RPA-based methods with realistic interactions: why and how

INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY

Panagiota Papakonstantinou

Atelier ESNT
``Linear response theory: from infinite matter to finite nuclei``
Saclay, 30/5-1/6/2012

>> Material mainly from:

...

PP, R.Roth, PLB 671 (09) 356

PP, R.Roth, PRC 81 (10) 024317

H.Hergert, PP, R.Roth (11) 064317

...

UCOM and SRG Hamiltonians based on AV18

in RPA, **SRPA, QRPA**

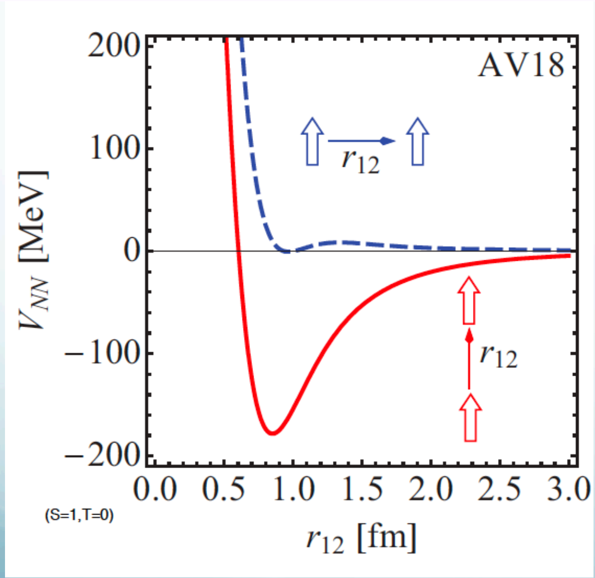
The NN interaction vs mean-field approaches

The NN interaction

- Short-range repulsion
- Tensor interaction
- ... but not evident in low-momentum nuclear phenomena

Mean-field approaches

- *Almost* independent particles + V_{res}
- Shell model, Hartree-Fock, RPA, ...
- E/A, $\varepsilon_i \approx \varepsilon_F$, $\langle r^2 \rangle$, bulk properties of GRs, ...



Effective interactions, functionals

- Phenomenological fits...
- ... Or derived from realistic interactions

→Unitary transformations

Unitarily transformed interactions

- **UCOM$_{var}$**
  - Correlation functions determined variationally
  - Two-body only; already used in many applications
- **SRG**
  - Transformation to diagonal form in a given basis (here KE, momentum)
  - All or only the S-waves transformed; +**3N term**
- **UCOM(SRG)**
  - Correlation functions determined by SRG
  - All or only the S-waves transformed; +**3N term**
- **3N term**: simple phenomenological contact term
  - To reproduce energy and radii in PT

A.Guenther et al., PRC82, 024319

Roth,Hergert,PP,Neff,Feldmeier,PRC72,034002
Roth,PP,Paar,Hergert,Neff,Feldmeier,PRC73,044312
Paar,PP,Hergert,Roth,PRC74,014318,
PP,Roth,Paar,PRC75,014310
PP,Roth,PLB671,356
PP,Roth,PRC81,024317
Hergert,PP,Roth,PRC83,064317
++
++

Review:
Roth,Neff,Feldmeier,
Prog.Part.Nucl.Phys.
65,50 (2010)

Argonne V18 transformed and used here

Unitary correlation operator method

- Explicit correlations by means of unitary operators imprinted in the wavefunction or the operators

$$|\tilde{\Psi}\rangle = C_\Omega C_r|\Psi\rangle = U|\Psi\rangle$$

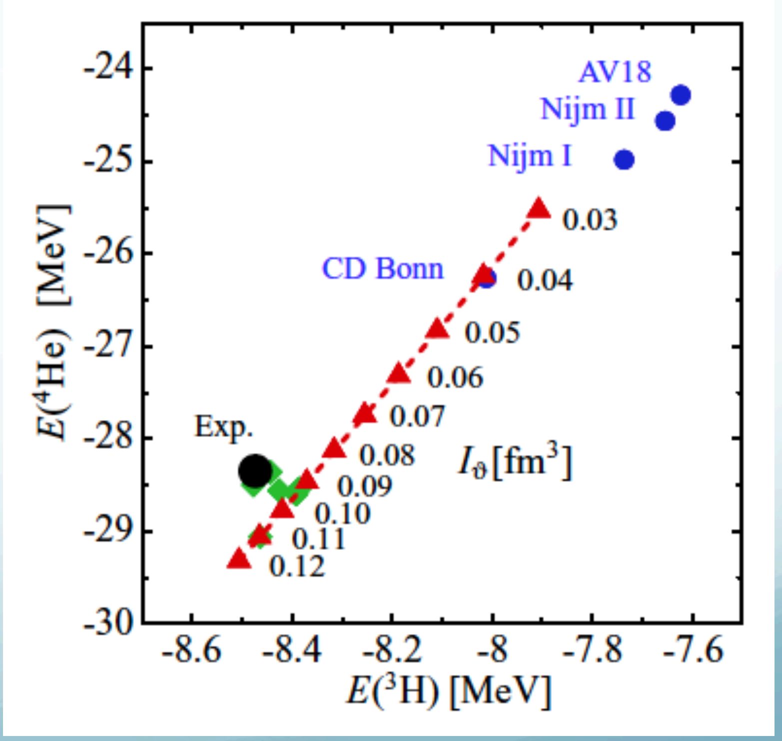
$$\tilde{A} = U^{-1}AU = U^\dagger AU$$

➔ $$\langle\tilde{\Psi}|A|\tilde{\Psi}\rangle = \langle\Psi|\tilde{A}|\Psi\rangle$$

- A : e.g. Hamiltonian ➔ H_{eff}
- U determined variationally

In practice: truncate at 2N nucleon level and adjust range of tensor correlator using exact calculations

➔ One parameter



Similarity renormalization group

- Flow equations $$\frac{d\tilde{A}_\alpha}{d\alpha} = [\eta_\alpha, \tilde{A}_\alpha]$$
- Towards diagonal Hamiltonian in momentum space: KE as generator

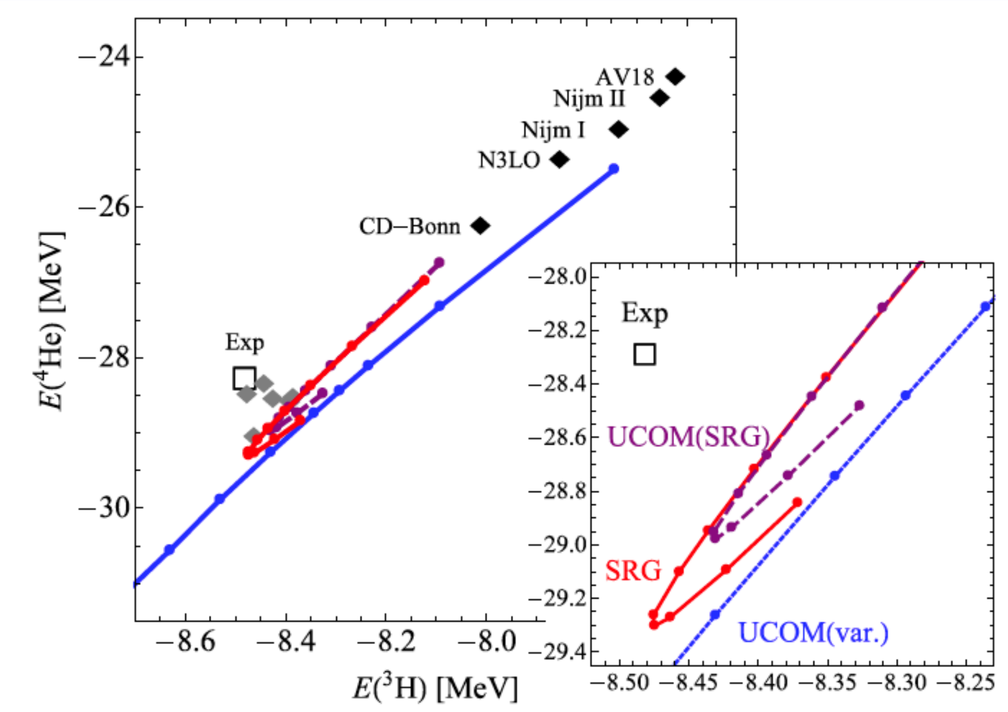
$$\eta_\alpha = (2\mu)^2 [T_{\rm int}, \tilde{H}_\alpha]$$

- Also unitary transformation $$\tilde{A}_\alpha = U_\alpha^\dagger A U_\alpha$$

In practice: again truncate at 2N nucleon level; adjust flow parameter, e.g. using exact calculations; possibly 3N force for saturation

one -> two parameters

Tjon line - comparison

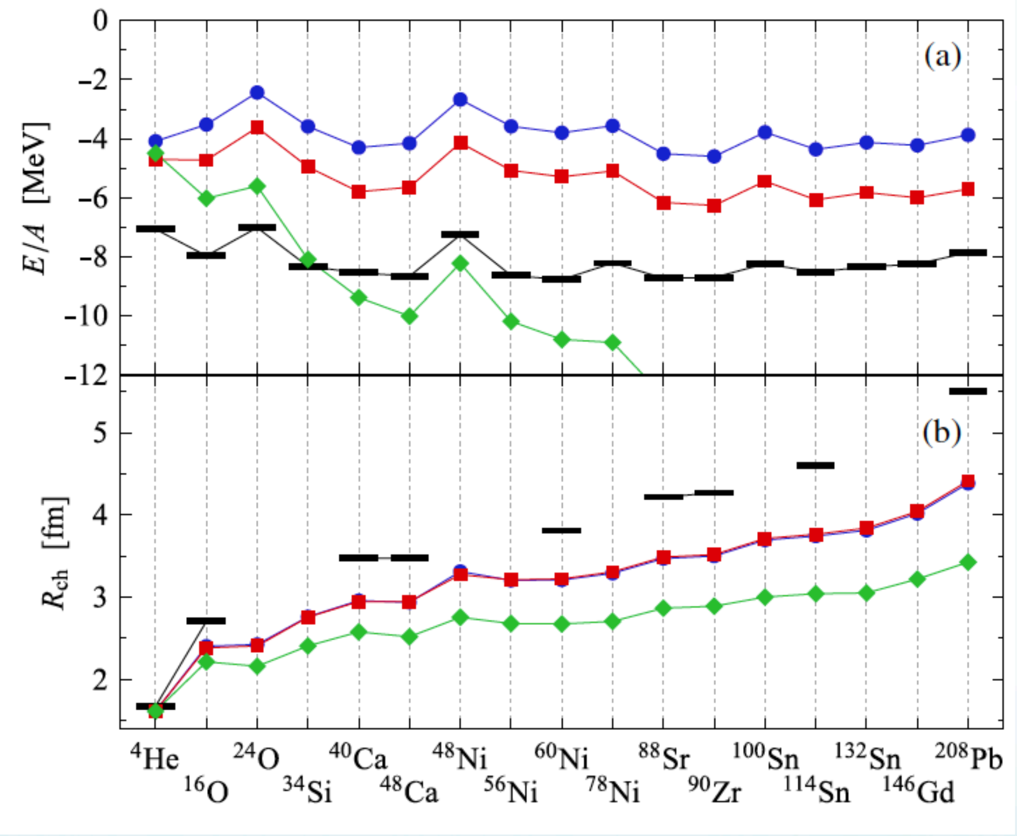


UCOM(var.): $I_\vartheta = 0.09\ \text{fm}^3$

UCOM(SRG): $\alpha = 0.04\ \text{fm}^4$

SRG: $\alpha = 0.03\ \text{fm}^4$.

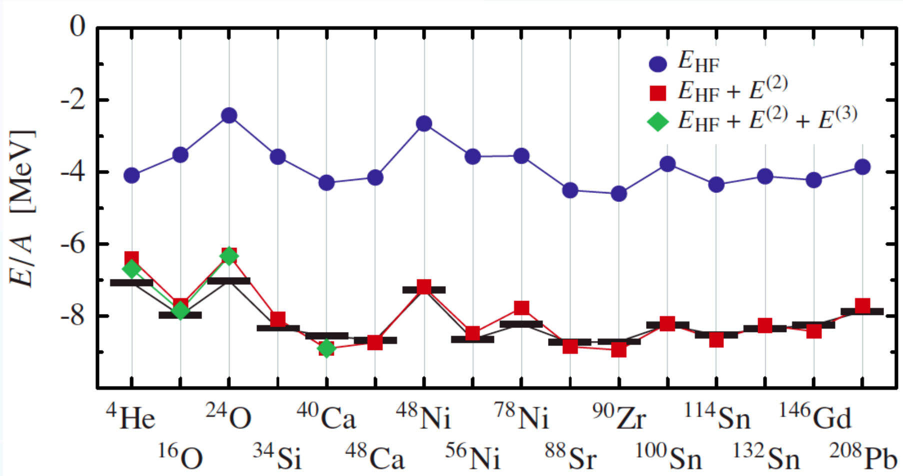
Hartree-Fock - comparison

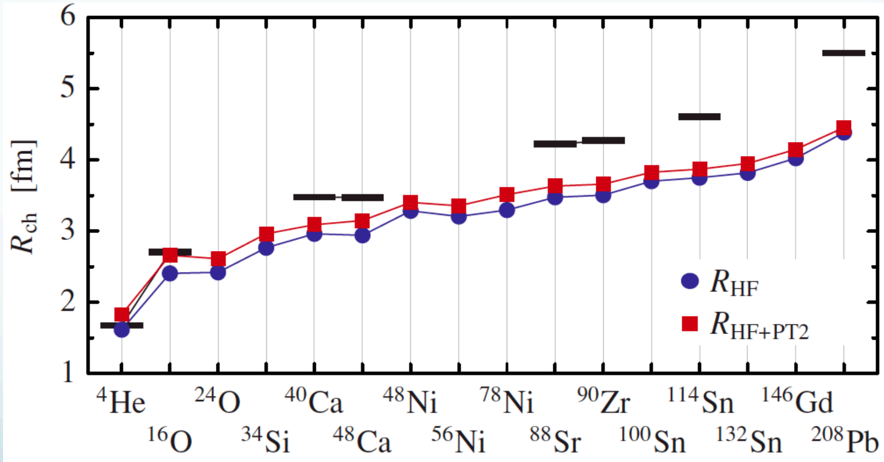


to UCOM(var.) interaction (●), the UCOM(SRG) interaction (■), and the SRG interaction (♦).

Ground-state properties with UCOM

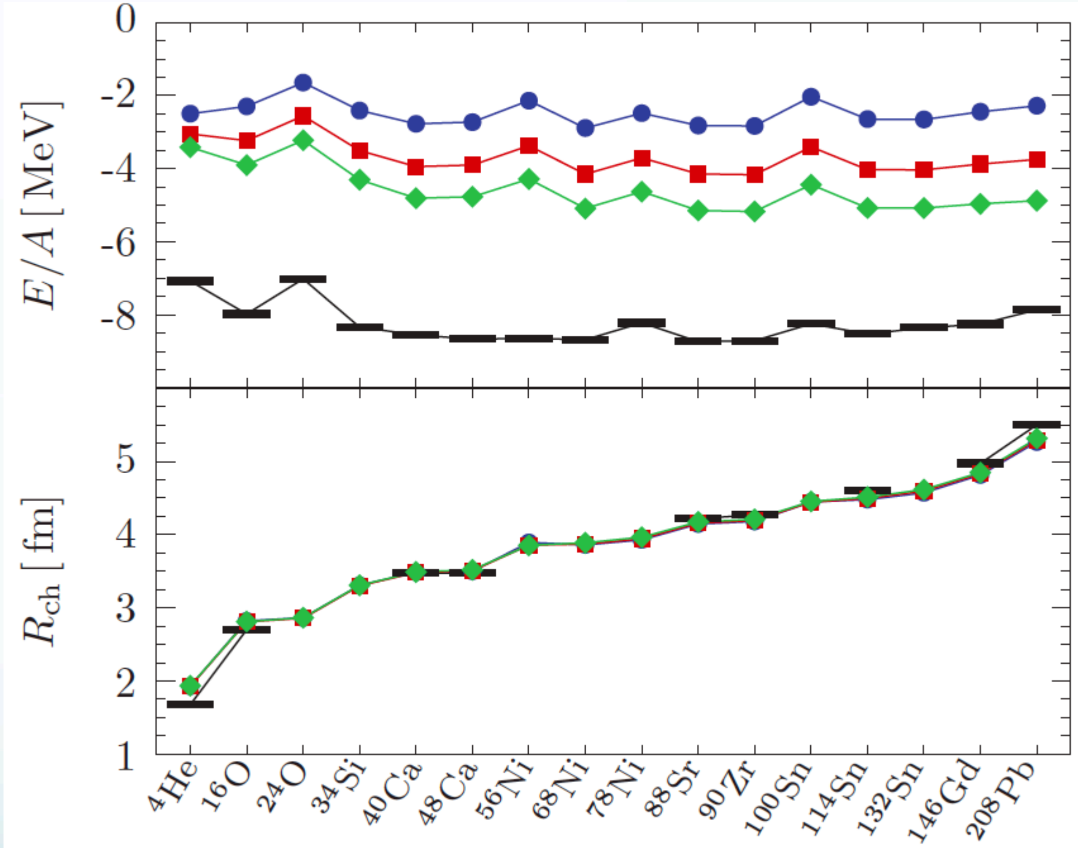
- Good energies within perturbation theory
- Small radii
- Single-particle HF spectra: large spacings
- Low efective mass, ...





Ground-state properties with SRG+DDI

- Quality of total energies as with UCOM (good within PT).
- Good radii with the help of the DDI
- Single-particle spectra compressed thanks to DDI



(λ fm($^{-1}$), C_{3N} (GeV fm^6)) = (2.40, 2.94) (●), (2.02, 3.87) (■), and (1.78, 4.41) (♦).

$\lambda = \alpha^{-4}$

This talk...

- A transformed Argonne V18 interaction is used

  Realistic to the 2-body level

- **UCOM + SRPA**

  successes and limitations with a two-body realistic interaction; what we learned from the first « self-consistent » applications of standard SRPA in nuclei

- **SRG + QRPA**

  further prospects with three-body terms

- Lessons to and from phenomenology (?), Outlook

UCOM-SRPA

-

Large-scale, « self-consistent » Second RPA

- **Original SRPA applications**:
  - Phenomenological s.p. energies and residual interaction
  - A few (relatively speaking…) 2p2h configurations in the vicinity of a resonance
- **Nowadays possible**:
  - Large-scale:
    - Choose a s.p. space large enough for convergence (eg 12 HO shells) – solve HF
    - Include all ph and 2p2h configurations available
  - « Self-consistent »
    - 2B interaction sole input
    - No conceptual problems, if input has not been fitted to RPA

SRPA - formalism

- 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:

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

- 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

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

Solving SRPA

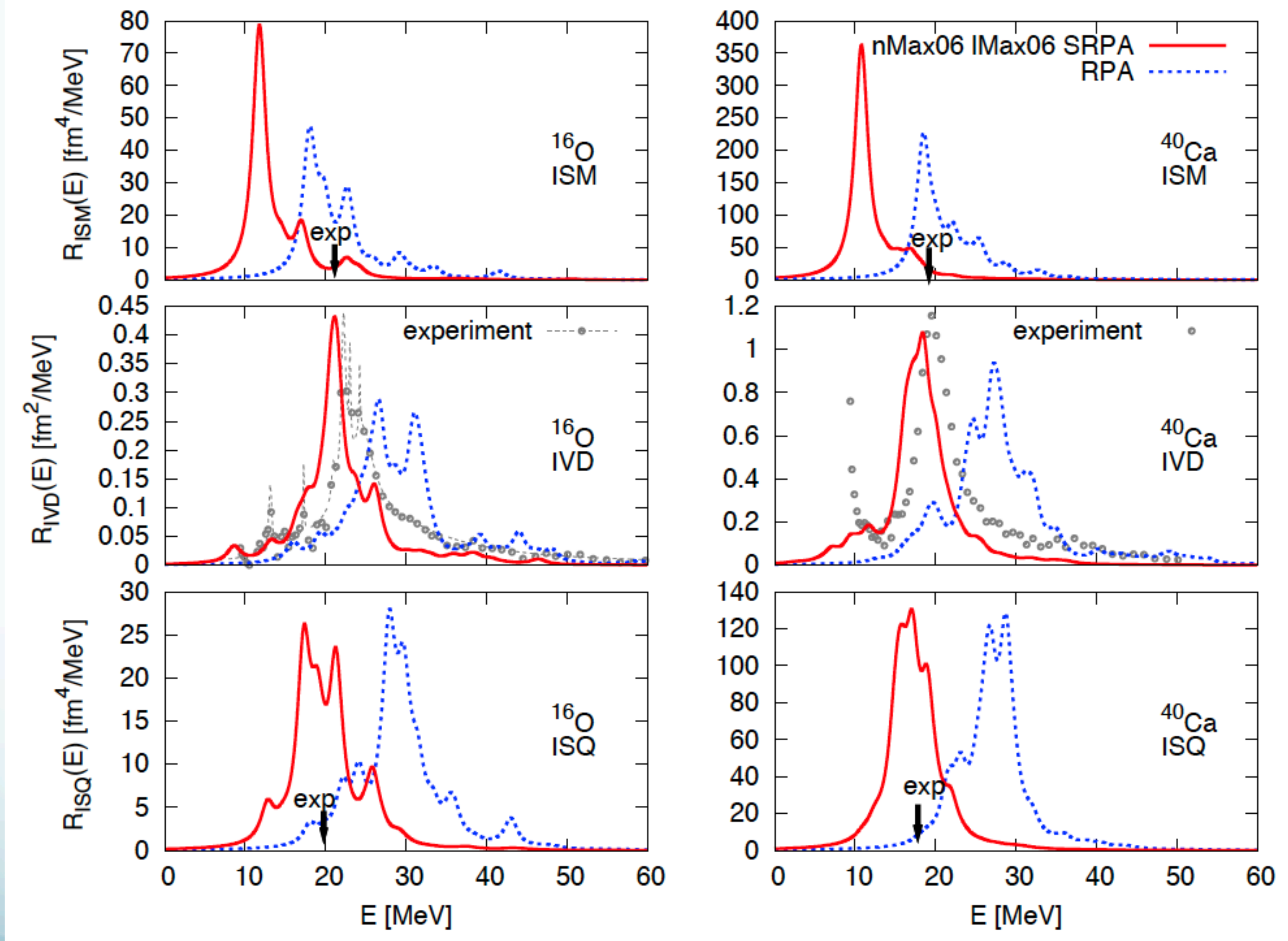
- Large model spaces:
  - Number of states up to $\approx 10^6$ for the present cases – can get larger
  - But 1) SRPA matrix is sparse and
    2)reduction to half the size is always possible *[PP, EPL78,12001]*
- Use Lanczos
  - Find only the lowest eigenvalues $|\epsilon_\nu|$
  - ... or the ones closest to a set value E_0, e.g.

$$\mathrm{HX}_\nu = \epsilon_\nu \mathrm{X}_\nu \iff \mathrm{H}'\mathrm{X}_\nu = \epsilon'_\nu \mathrm{X}_\nu \ , \quad \left\{ \begin{array}{l} \mathrm{H}' \equiv \mathrm{H} - E_0 \mathrm{I} \\ \epsilon'_\nu \equiv \epsilon_\nu - E_0 \end{array} \right\}$$

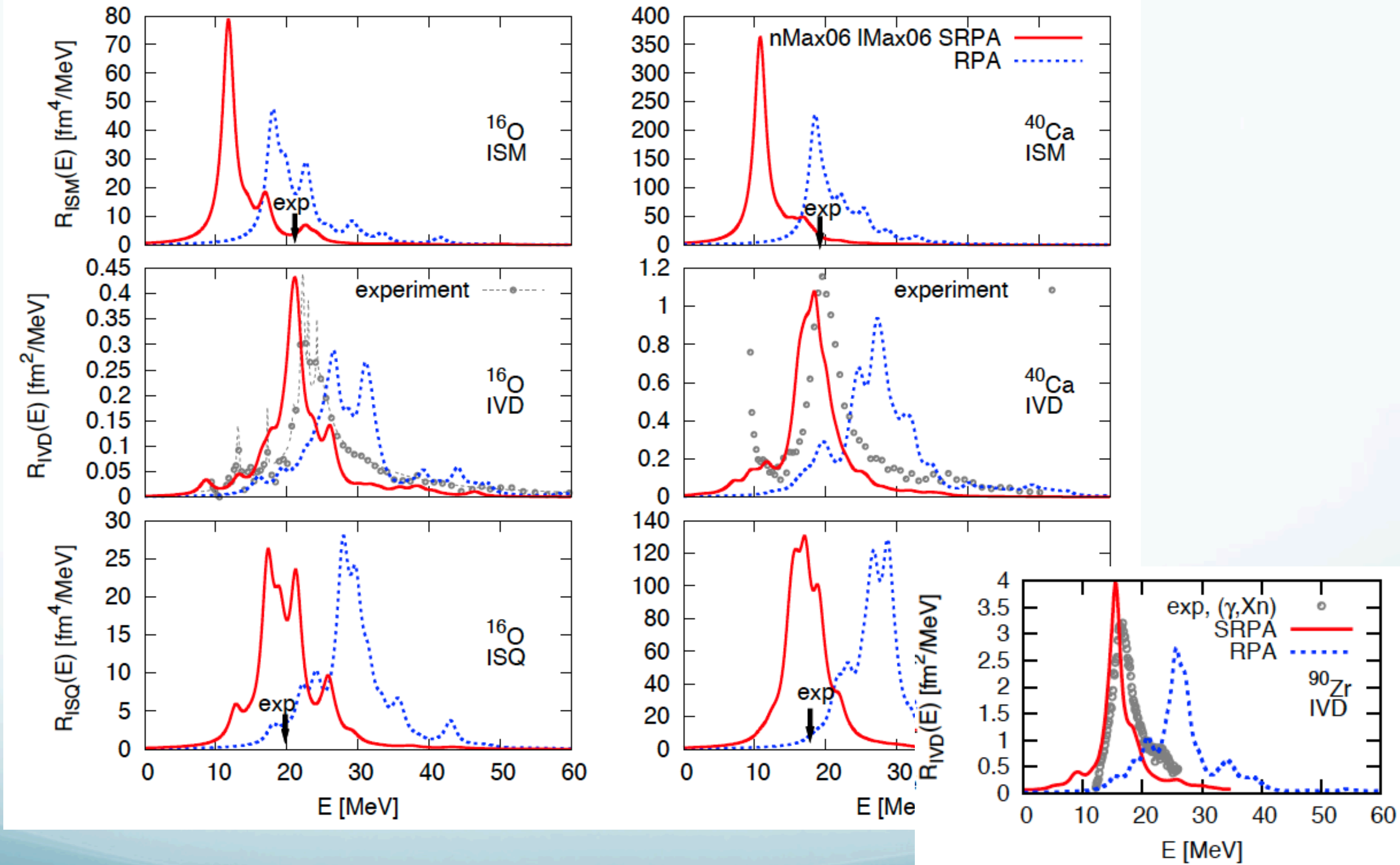
- Alternatively, reduce to an $\omega-$dependent problem of RPA size
  - ... especially if you ignore interactions within 2p2h space:

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

UCOM:: RPA and SRPA

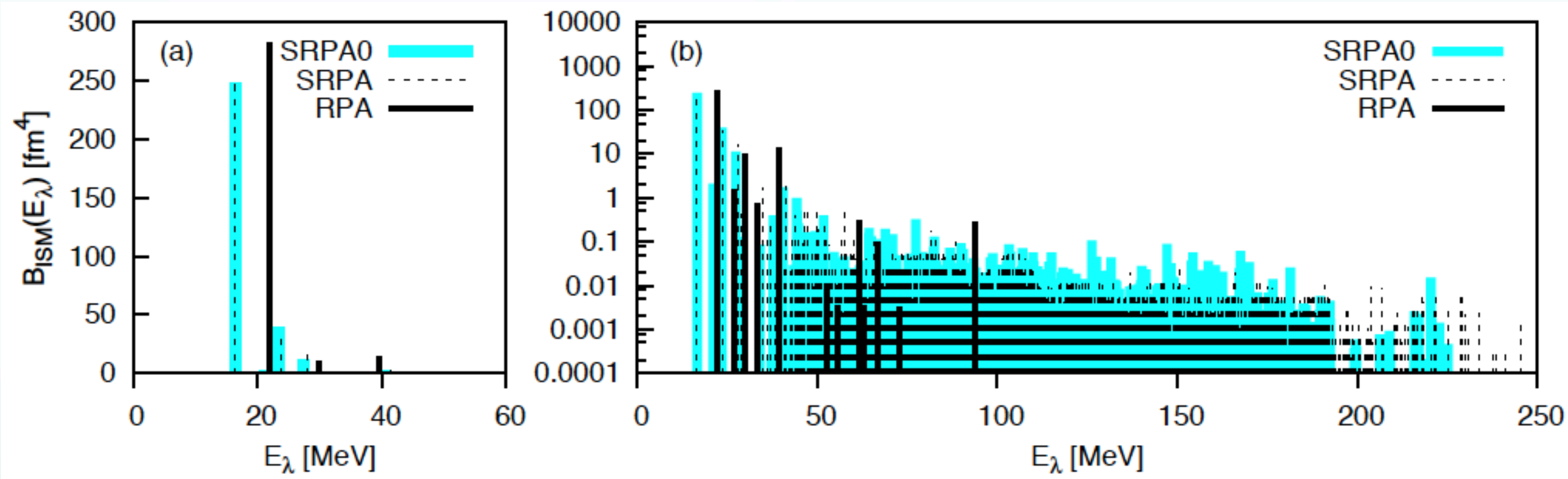


UCOM:: RPA and SRPA



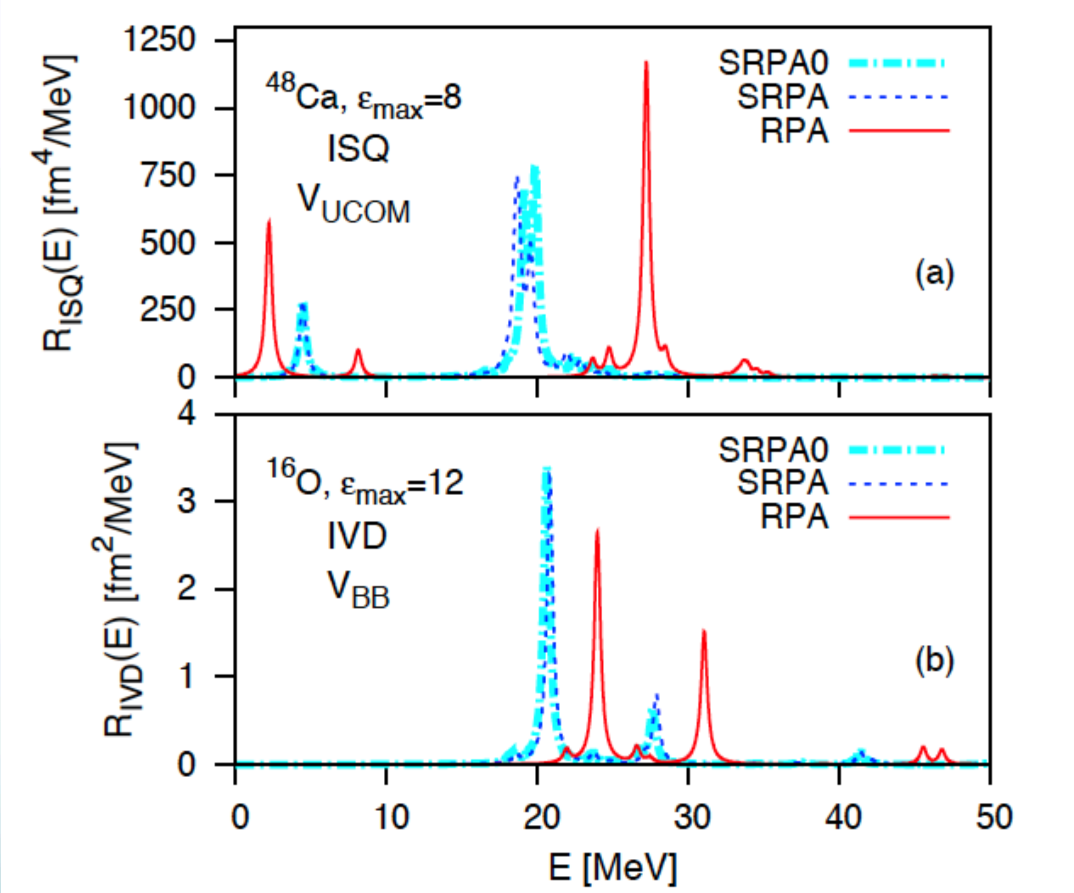
SRPA eigenstates

SRPA and its diagonal approximation vs RPA:

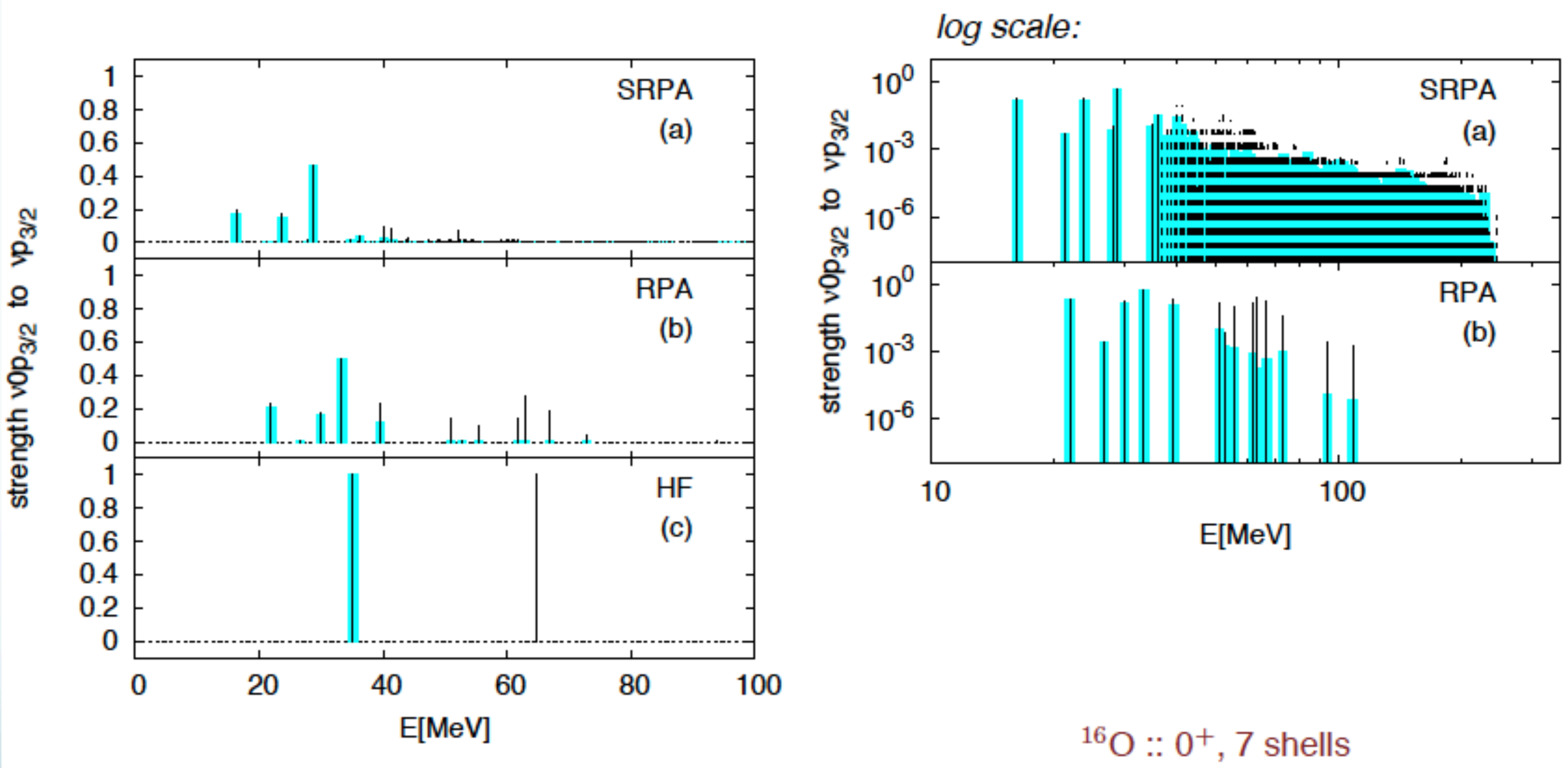


16O with UCOM-AV18 in 7 shells

Diagonal approximation

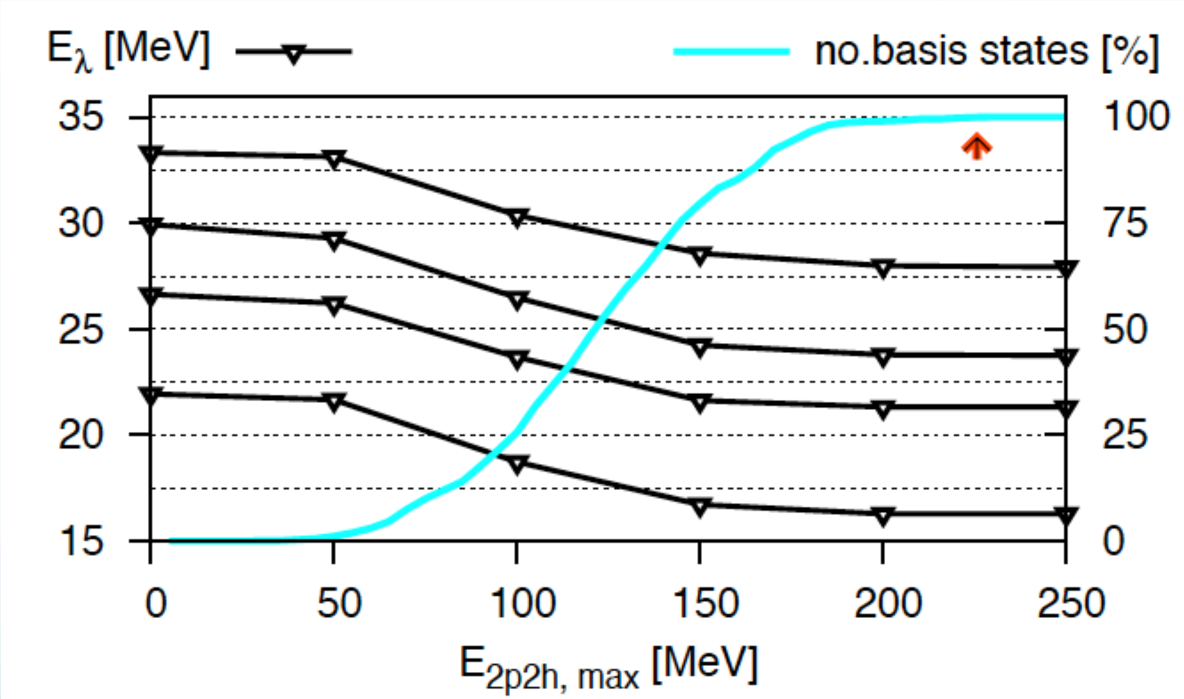


Fragmentation of ph states



^{16}O :: 0^{+}, 7 shells

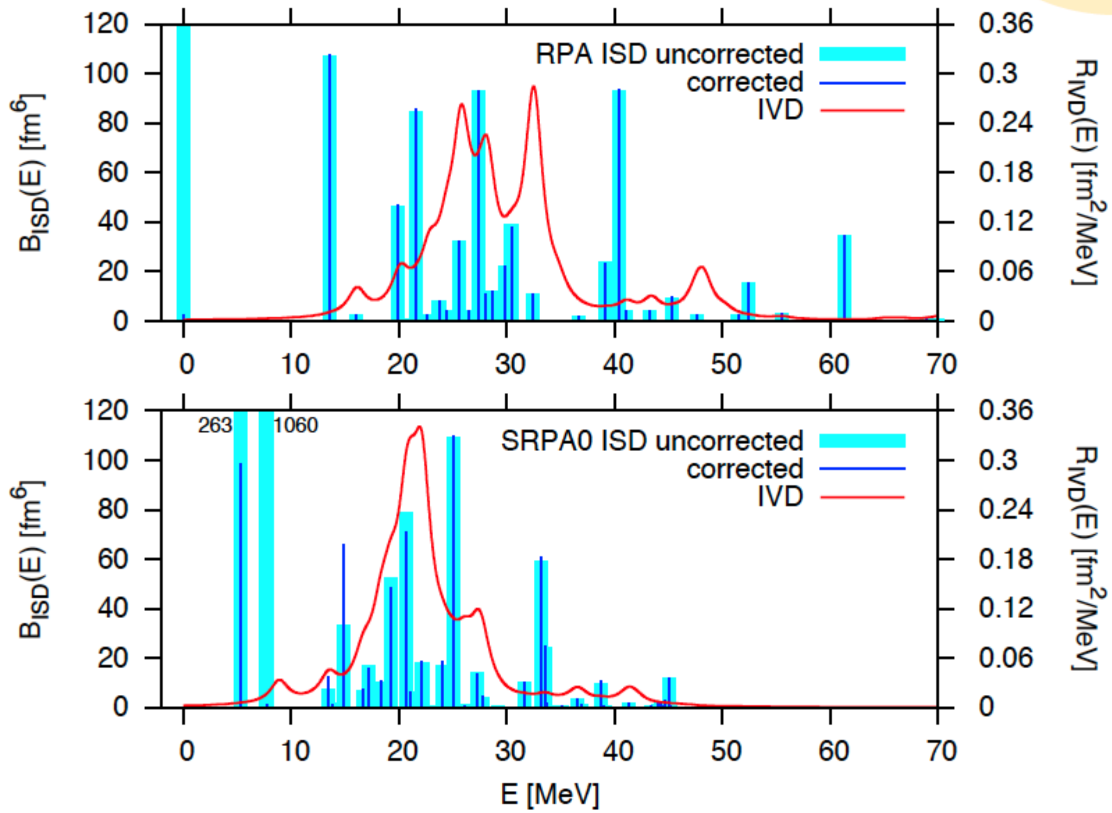
Truncation in 2p2h energy



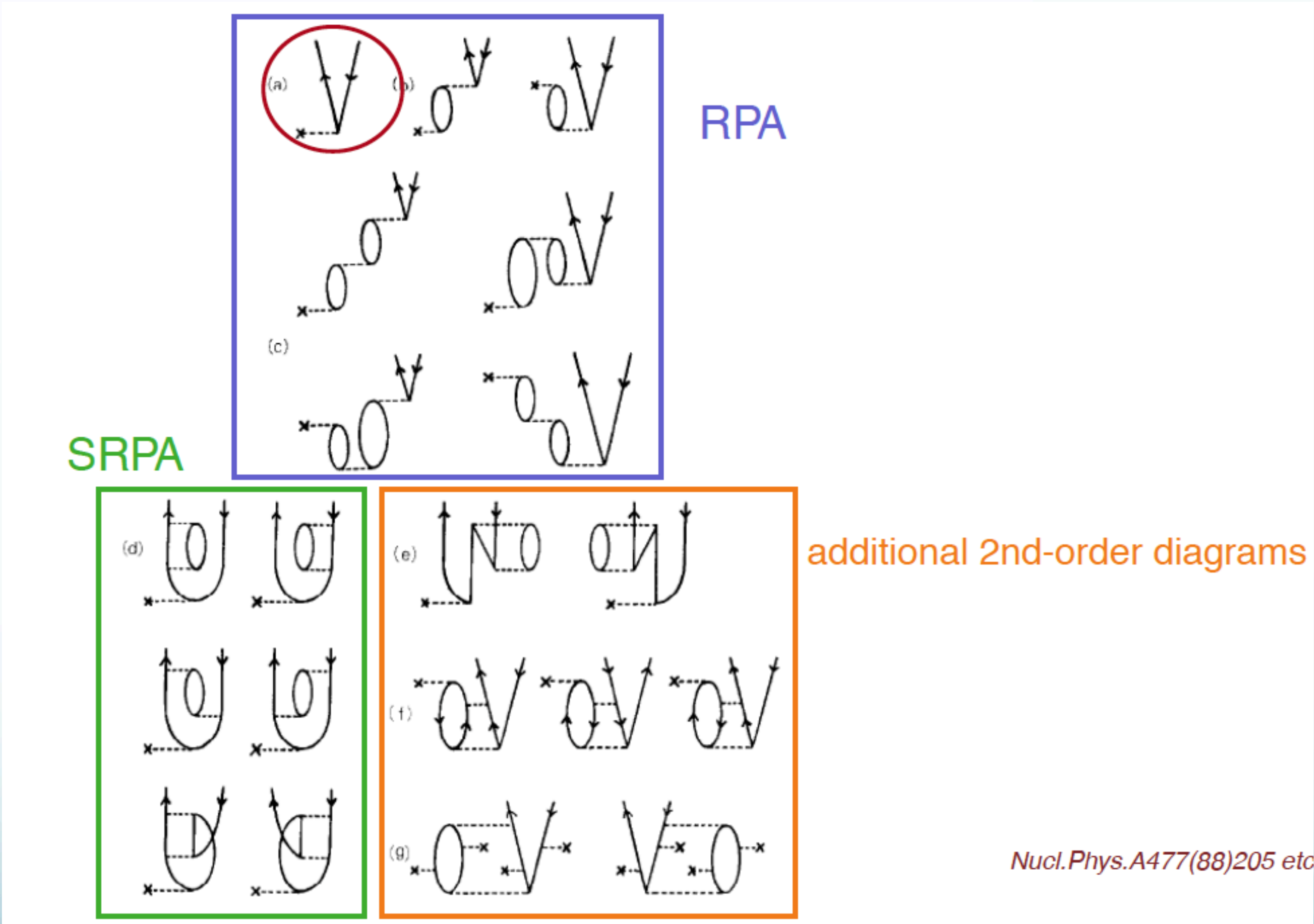
Spurious states

ISD corrected radial operator $r^3 - \frac{5}{3}\langle r^2 \rangle r$ vs r^3

^{16}O
$N_{\max} = 12$

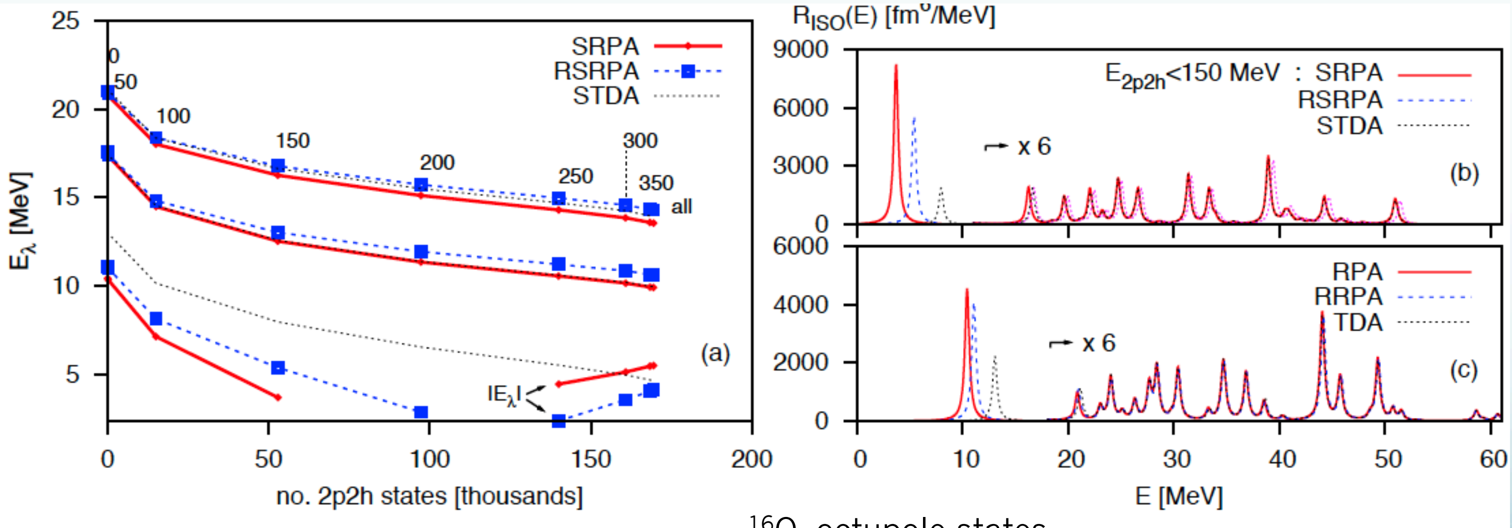


RPA, SRPA, and extensions



Role of ground-state correlations

- Use a more consistent second-order framework
- For the moment, possible tests:
  - Ignore SRC altogether -- TDA, STDA (B=0) or
  - Renormalize matrix elements using occ. probabilities from eg the shell model



^{16}O, octupole states

SRPA with UCOM

- A « self consistent » application - though formalism inconsistent
- No conceptual problems: finite range, not fitted at RPA level
- Promising for very collective vibrations
  - extended model space compensating for « low effective mass »
  - Quenching mechanism, ...
- Instabilities at low energies

(Q)RPA with SRG+DDI

Ground states of Ca isotopes

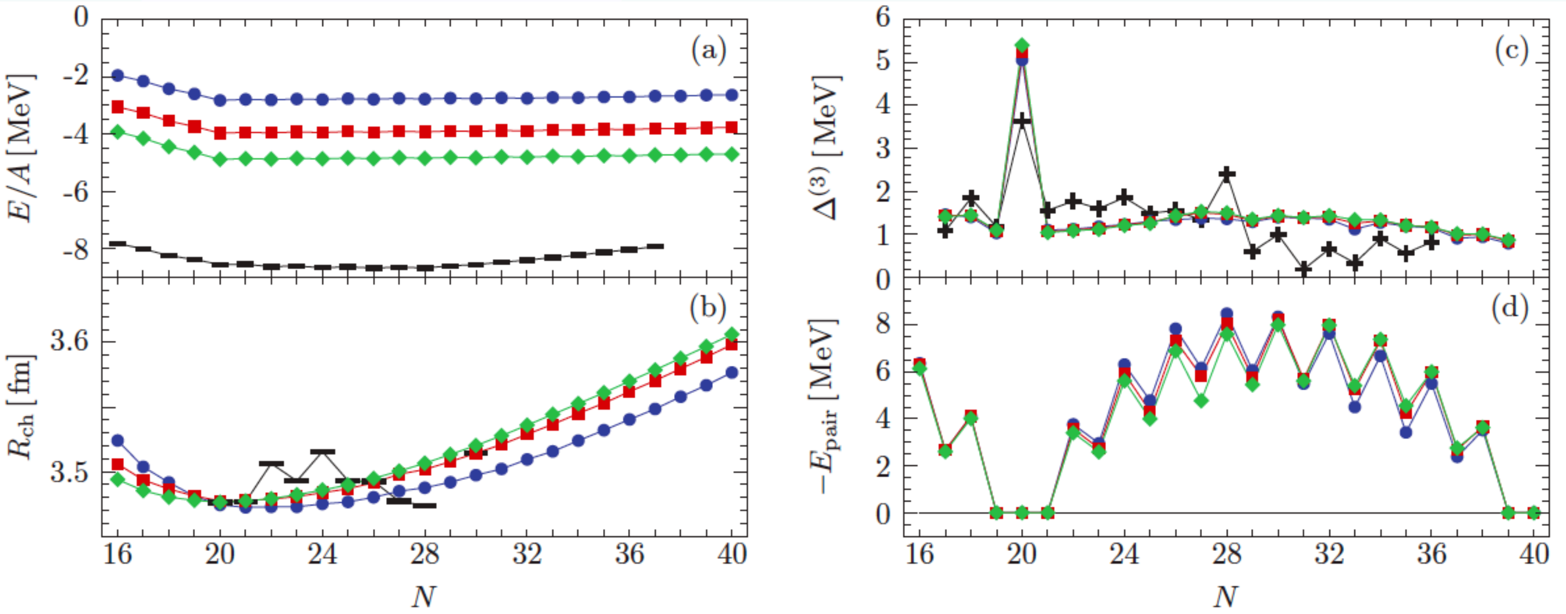


FIG. 4. (Color online) Ground-state properties of the calcium isotopes for V_{SRG}+DDI with (λ (fm^{-1}), C_{3N} (GeV fm^6)) = (2.40, 2.94) (●), (2.02, 3.87) (■), and (1.78, 4.41) (♦): (a) ground-state energies per nucleon, (b) charge radii, (c) odd-even mass differences, and (d) pairing energies. Experimental values [34,35] are indicated by black bars or crosses.

Sensitivity of results – RPA examples

Flow parameter

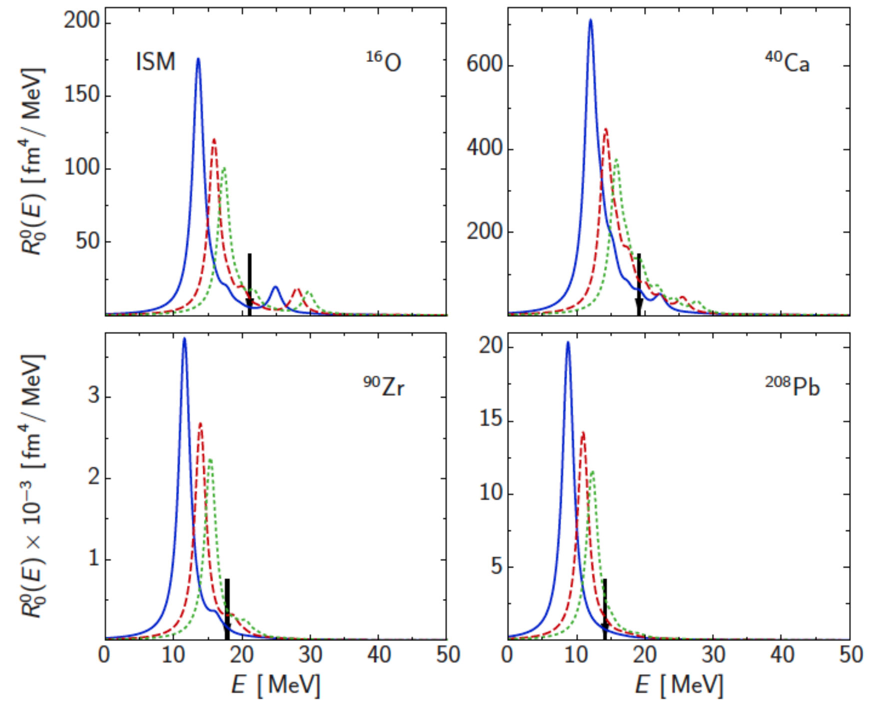


Figure 7.6: Same as in Figure 7.5 for the S-SRG interaction with $C_{3N} = 2.0\,\text{GeV fm}^6$, $e_{max} = 10$, and (——) $\alpha = 0.03\,\text{fm}^4$, (– – –) $\alpha = 0.06\,\text{fm}^4$, (······) $\alpha = 0.10\,\text{fm}^4$.

3N strength

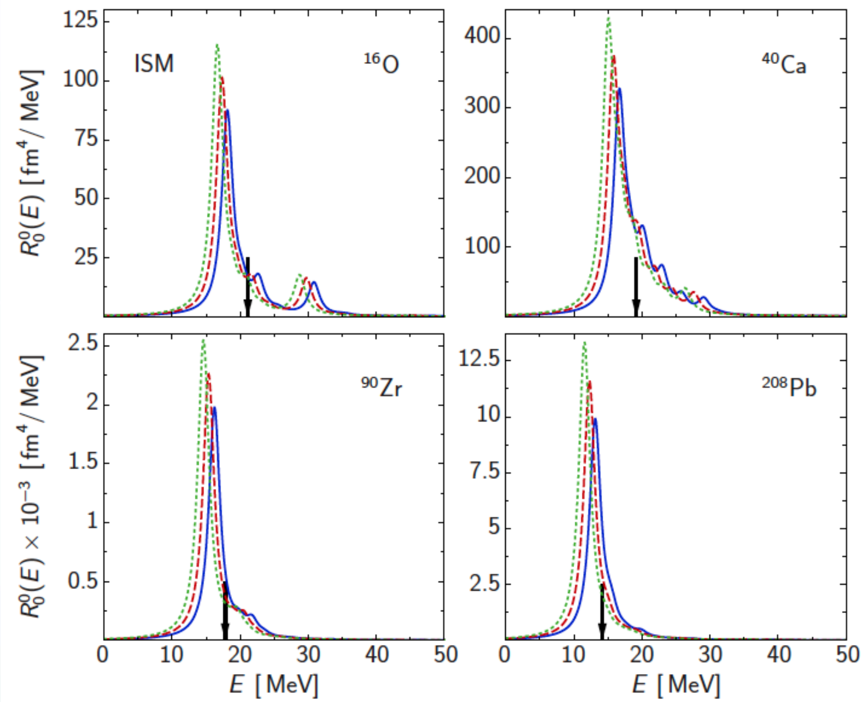
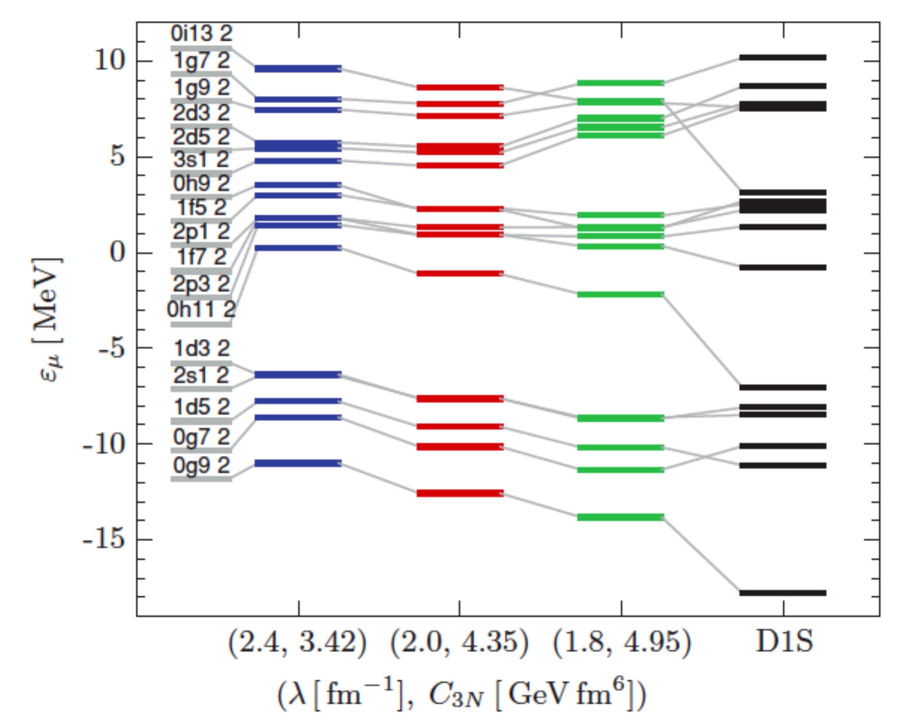


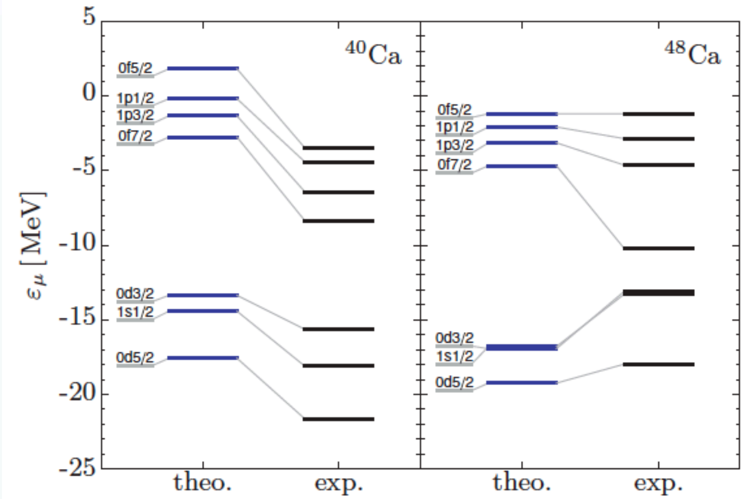
Figure 7.4: Same as in Figure 7.3 for the S-SRG interaction with $\alpha = 0.10\,\text{fm}^4$, $e_{max} = 10$, and (——) $C_{3N} = 1.5\,\text{GeV fm}^6$, (– – –) $C_{3N} = 2.0\,\text{GeV fm}^6$, (······) $C_{3N} = 2.5\,\text{GeV fm}^6$.

A.Guenther, Ph.D. Thesis (TUD,2011)

Single-particle spectra, spin-orbit splittings

^{120}Sn





(2.02,3.9)

$$\lambda = \alpha^{-4}$$

Sum rules

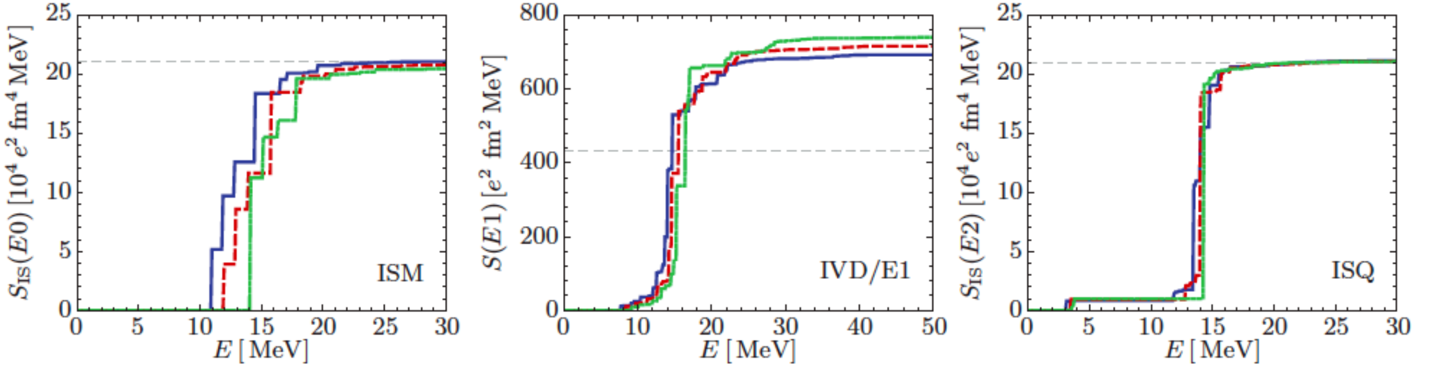
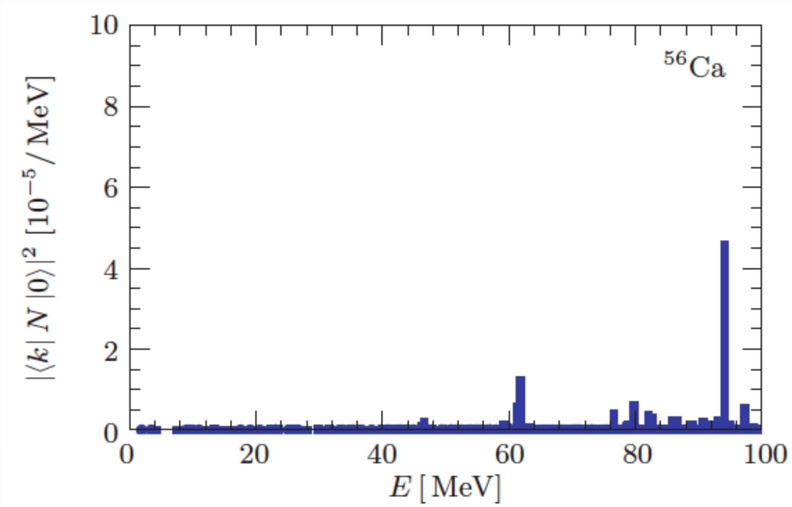
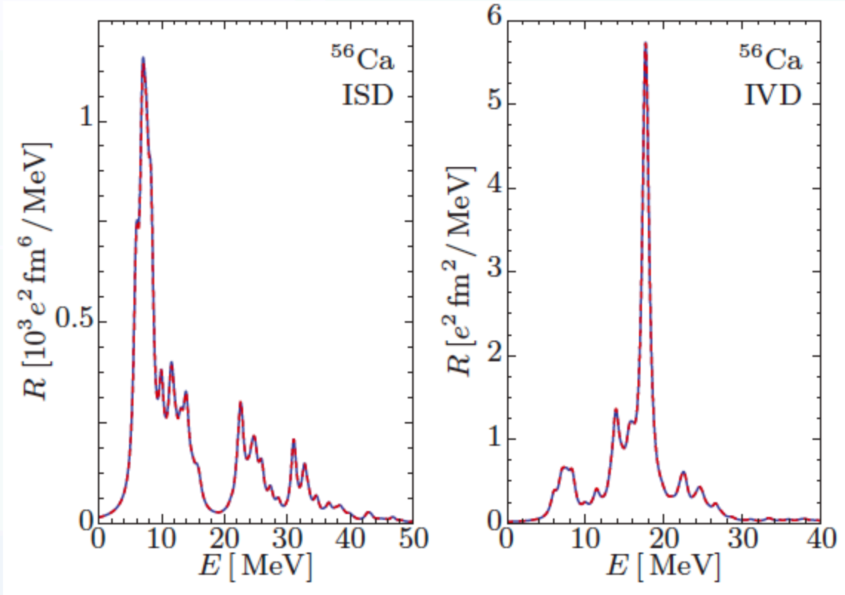


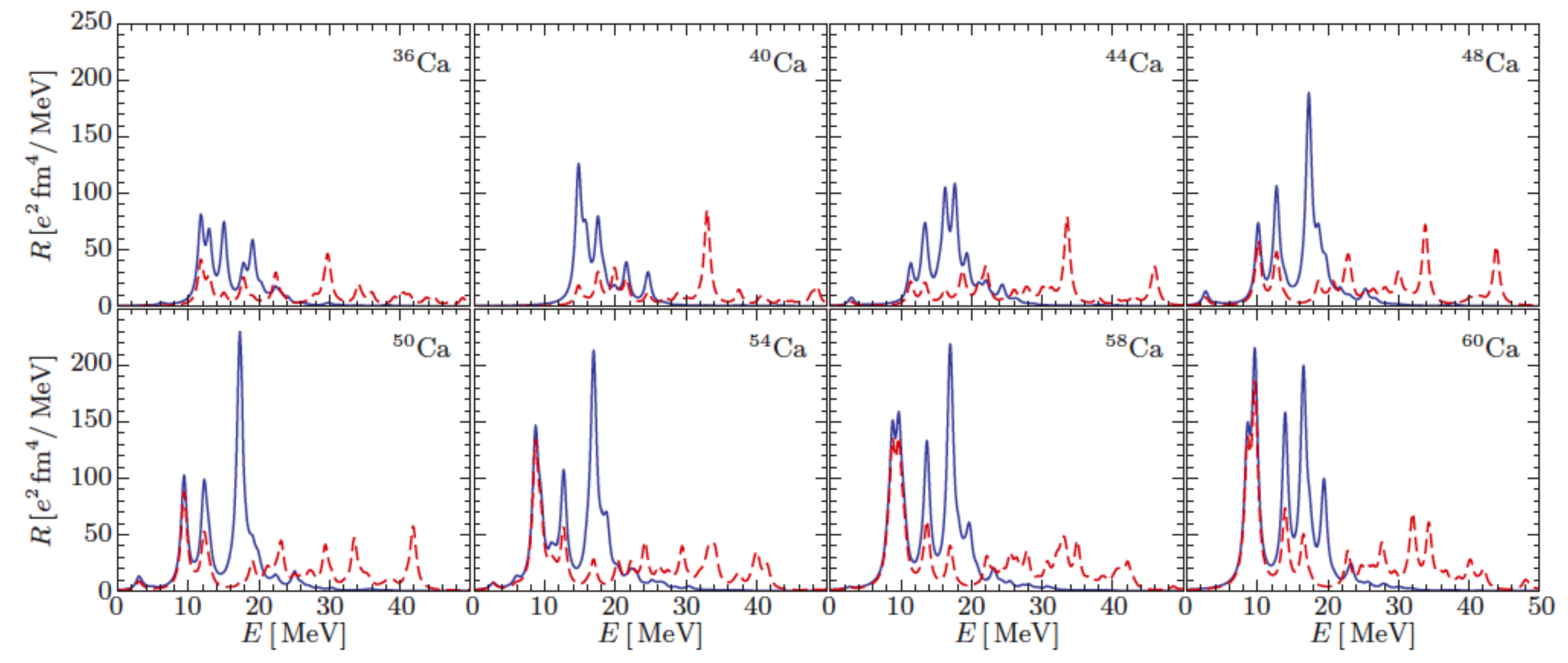
FIG. 7. (Color online) Running energy-weighted sums of ^{120}Sn for V_{SRG}+DDI with (λ (fm^{-1}), C_{3N} (GeV fm^6)) = (2.40, 3.42) (——), (2.02, 4.35) (– – –), and (1.78, 4.95) (......). The light gray dashed lines indicate the values of the classical sum rules (see text).

Spurious states



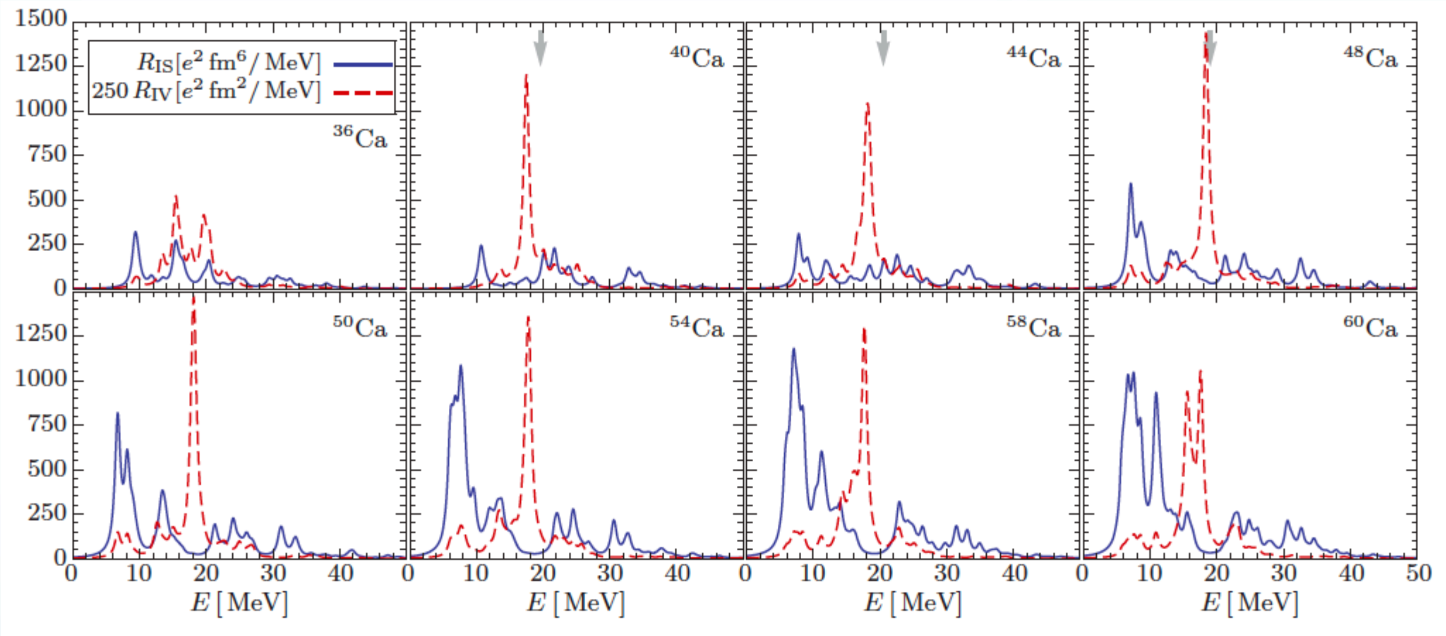


Monopole response

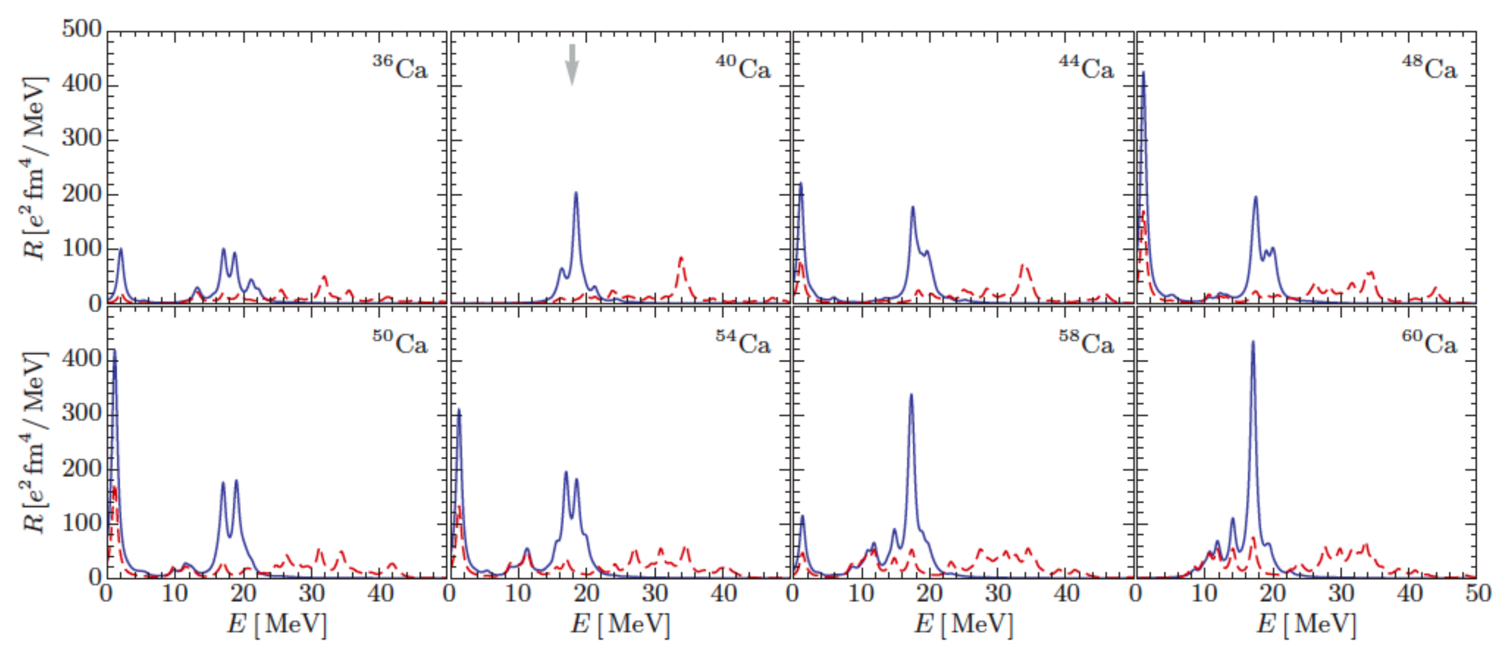


IS **IV**

Dipole response



Quadrupole response



Some questions, speculations, oddities…

3N or DDI term…

- … In SRG: a couple of times smaller than 10^4MeVfm^{-3}, in UCOM(SRG) an order of magnitude smaller…
- And linear dependence on density (practical whan beyond HF)
- Role of complexity / richness of two-body interaction?

Fragmentation of GQR?

Physics Letters B 698 (2011) 191–195

Contents lists available at ScienceDirect

Physics Letters B

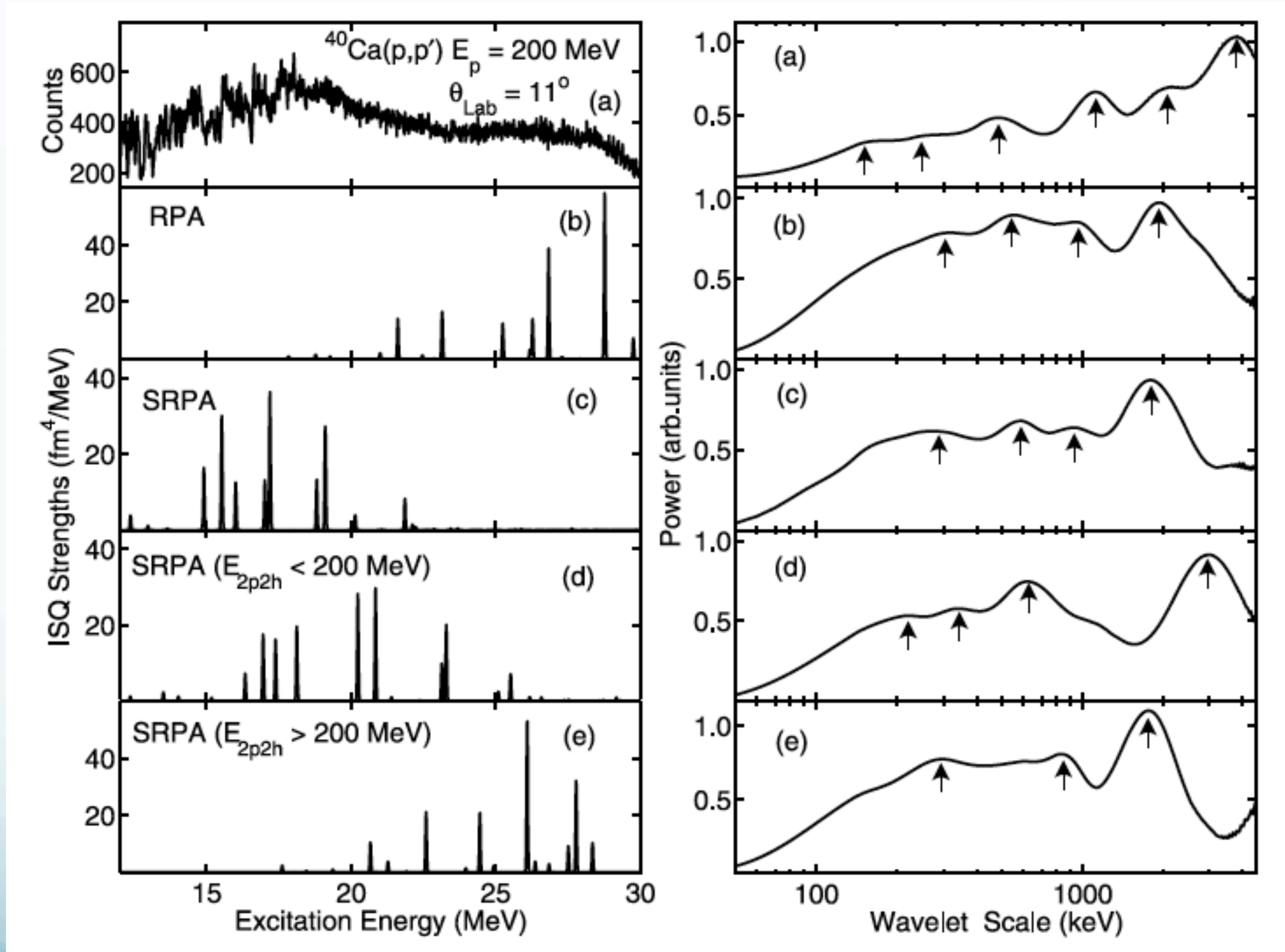
www.elsevier.com/locate/physletb

ELSEVIER

Fine structure of the isoscalar giant quadrupole resonance in ^{40}Ca due to Landau damping?

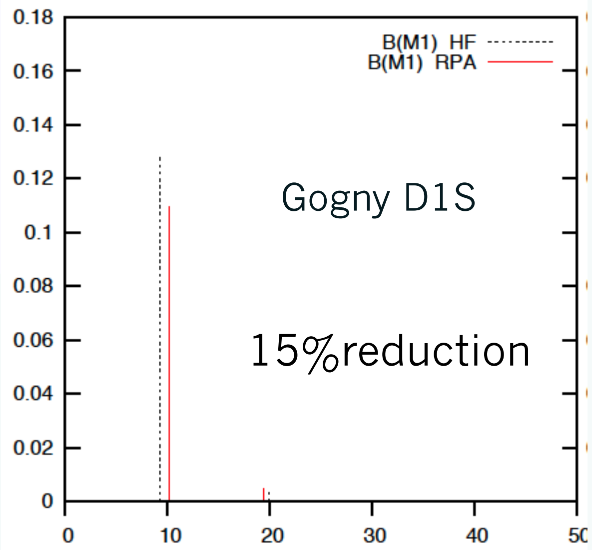
I. Usman [a,b], Z. Buthelezi [a], J. Carter [b], G.R.J. Cooper [c], R.W. Fearick [d], S.V. Förtsch [a], H. Fujita [a,b], Y. Fujita [e], Y. Kalmykov [f], P. von Neumann-Cosel [f,*], R. Neveling [a], P. Papakonstantinou [f], A. Richter [f,g], R. Roth [f], A. Shevchenko [f], E. Sideras-Haddad [b], F.D. Smit [a]

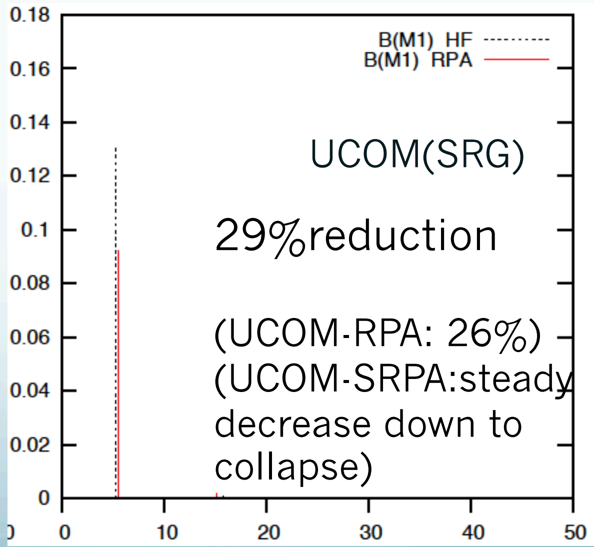
Fragmentation of GQR?



Magnetic transitions?

- Exp: 1_1^+ of ^{48}Ca appears at 10.22MeV with B(M1) $=0.043e^2fm^2$
- IPM (HF): a purely $0f_{7/2}$ -> $0f_{5/2}$ spin transition, almost **4** times stronger than measured.





Summary

- Prospects for an « ab initio » description of nuclear response:
  - With extended methods inspired by RPA
  - With (quasi-)realistic interactions
- We have come a long way in our efforts to tame the realistic NN(N(N)...) interaction and we have a long way to go.
  - Realistic 3N forces
  - Demanding for the many-body methods
- Consistent results obtained so far promote our understanding of the nuclear effective interaction and the above methods

Much to learn together with more phenomenological approaches
How can we help?

Possible directions...

- Fancier extended methods...
- Eg. extended RPA without inconsistencies

M.Tohyama, S.Takahara, P. Schuck, EPJA21,217

- Rearrangement terms of the density-dependent interaction

M.Grasso, D.Gambacurta, F.Catara, JPG38,035103

- **Realistic three-body force**, e.g., normal-ordered

R.Roth et al., 1112.0287

- Extended RPA versions **with pairing**? Phonon coupling?
- **Nuclear matter** calculations

Thank you!

- ... For your attention and the opportunity to be here...

- And thanks for the collaboration to:

  - R.Roth and the tnp++ group: A.Guenther, S.Reinhardt, B.Erler, ... (TU Darmstadt)
  - H.Hergert (OSU)
  - V.Yu.Ponomarev, J.Wambach (TUD)
  - T.Neff, H.Feldmeier (GSI)

  ...