Large-scale Second-RPA calculations for collective excitations

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Overview

- **Introduction – Motivation**
  - ... and some formalism
- **Large-scale Second RPA**
  - Technical issues
  - Physical aspects via illustrative examples
  - Stability problems and missing correlations
- **Open questions**
  - Range and conditions of validity of SRPA?
  - Any implications for first RPA?
  - ...

About this work

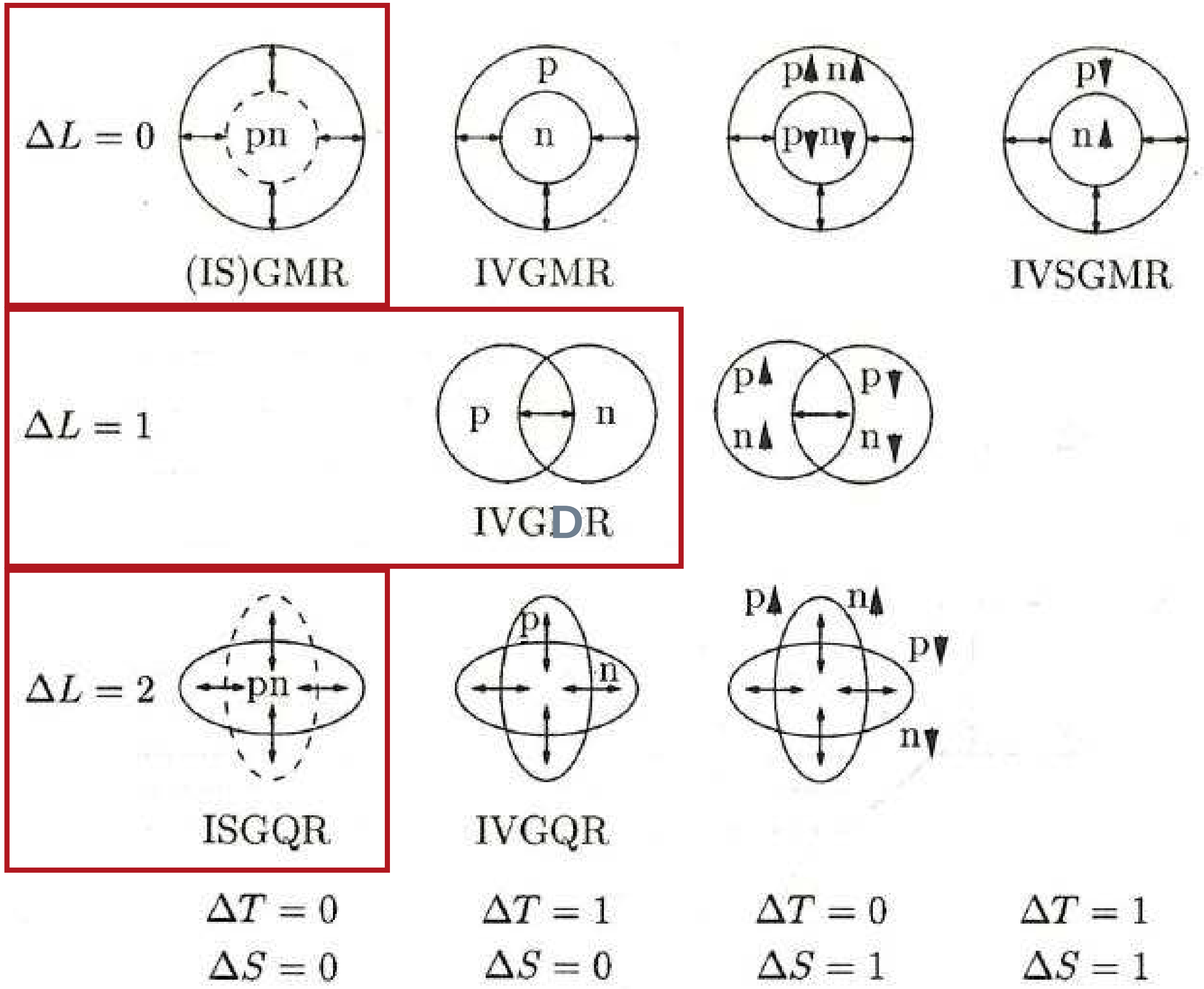
(S)RPA for excited states

- ... on top of a mean-field ground state – Hartree Fock
- ... mostly from a nuclear point of view
- Spherical, closed-shell nuclei will be considered (good angular momentum, no pairing)

■ **Why go beyond first-order RPA?**

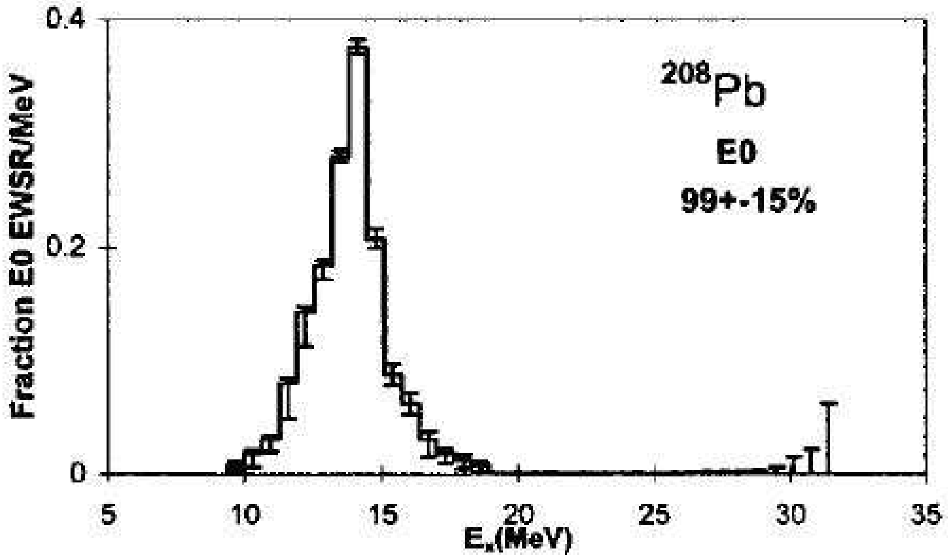
- Decay of collective excitations, but also...
- **... convergence and the problem of the (nuclear) interaction**

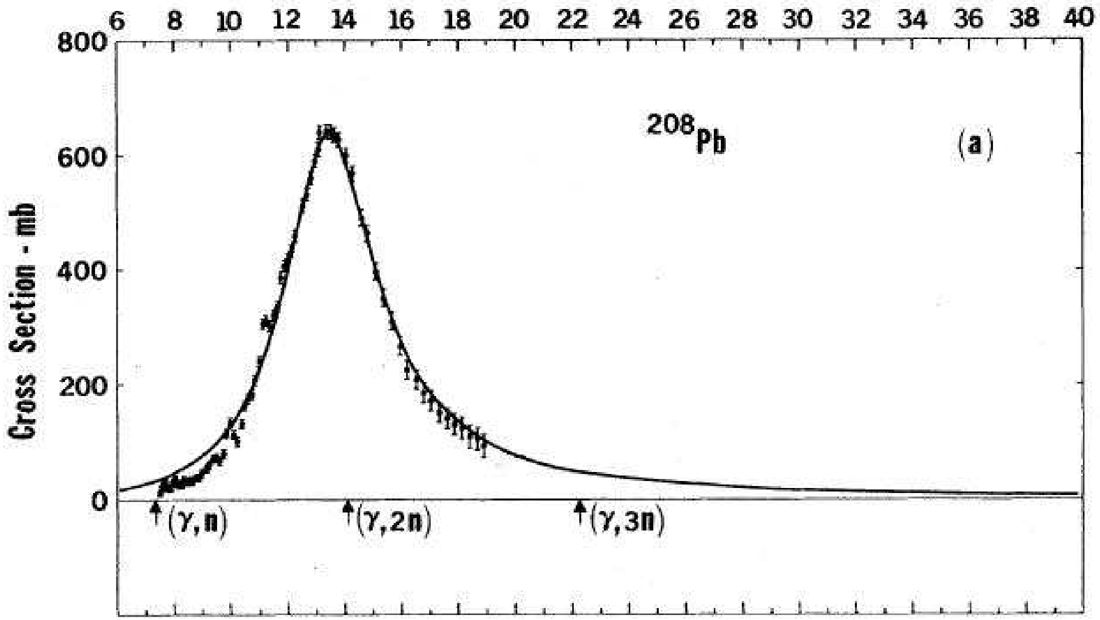
Nuclear Giant Resonances

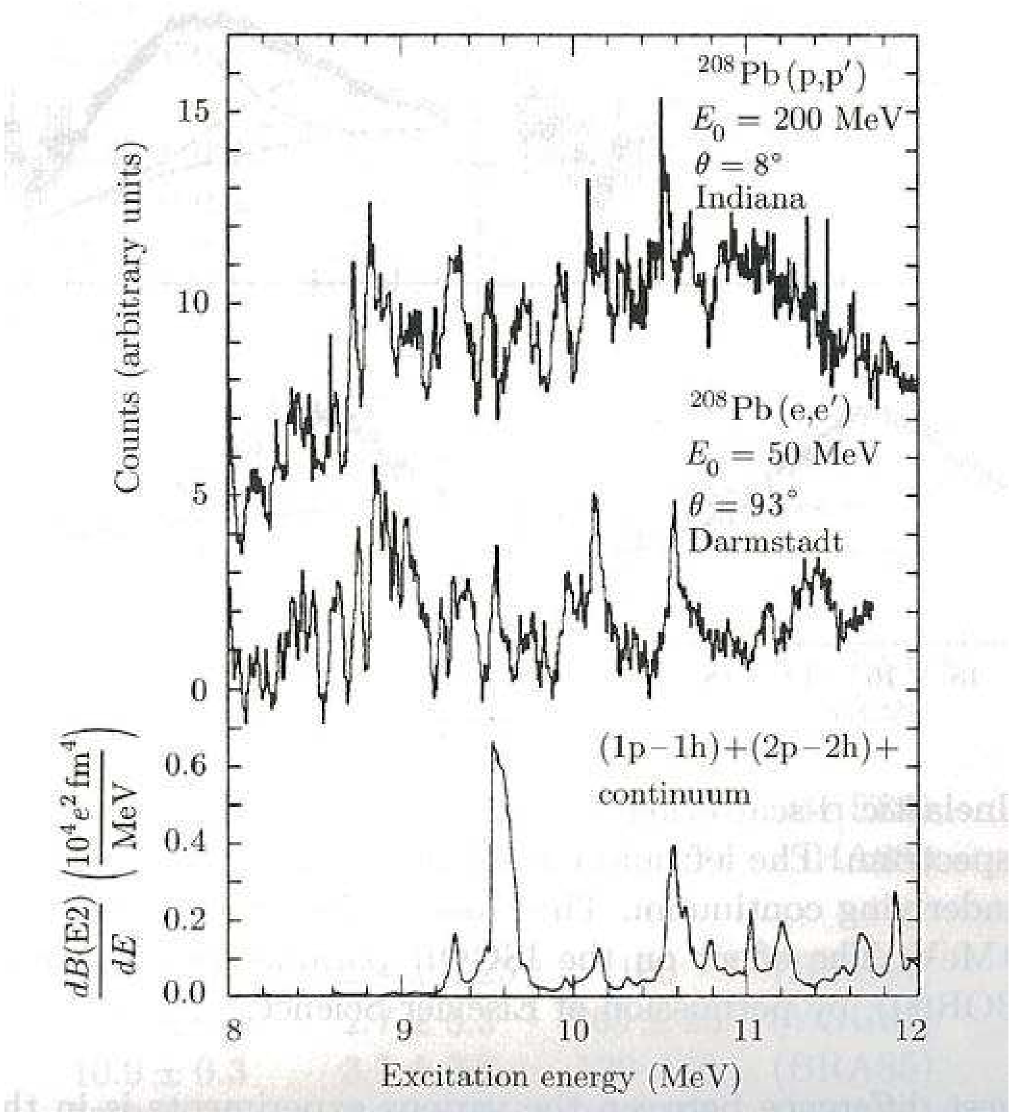


from Harakeh and Van der Woude book

Giant Resonances – ^{208}Pb







To (over)simplify

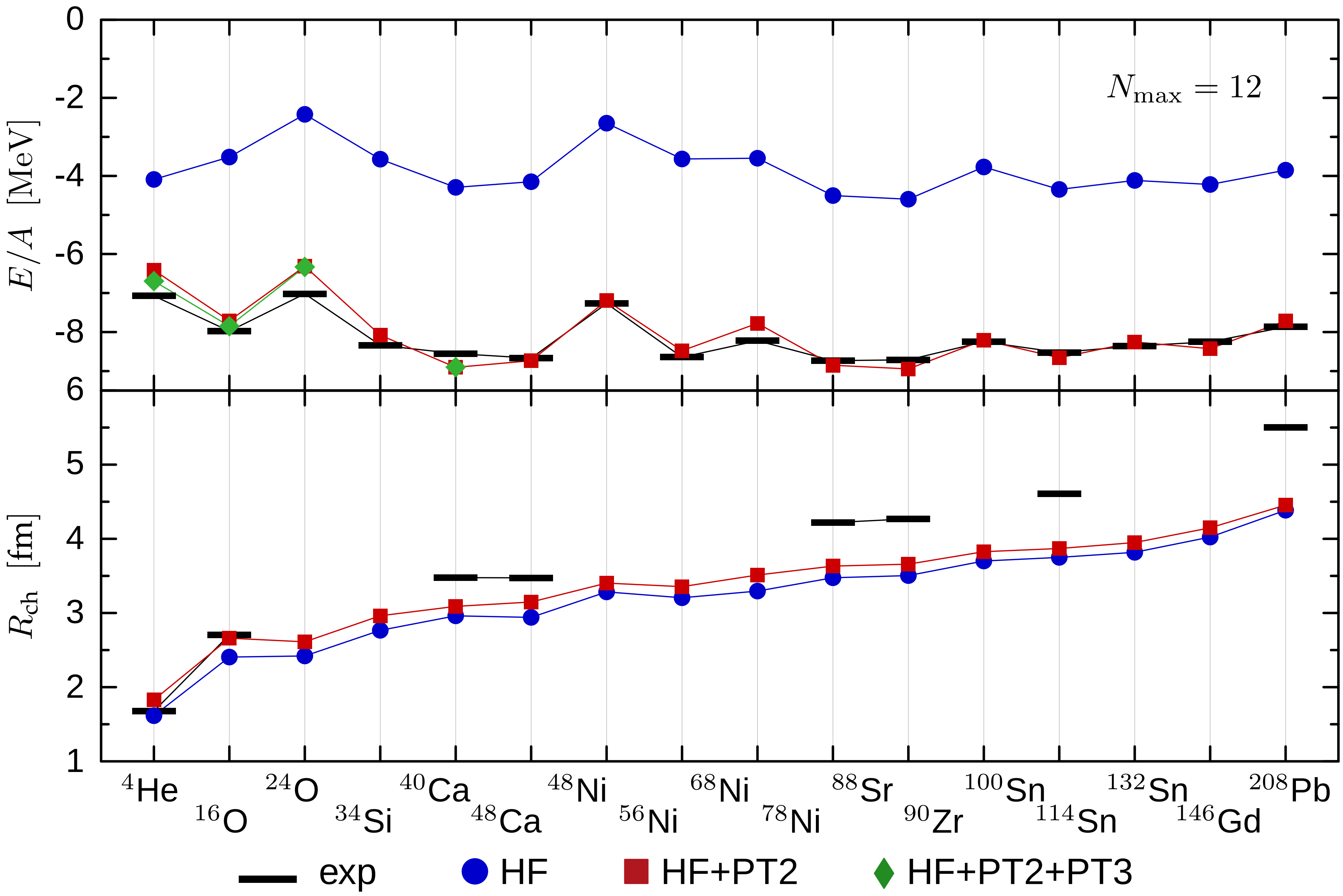
phenomenological effective interactions

- start with some ansatz, e.g. $V_0 \mathrm{e}^{-r^2/\mu^2} + \cdots$, or $V_0 \delta(\vec{r}) + \cdots$ and determine parameters by fitting HF, RPA results to data
- Streamlined over the years for **global properties** – energy and strength of GRs

realistic effective interactions

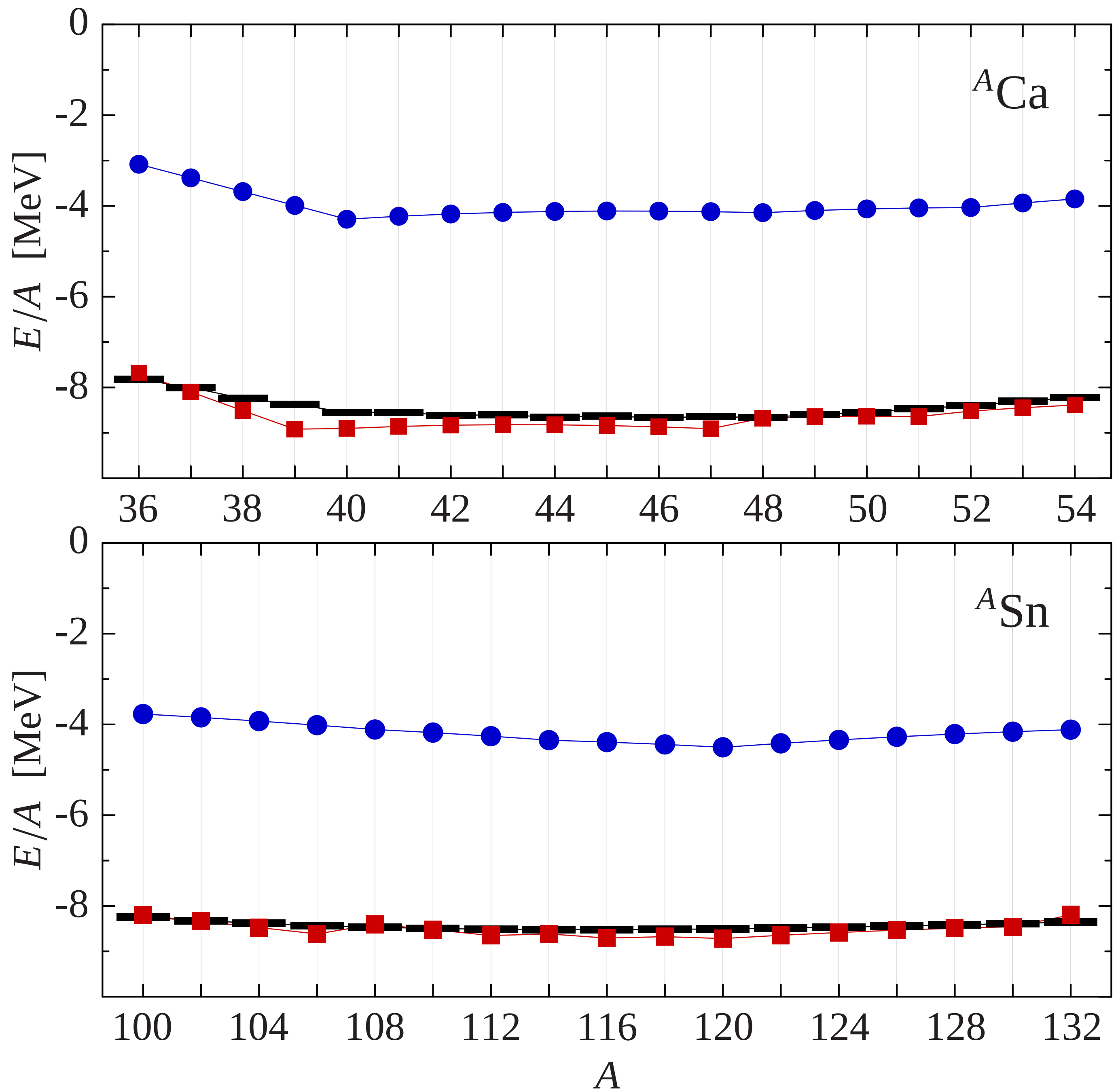
- start with the bare NN interaction and renormalize it properly, using, e.g., the UCOM, SRG, ...
- perturbative interactions, retaining the complexities of the bare NNI – but **not tailored for HF, RPA**

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

Large-scale, ”self-consistent” Second RPA

A typical SRPA application:

- phenomenological s.p. energies and residual interaction
- a few (relatively speaking...) $2p2h$ configurations in the vicinity of a resonance

In this work:

- Large-scale:
  - choose a s.p. space large enough for good convergence (e.g. 12 HO shells) – solve HF
  - include all ph and $2p2h$ configurations available
- ”self-consistent”:
  - 2B interaction sole input – used to describe ground state and residual couplings

Quantities of interest

- Strength function – response to an external field $F^\dagger$:

$$S_F(E) = \sum_\nu |\langle \nu | F^\dagger | 0 \rangle|^2 \delta(E_\nu - E)$$

- Sum rules

$$m_k = \int_0^\infty S_F(E) E^k dE$$

- We consider electrical multipole fields inducing small-amplitude oscillations of the density: compression, surface deformation, etc.
- $F^\dagger$ will be a single-particle operator, able to excite, e.g., ph configurations when acting on the Hartree-Fock ground state.

Equations of Motion Method

- Schrödinger equation:

$$H|\nu\rangle = E_\nu|\nu\rangle$$

- Define creation / annihilation operators

$$|\nu\rangle = Q_\nu^\dagger|0\rangle \quad ; \quad Q_\nu|0\rangle = 0$$

- Rewrite:

$$\langle 0|[R,[H,Q_\nu^\dagger]]|0\rangle = E_\nu\langle 0|[R,Q_\nu^\dagger]|0\rangle \quad ; \quad \forall R$$

- E.g.: $R = a_p^\dagger a_h$, ph operator, $Q_\nu = \sum_{ph} X_{ph} a_p^\dagger a_h - Y_{ph} a_h^\dagger a_p$, and $|0\rangle = |\mathrm{HF}\rangle$: HF-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:

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

- 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

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:

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

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

$\mathcal{A}_{12}$: 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

Reduction of the RPA problem

[P.P.,EPL78(07)12001]

- 2Nx2N RPA problem, with A and B NxN symmetric:

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} = \epsilon_\nu \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix}$$

- Reduction to NxN is always possible in various ways

... even when $A \pm B$ are not positive definite

- How:

if $A + B$ decomposable as $A + B = CDE$ (all real, E has inverse),$^{(**)}$

then solve $HR_\nu = \epsilon_\nu^2 R_\nu$ where $H = E(A - B)CD$ is $N \times N$

For real, positive solutions, recover X, Y as

$$X_\nu = \tfrac{1}{2}[\epsilon_\nu^{1/2} E^{-1} + \epsilon_\nu^{-1/2} CD] R_\nu$$

$$Y_\nu = \tfrac{1}{2}[\epsilon_\nu^{1/2} E^{-1} - \epsilon_\nu^{-1/2} CD] R_\nu$$

$^{(**)}$ *completely analogous expressions can be derived if we decompose $A - B$ instead*

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- $A + B$ positive-definite: Use Cholesky (find square root):

$A + B = CDE = LL^T$ ($C = E^T = L$ lower-triangular, $D = I$)

then solve $HR_\nu = \epsilon_\nu^2 R_\nu$ where $H = L^T(A - B)L$ is $N \times N$ symmetric

Recover X, Y as

$$X_\nu = \frac{1}{2}[\epsilon_\nu^{1/2} L^{T^{-1}} + \epsilon_\nu^{-1/2} L] R_\nu$$

$$Y_\nu = \frac{1}{2}[\epsilon_\nu^{1/2} L^{T^{-1}} - \epsilon_\nu^{-1/2} L] R_\nu$$

[Chi, NPA146(70)449]

Reduction of the RPA problem

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- Reduction to NxN is always possible in various ways

  ... even when $A \pm B$ are not positive definite

- Unsure about $A + B$: Use "Generalized" Cholesky :

  $A + B = CDE = LDL^T$ ($C = E^T = L$ triang., $D =$diagonal with ± 1)

  then solve $HR_\nu = \epsilon_\nu^2 R_\nu$ where $H = E(A - B)CD$ is $N \times N$ symmetric

  For real, positive solutions, recover X, Y as

$$X_\nu = \frac{1}{2}[\epsilon_\nu^{1/2} L^{T^{-1}} + \epsilon_\nu^{-1/2} L] R_\nu$$

$$Y_\nu = \frac{1}{2}[\epsilon_\nu^{1/2} L^{T^{-1}} - \epsilon_\nu^{-1/2} L] R_\nu$$

decomposition algorithm
as efficient as Cholesky

Reduction of the RPA problem

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- Reduction to NxN is always possible in various ways

... even when $A \pm B$ are not positive definite

- Simplest way: (saves matrix operations)

$$[(A-B)(A+B)]R_\nu = \epsilon_\nu^2 R_\nu \text{ , with } R_\nu = \epsilon_\nu^{-1/2}(X_\nu + Y_\nu)$$

For real, positive solutions,

$$X_\nu = \tfrac{1}{2}[\epsilon_\nu^{1/2} I + \epsilon_\nu^{-1/2}(A+B)]R_\nu$$

$$Y_\nu = \tfrac{1}{2}[\epsilon_\nu^{1/2} I - \epsilon_\nu^{-1/2}(A+B)]R_\nu$$

Second RPA

- Large model spaces:
  - Number of states up to $\approx 10^6$ for the present cases – can get larger
  - But SRPA matrix is sparse and reduction to half the size is always possible

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- Use Lanczos
  - Find only the lowest eigenvalues $|\epsilon_\nu|$
  - ... or the ones closest to a set value E_0, e.g.

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

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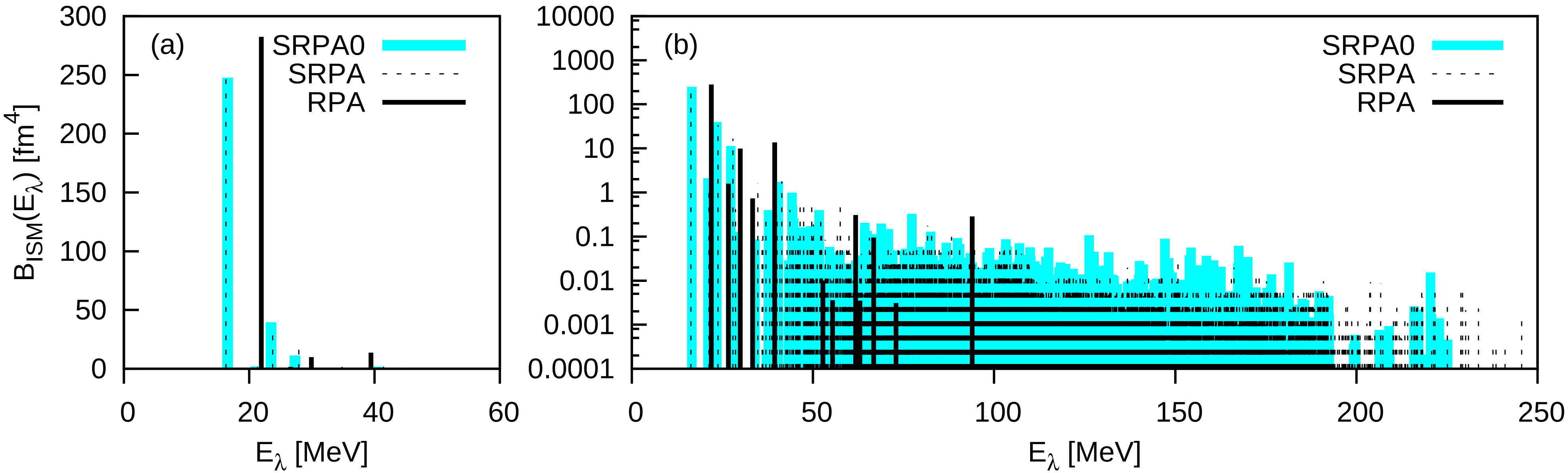
- Alternatively, reduce to an $\omega-$dependent problem of RPA size
  - ... especially if you ignore interactions within 2p2h space:

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

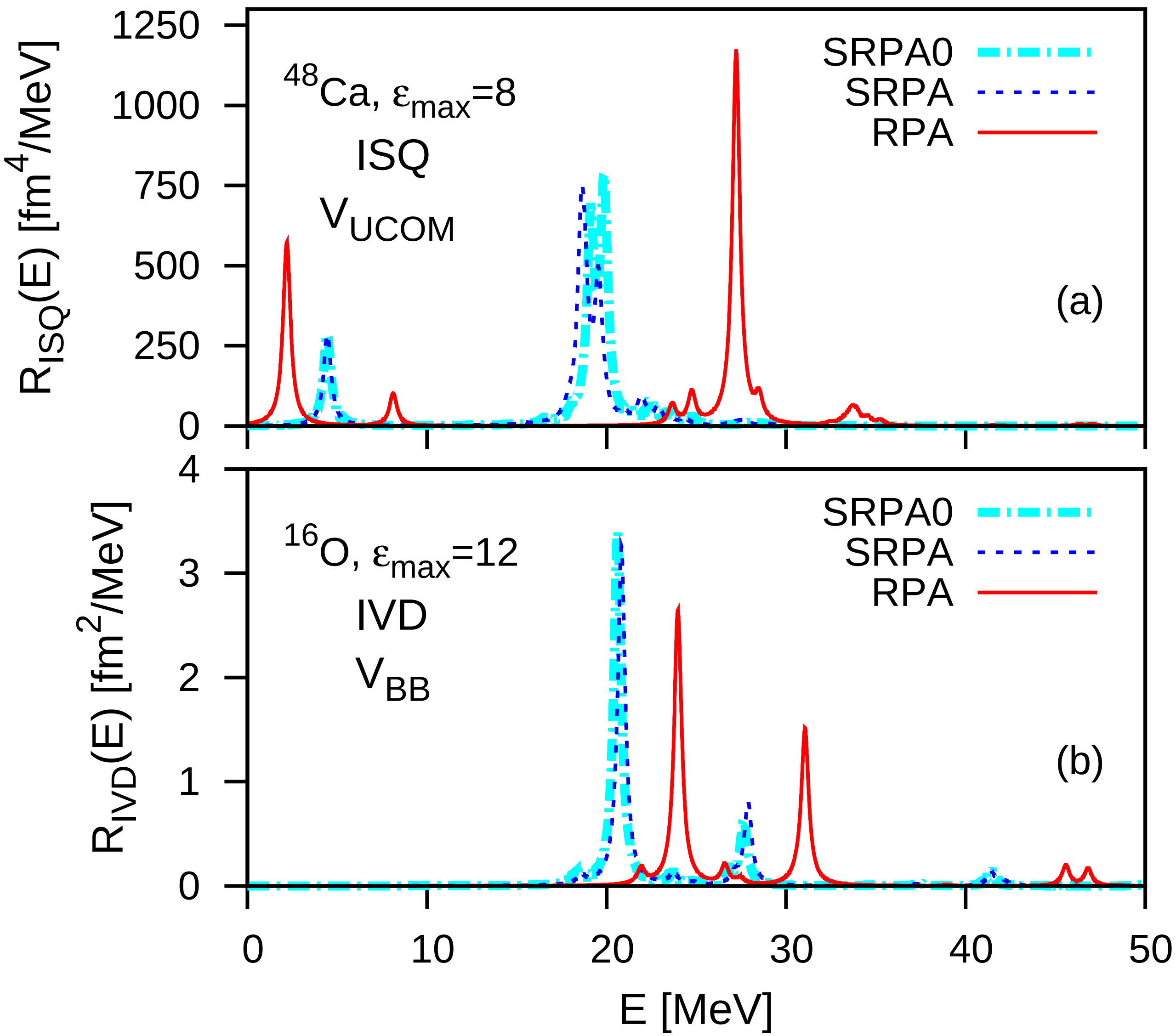
SRPA Eigenstates

SRPA and its diagonal approximation ("SRPA0") vs RPA



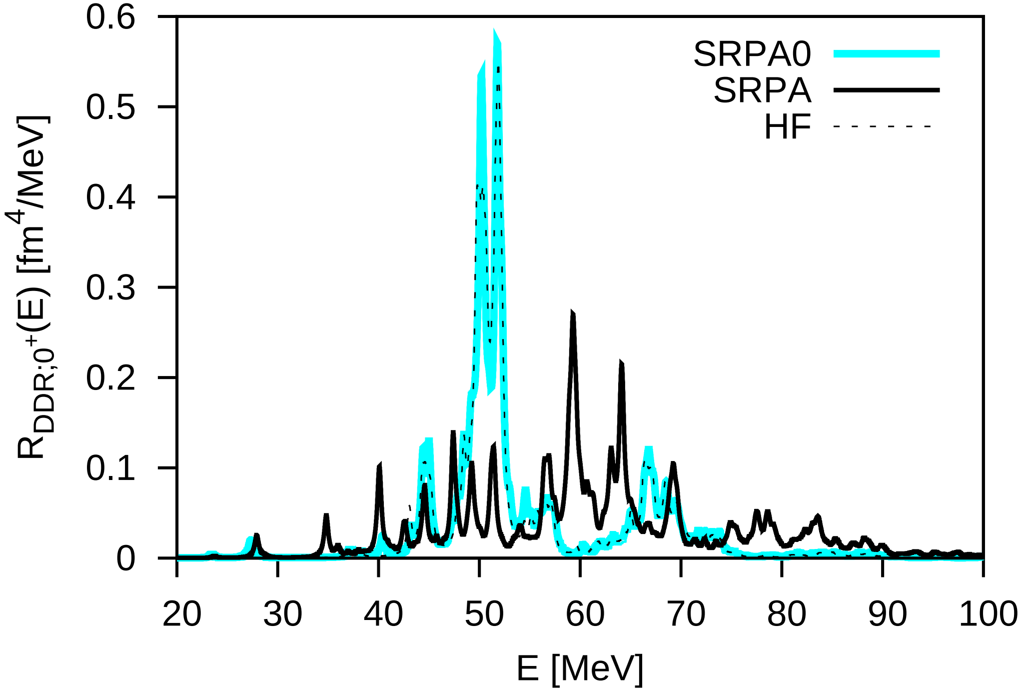
^{16}O with UCOM-AV18 in 7 shells

Diagonal Approximation

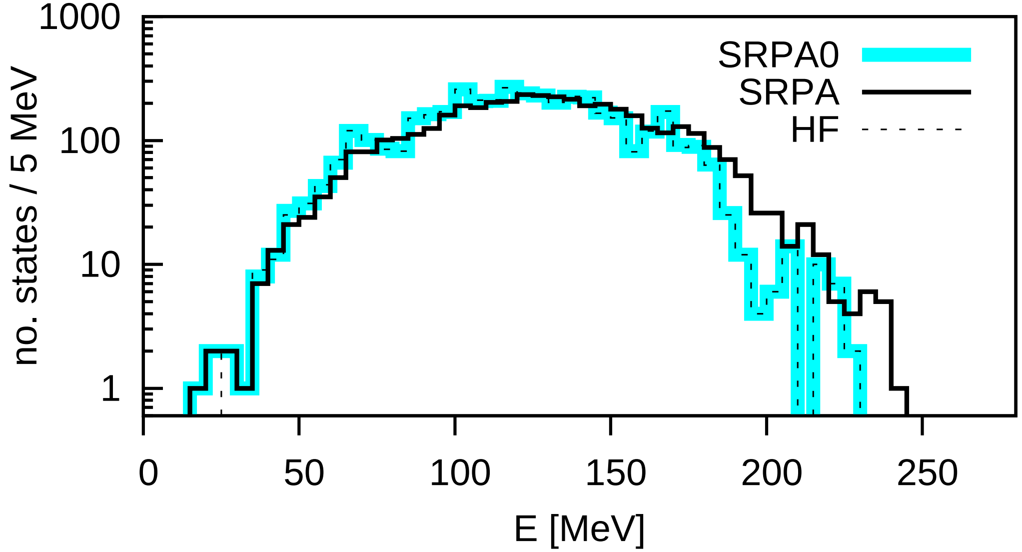


Diagonal Approximation

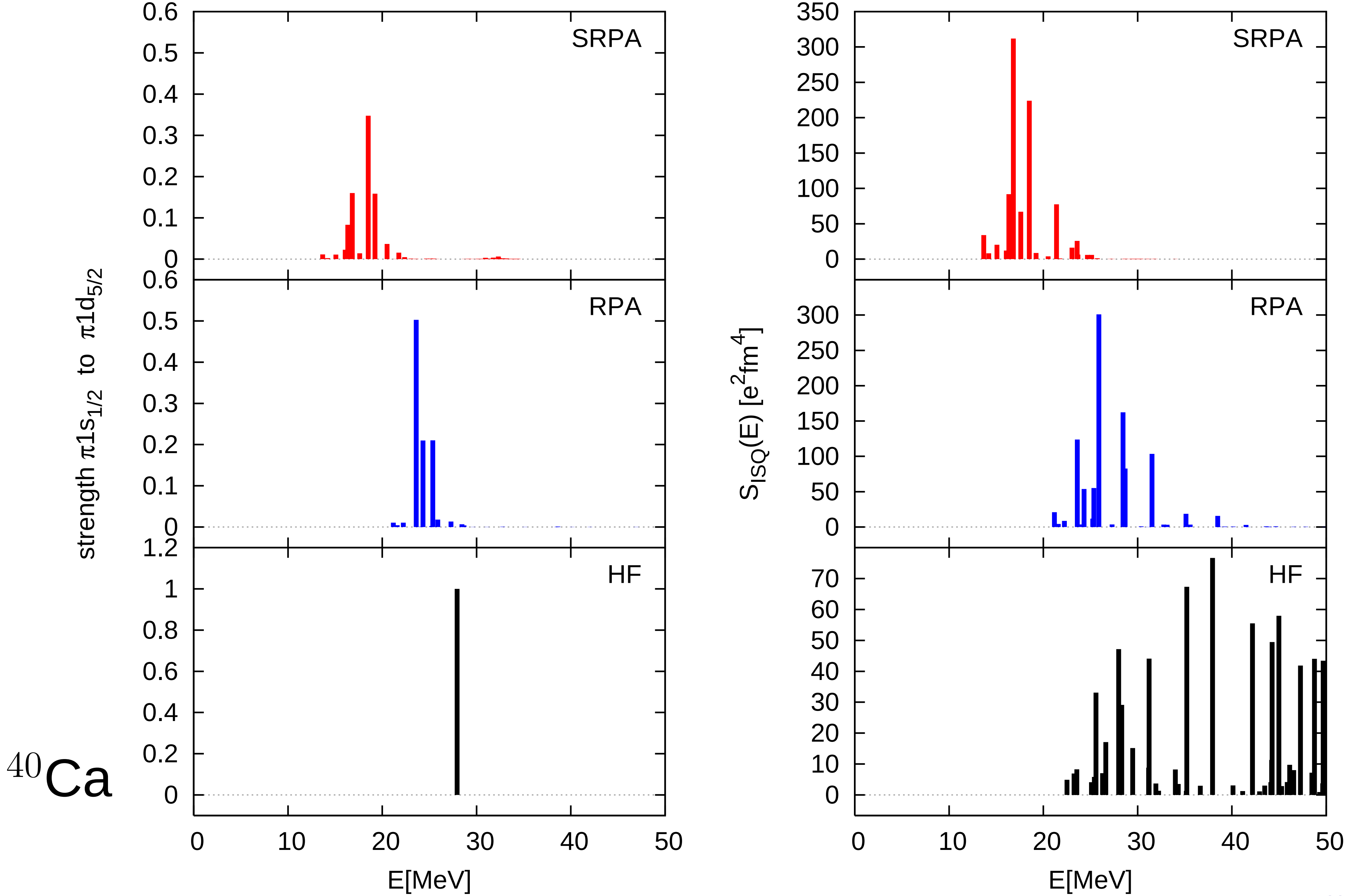
Double resonances:



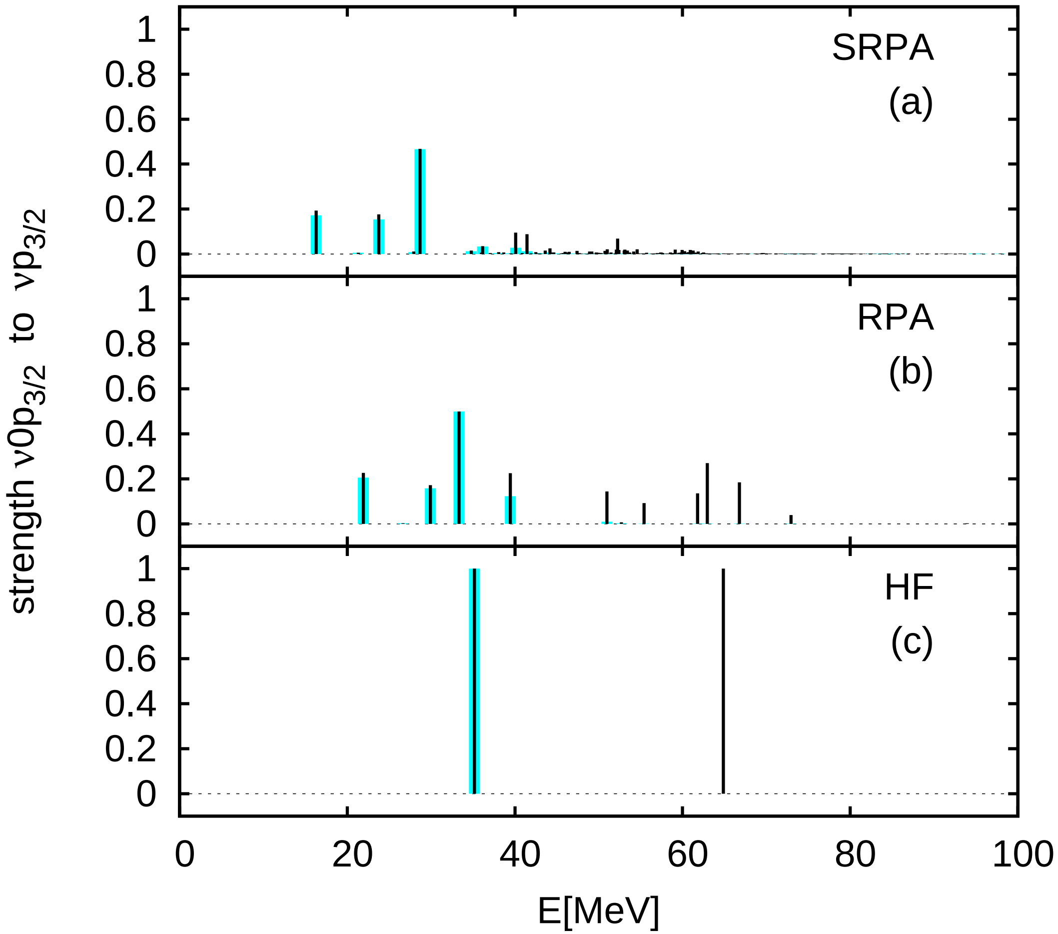
Density of eigenstates:



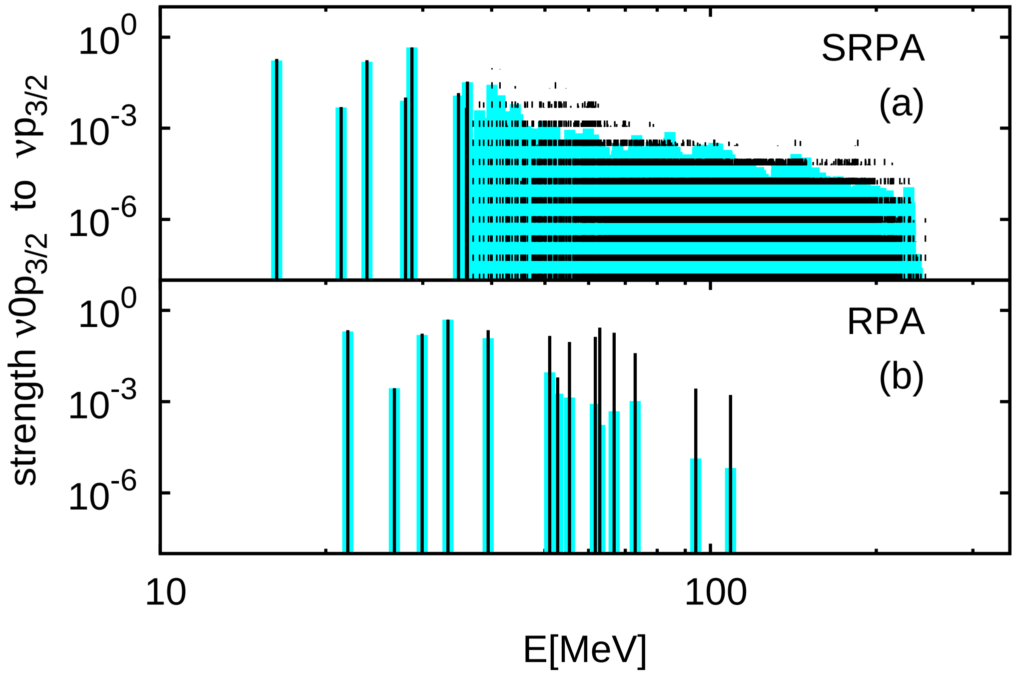
Fragmentation of ph states



Fragmentation of ph states

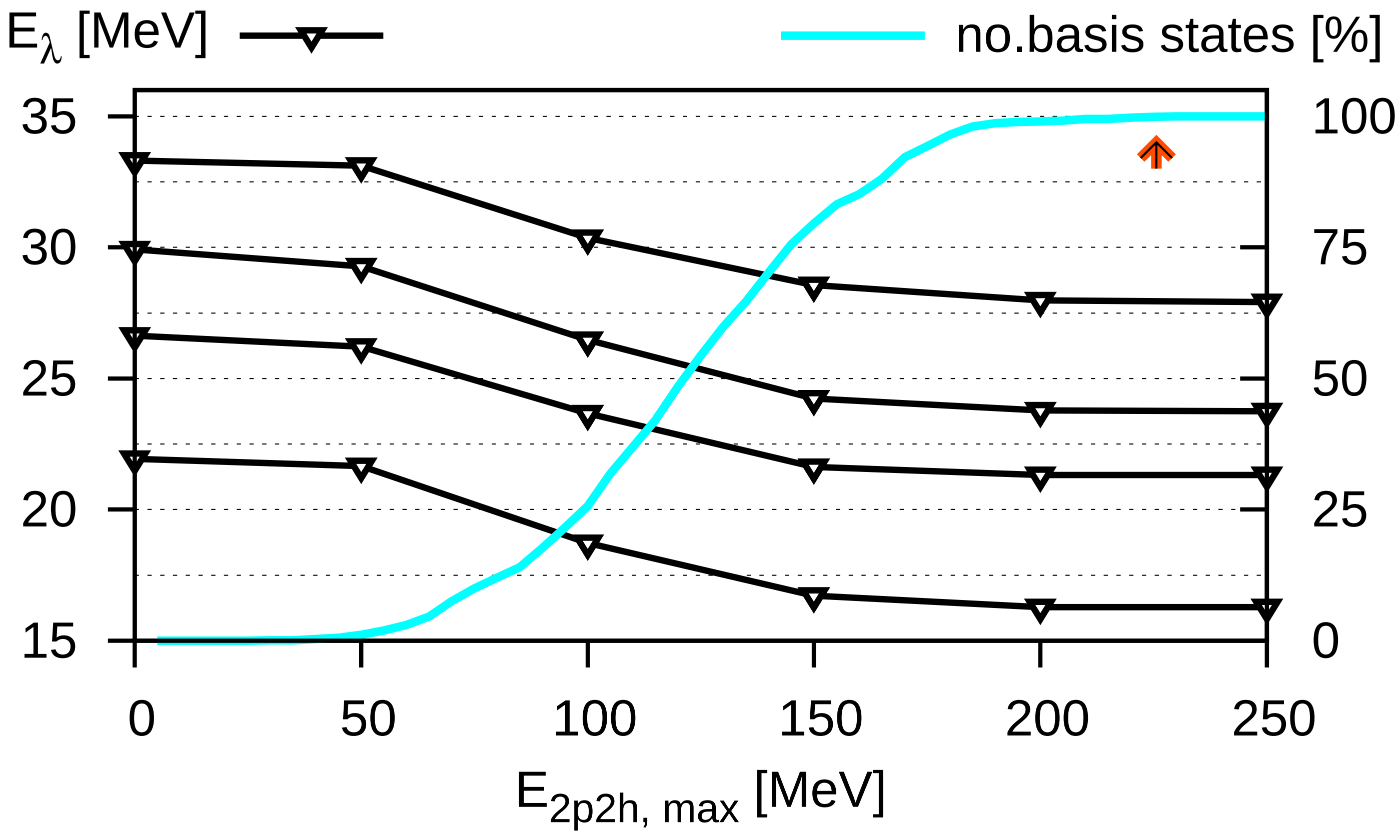


log scale:

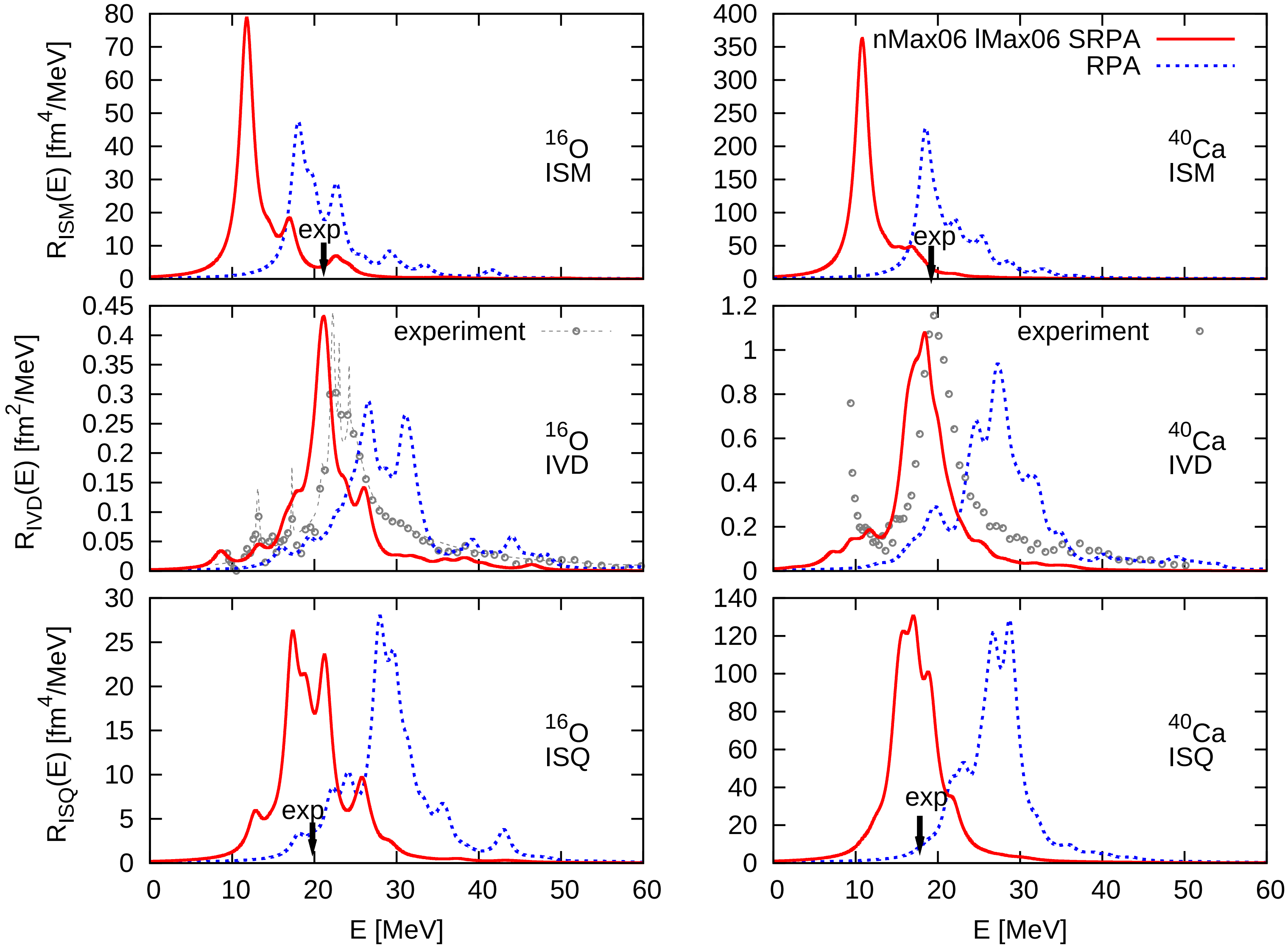


^{16}O :: 0^+, 7 shells

Truncation in 2p2h energy



UCOM :: RPA and SRPA



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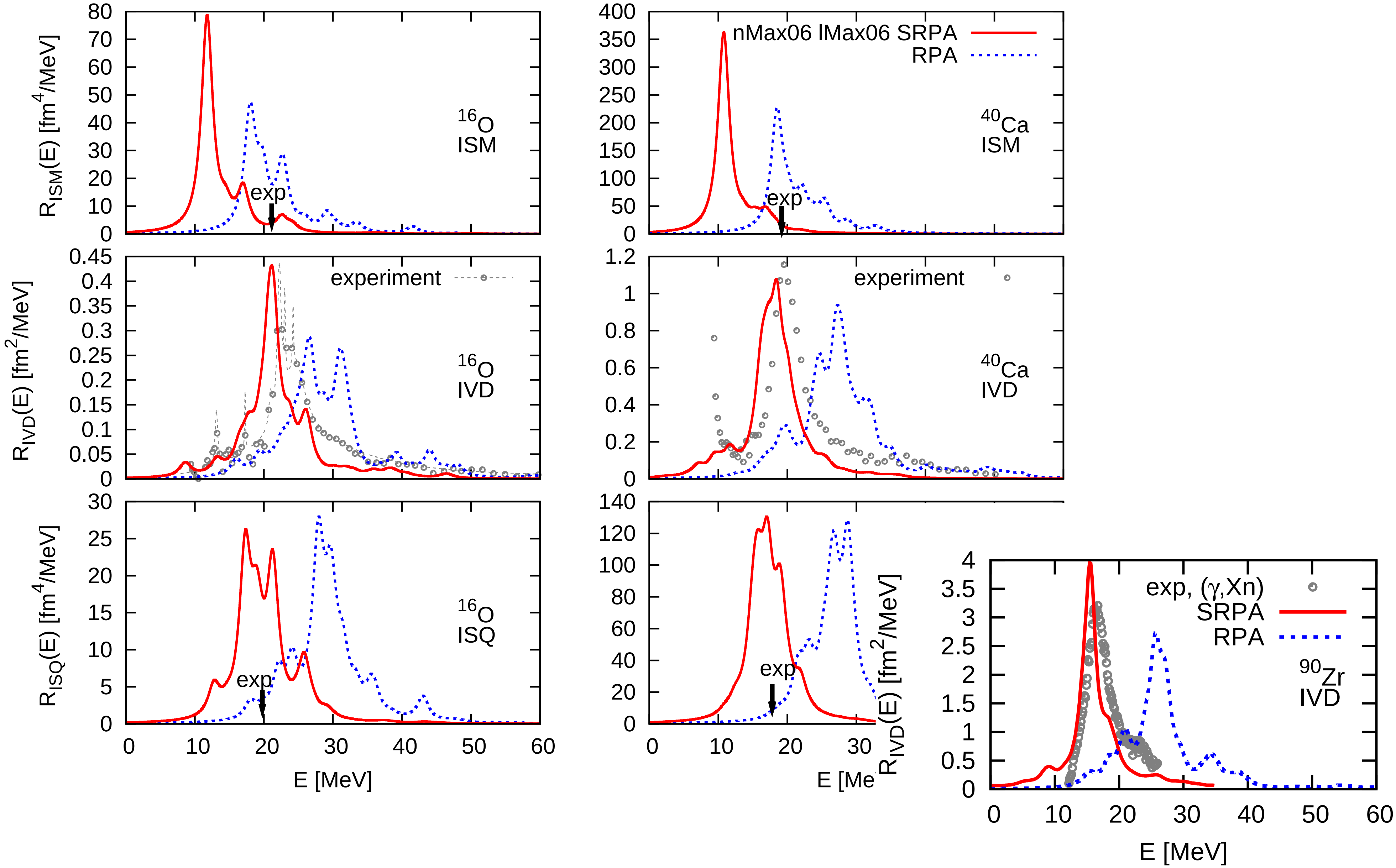
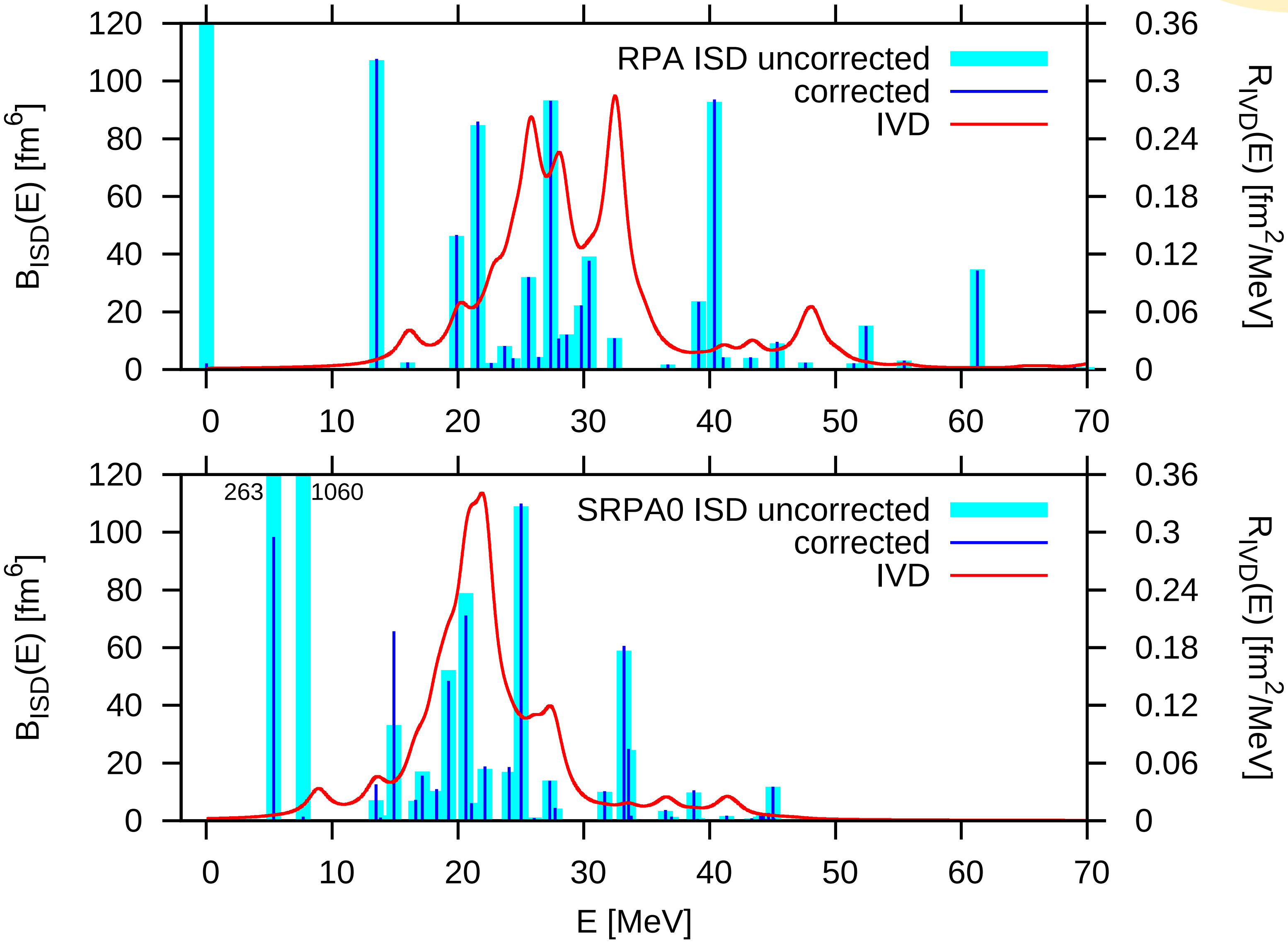


Spurious states

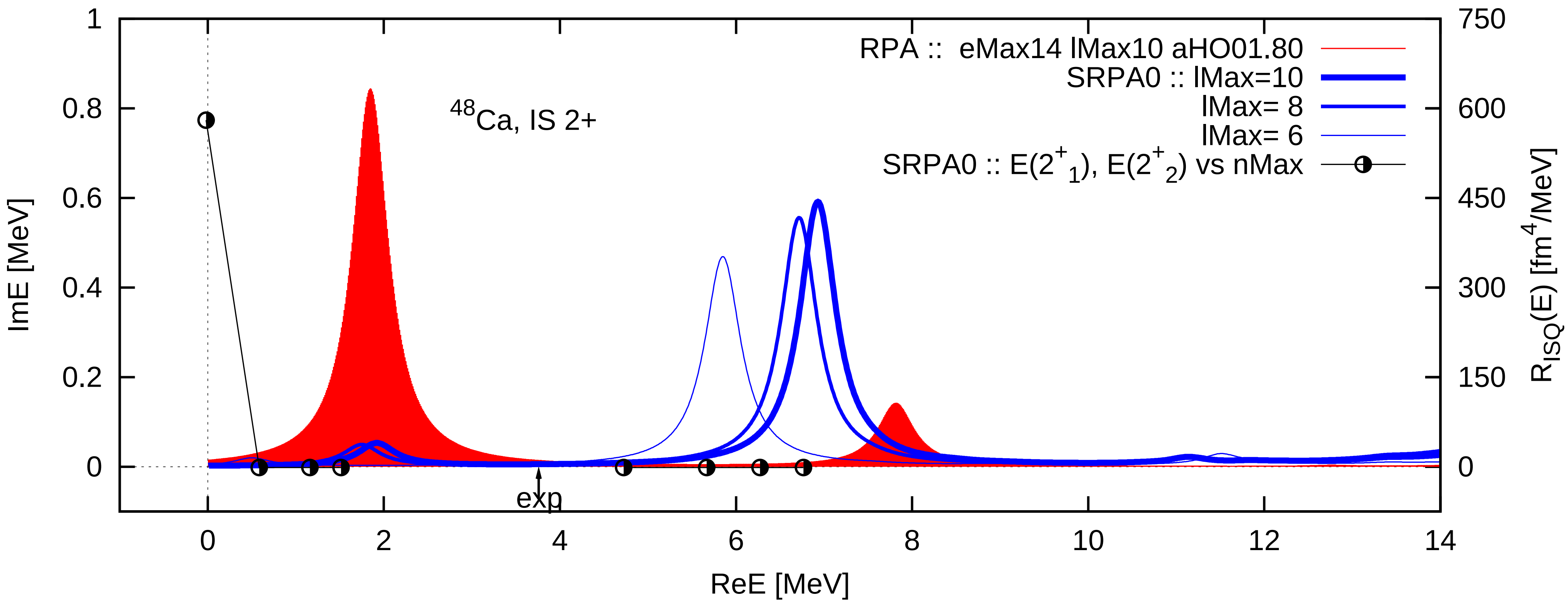
ISD corrected radial operator $r^3 - \frac{5}{3}\langle r^2 \rangle r$ vs r^3

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

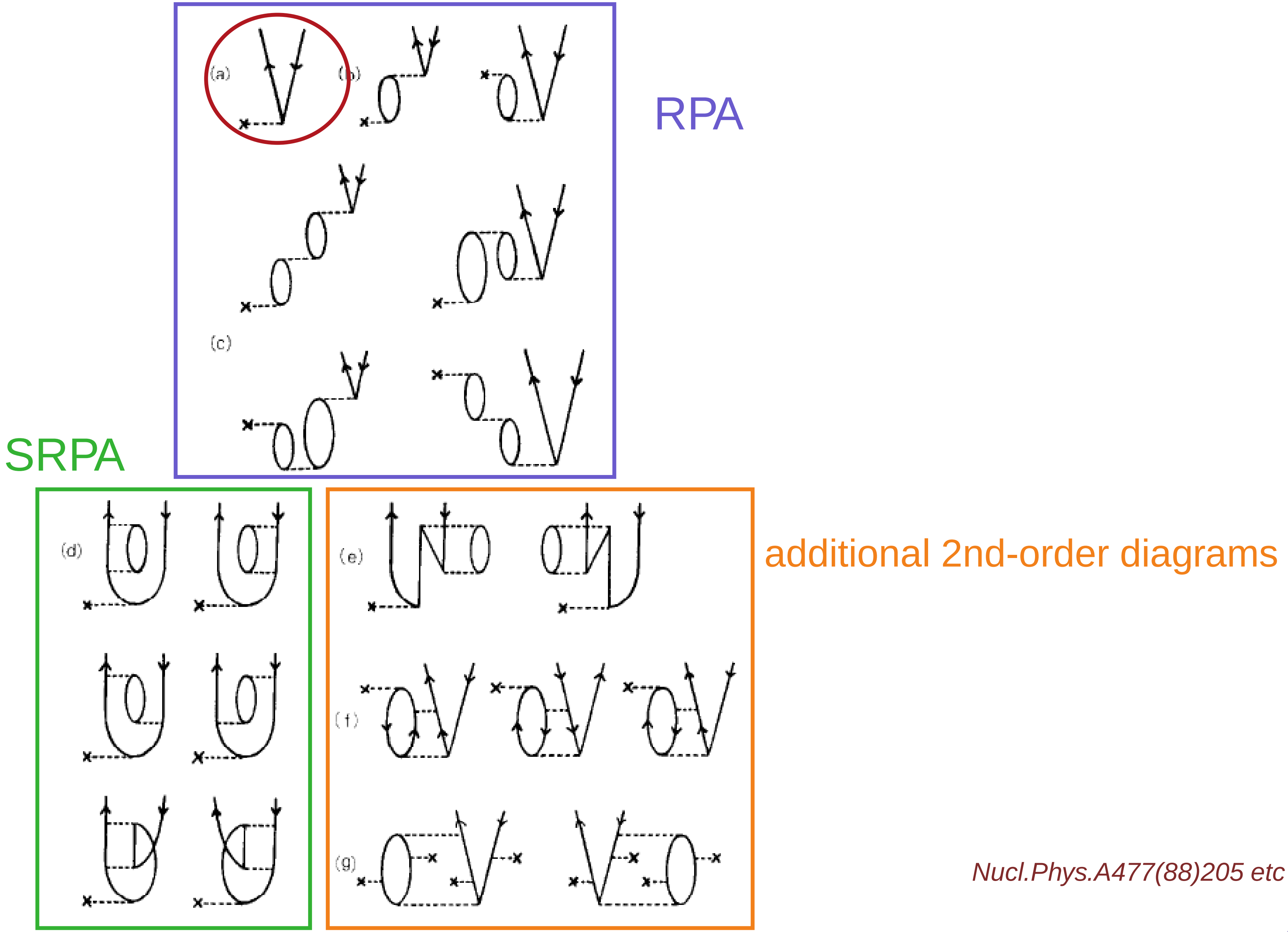


Low-lying states

SRPA0: convergence and stability of low-lying ISQ states



RPA, SRPA, and extensions



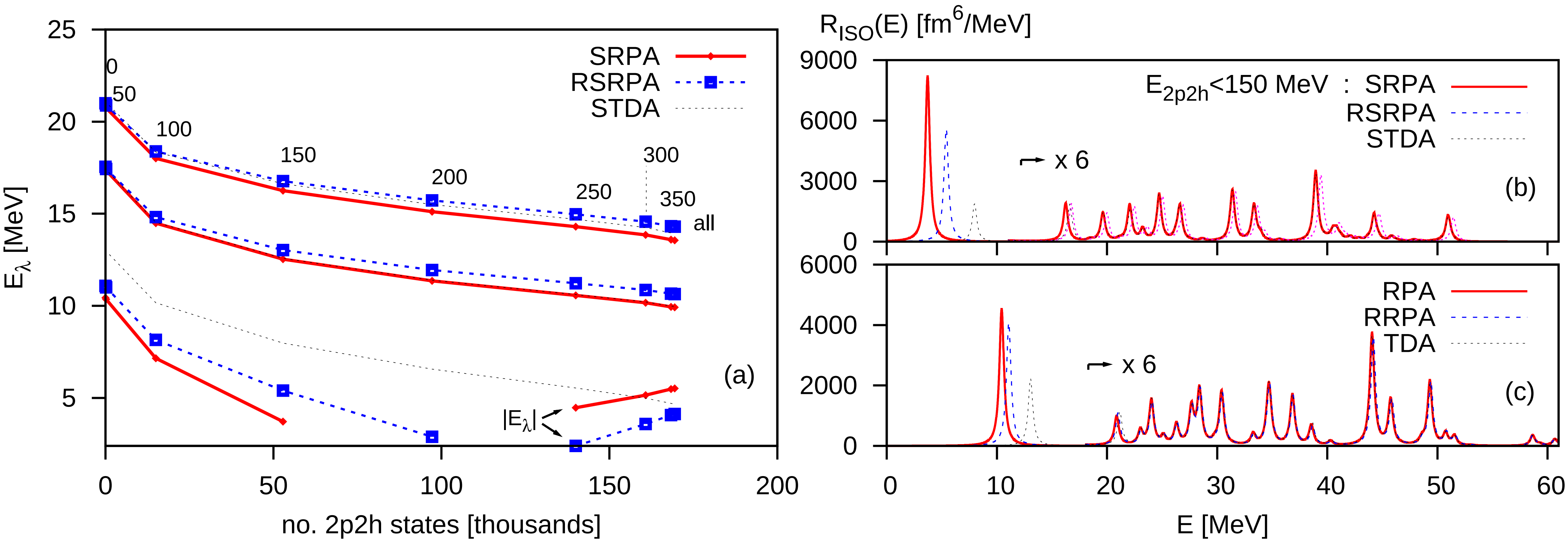
Nucl.Phys.A477(88)205 etc

Role of ground-state correlations

- Use a more consistent extended-RPA formalism
- For the moment, possible tests:
  - ignore GSC altogether - TDA and STDA ($B = 0$)
  - renormalize matrix elements: e.g., $\times D_{ph}^{1/2}$ ($D_{ph} \equiv n_h - n_p$)
  - here occupation probabilities from shell model

Ground State Correlations

^{16}O octupole states



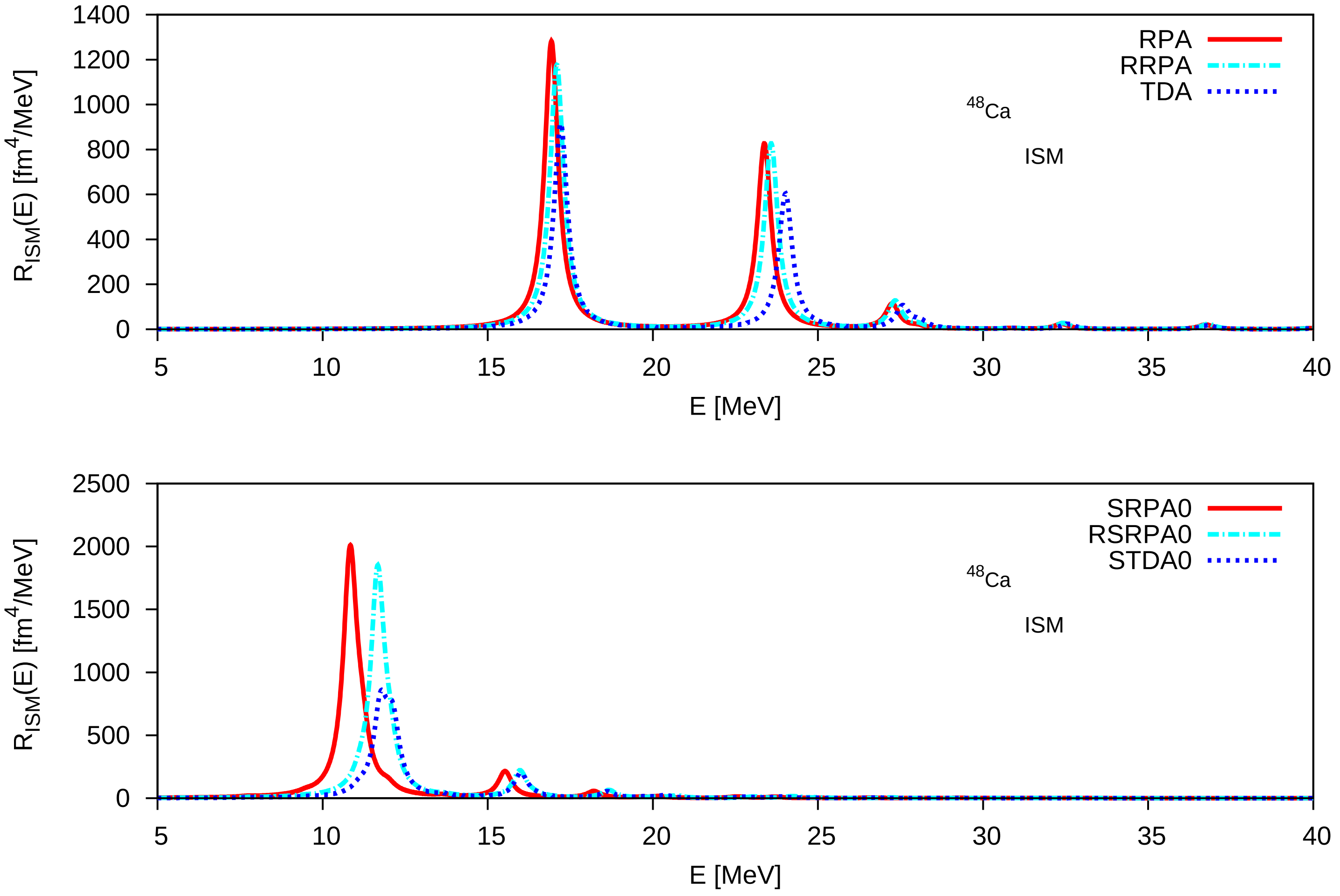
Ground State Correlations

^{48}Ca quadrupole states

	E_1	E_2	E_{GQR}	$B(E_1)$	$B(E_2)$	$B(\mathrm{GQR})$
RPA	2.19	8.12	27.22	450.05	79.18	915.2
RRPA	2.42	8.16	27.41	373.09	69.36	892.2
TDA	2.61	8.39	27.42	127.05	46.06	813.1
SRPA	-4.44	$i\times$0.803	19.51	223.18	—	1021.3
RSRPA	-3.14	1.34	20.18	161.95	22.25	991.3
STDA	-4.26	0.46	19.72	182.28	41.14	831.1

Ground State Correlations

monopole states

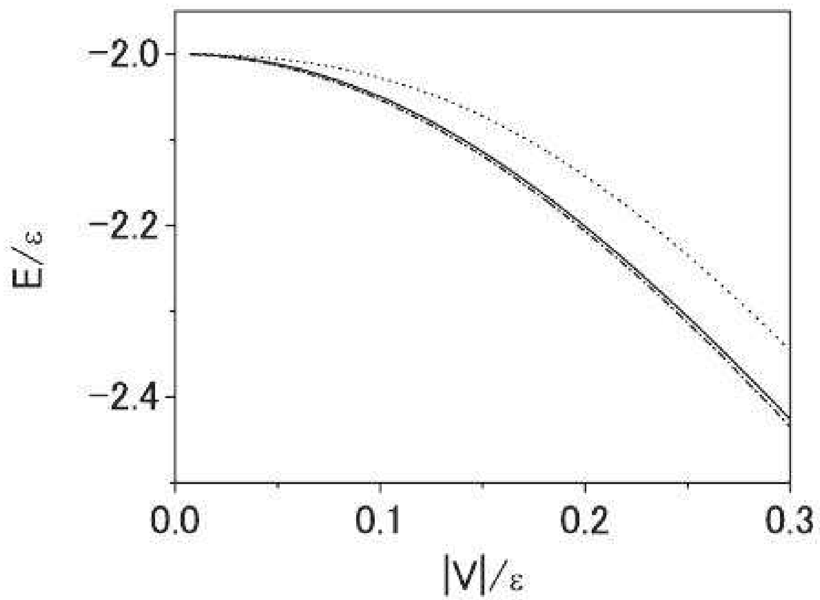


Validity of SRPA?

M.Tohyama, PRC75 (07) 044310

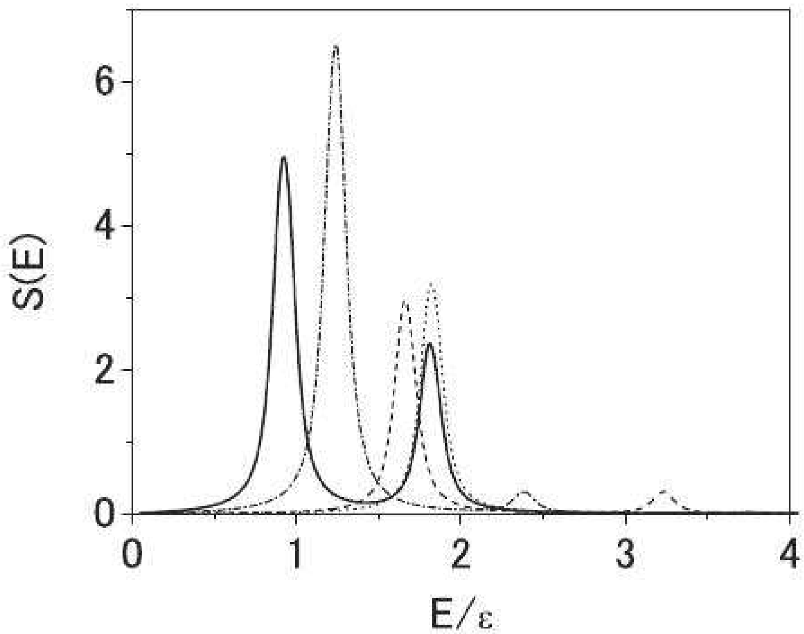
$$H = \epsilon J_z + \frac{V}{2}(J_+^2 + J_-^2) + \frac{U}{2}[J_z(J_+ + J_-) + (J_+ + J_-)J_z],$$

TDDM ——
HF · · ·
exact - · - · -



$U = V/2$

STDDM ——
RPA · · ·
SRPA - - -
exact - · - · -



$N = 4$ and $U/\epsilon = V/2\epsilon = -0.15$

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TDDM ——
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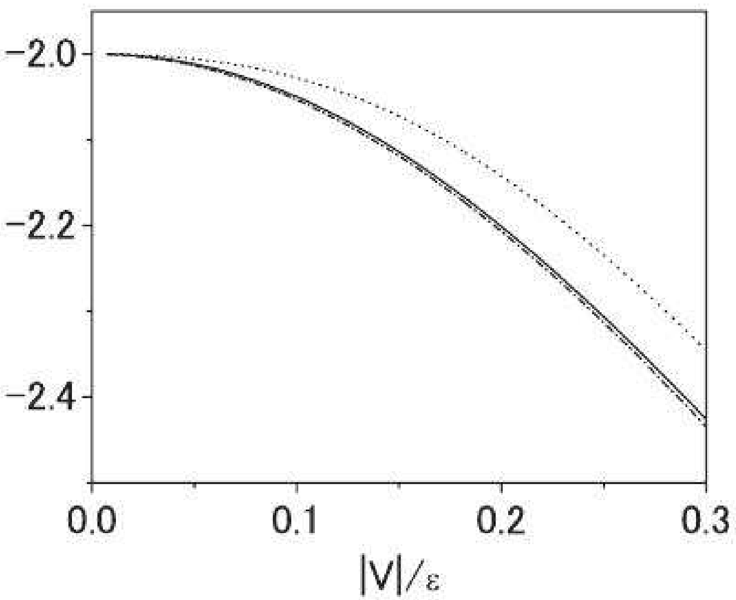
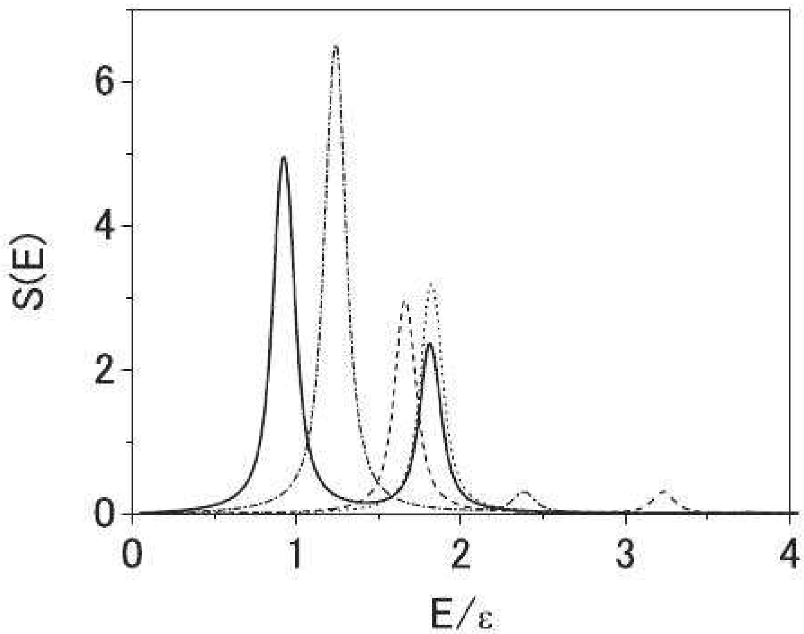


STDDM ——
RPA · · ·
SRPA - - -
exact - · - ·



$U = V/2$

$N = 4$ and $U/\epsilon = V/2\epsilon = -0.15$

strong correlations: all methods fail

Validity of SRPA?

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TDDM	——
HF	· · ·
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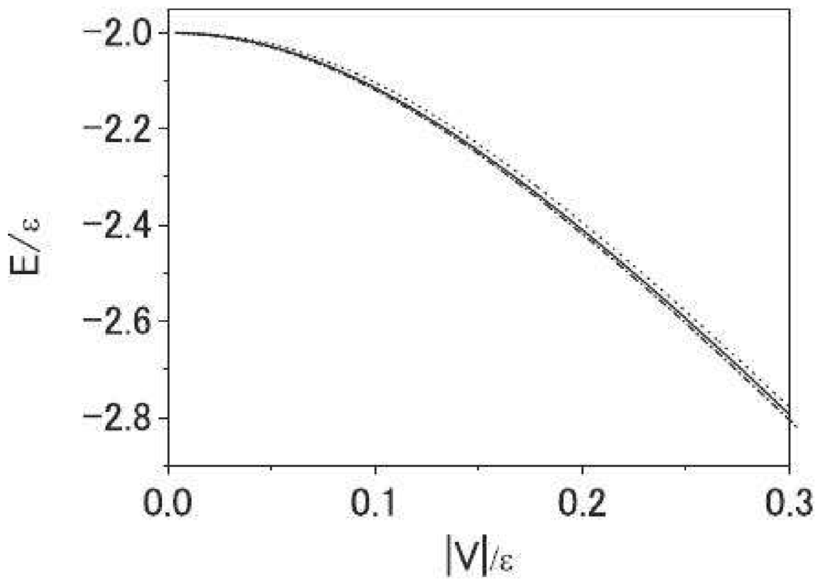
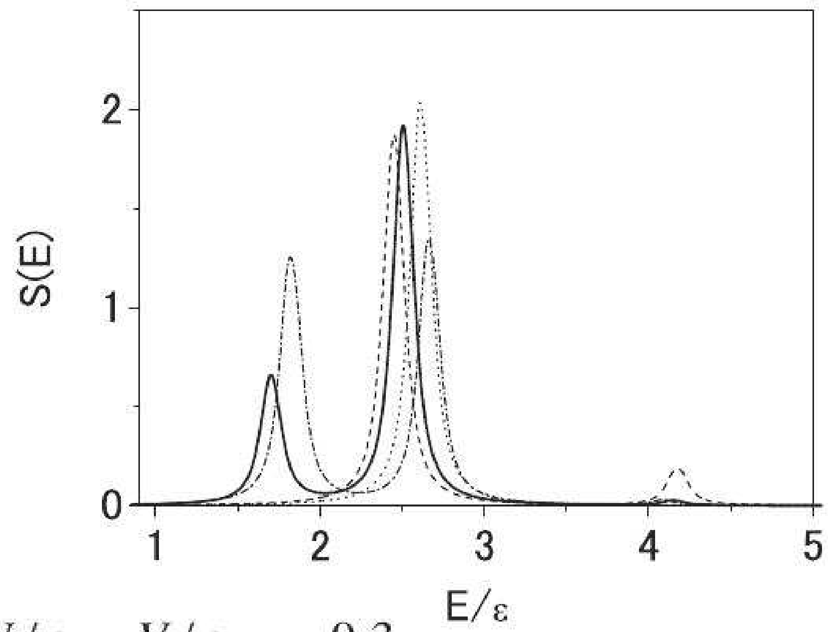


$U = V$

STDDM	——
RPA	· · ·
SRPA	- - -
exact	- · - ·



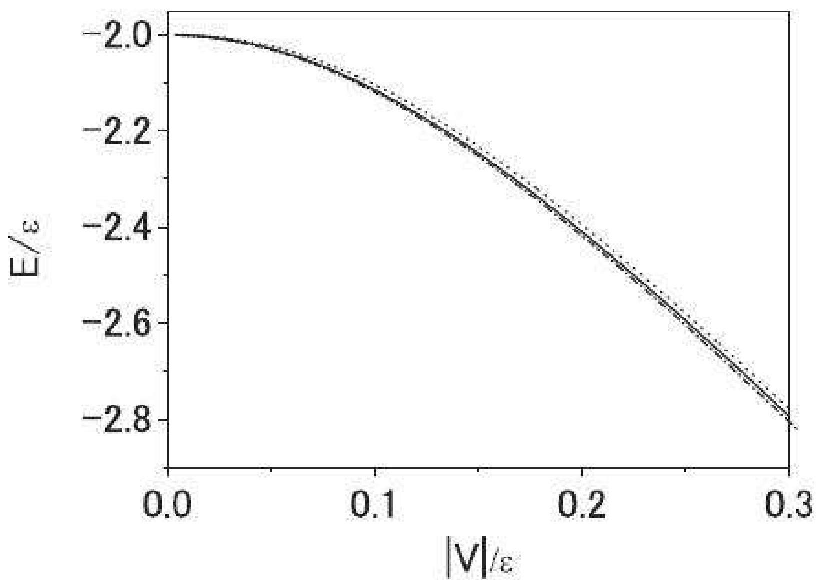
$U/\epsilon = V/\epsilon = -0.3$

Validity of SRPA?

M.Tohyama, PRC75 (07) 044310

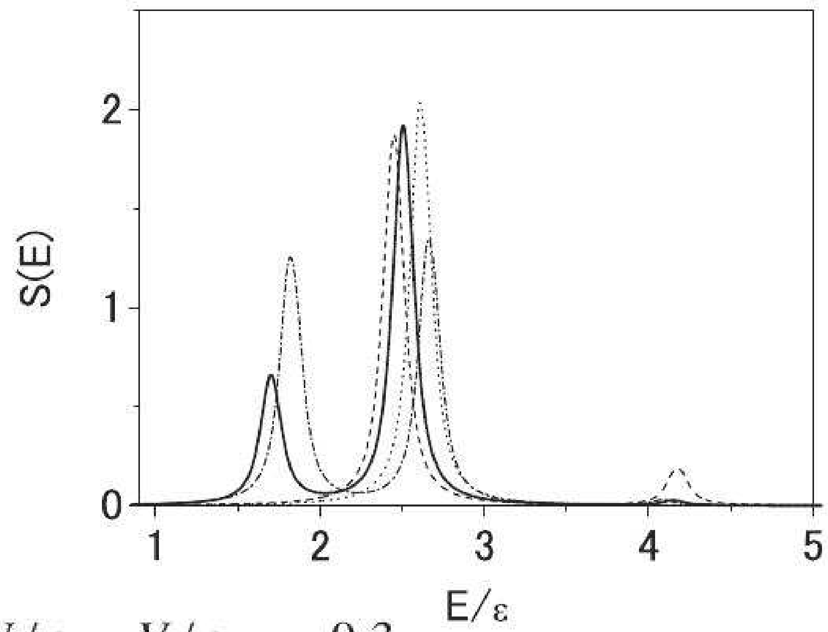
$$H = \epsilon J_z + \frac{V}{2}(J_+^2 + J_-^2) + \frac{U}{2}[J_z(J_+ + J_-) + (J_+ + J_-)J_z],$$

TDDM ——
HF · · ·
exact - · - ·



$U = V$

STDDM ——
RPA · · ·
SRPA - - -
exact - · - ·



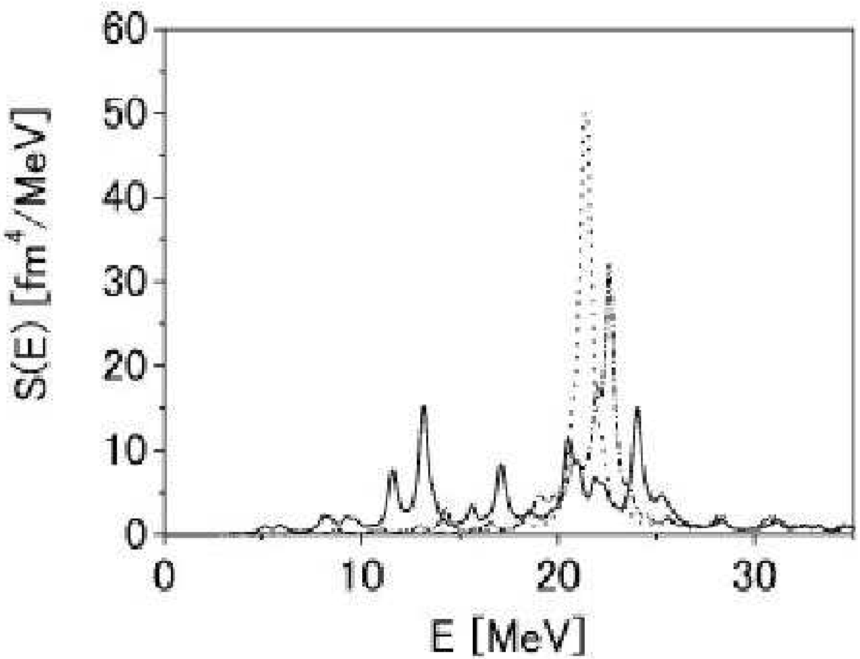
$U/\epsilon = V/\epsilon = -0.3$

weak correlations: 1-phonon state OK?

Validity of SRPA?

M.Tohyama, PRC75 (07) 044310

GQR of ^{16}O



STDDM ——
RPA · · ·
SRPA - · - ·

Conclusions – nuclear

Extended-RPA calculations using
correlated realistic interactions

Effective interactions for extended RPA?

- ✔ Avoiding conceptual problems
- ✔ More fundamental treatment of nucleon self energy, m^* (ISQ, IVD)
- ✘ Two-body UCOM: Soft nuclei due to residual three body effects?
- Second RPA:
  - ✔ Great improvement over RPA results
  - ✔ model space should be flexible enough to describe residual LRC
  - ✘ Instabilities and inconsistencies
- Extensions of the present simple SRPA method

Summary

Large-scale Second RPA calculations
for collective states

Role of model space and interaction

✔ Large-scale: no arbitrary truncations of model space

✔ “Self-consistent”: NN interaction only input

- Second RPA:
  - ✔ Shift and fragmentation of resonances
  - ✘ Instabilities and inconsistencies
  - ... but GRs rather stable? (Except compression mode)
- Extensions of the present simple SRPA method?

Thank you!

Work in collaboration with:

- R. Roth and the TNP++ group, J.Wambach, V.Yu.Ponomarev, ...

  Institut für Kernphysik, TU Darmstadt, Germany

- H. Feldmeier, K. Langanke, G. Martinez-Pinedo, T. Neff, ...

  GSI, Darmstadt, Germany

Some related references

- P. P., R. Roth, to appear in PRC (2010)
- P. P., R. Roth, PLB**671**, 356 (2009)
- and many more: **http://crunch.ikp.physik.tu-darmstadt.de/tnp/**
  http://crunch.ikp.physik.tu-darmstadt.de/˜panagiota/

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