Description of Nuclear Collectivity Using Correlated Realistic Interactions

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Overview

- Introduction
  - The Unitary Correlation Operator Method (UCOM)
- Ground-state properties
  - Hartree-Fock and Perturbation Theory
- Collective excitations
  - RPA and beyond: Extended RPA and Second RPA
  - The UCOM Hamiltonian as an effective interaction
- Summary

Introduction

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

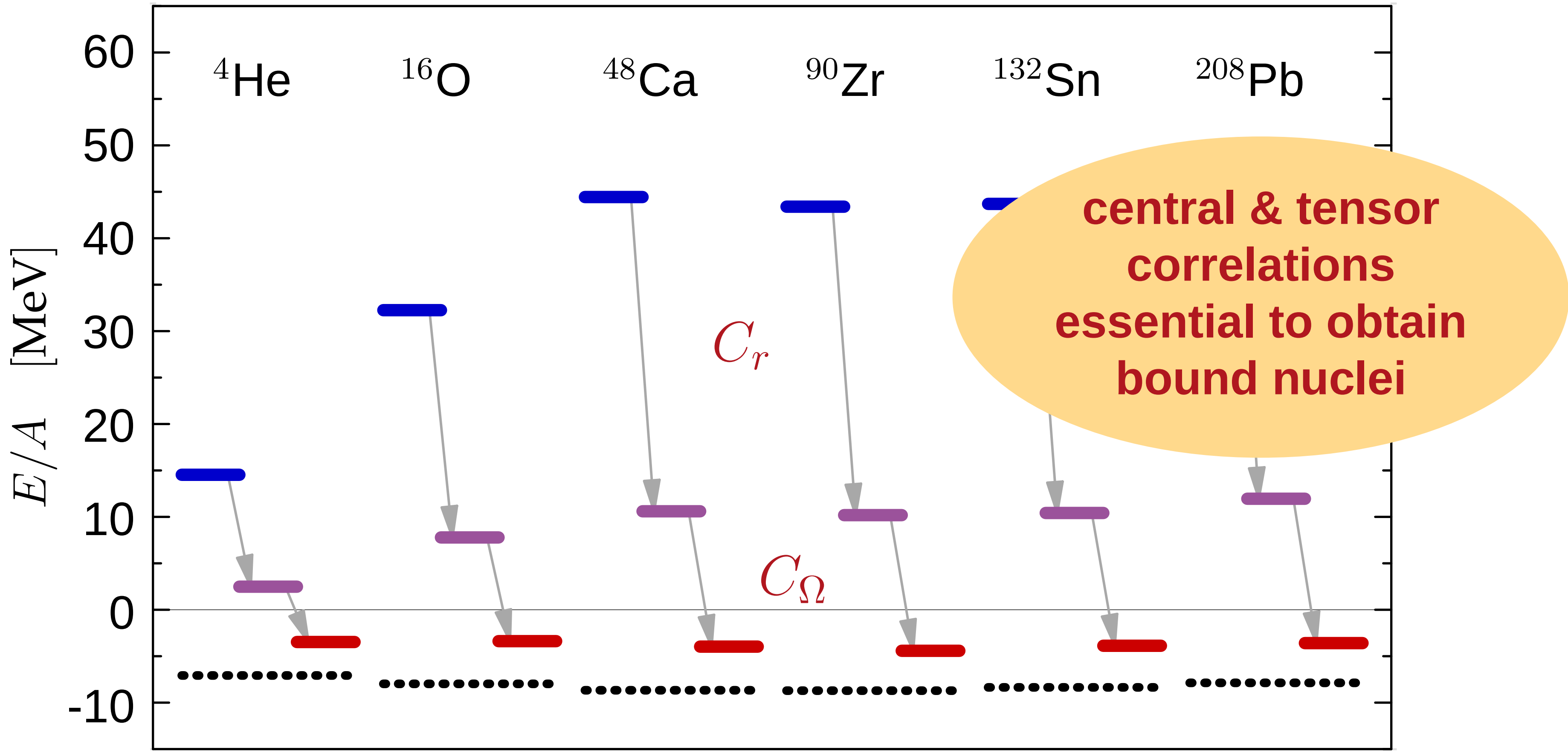
$$\langle \tilde{\Psi} | O | \tilde{\Psi} \rangle = \langle \Psi | C^\dagger O C | \Psi \rangle = \langle \Psi | \tilde{O} | \Psi \rangle$$

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

Introduction

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

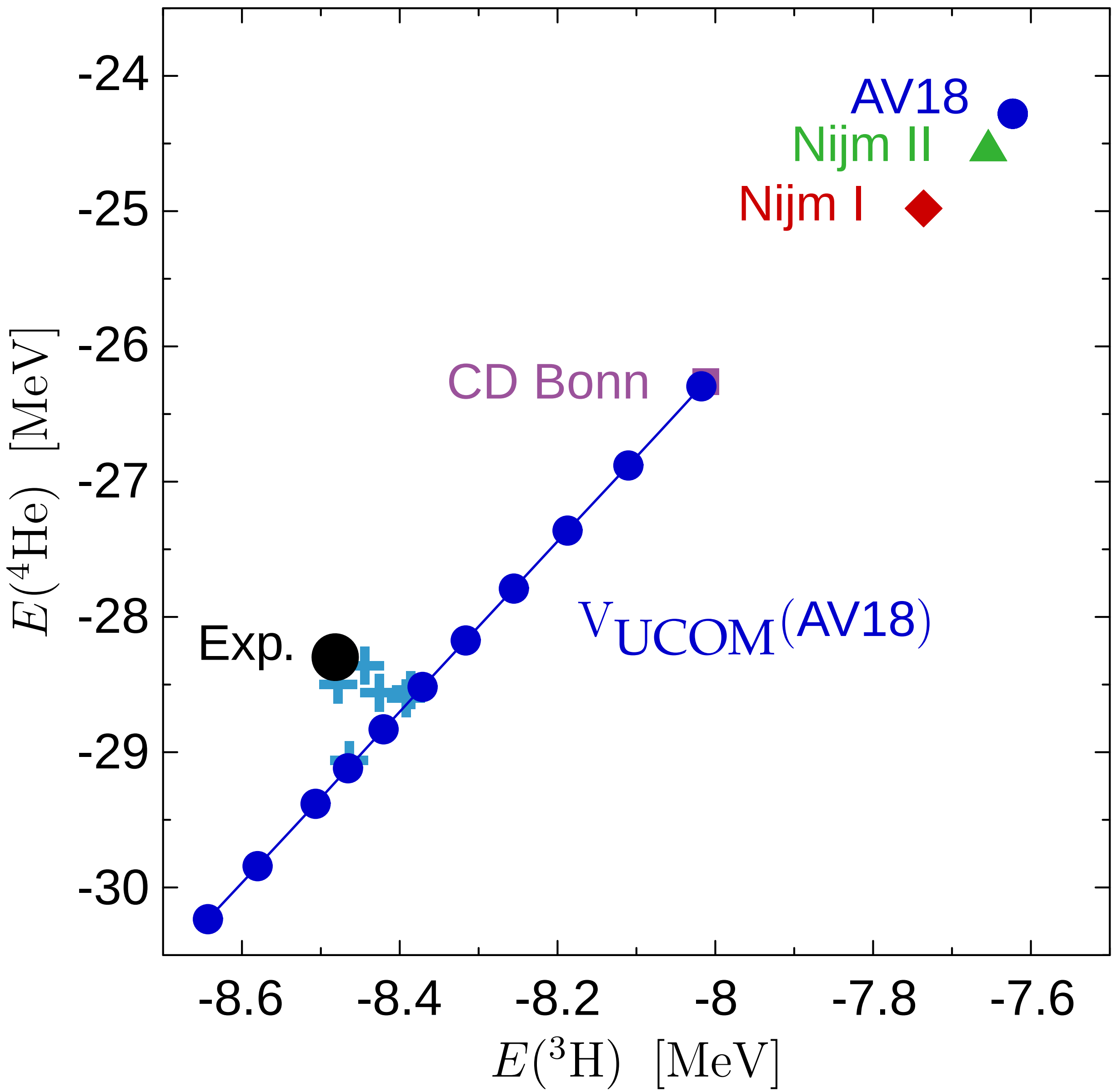


Introduction

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

- Ground state properties and excited states of closed-shell nuclei:
  - Hartree-Fock calculations
  - Second-order perturbation theory
  - Versions of the RPA: Standard, Extended, Second RPA
- ...and open-shell ones:
  - Hartree-Fock-Bogolyubov, Quasi-particle RPA...
- In what follows, a UCOM Hamiltonian based on the Argonne V18 NN interaction is used

Tjon Line and Correlator Range



- Tjon line: E(^{4}He) vs E(^{3}H) for phase-shift equivalent NN interactions
- Change of tensor-correlator range results in shift along the Tjon line

minimize net three-body force by choosing correlator giving energies close to the experimental point

Ground-State Properties

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 + PT

LRC: extending the model space

Second-order perturbation theory

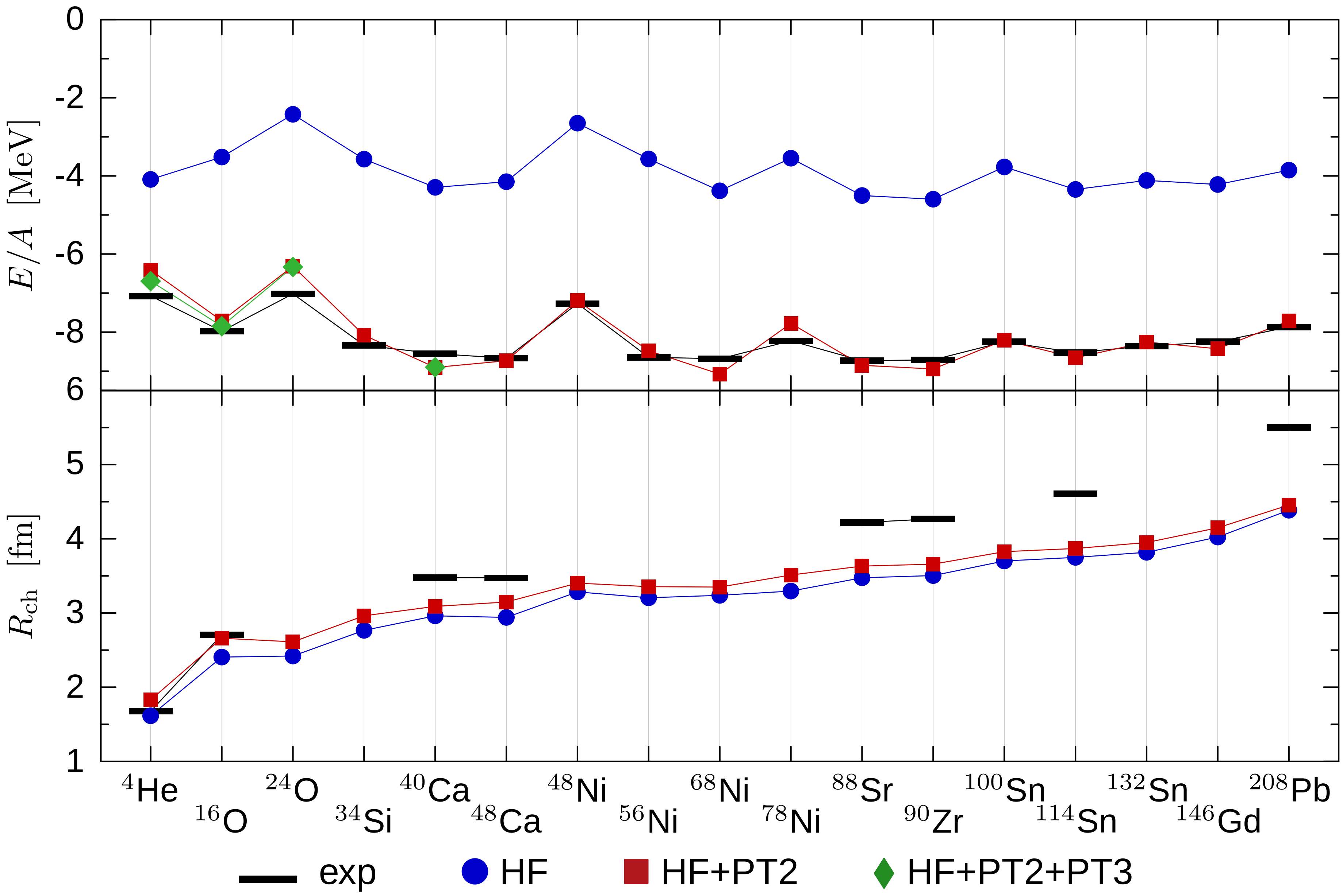
- Binding-energy correction:

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

- Modified density matrix and occupation numbers

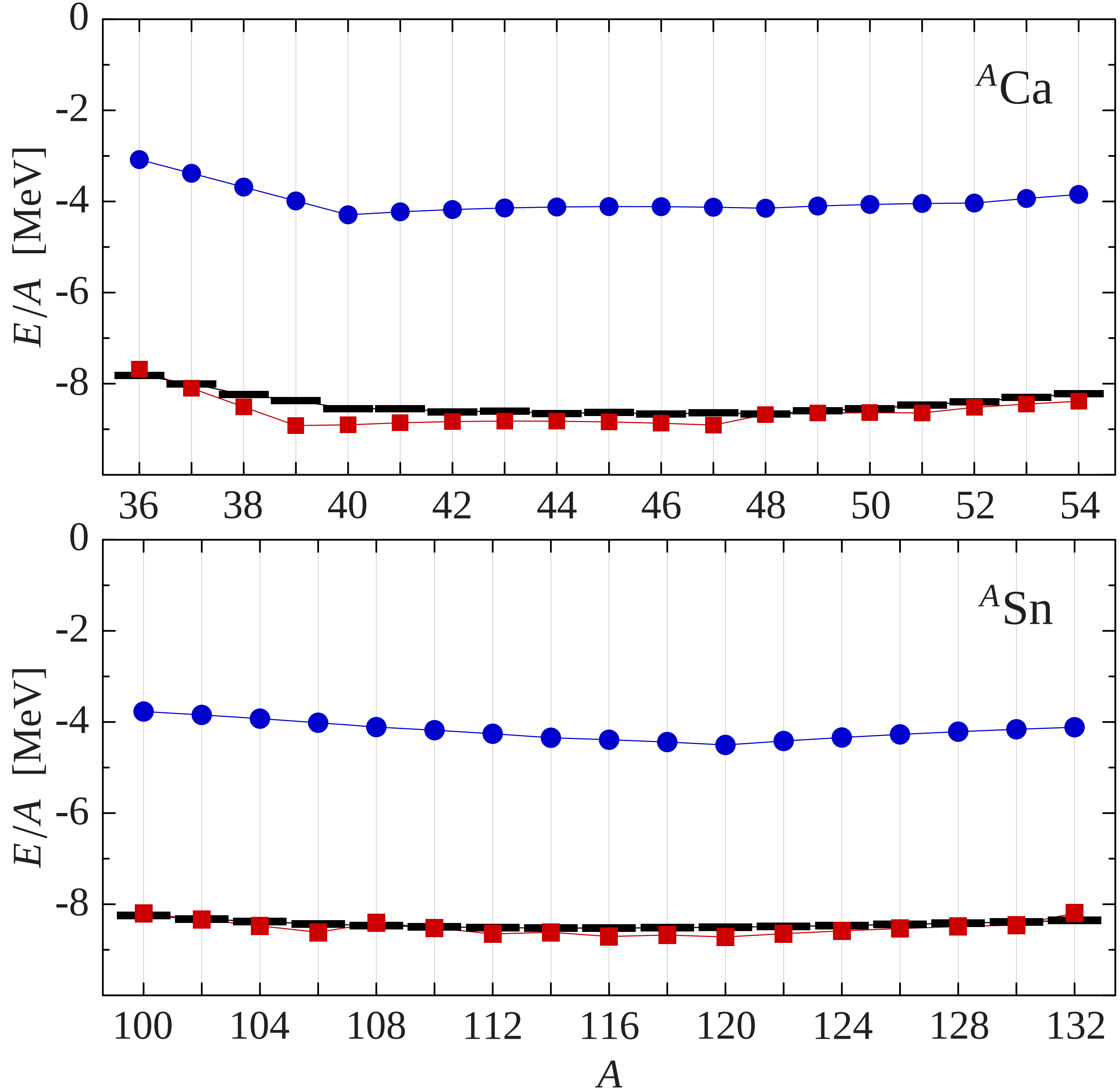
☞ Modified charge radii

UCOM-HF + PT



0
-2
-4
-6
-8
6
5
4
3
2
1
E/A [MeV]
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
HF+PT2
HF+PT2+PT3

UCOM-HF + PT



^{A}Ca
^{A}Sn
E/A [MeV]
0
-2
-4
-6
-8
36
38
40
42
44
46
48
50
52
54
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

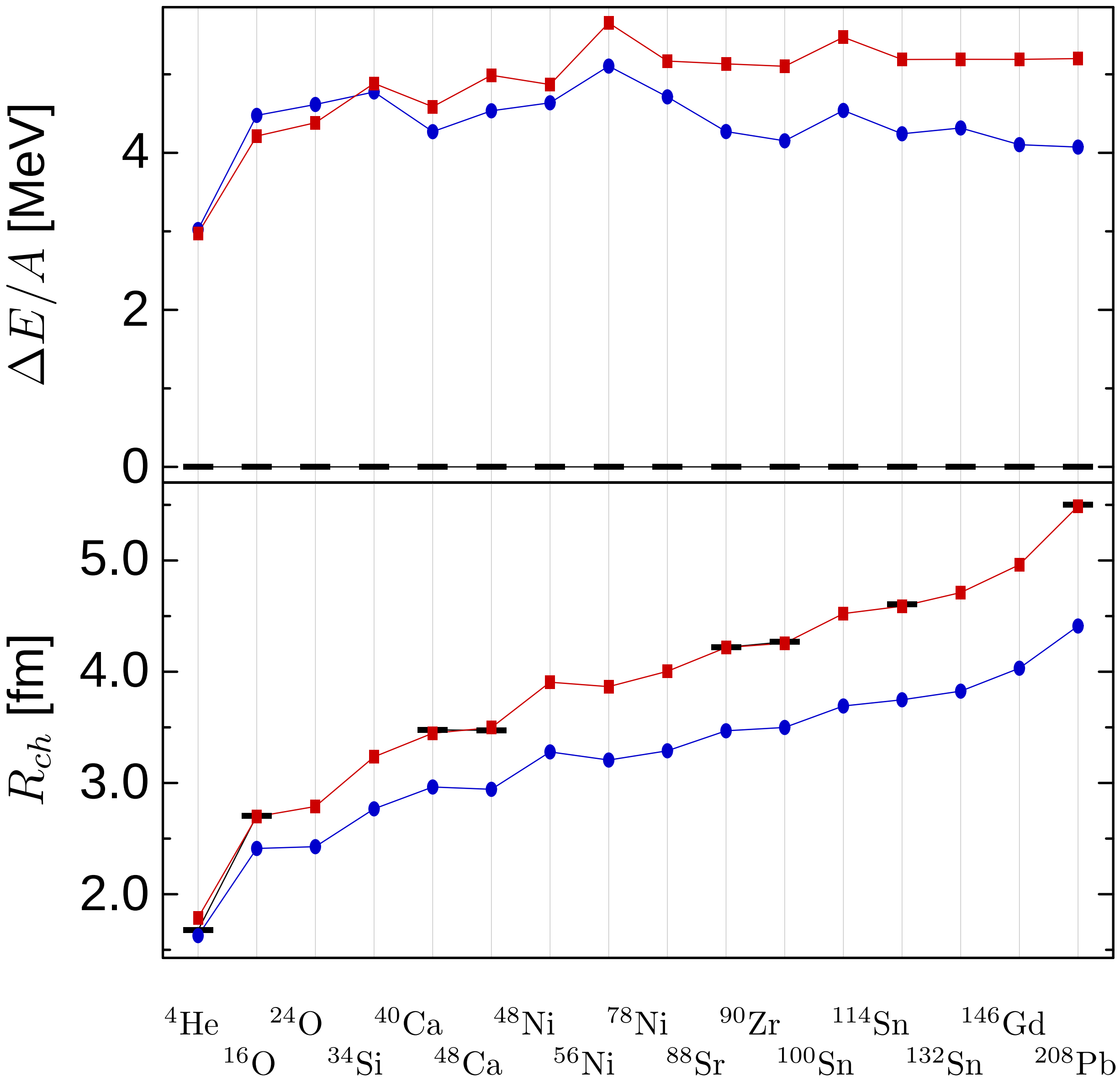
- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, CI, CC,...

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



Collective Excitations:
RPA and beyond

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:

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

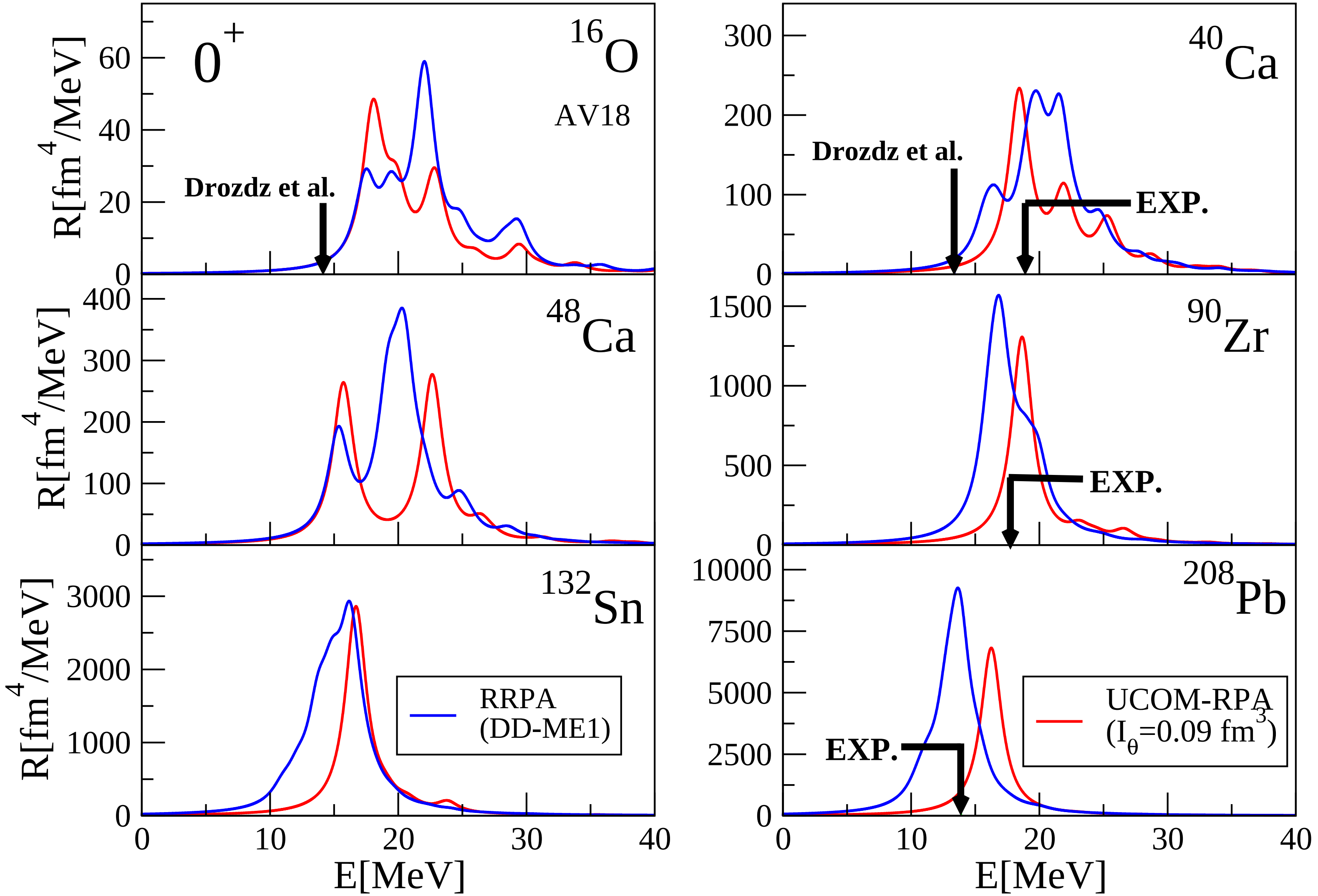
$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(e_p - e_h) + H_{hp',ph'} \;\; ; \;\; B_{ph,p'h'} = H_{hh',pp'} \;\; ; \;\; H = H_{\mathrm{int}} = T_{\mathrm{rel}} + V_{\mathrm{UCOM}}$$

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

Standard RPA

Isoscalar monopole response

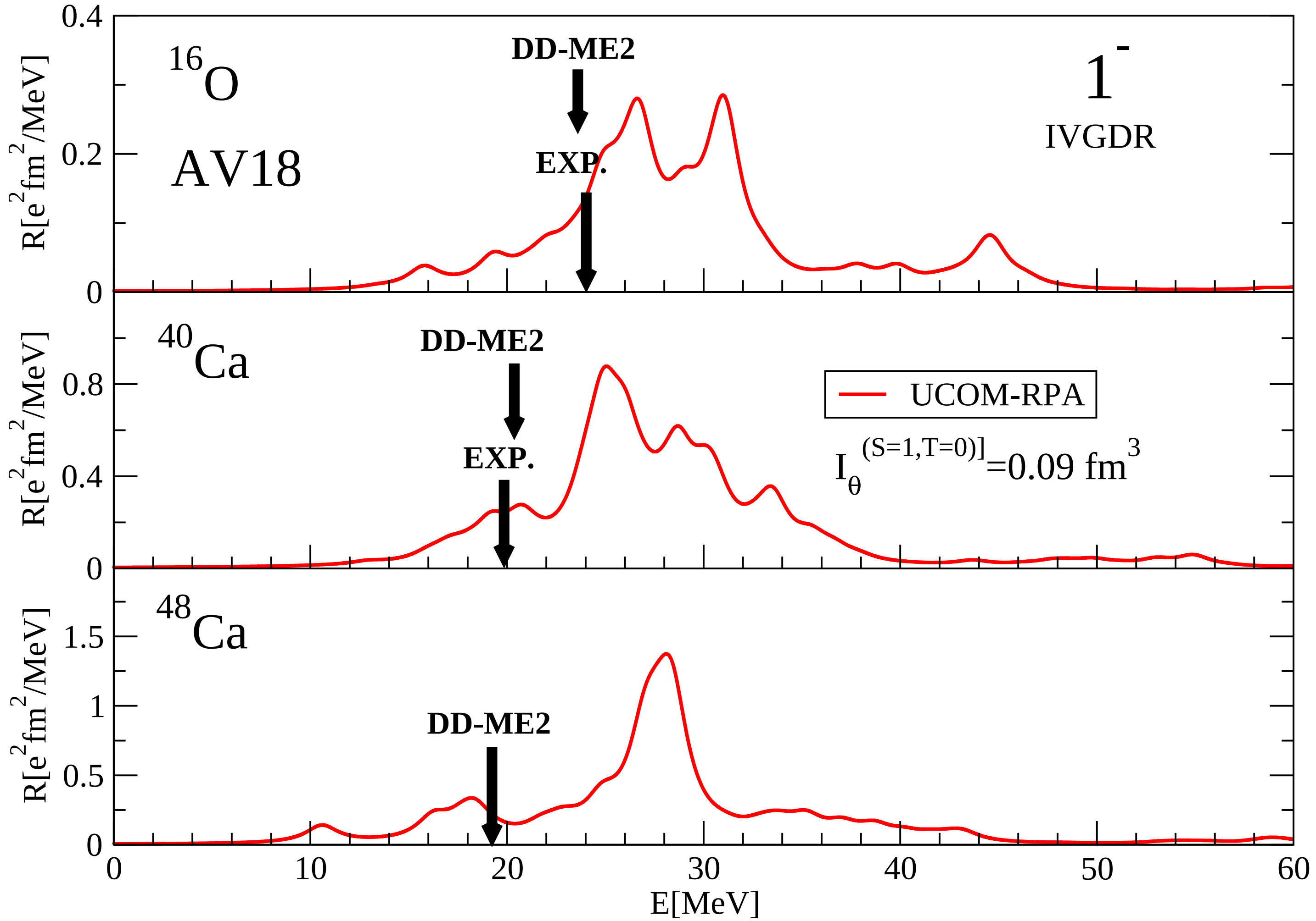
$N_{\mathrm{max}} = 12$



Standard RPA

Isovector dipole response

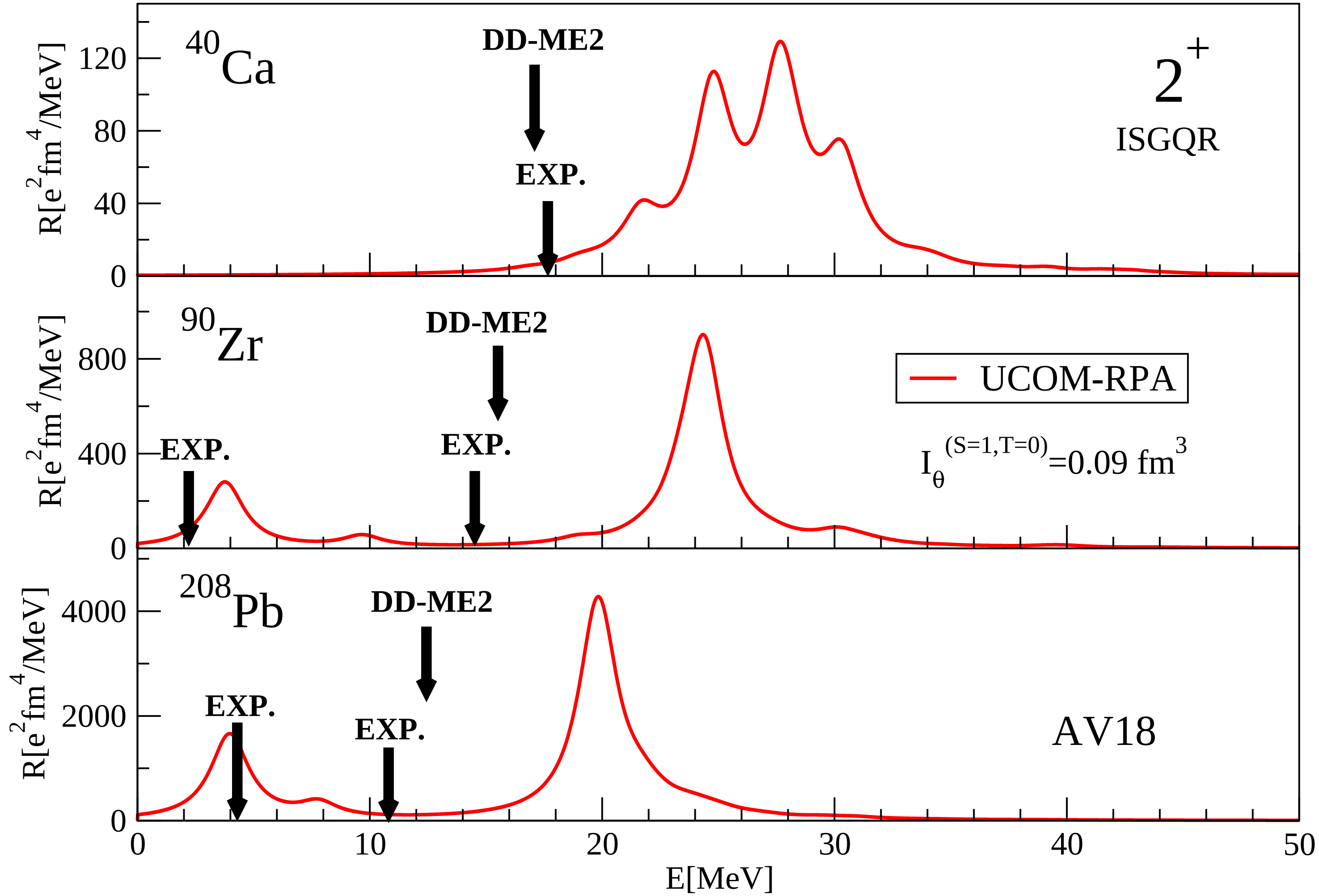
$N_{\text{max}} = 12$



Standard RPA

Isoscalar quadrupole response

$N_{\max} = 12$



Beyond Standard 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

[Catara et al.: PRB58(98)16070;
Voronov et. al.: Phys.Part.Nucl.31(00)904]

- Vibration creation operator:

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

- Excitations are built on the RPA vacuum. In general,

$$O_{ph} = \sum_{p'h'} N_{ph,p'h'} a_{p'}^\dagger a_{h'}$$

- ERPA is formulated in the natural-orbital basis:

$$O_{ph} \rightarrow D_{ph}^{-1/2} a_p^\dagger a_h \quad ; \quad D_{ph} \equiv n_h - n_p$$

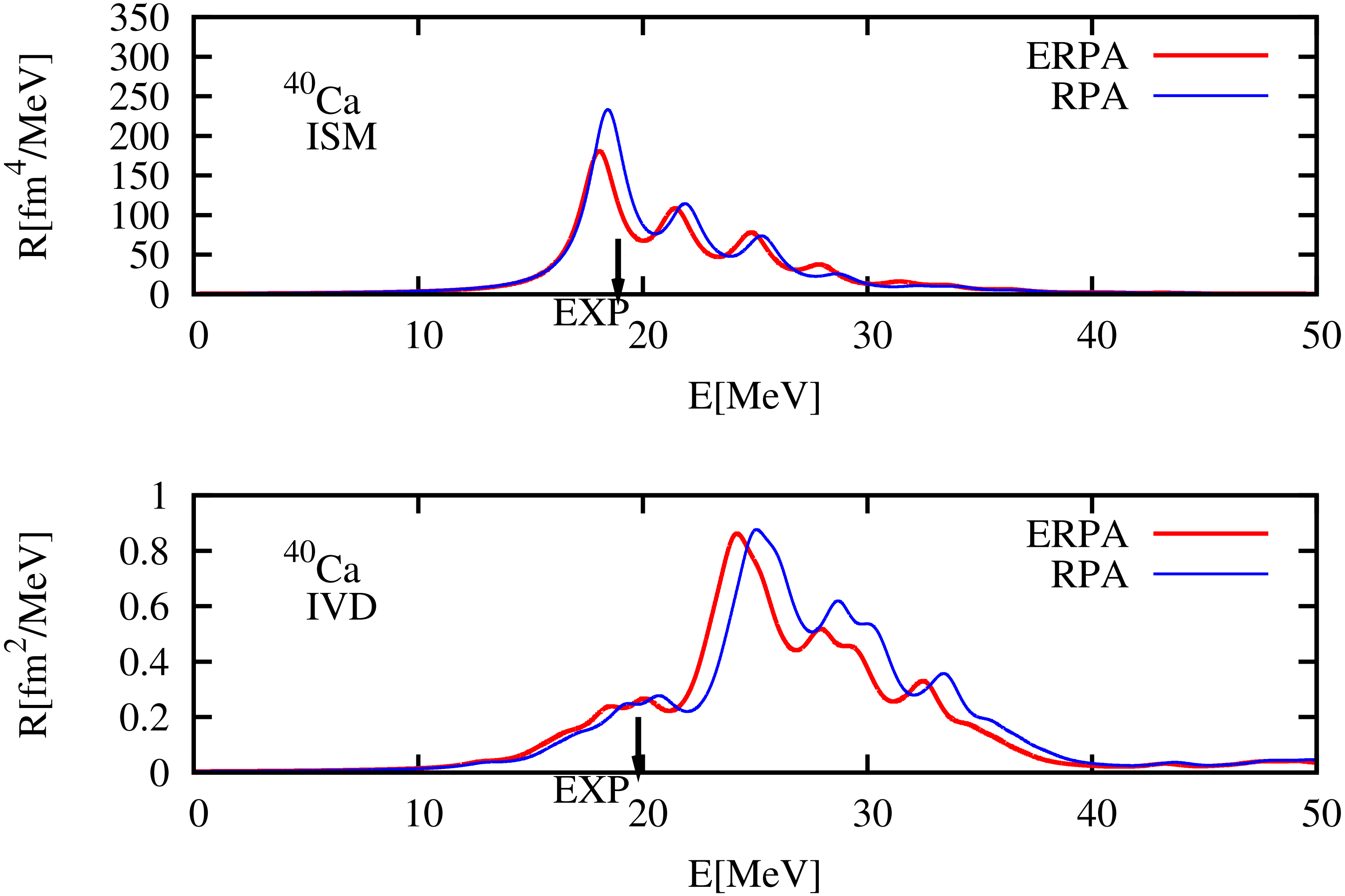
ERPA equations: solved iteratively

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

$$A_{ph,p'h'} = \delta_{hh'} e_{pp'} - \delta_{pp'} e_{hh'} + D_{ph}^{1/2} D_{p'h'}^{1/2} H_{hp',ph'} \quad ; \quad B_{ph,p'h'} = D_{ph}^{1/2} D_{p'h'}^{1/2} H_{hh',pp'}$$

$$e_{ij} = \sum_k n_k H_{ik,jk}$$

Extended RPA



Second RPA

- Vibration creation operator: Includes $2p2h$ configurations

$$Q_\nu^\dagger = \sum_{ph} X_{ph}^\nu O_{ph}^\dagger - \sum_{ph} Y_{ph}^\nu O_{ph} + \sum_{p_1h_1p_2h_2} \mathcal{X}_{p_1h_1p_2h_2}^\nu O_{p_1h_1p_2h_2}^\dagger$$
$$-\sum_{p_1h_1p_2h_2} \mathcal{Y}_{p_1h_1p_2h_2}^\nu O_{p_1h_1p_2h_2}$$

- The SRPA vacuum is approximated by the HF ground state:

$$\langle \mathrm{SRPA}| \ldots |\mathrm{SRPA}\rangle \rightarrow \langle \mathrm{HF}| \ldots |\mathrm{HF}\rangle$$

- SRPA equations in $ph \oplus 2p2h-$space:

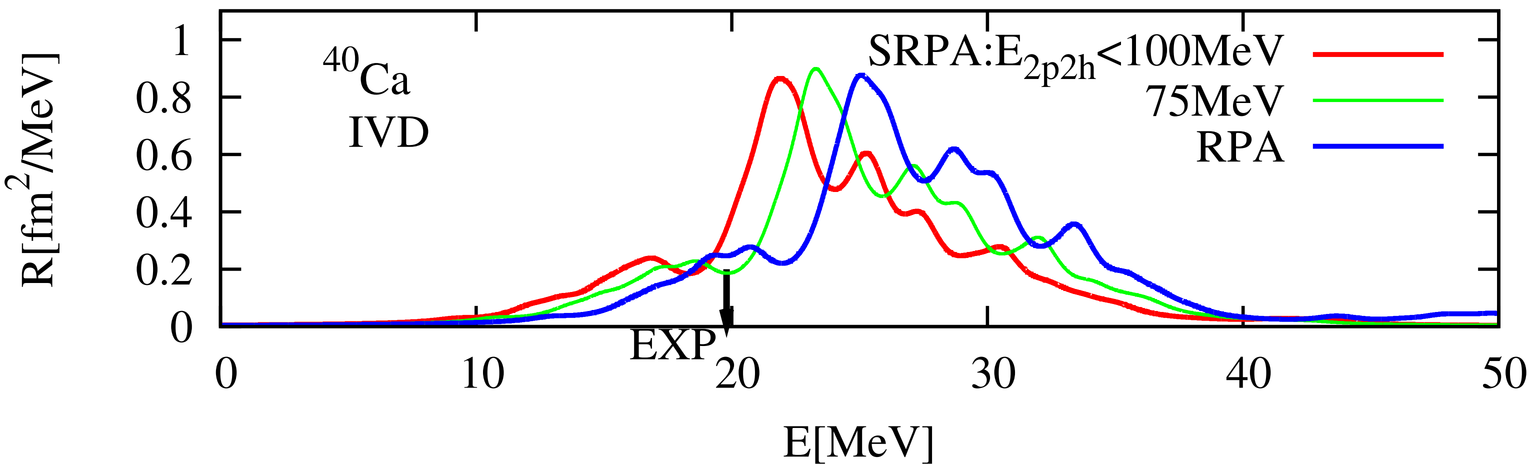
$$\left(\begin{array}{cc|cc} A & \mathcal{A}_{12} & B & 0 \\ \mathcal{A}_{21} & \mathcal{A}_{22} & 0 & 0 \\ \hline -B^* & 0 & -A^* & -\mathcal{A}_{12}^* \\ 0 & 0 & -\mathcal{A}^* & -\mathcal{A}_{22}^* \end{array}\right) \left(\begin{array}{c} X^\nu \\ \mathcal{X}^\nu \\ \hline Y^\nu \\ \mathcal{Y}^\nu \end{array}\right) = \hbar\omega_\nu \left(\begin{array}{c} X^\nu \\ \mathcal{X}^\nu \\ \hline Y^\nu \\ \mathcal{Y}^\nu \end{array}\right)$$

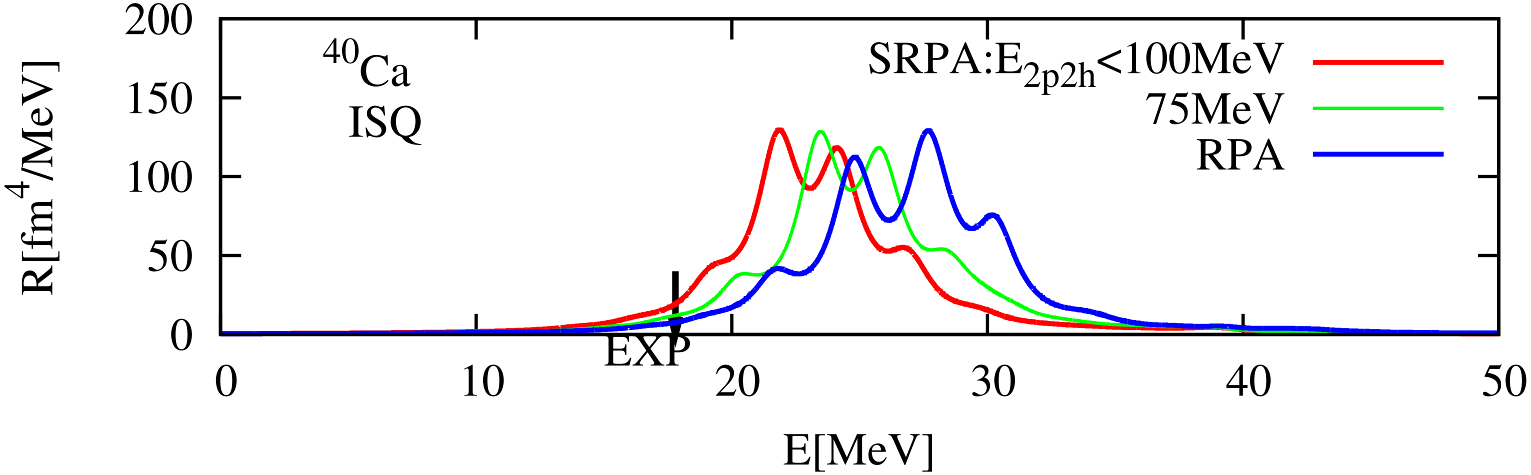
$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(e_p - e_h) + H_{hp',ph'} \;\; ; \;\; B_{ph,p'h'} = H_{hh',pp'} \;\; ; \;\; H = H_{\mathrm{int}} = T_{\mathrm{rel}} + V_{\mathrm{UCOM}}$$

$\mathcal{A}_{12}$: interactions between ph and $2p2h$ states

$\mathcal{A}_{22}$: $\delta_{p_1p_1'}\delta_{h_1h_1'}\delta_{p_1p_1'}\delta_{h_1h_1'}(e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2})$ + interactions among $2p2h$ states

Second RPA - Preliminary





Summary

Nuclear collective excitations
using the V_{UCOM}

- Standard RPA
  - GMR properties well reproduced
  - GDR, GQR centroids overestimated
  - Properties of the V_{UCOM} as an “effective interaction”
- “Extended” RPA
  - Small effect of explicit ground-state correlations
- Second RPA
  - Preliminary results show sizable effect of extended space

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

Thank you!

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References and further information

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