# Nuclear Structure in the UCOM Framework

## Many-Body Calculations: HF, RPA and beyond

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# Introduction

Correlated realistic interactions $V_{\mathrm{UCOM}}$

- 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

$$\langle\tilde{\Psi}|O|\tilde{\Psi}\rangle = \langle\Psi|C^\dagger O C|\Psi\rangle = \langle\Psi|\tilde{O}|\Psi\rangle$$

realistic NN interaction $\longrightarrow$ correlated interaction

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

$\longrightarrow$ H.Hergert's talk, HK18.4 Di 14:45 B

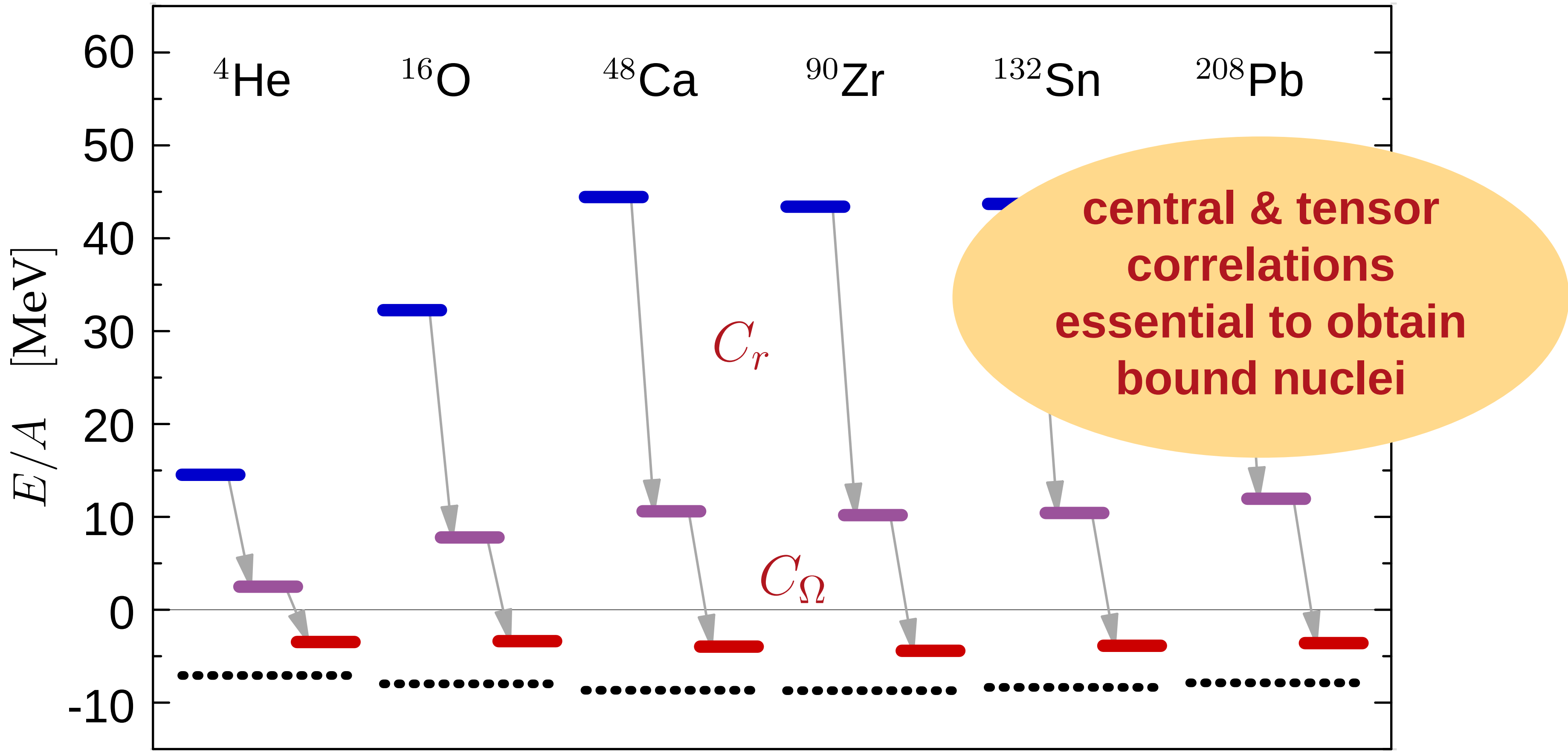
# Overview

Use of the $V_{\mathrm{UCOM}}$ 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



# UCOM-Hartree-Fock

# UCOM-HF

## Standard Hartree-Fock

- Ground state approximated by a single Slater determinant

$$|\mathrm{HF}\rangle = \mathcal{A}\{|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots |\phi_A\rangle\}$$

no correlations

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

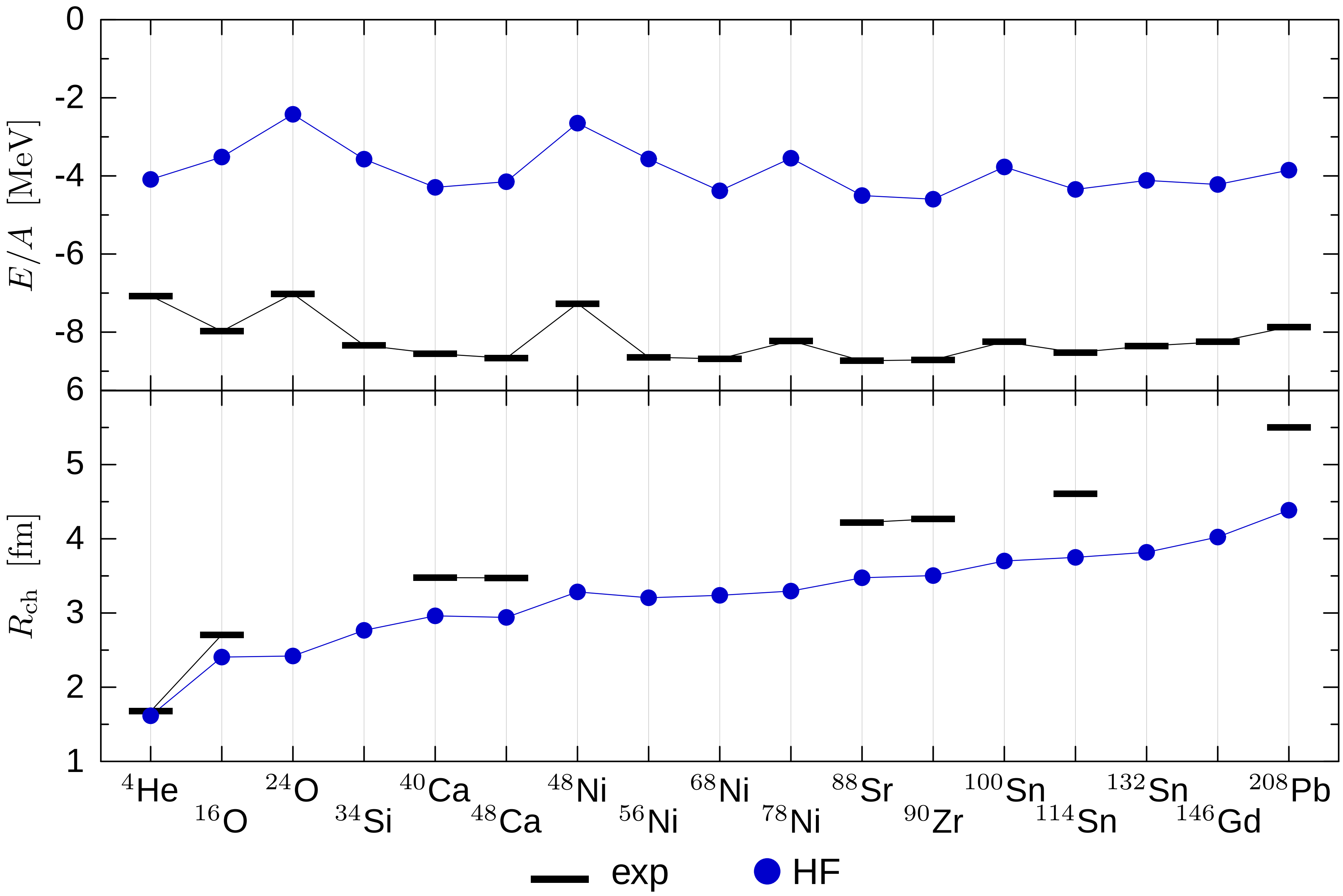
$$|\phi_i\rangle = \sum_\alpha D_{i\alpha}|\alpha\rangle \quad ; \quad |\alpha\rangle = |n, (\ell\tfrac{1}{2})jm, \tfrac{1}{2}m_t\rangle$$

- Expansion coeff's $D_{i\alpha}$ determined by minimizing the energy

$$E_{\mathrm{HF}} = \langle \mathrm{HF}|\hat{H}_{\mathrm{int}}|\mathrm{HF}\rangle = \tfrac{1}{2}\sum_{i,j=1}^{A}\langle\phi_i\phi_j|T_{\mathrm{rel}} + V_{\mathrm{UCOM}}|\phi_i\phi_j\rangle$$

inclusion of SRC

# UCOM-HF

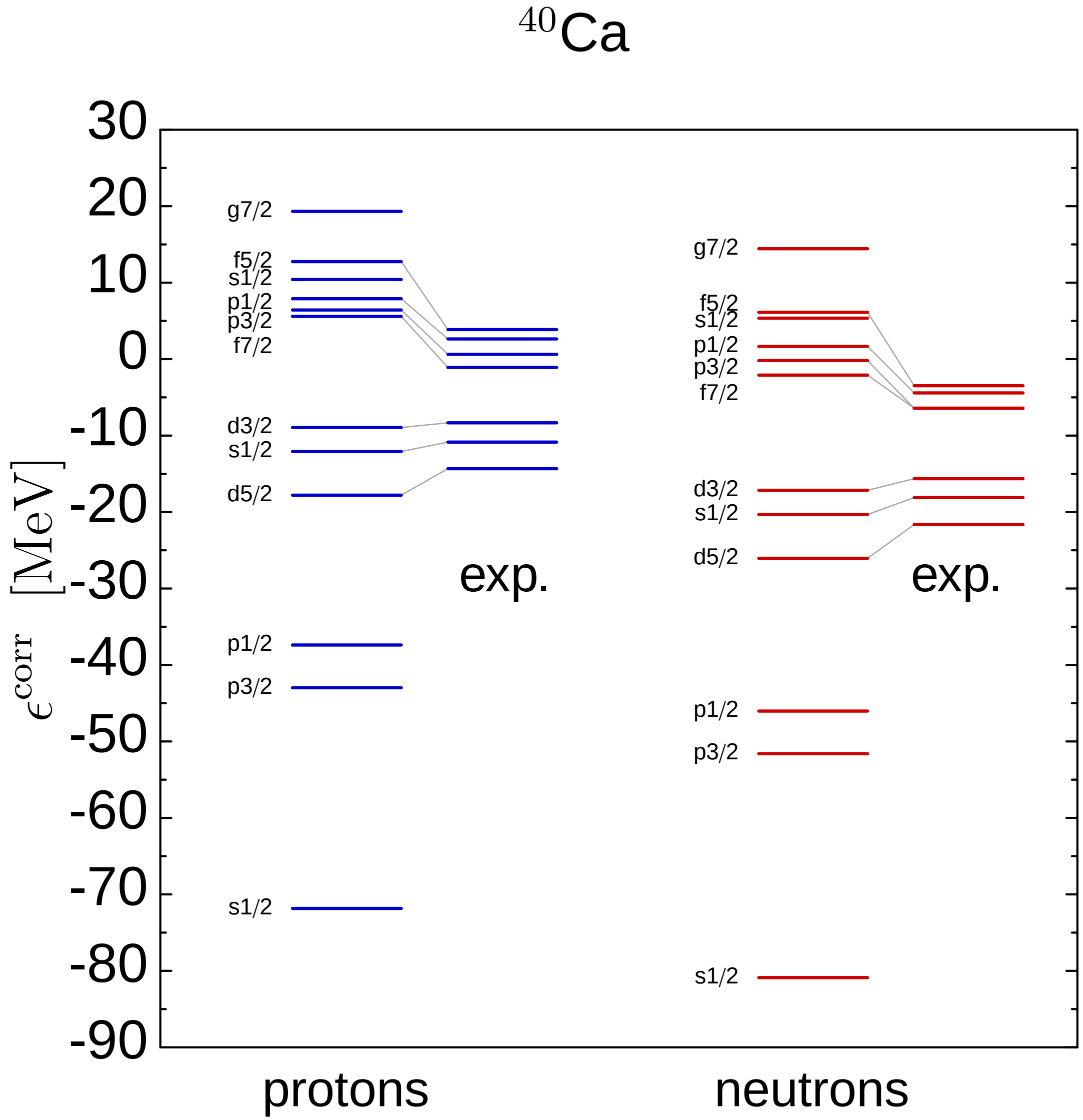


0
-2
-4
-6
-8
$E/A$ [MeV]
6
5
4
3
2
1
$R_{ch}$ [fm]
$^{4}$He
$^{16}$O
$^{24}$O
$^{34}$Si
$^{40}$Ca
$^{48}$Ca
$^{48}$Ni
$^{56}$Ni
$^{68}$Ni
$^{78}$Ni
$^{88}$Sr
$^{90}$Zr
$^{100}$Sn
$^{114}$Sn
$^{132}$Sn
$^{146}$Gd
$^{208}$Pb
exp
HF

# UCOM-HF

## Single-particle energies

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



# 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

# UCOM-HF + PT

LRC: extending the model space

## Second-order perturbation theory

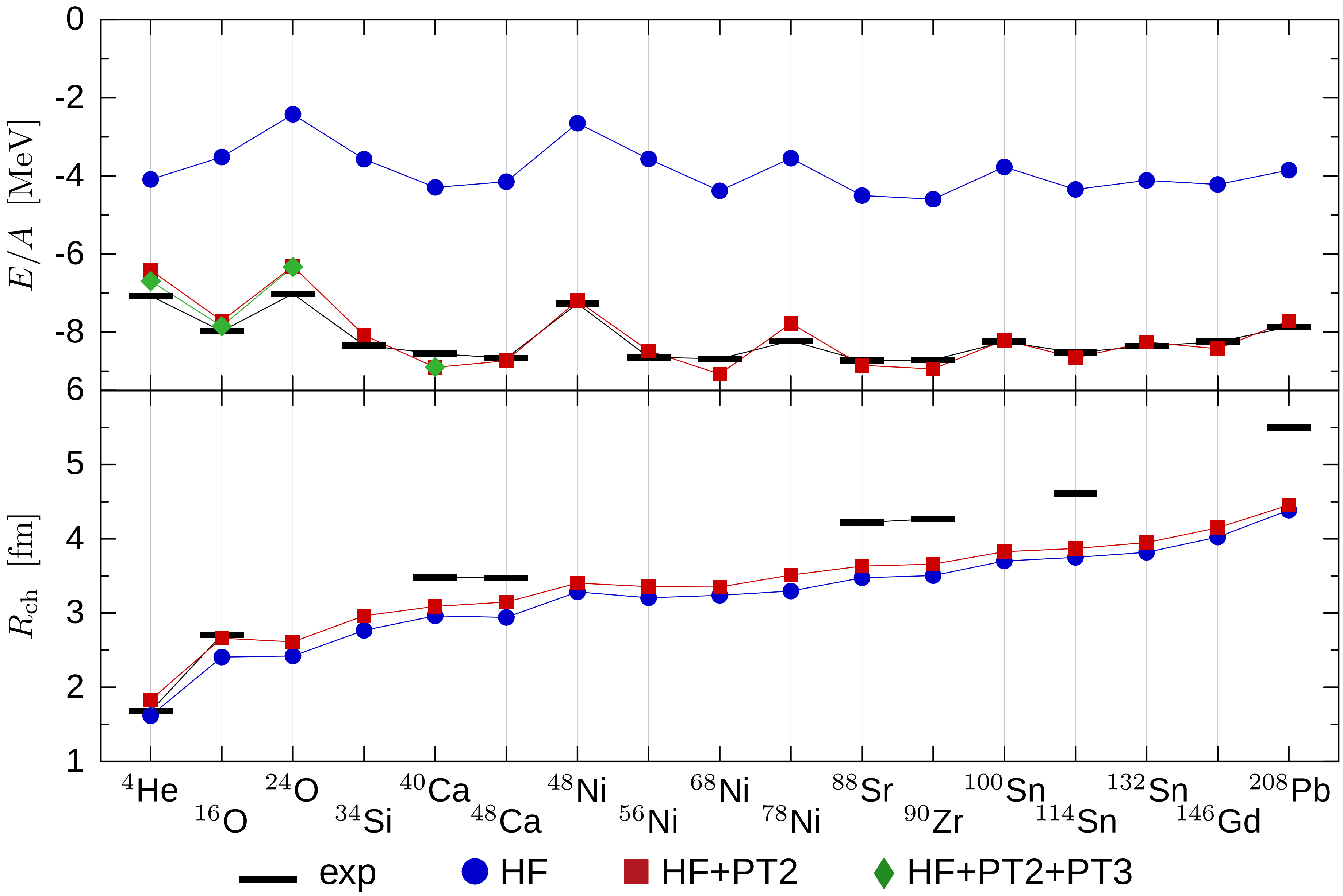
- Binding-energy correction:

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

- Modified density matrix and occupation numbers

☞ Modified charge radii

# UCOM-HF + PT



$E/A$ [MeV]
$R_{ch}$ [fm]
0
-2
-4
-6
-8
6
5
4
3
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1
$^{4}$He
$^{16}$O
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$^{34}$Si
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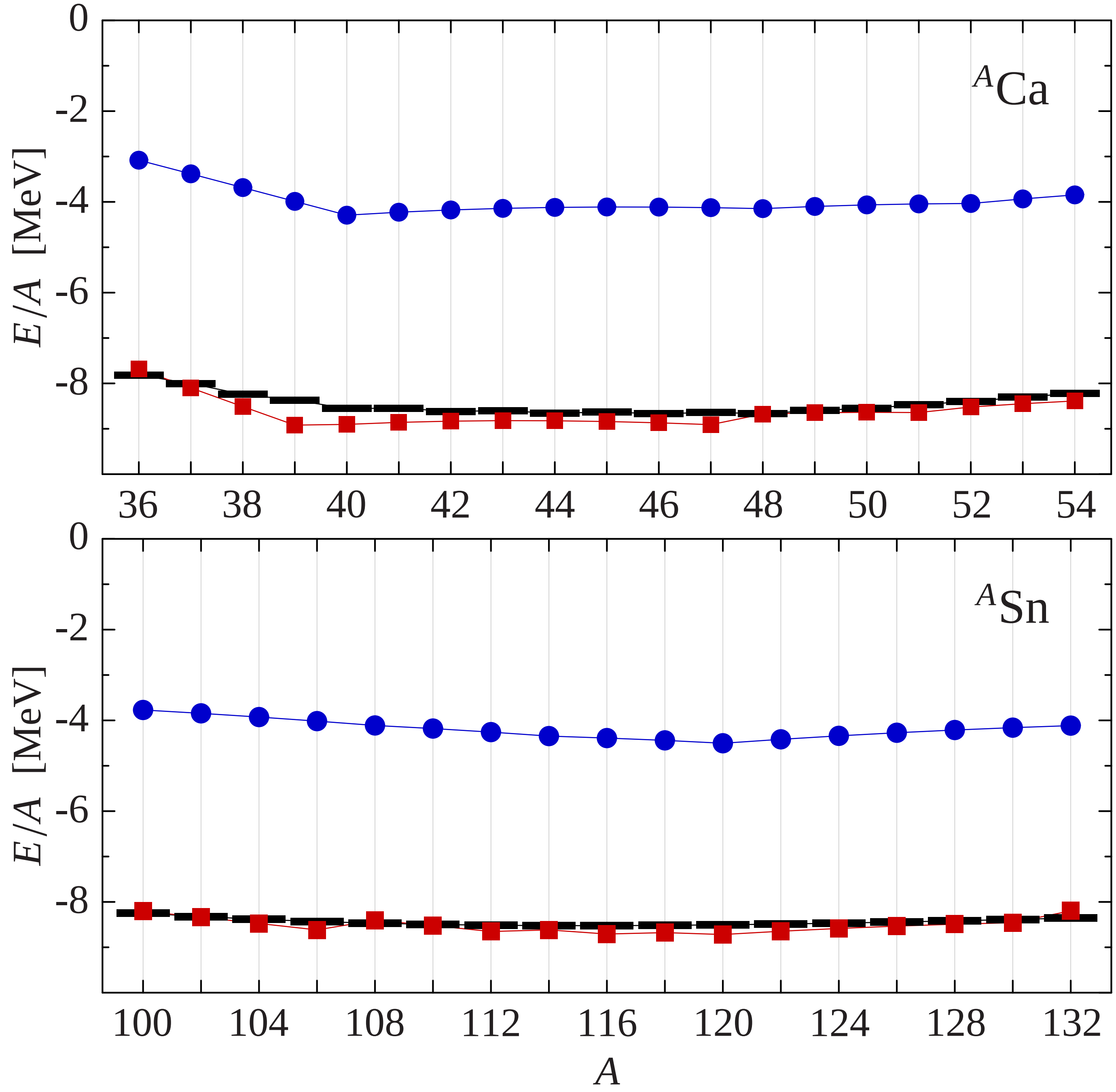
$^{68}$Ni
$^{78}$Ni
$^{88}$Sr
$^{90}$Zr
$^{100}$Sn
$^{114}$Sn
$^{132}$Sn
$^{146}$Gd
$^{208}$Pb
exp
HF
HF+PT2
HF+PT2+PT3

# UCOM-HF + PT



0
-2
-4
-6
-8
E/A [MeV]
$^{A}$Ca
36
38
40
42
44
46
48
50
52
54
0
-2
-4
-6
-8
E/A [MeV]
$^{A}$Sn
100
104
108
112
116
120
124
128
132
A

# Missing Pieces

**long-range correlations**

**genuine three-body forces**

**three-body cluster contributions**

## Beyond Hartree-Fock

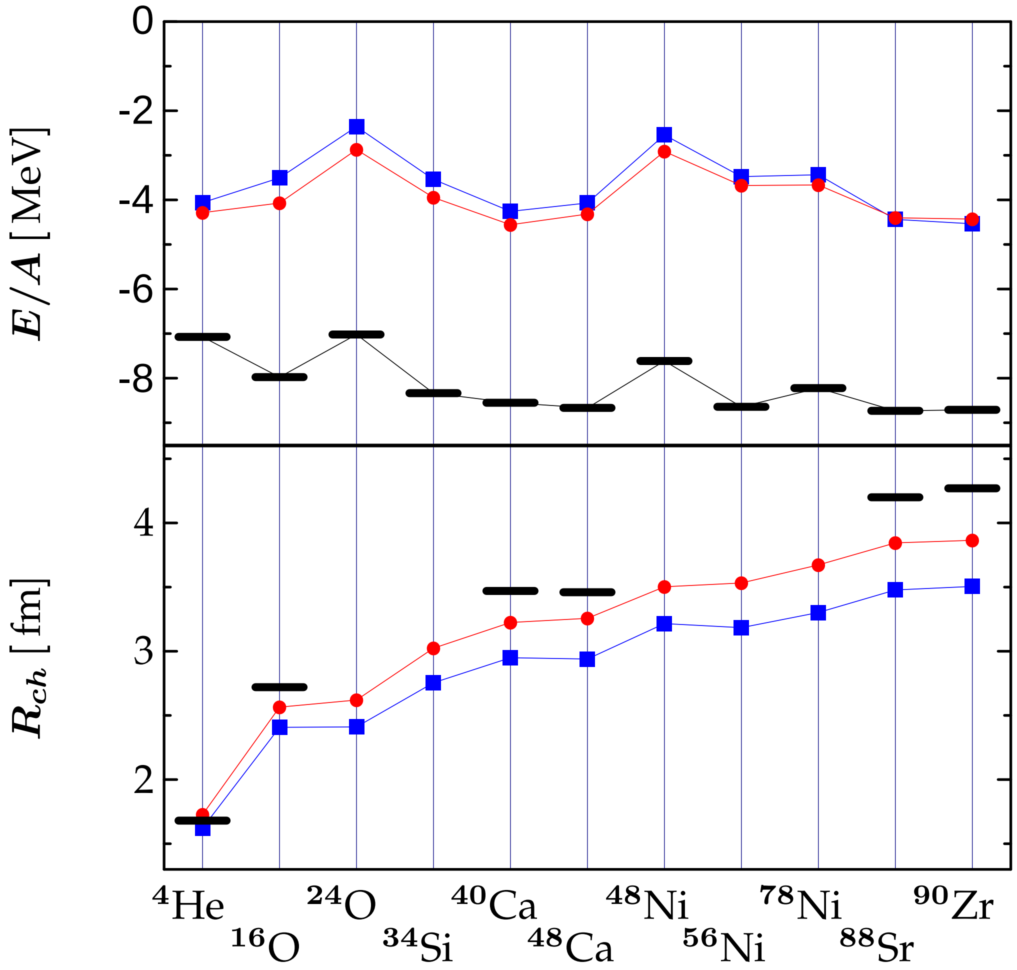
- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, CI, CC,...

## 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

# UCOM-HF + PT

## Three-body force - In progress



# Standard RPA

# Standard RPA

- Vibration creation operator:

$$Q_\nu^\dagger = \sum_{ph} X_{ph}^\nu O_{ph}^\dagger - \sum_{ph} Y_{ph}^\nu O_{ph} \quad ; \quad Q_\nu|\mathrm{RPA}\rangle = 0 \quad ; \quad Q_\nu^\dagger|\mathrm{RPA}\rangle = |\nu\rangle$$

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

$$\langle \mathrm{RPA}|\ldots|\mathrm{RPA}\rangle \rightarrow \langle \mathrm{HF}|\ldots|\mathrm{HF}\rangle \quad ; \quad O_{ph} \rightarrow a_p^\dagger a_h$$

- RPA equations in $ph-$space:

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

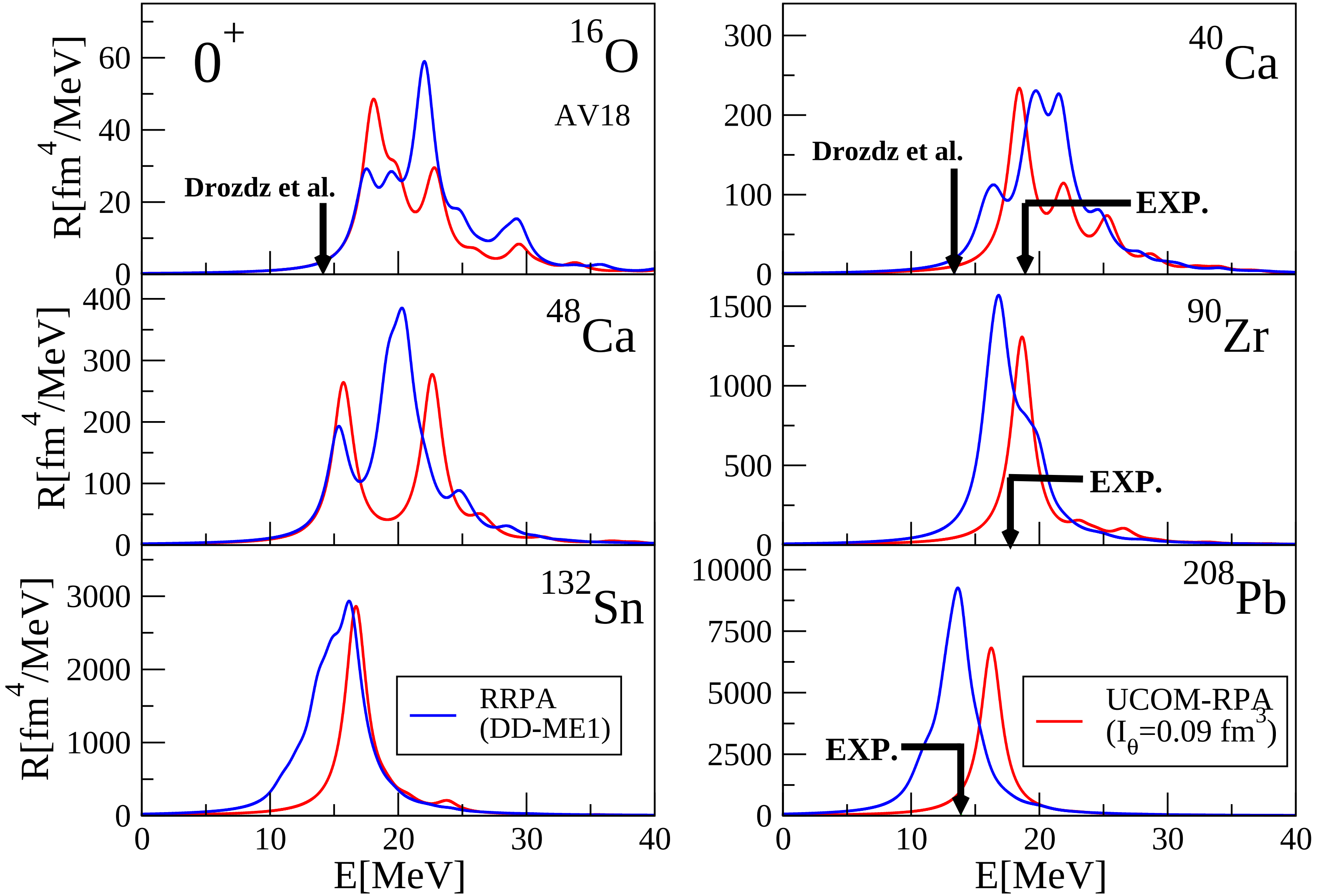
$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(e_p - e_h) + H_{hp',ph'} \ ; \ B_{ph,p'h'} = H_{hh',pp'} \ ; \ H = H_{\mathrm{int}} = T_{\mathrm{rel}} + V_{\mathrm{UCOM}}$$

☞ Self-consistent HF+RPA: spurious state and sum rules

# Standard RPA

## Isoscalar monopole response

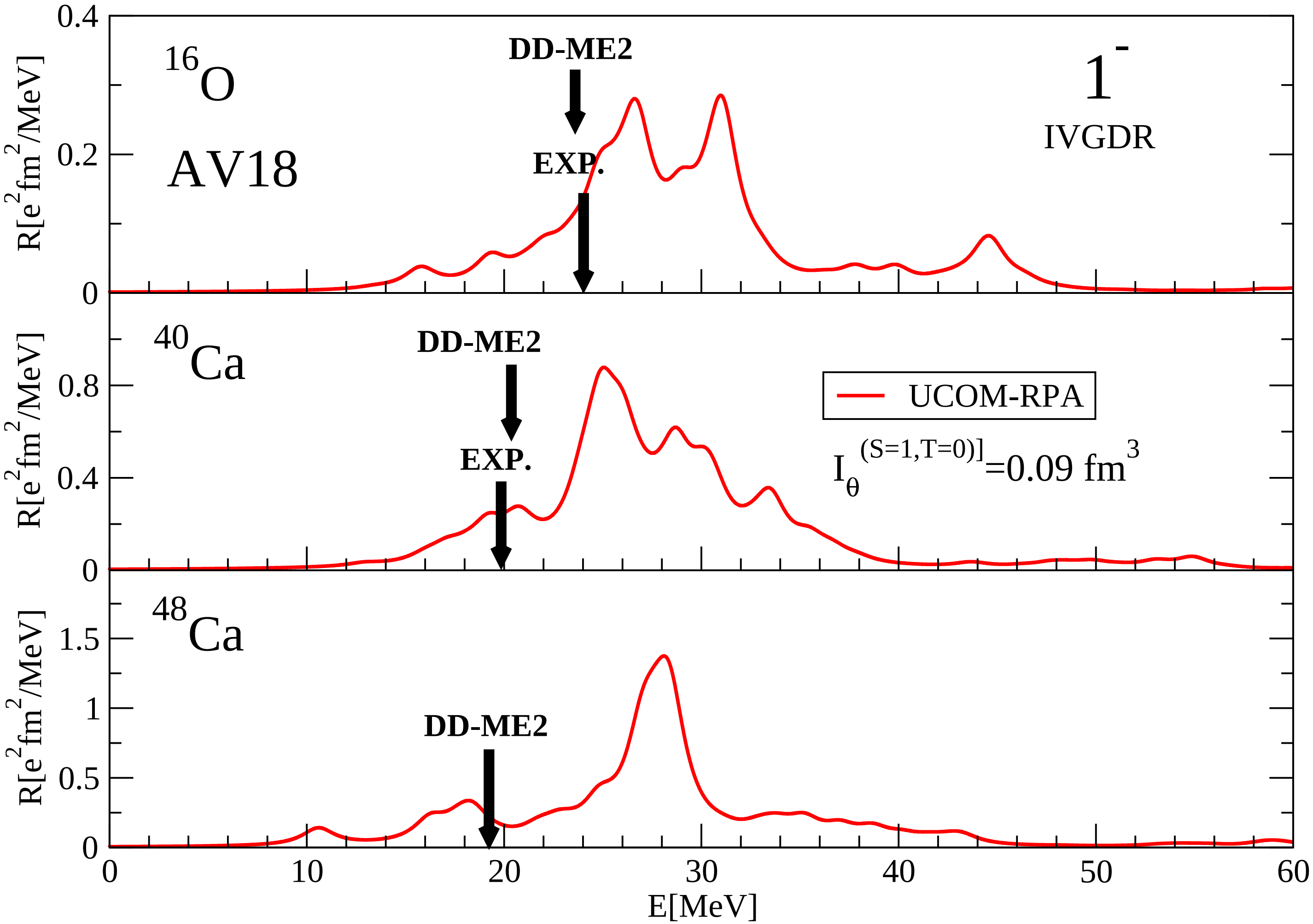
$N_{\mathrm{max}} = 12$



# Standard RPA

## Isovector dipole response

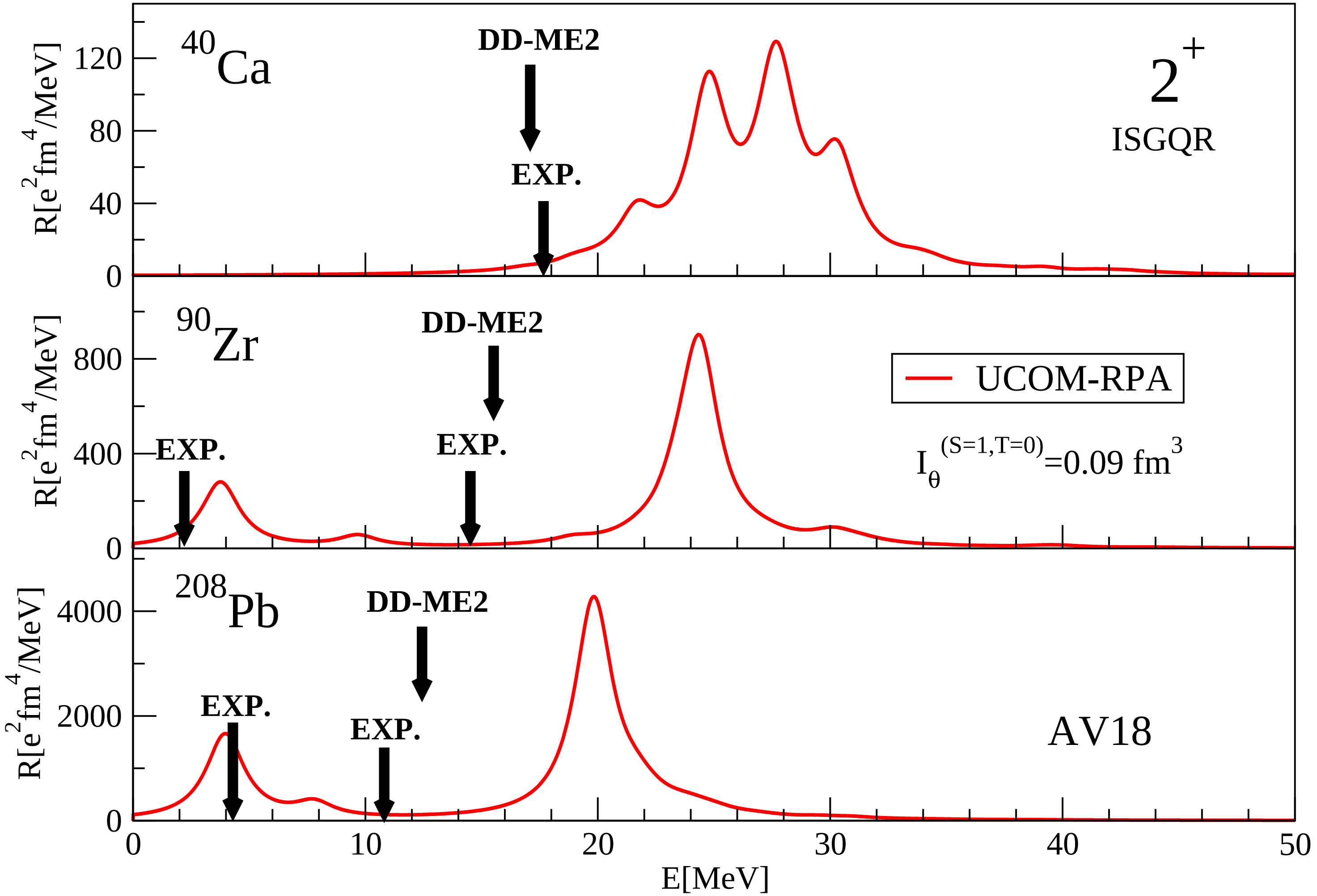
$N_{\max} = 12$



# Standard RPA

## Isoscalar quadrupole response

$N_{\max} = 12$



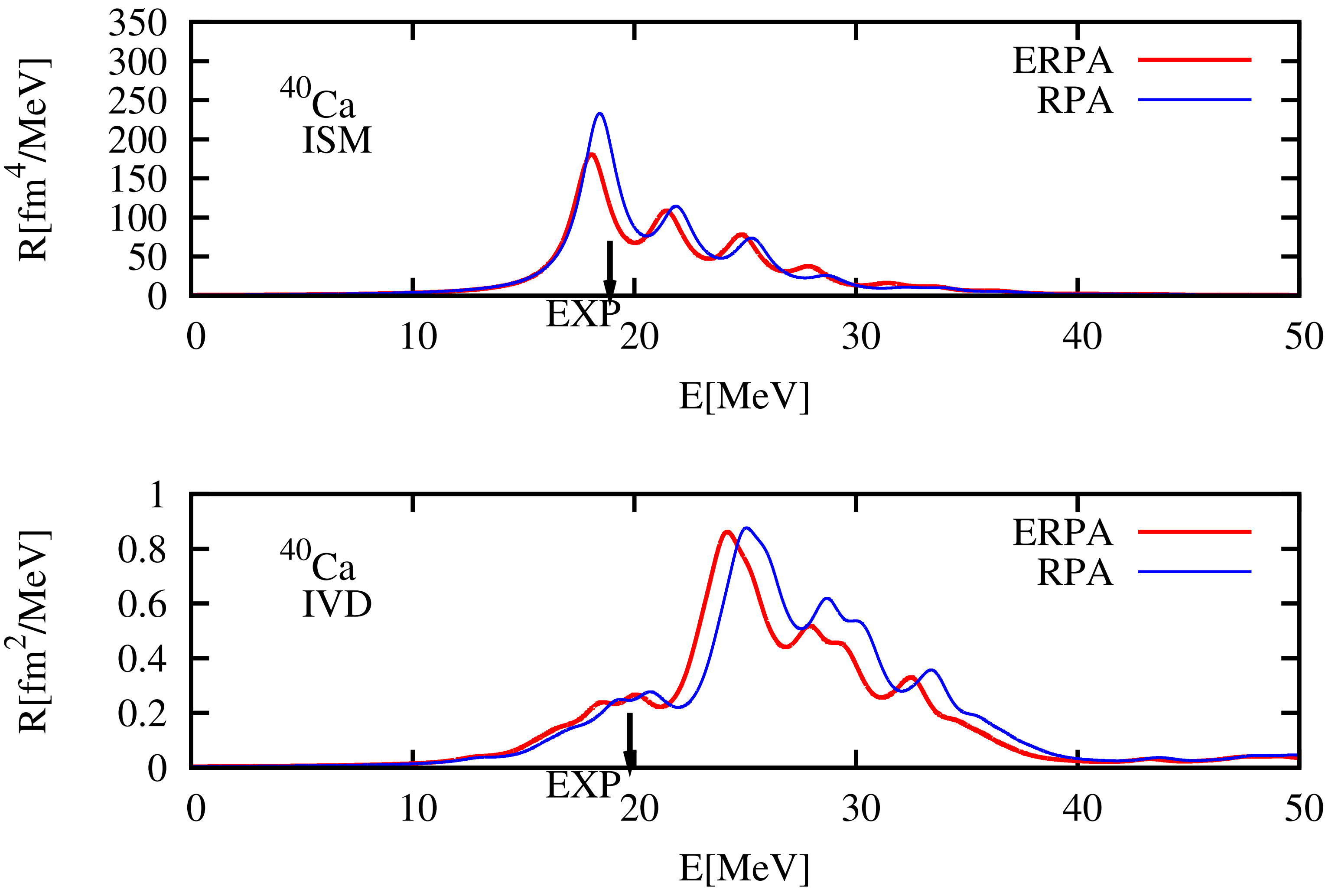
# “Extended” RPA

# Extended RPA

**The HF+RPA method is based mainly on the following approximations:**

- ☞ Coupling to higher order excitations $(np - nh)$ is neglected → Second RPA
- ☞ The ground state does not deviate much from the HF ground state → Renormalized RPA, “Extended” RPA, ...

# Extended RPA



# Summary

Use of the $V_{\mathrm{UCOM}}$ 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 $V_{\mathrm{UCOM}}$ 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

# Thank you!

## Work in collaboration with:

- R. Roth, N. Paar, H.Hergert, A. Zapp

  Institut für Kernphysik, TU Darmstadt

- T. Neff

  NSCL, Michigan State University

- H. Feldmeier

  Gesellschaft für Schwerionenforschung (GSI)

## Recent References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