation amplitudes $t_{ij}^{ab}$ may be determined from

$$0 = \langle \Phi_i^a | H | \Phi_0 \rangle, \quad 0 = \langle \Phi_{ij}^{ab} | H | \Phi_0 \rangle;$$

known as the $T_1$ and the $T_2$ amplitude equations. Writing the Hamiltonian in normal-ordered form

$$H = \sum_{pq} f_{pq} \{ a_p^\dagger a_q \} + \frac{1}{4} \sum_{pqrs} \langle pq || rq \rangle \{ a_p^\dagger a_q^\dagger a_s a_r \} + \langle \Phi_0 | H | \Phi_0 \rangle$$
Coupled Cluster Amplitude Equations

\[ 0 = \langle ab | ij \rangle + \sum_c \left( f_{bc} t_{cij}^{bc} - f_{ac} t_{cij}^{ac} \right) - \sum_k \left( f_{ik} t_{kj}^{ik} - f_{jk} t_{kj}^{jk} \right) + \]

\[ \frac{1}{2} \sum_{kl} \langle kl | ij \rangle t_{ij}^{ab} + \frac{1}{2} \sum_{cd} \langle ab | cd \rangle t_{cd}^{cd} + P(ij) P(ab) \sum_{kc} \langle kb | cj \rangle t_{cij}^{ab} + P(ij) \sum_c \langle ab | cj \rangle t_{cij}^{ac} - P(ab) \sum_k \langle kb | ij \rangle t_{kij}^{ab} + \]

Nonlinear terms in t2
(4th order)

T2 amplitudes from:

\[ P(ab) \frac{1}{2} \sum_{kcd} \langle kl | cd \rangle t_{cd}^{cd} t_{cd}^{kcd} - P(ij) \frac{1}{2} \sum_{kcd} \langle kl | cd \rangle t_{cd}^{cd} t_{cd}^{kcd} + \]

\[ P(ab) \frac{1}{2} \sum_k \langle kl | cij \rangle t_{cij}^{ab} + P(ij) \frac{1}{2} \sum_{cd} \langle ab | cd \rangle t_{cd}^{cd} - P(ij) P(ab) \sum_{ke} \langle kb | ic \rangle t_{cij}^{ab} + \]

\[ P(ab) \sum_k f_{ik} t_{kj}^{ik} + P(ij) \sum_k f_{jk} t_{kj}^{jk} - P(ij) \sum_{kcd} \langle kl | cd \rangle t_{cd}^{cd} t_{cd}^{kcd} + P(ab) \sum_{kcd} \langle kl | cd \rangle t_{cd}^{cd} t_{cd}^{kcd} - P(ij) \sum_{kcd} \langle kl | cd \rangle t_{cd}^{cd} t_{cd}^{kcd} + \]

Question: Is this model independence also seen in A > 2 calculations?


Modern N-N interactions reproduce two-particle scattering data + deuteron properties.

They all differ in strength of tensor force and treatment of the hard-core.

V-lowk from different N-N models have the same on-shell and half-off-shell behaviour.

At the two-body level V-lowk is model-independent.

Question: Is this model independence also seen in A > 2 calculations?

Comparison with Shell Model/Configuration Interaction

In Shell Model approach a linear excitation operator is used instead of an exponential. \( \Psi = (1 + C)\Phi_0 = (1 + C_1 + C_2 + \ldots)\Phi_0 \)

- If truncated disconnected diagrams enter. And it is not size consistent.
- Dimension increases dramatically with number of active particles.
Coupled Cluster Results for $^{16}\text{O}$

$V_{\text{lowk}}^{^{16}\text{O}}$ results using N3LO and CD-Bonn
Two-body matrix elements are calculated numerically in an arbitrary two-particle Gamow basis by truncating the completeness expansion up to $N$ harmonic oscillator two-body states

$$
\langle ab|V_{osc}|cd\rangle \approx \sum_{\alpha \leq \beta} \sum_{\gamma \leq \delta} \langle ab|\alpha \beta\rangle \langle \alpha \beta|V_{low-k}|\gamma \delta\rangle \langle \gamma \delta|cd\rangle.
$$

(1)

The Gamow-Hartree-Fock basis may then be constructed,

$$
\langle p|h_{HF}|q\rangle = \langle p|t|p\rangle \delta_{p,q} + \sum_{i<e_f} \langle pi|V_{osc}|qi\rangle
$$

(2)
Coupled Cluster Results for $^{16}$O with three-body force

Initial V3-CCSD results
(proof of principle, Papenbrock, Hagen, et al)

(1): V2 only
(2): (1)+v3 normal ordered contribution to vacuum energy
(3): (1)+(2)+ v3 contribution to CCSD energy
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(6): (1)+(2)+(3)+(4)+(5)+ t1 and t2 amplitudes consistently calculated with v3

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Motivation

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CCSD

CCSD at the dripline

Conclusion

Coupled Cluster Equations

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

Correlated Ground-State wave function

Correlation operator

Reference Slater determinant

Energy

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

Amplitude equations

\[ \langle \Phi_{ij\Lambda}^{ab\Lambda} | \exp(-T)H \exp(T) | \Phi \rangle = \langle \Phi_{ij\Lambda}^{ab\Lambda} | \overline{H} | \Phi \rangle = 0 \]

• Nomenclature
  • Coupled-clusters in singles and doubles (CCSD)
  • …with triples corrections CCSD(T);