Nuclear Structure in the UCOM Framework
Many-Body Calculations: HF, RPA and beyond

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Correlated realistic interactions $V_{UCOM}$

- Short-range central and tensor correlations (SRC) described by a unitary correlation operator $C = C_\Omega C_r$
- Introduce SRC to uncorrelated $A$-body state or an operator of interest
\[
\langle \tilde{\Psi} | O | \tilde{\Psi} \rangle = \langle \Psi | C^\dagger OC | \Psi \rangle = \langle \Psi | \tilde{O} | \Psi \rangle
\]

realistic NN interaction $\rightarrow$ correlated interaction

- Same for all nuclei
- Phase-shift equivalent to the original NN interaction
- Suitable for use within simple Hilbert spaces

$\rightarrow$ H.Hergert’s talk, HK18.4 Di 14:45 B
Overview

Use of the $V_{UCOM}$ in many-body calculations across the nuclear chart:

- A UCOM Hamiltonian based on the Argonne V18 NN interaction is used
- **Ground state** properties and **excited states** of closed-shell nuclei:
  - Hartree-Fock calculations
  - Second-order perturbation theory
  - Versions of the RPA
Motivation

- expectation value of Hamiltonian (with AV18) for Slater determinant of harmonic oscillator states

![Graph showing binding energies of different nuclei, with annotations for central and tensor correlations essential to obtain bound nuclei.]

$E/A$ [MeV]
UCOM-Hartree-Fock
Standard Hartree-Fock

- Ground state approximated by a single Slater determinant

\[ |\text{HF}\rangle = \mathcal{A}\{|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots |\phi_A\rangle\} \] no correlations

- Single-particle states are expanded in a H.O. basis

\[ |\phi_i\rangle = \sum_\alpha D_{i\alpha} |\alpha\rangle ; \quad |\alpha\rangle = |n, (\ell \frac{1}{2}) jm, \frac{1}{2} m_t\rangle \]

- Expansion coeff’s \( D_{i\alpha} \) determined by minimizing the energy

\[ E_{\text{HF}} = \langle \text{HF}|\hat{H}_{\text{int}}|\text{HF}\rangle = \frac{1}{2} \sum_{i,j=1}^{A} \langle \phi_i \phi_j | T_{\text{rel}} + V_{\text{UCOM}} | \phi_i \phi_j \rangle \] inclusion of SRC
Single-particle energies

- Reasonable agreement with experimental levels
- Energy of highest occupied state reproduced
- Density of levels low

![Graph of single-particle energies for \(^{40}\text{Ca}\)](image-url)
Missing Pieces

long-range correlations

genuine three-body forces

three-body cluster contributions

Beyond Hartree-Fock

■ improve many-body states such that long-range correlations are included

■ many-body perturbation theory (MBPT), configuration interaction (CI), coupled-cluster (CC),...
Perturbation Theory
Second-order perturbation theory

- **Binding-energy correction:**

\[
E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occ}} \sum_{a,b}^{\text{unocc}} \frac{|\langle ij | H_{\text{int}} | ab \rangle|^2}{e_a + e_b - e_i - e_j}; \quad H_{\text{int}} = T_{\text{rel}} + V_{\text{UCOM}}
\]

- **Modified density matrix and occupation numbers**

- **Modified charge radii**
$^{40}$Ca and $^{128}$Sn.
Missing Pieces

Beyond Hartree-Fock
- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, CI, CC,...

Net Three-Body Force
- small effect on binding energies for all masses
- cancellation does not work for all observables
- construct simple effective three-body force
Three-body force - In progress
Standard RPA
Standard RPA

- **Vibration creation operator**:

  \[
  Q^\dagger_\nu = \sum_{ph} X^\nu_{ph} O^\dagger_{ph} - \sum_{ph} Y^\nu_{ph} O_{ph}; \quad Q_\nu \mid \text{RPA} \rangle = 0; \quad Q^\dagger_\nu \mid \text{RPA} \rangle = \mid \nu \rangle
  \]

- **Standard RPA** - the RPA vacuum is approximated by the HF ground state:

  \[
  \langle \text{RPA} \mid \ldots \mid \text{RPA} \rangle \rightarrow \langle \text{HF} \mid \ldots \mid \text{HF} \rangle; \quad O_{ph} \rightarrow a^\dagger_p a_h
  \]

- **RPA equations** in \( ph \)-space:

  \[
  \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \hbar \omega_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}
  \]

  \[
  A_{ph, p'h'} = \delta_{pp'} \delta_{hh'} (e_p - e_h) + H_{hp', ph'}; \quad B_{ph, p'h'} = H_{hh', pp'}; \quad H = H_{\text{int}} = T_{\text{rel}} + V_{\text{UCOM}}
  \]

- **Self-consistent HF+RPA**: spurious state and sum rules
Isoscalar monopole response

$N_{\text{max}} = 12$

- $^{0^+}_{16}\text{O}$
  - AV18
  - Drozdz et al.

- $^{48}_{40}\text{Ca}$
  - RRPA (DD-ME1)
  - EXP.

- $^{132}_{90}\text{Zr}$
  - EXP.

- $^{208}_{132}\text{Sn}$
  - UCOM-RPA ($I_0=0.09 \text{ fm}^3$)
  - EXP.
Standard RPA

Isovector dipole response

$N_{\text{max}} = 12$

16 O

AV18

$^{16}$O

DD-ME2

EXP.

$^{1^{-}}$

IVGDR

$^{40}$Ca

$^{40}$Ca

DD-ME2

EXP.

$N_{\text{max}} = 12$

$^{48}$Ca

DD-ME2

$N_{\text{max}} = 12$

$^{48}$Ca

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$N_{\text{max}} = 12$
Isoscalar quadrupole response

\[ N_{\text{max}} = 12 \]

\[ \frac{90}{Zr} \]

\[ \frac{208}{Pb} \]

\[ \frac{40}{Ca} \]

\[ I_\theta^{(S=1,T=0)} = 0.09 \text{ fm}^3 \]

\[ \text{DD-ME2} \]

\[ \text{UCOM-RPA} \]

\[ \text{EXP.} \]
“Extended” RPA
The HF+RPA method is based mainly on the following **approximations**:

- Coupling to higher order excitations \((np - nh)\) is neglected
- The ground state does not deviate much from the HF ground state
Extended RPA

$^{40}$Ca

**ISM**

**ERPA**

**RPA**

$R [fm^4/\text{MeV}]$

$E [\text{MeV}]$

$R [fm^2/\text{MeV}]$

$E [\text{MeV}]$
Use of the $V_{UCOM}$ in many-body calculations across the nuclear chart:

- **Ground-state** properties: HF, PT
  - Binding energies, radii, ...
- **Excited states**: RPA, ERPA
  - Properties of collective excitations
- **Properties** of the $V_{UCOM}$ as an “effective interaction”
  - Effective mass, compressibility

☞ Role of residual long-range correlations and three-body terms

See also: H.Hergert’s talk, HK18.4 Di 14:45 B
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Recent References


- http://crunch.ikp.physik.tu-darmstadt.de/tnp/