RPA Methods and Modern Effective Interactions

– Recent results and outlook –

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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

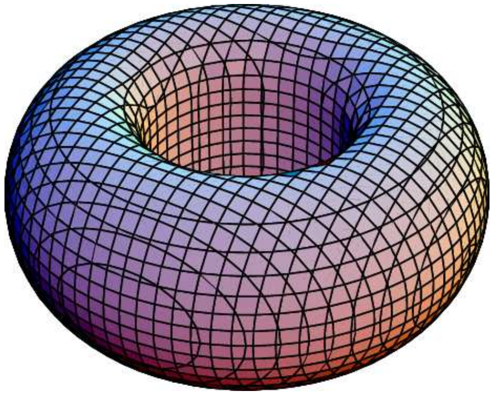
- Nuclear structure and dynamics starting from a realistic NN interaction?
  - Modern NN potentials reproduce precise deuteron and scattering data
  - Potentials based on chiral EFT
- Exact calculations possible for light nuclei and nuclear matter
  - For heavy nuclei the size of the model space becomes prohibitive
  - Strong correlations cannot be described by simple model states
- ”Effective interactions” based on realistic potentials?

Correlated realistic interactions V_{UCOM}

- Short-range central and tensor correlations described by a unitary correlation operator $C = C_\Omega C_r$

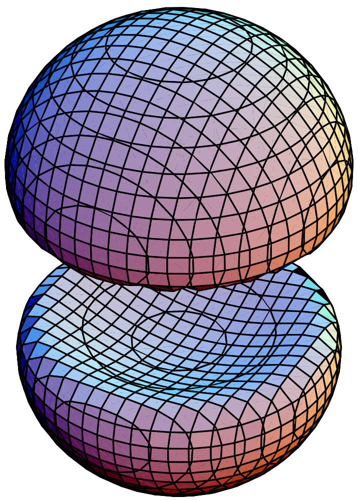
Deuteron: Manifestation of Correlations

- Spin-projected two-body density for Argonne V18 potential



$M_S = 0$

$\frac{1}{\sqrt{2}}(\,|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\,)$



$M_S = \pm 1$

$|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$

Fully suppressed at
short particle distances $|\vec{r}|$:
central correlations

Strong dependence
on relative spin orientation:
tensor correlations

The Unitary Correlation Operator Method

Correlated realistic interactions V_{UCOM}

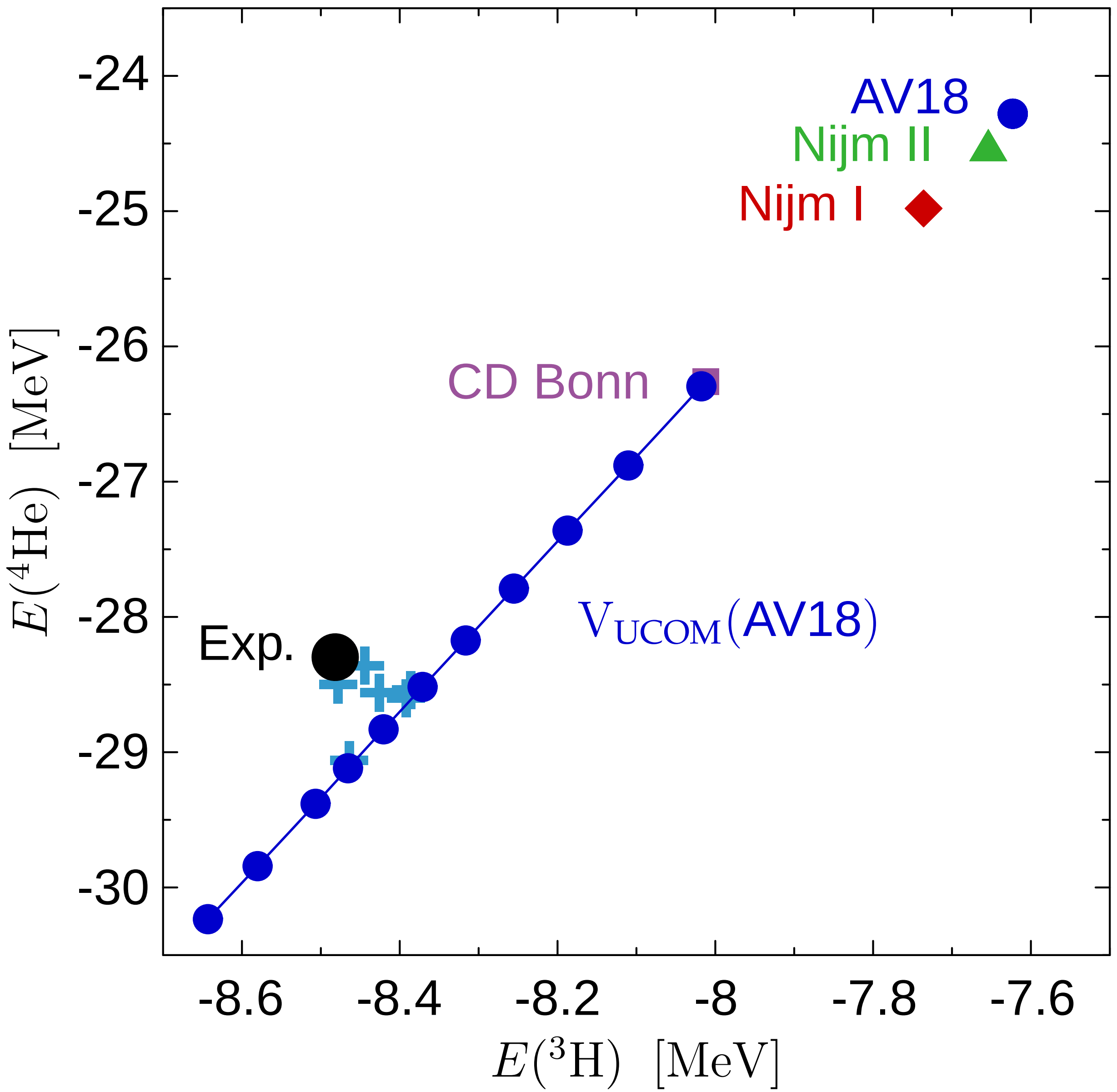
- Short-range central and tensor correlations (SRC) described by a unitary correlation operator $C = C_{\Omega} C_r$
- Introduce SRC to uncorrelated A-body state or an operator of interest

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

realistic NN interaction → correlated interaction

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

Tjon Line and Correlator Range

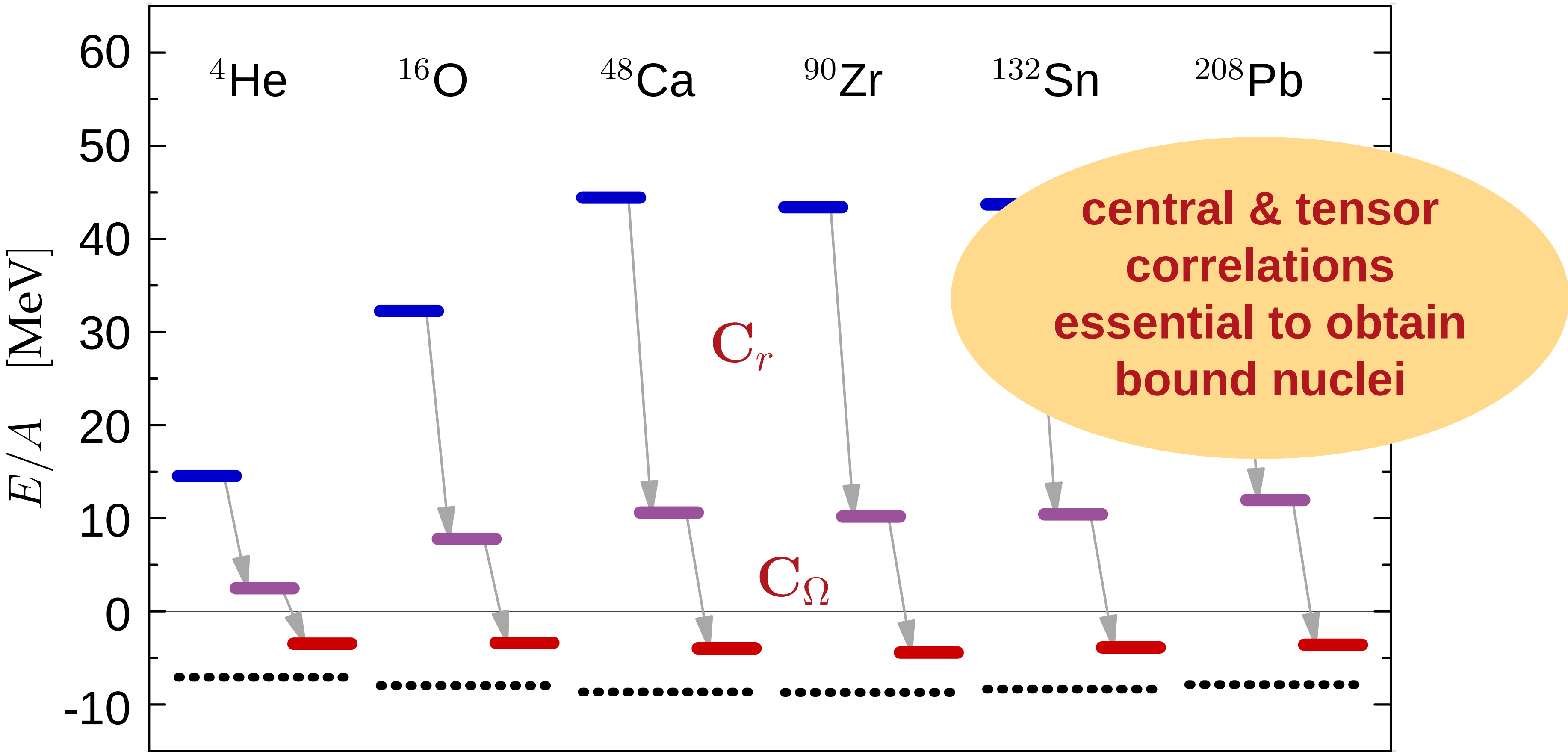


- Tjon line: E(^{4}He) vs E(^{3}H) for phase-shift equivalent NN interactions
- Change of tensor-correlator range results in shift along the Tjon line

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

Simplistic “Shell-Model” Calculation

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



Overview

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 and 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

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

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

↓ inclusion of SRC

UCOM-HF + PT

LRC: extending the model space

Second-order perturbation theory

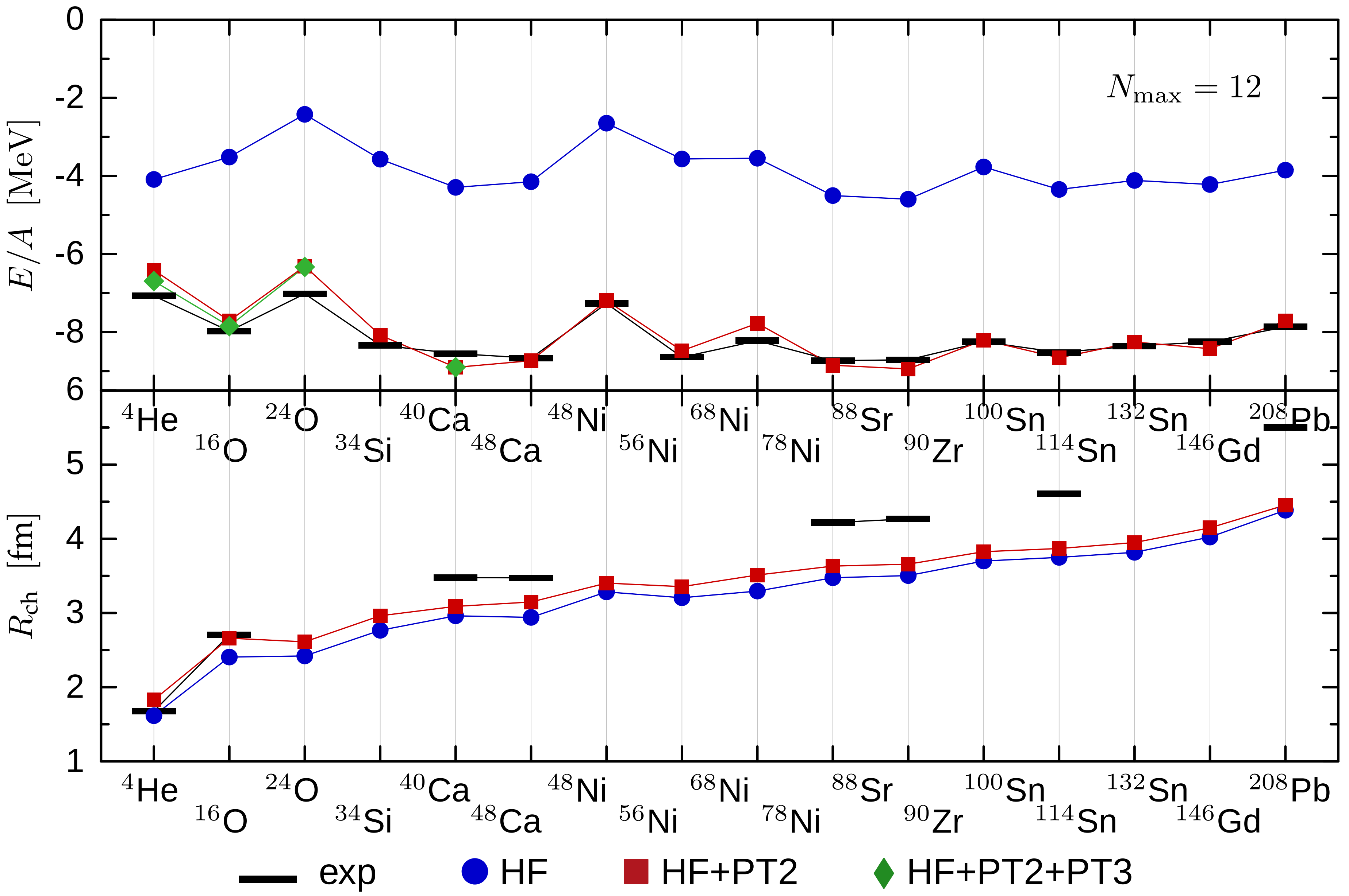
- Binding-energy correction:

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

- Modified density matrix and occupation numbers

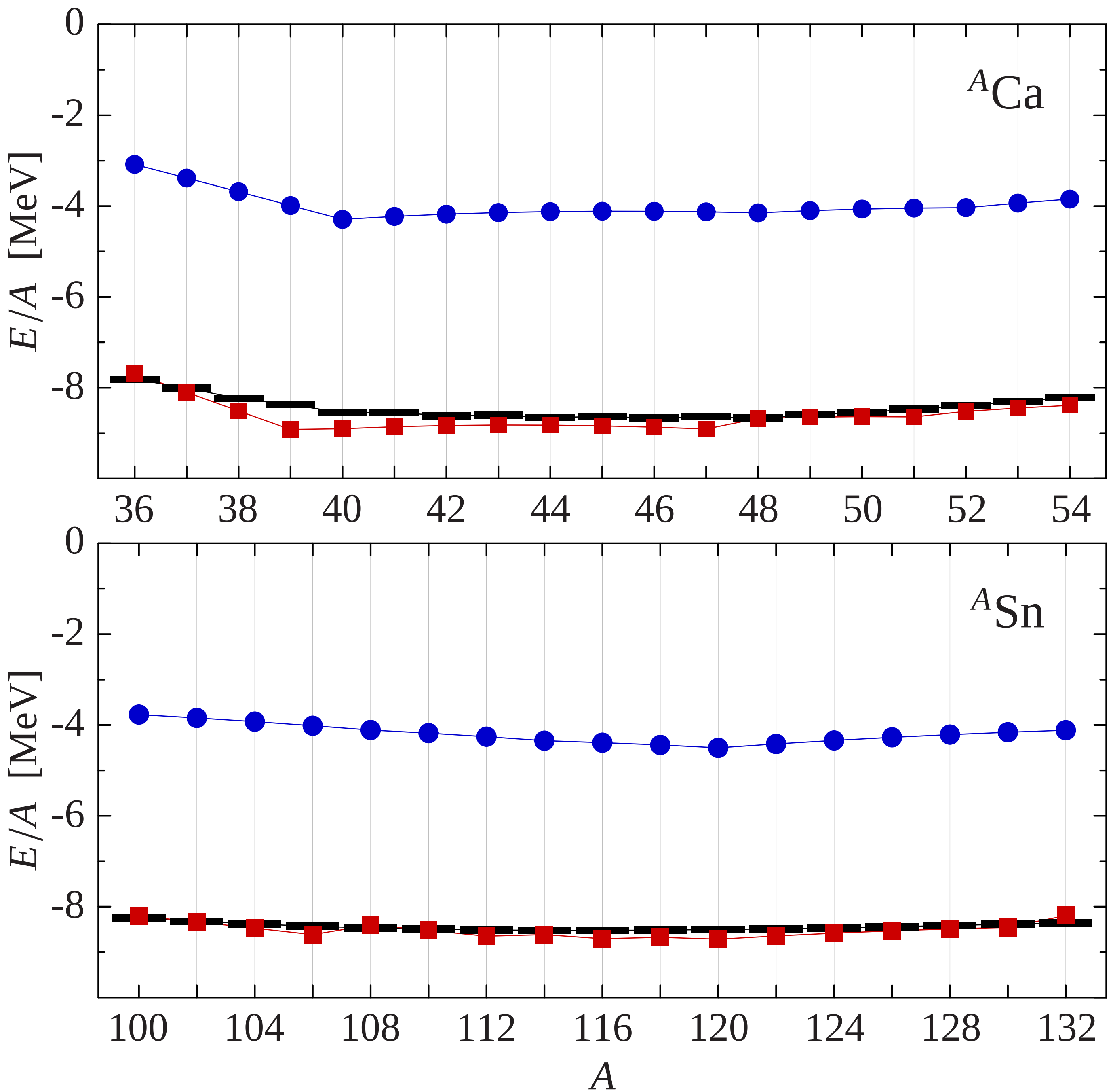
☞ Modified charge radii

UCOM-HF + PT



$N_{max} = 12$
E/A [MeV]
R_{ch} [fm]
0
-2
-4
-6
-8
6
5
4
3
2
1
^{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



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

Collective Excitations

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:

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

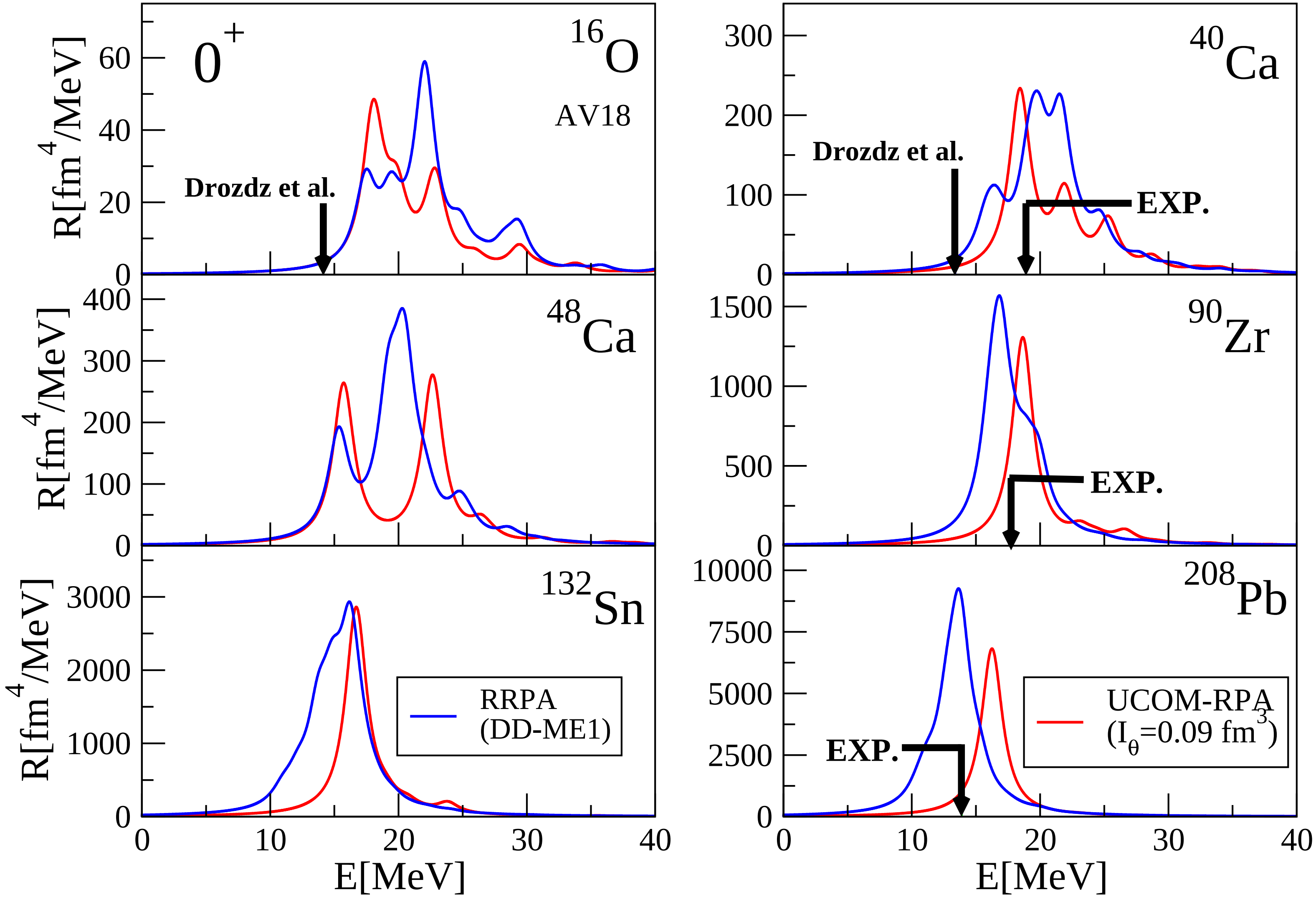
$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(e_p - e_h) + H_{hp',ph'} \; ; \; B_{ph,p'h'} = H_{hh',pp'} \; ; \; H = H_{\mathrm{int}} = T_{\mathrm{rel}} + V_{\mathrm{UCOM}}$$

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

Standard RPA

Isoscalar monopole response

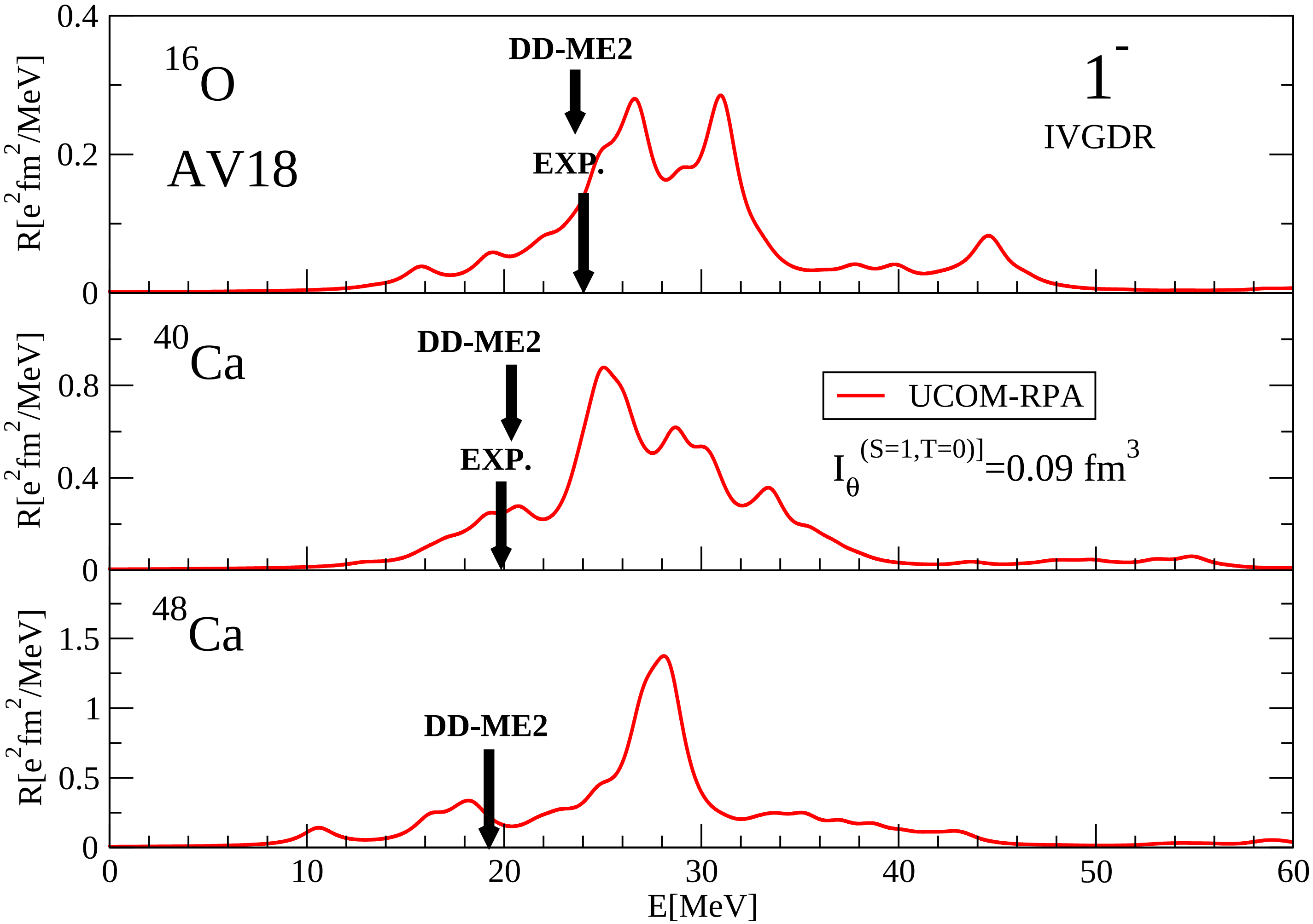
$N_{\max} = 12$



Standard RPA

Isovector dipole response

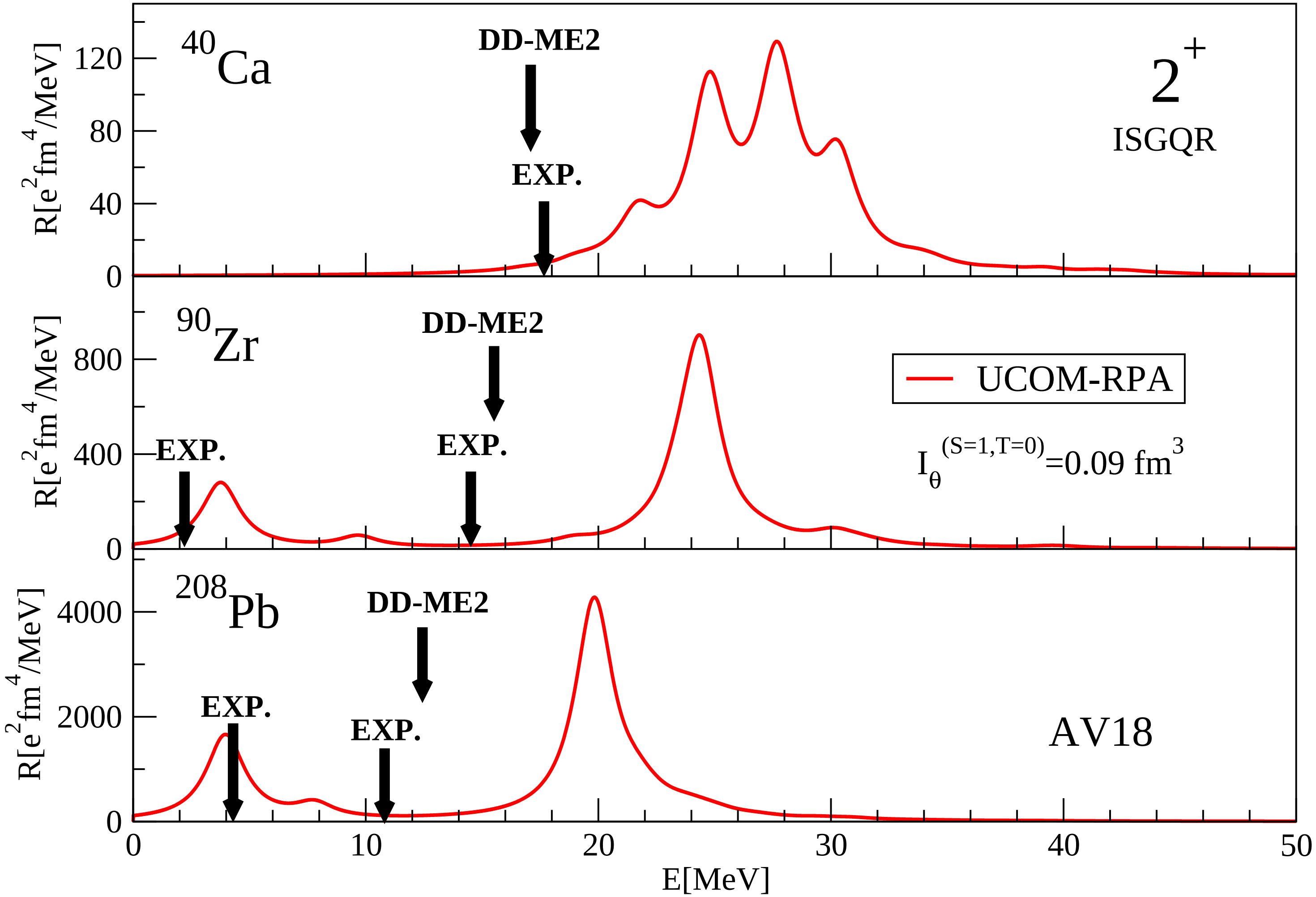
$N_{\text{max}} = 12$



Standard RPA

Isoscalar quadrupole response

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



Beyond Standard RPA

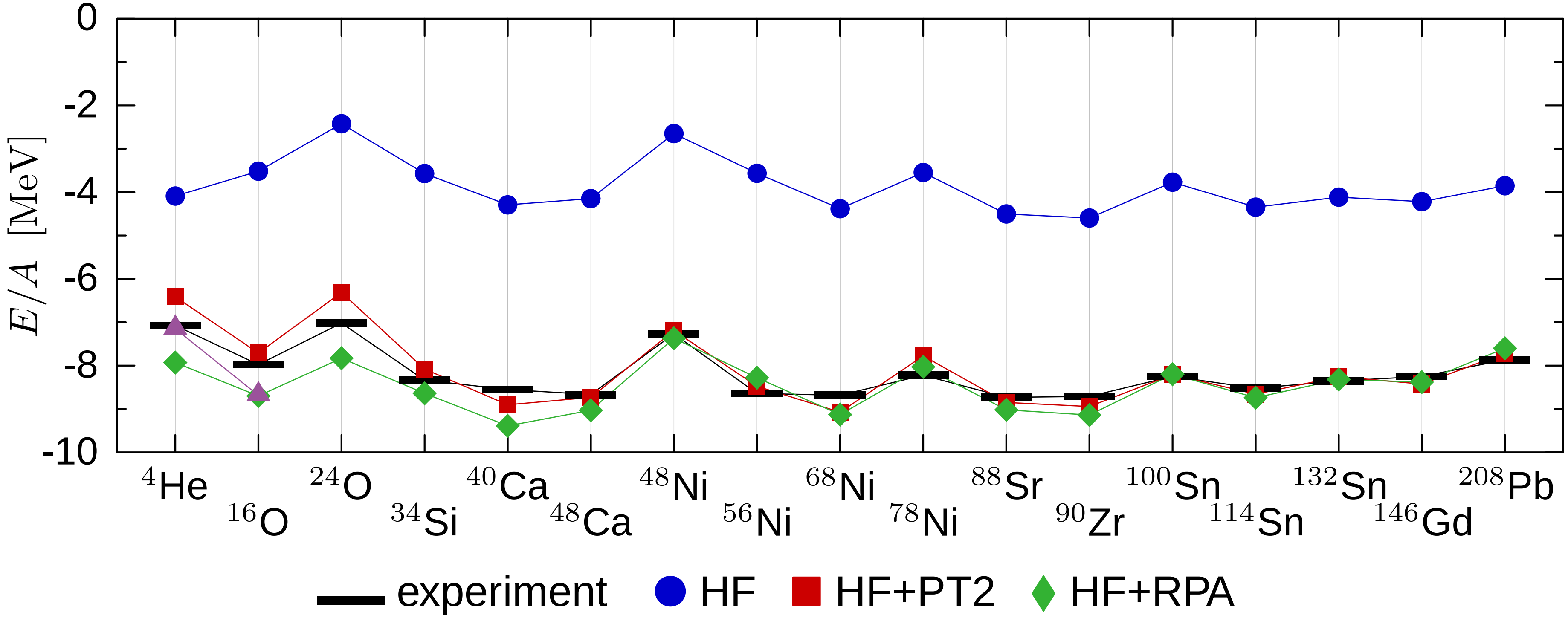
The HF+RPA method is based mainly on the following approximations:

☞ 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, ...

RPA Ground State Correlations

- evaluate correlation energy beyond Hartree-Fock via **ring summation** using RPA amplitudes
- include all parities and charge exchange and correct for double-counting of 2nd order term



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

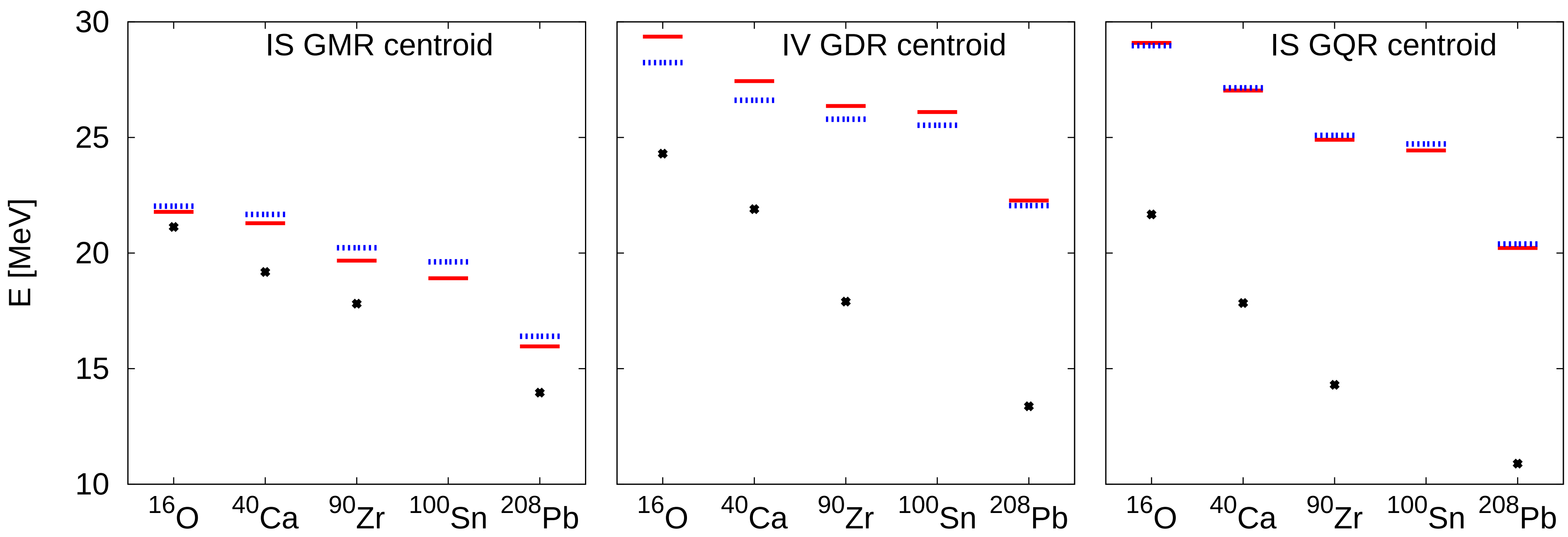
$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \hbar\omega_\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

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

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

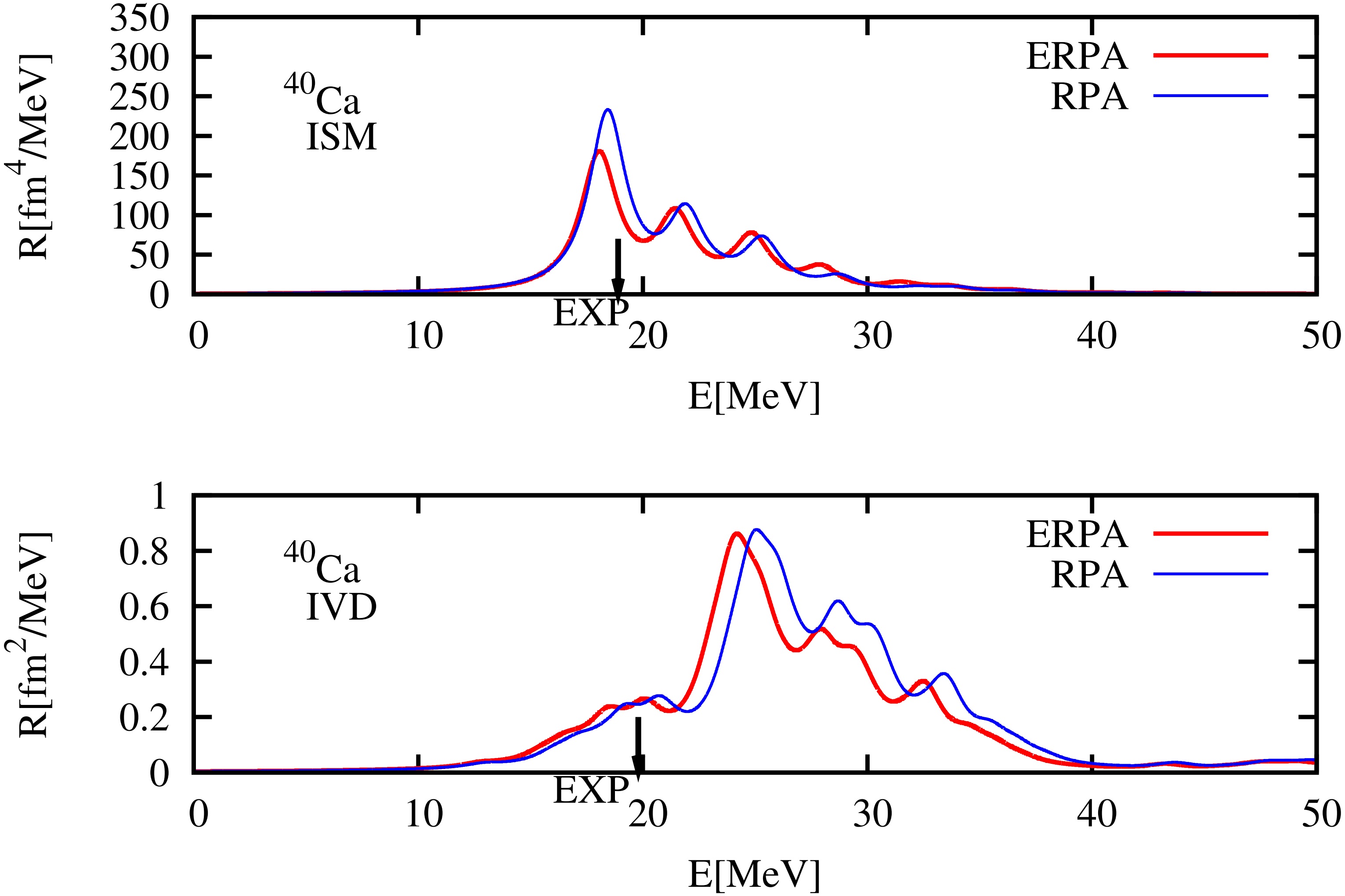
Extended RPA

Centroid energies — RPA ···· ERPA ▪ exp



Fermi-sea depletion: 2.6-5.0%

Extended RPA



Second RPA

- Vibration creation operator: Includes $2p2h$ configurations

$$Q_\nu^\dagger = \sum_{ph} X_{ph}^\nu O_{ph}^\dagger - \sum_{ph} Y_{ph}^\nu O_{ph} + \sum_{p_1 h_1 p_2 h_2} \mathcal{X}_{p_1 h_1 p_2 h_2}^\nu O_{p_1 h_1 p_2 h_2}^\dagger$$
$$- \sum_{p_1 h_1 p_2 h_2} \mathcal{Y}_{p_1 h_1 p_2 h_2}^\nu O_{p_1 h_1 p_2 h_2}$$

- 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:

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

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

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

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

Second RPA

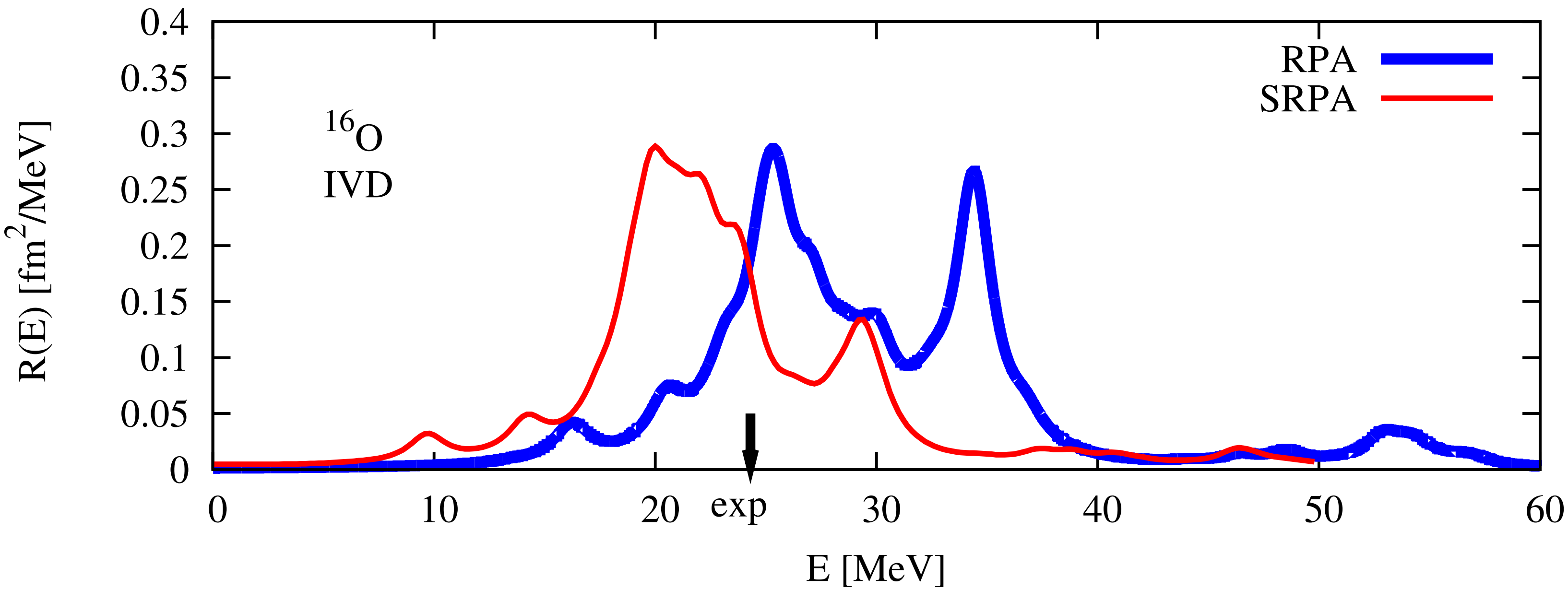
- Large model spaces:
  - Up to half a million states for the cases presented here!
  - Even larger for larger nuclei, bases, other excitations
- Use Lanczos
  - Find only the lowest eigenvalues $|\omega_\nu|$
  - ... or the ones closest to a set value E_0

$$\mathrm{R}\mathrm{X}_\nu = \omega_\nu \mathrm{X}_\nu \quad \Longleftrightarrow \quad \mathrm{R}'\mathrm{X}_\nu = \omega'_\nu \mathrm{X}_\nu \ , \qquad \left\{ \begin{array}{c} \mathrm{R}' \equiv \mathrm{R} - E_0 \mathrm{I} \\ \omega'_\nu \equiv \omega_\nu - E_0 \end{array} \right\}$$

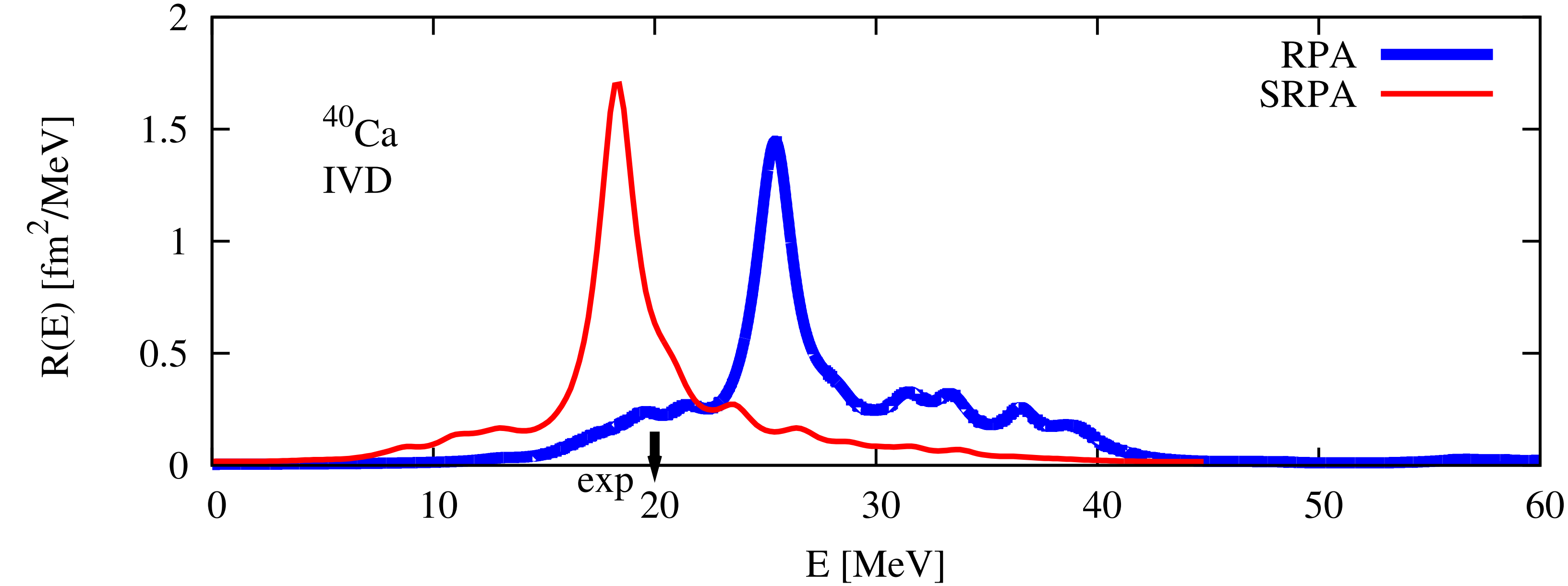
- Reduce to an $\omega-$dependent problem of RPA size
  - ... especially if you ignore interactions within 2p2h space:

$$A_{php'h'} \longrightarrow A_{php'h'}(\omega) = A_{php'h'} + \sum_{PHP'H'} \frac{A^*_{ph\,PHP'H'} A_{p'h'\,PHP'H'}}{\hbar\omega - (\epsilon_P + \epsilon_{P'} - \epsilon_H - \epsilon_{H'}) + \mathrm{i}\eta}$$

Second RPA

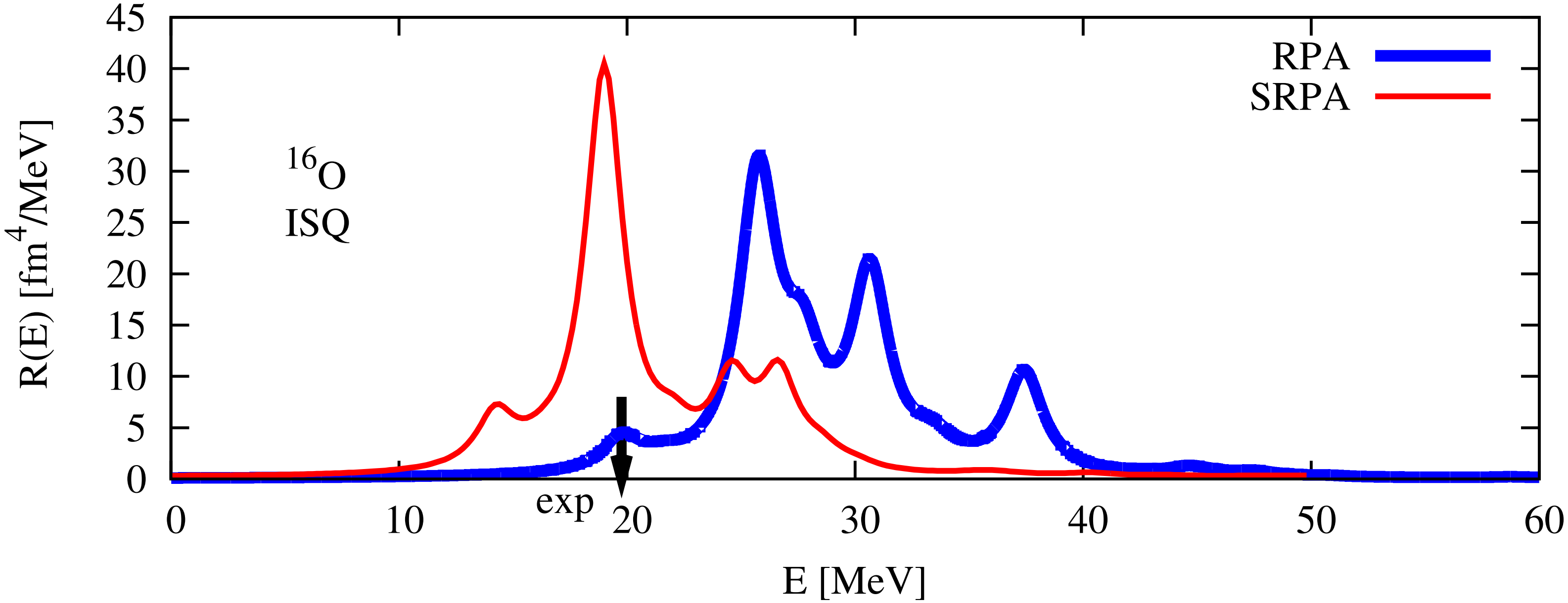


0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
R(E) [fm²/MeV]
RPA
SRPA
16O
IVD
exp
0
10
20
30
40
50
60
E [MeV]

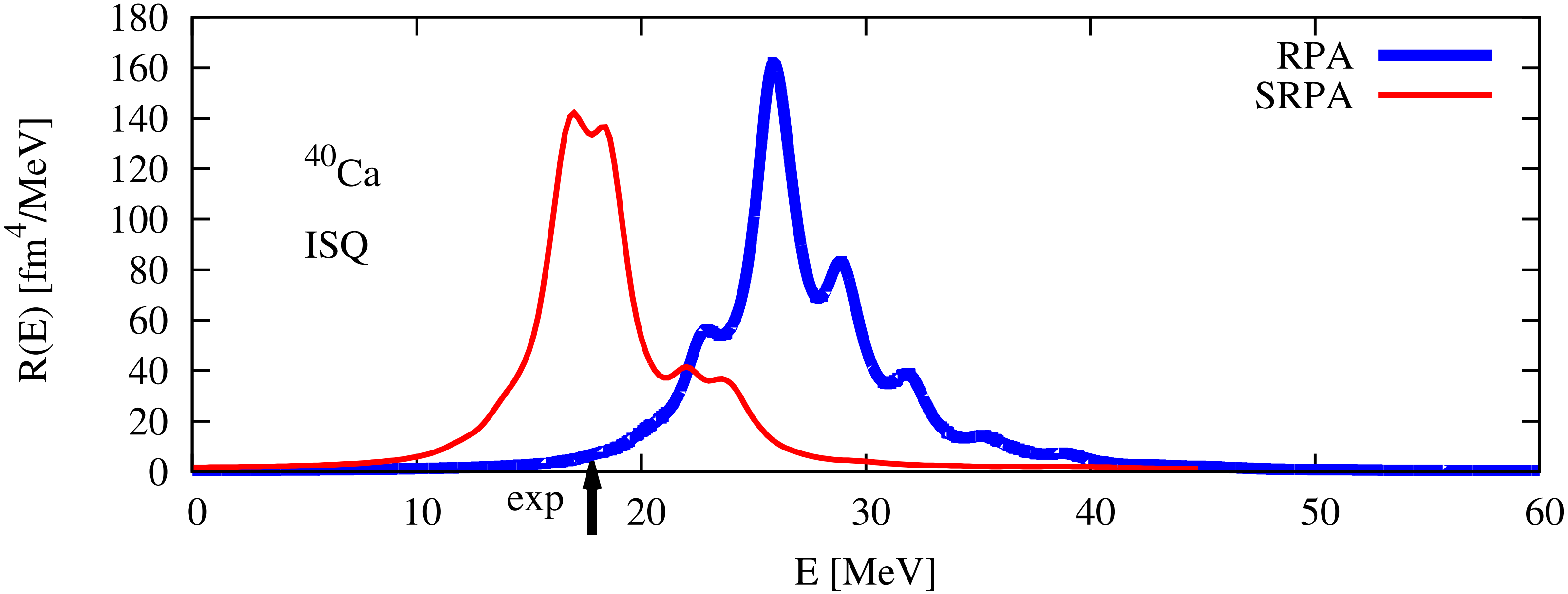


2
1.5
1
0.5
0
R(E) [fm²/MeV]
RPA
SRPA
40Ca
IVD
exp
0
10
20
30
40
50
60
E [MeV]

Second RPA

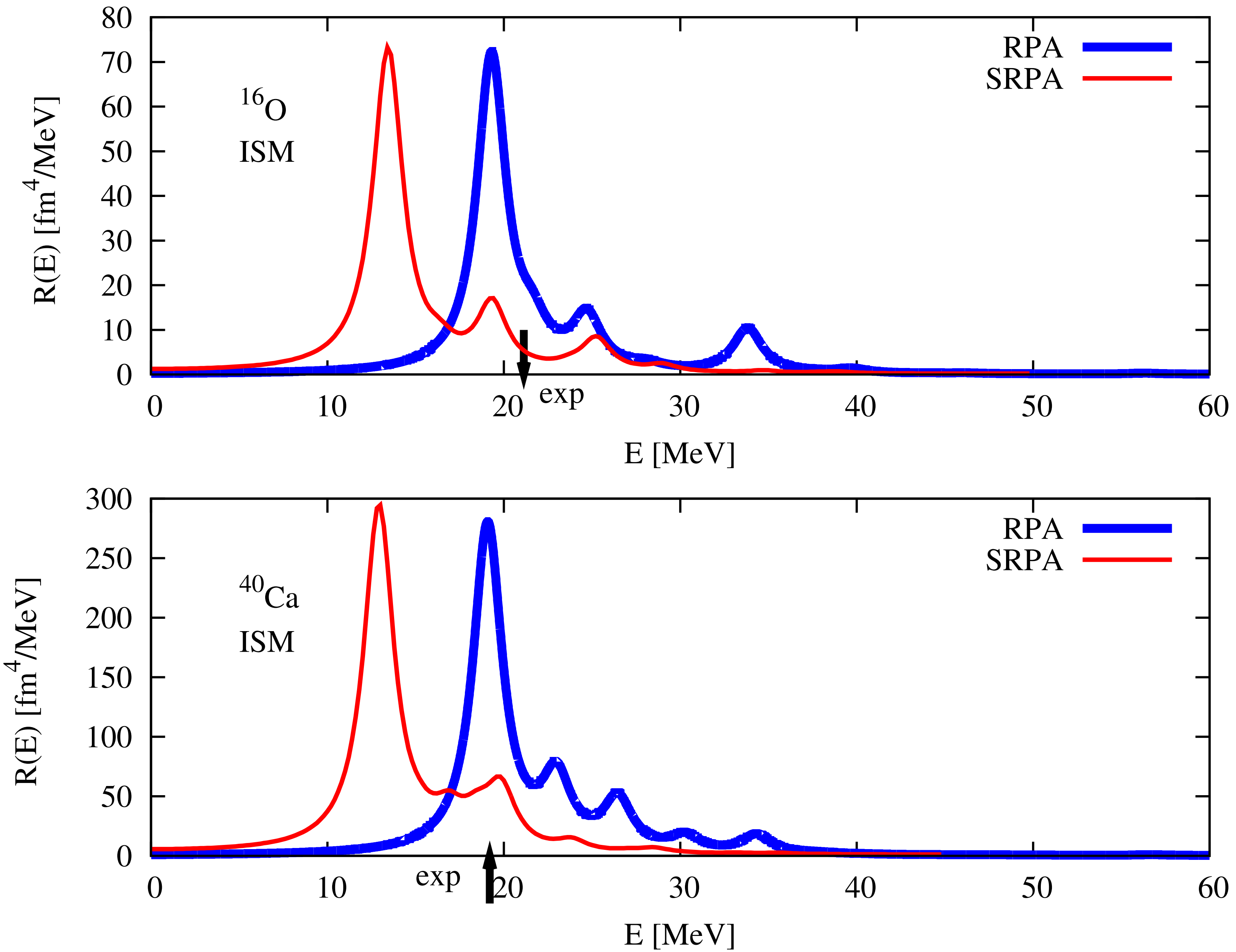


R(E) [fm^4/MeV]
E [MeV]
RPA
SRPA
16O
ISQ
exp



R(E) [fm^4/MeV]
E [MeV]
RPA
SRPA
40Ca
ISQ
exp

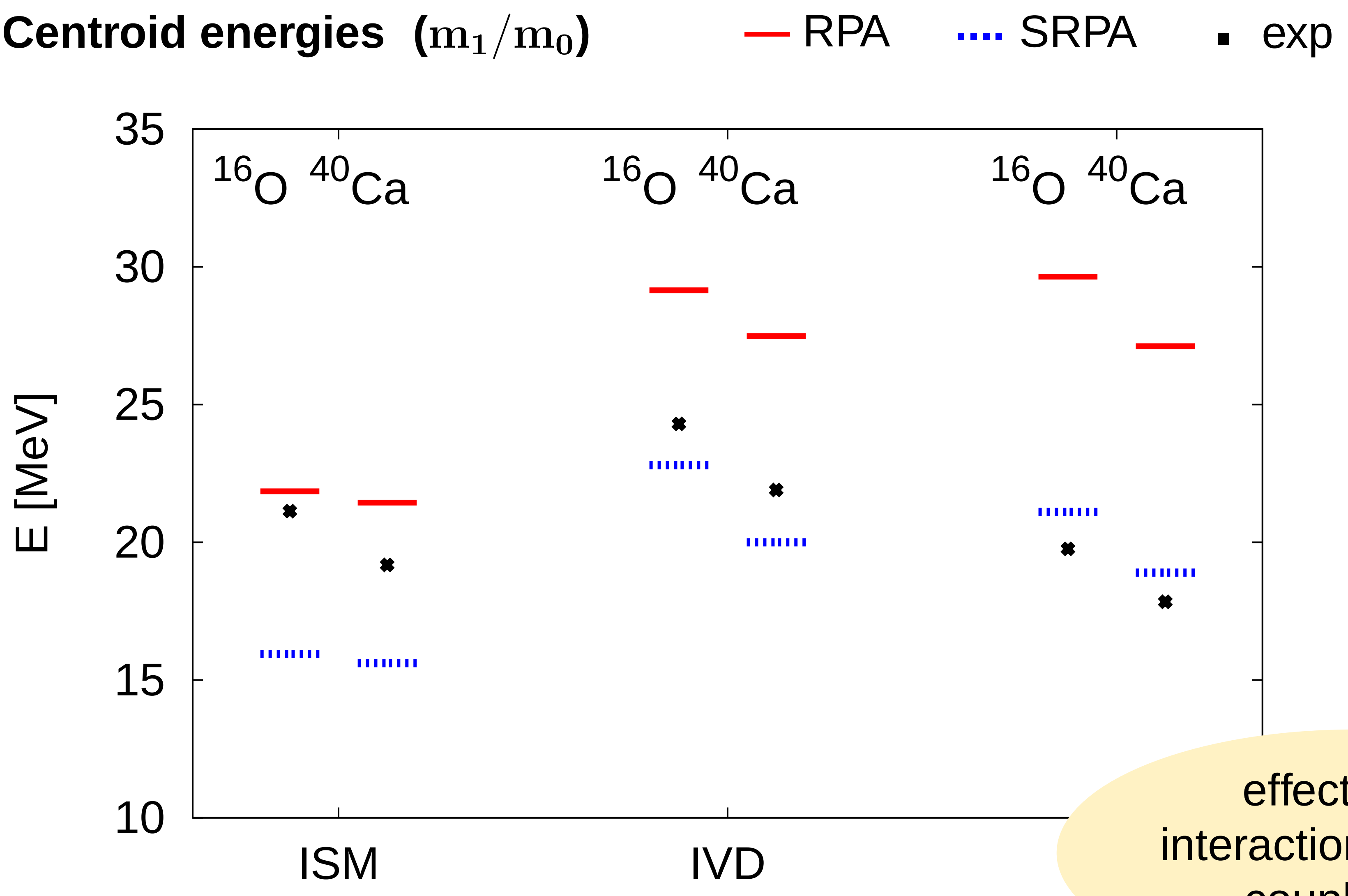
Second RPA



RPA
SRPA
^{16}O
ISM
exp
R(E) [fm^4/MeV]
E [MeV]
RPA
SRPA
^{40}Ca
ISM
exp
R(E) [fm^4/MeV]
E [MeV]

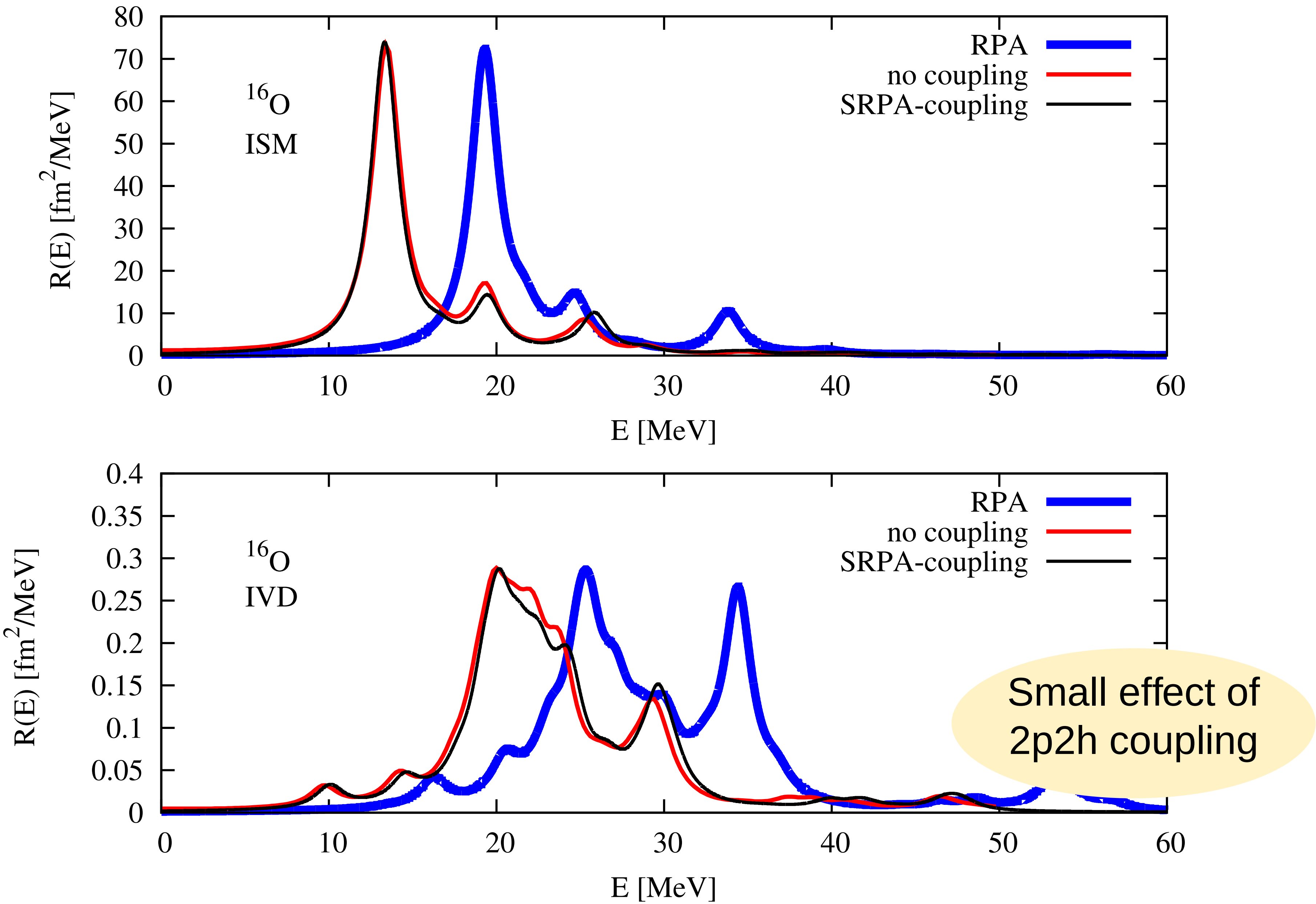
Second RPA

Centroid energies $(\mathbf{m_1/m_0})$

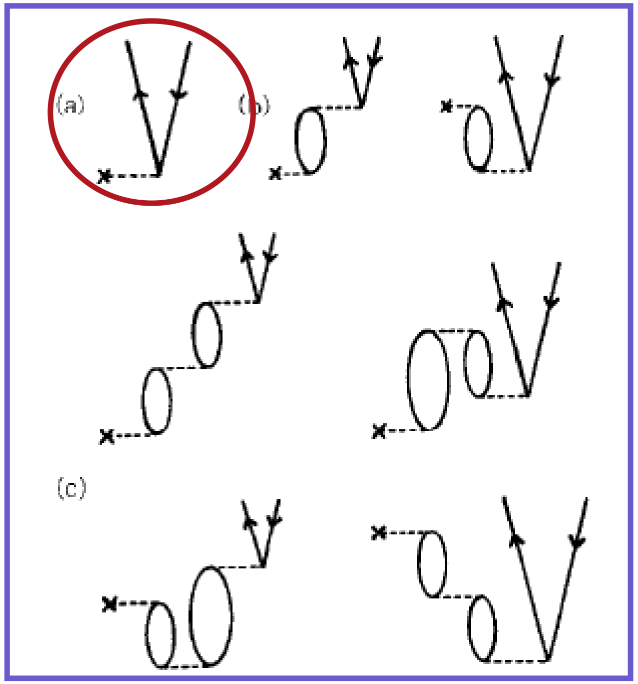


effect of 3b interactions? 2p-2h coupling??

Second RPA with 2p2h coupling

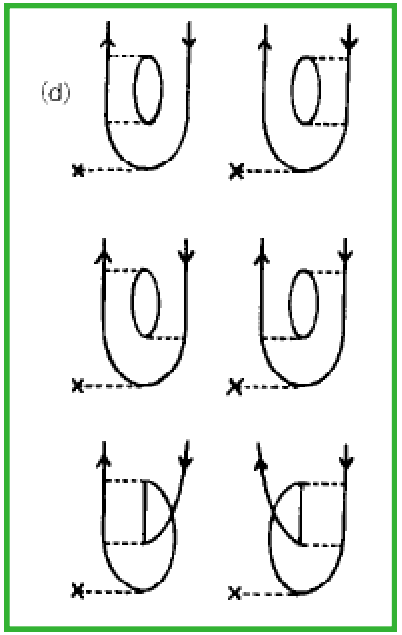


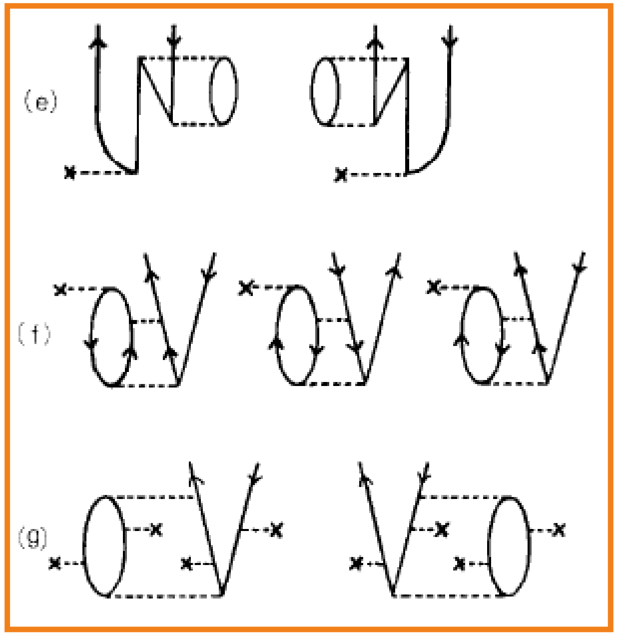
Second RPA – extensions?



RPA

SRPA





additional 2nd-order diagrams

Nucl.Phys.A477(88)205 etc

Summary

Use of V_{UCOM} in nuclear response
calculations across the nuclear chart:

- RPA: Properties of the V_{UCOM} as an effective interaction
  - Centroid energies overestimated (IVD, ISQ)
- Extended RPA: The role of RPA ground-state correlations
  - Weak effect on the properties of collective excitations
- SRPA: Sizable effect of coupling with 2p2h configurations
  - Important role of residual correlations
  - Discrepancies due to residual three body effects?

Second RPA – to consider

- Nuclei appear softer in Second RPA
  - Possibility to use a simple three-body force?
- Low-lying and other collective excitations
- Extensions of the SRPA?
  - Role of ground-state correlations in SRPA
  - Important missing diagrams?
  - Spurious states, sum rules...

Thank you!

Work in collaboration with:

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

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- N. Paar

  University of Zagreb, Croatia

- C. Barbieri, H. Feldmeier, T. Neff

  GSI, Darmstadt, Germany

Recent References

- P. Papakonstantinou, R. Roth, N.Paar, Phys. Rev. C**75**, 014310 (2007)
- N.Paar, P. Papakonstantinou, H.Hergert, R. Roth, Phys. Rev. C**74**, 014318 (2006)
- and many more: **http://crunch.ikp.physik.tu-darmstadt.de/tnp/**