

# [Second] RPA, linear-response theory, and nuclear sound

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TBW: Seven years ago

## ❖ SRPA:

- Range and conditions of validity
- (S)RPA vs linear-response theory vs density-functional theory

### Large-scale Second-RPA calculations for collective excitations

#### ■ Introduction – Motivation

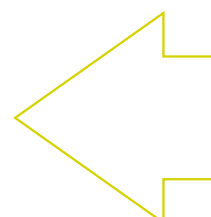
- ... and some formalism

#### ■ Large-scale Second RPA

- Technical issues
- Physical aspects via illustrative examples
- Stability problems and missing correlations

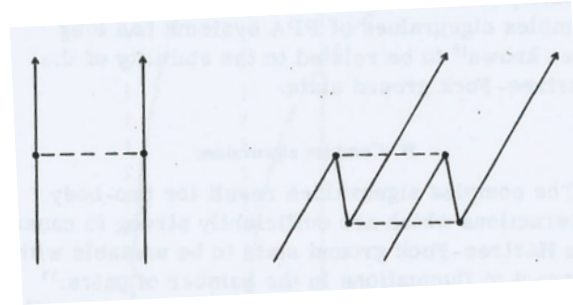
#### ■ Open questions

- Range and conditions of validity of SRPA?
- Any implications for first RPA?
- ...



## ❖ pp-RPA

- From  $A$  to  $A \pm 2$  system
- Pairing interaction
- Ladder diagrams



## ❖ ph-RPA

- Same number of particles
- Phonon excitations
- Ring diagrams

$\frac{1}{1 - \Sigma}$ , (4.97)

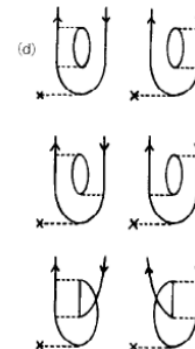
where  $\Sigma$  (the self energy) is given by

$\Sigma = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$  (4.98)

The diagrams in (4.98) are called 'ring' diagrams because of their ring-like structure. For historical reasons, this approximation for  $G$  is called the 'Random Phase Approximation' or 'RPA'.

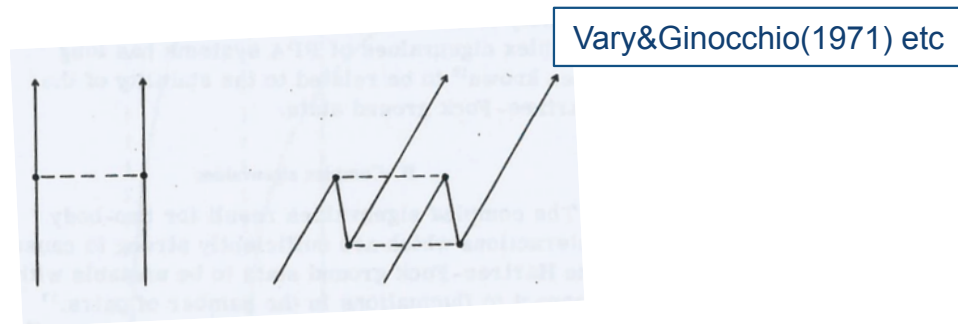
## ❖ ph-2p2h-RPA (Second RPA)

- Extension of ph-RPA
- Related to phonon-phonon coupling



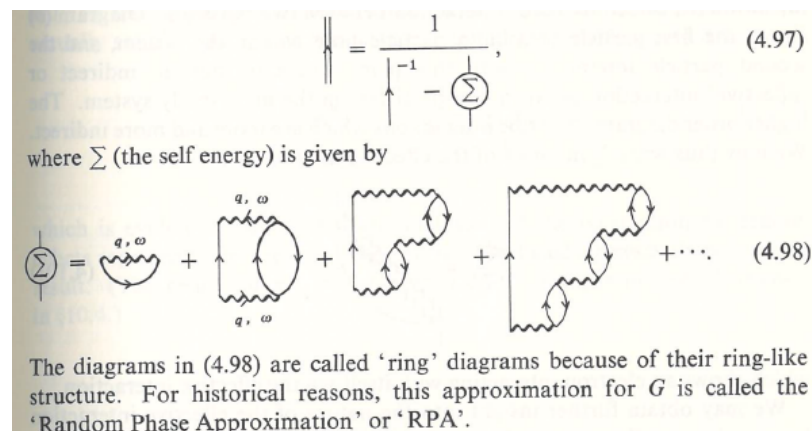
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## ❖ ph-RPA

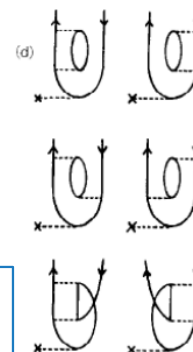
- Same number of particles
- Phonon excitations
- Ring diagrams



## ❖ ph-2p2h-RPA (Second RPA)

- Extension of ph-RPA
- Related to phonon-phonon coupling

- HF reference state
- Spherical systems ( $J$  good quantum number)
- Everything antisymmetrized



## ❖ Ground-state correlations

- Correction to the Hartree-Fock energy via the backward amplitudes
- Correction real in the absence of phase transitions (e.g. superfluidity in pp-RPA)

## ❖ Excited states

- pp-RPA: 2-particle transfer, spectroscopy
- ph-RPA, ph-2p2h-RPA: Vibrational states, sound waves

## ❖ Ground-state correlations

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## ❖ Excited states

- pp-RPA: 2-particle transfer, spectroscopy
- **ph-RPA, ph-2p2h-RPA: Vibrational states, sound waves**

- ❖ External potential field  $V$  probes system with ground-state density  $\rho_0(\mathbf{r})$

$$\sum_n (E_n - E_0) |\langle 0|V|n\rangle|^2 = \int d^3r \rho_0(\vec{r}) \frac{(\vec{\nabla} V)^2}{2m}$$

- Classical interpretation: relation between the average energy transferred and the impulse given to each nucleon
  - Plane-wave field  $\rightarrow$  f-sum rule [book: Pines&Nozières, 1966]
- 
- ❖ Sound modes in nuclei: >50% of EWSR  $\rightarrow$  “**Giant resonances**” [book: Harakeh&van der Woude, 2000]

- ❖ RPA for sound waves
  - Nuclear sound
  - ph-RPA as linear-response theory
  
- ❖ Second RPA – The past 7 years... and beyond
  - SRPA and Thouless' theorem
  - Implications for first-order RPA
  - Remarks on density-functional theory
  
- ❖ Summary



## ❖ The purist

- Thy shall not use SRPA based on the Hartree-Fock reference state. It suffers from inconsistencies and instabilities.

## ❖ The practitioner

- If you are interested in [giant resonances / collective phonons, plasmons, ... / excitations exhausting most of the EWSR] it's fine, it will even give you some fine structure and energy corrections

## ❖ The contrarian

- Then why would I use RPA at all?
- When should I use what? I'm confused.

- PP, R.Roth, “*Second random-phase approximation and realistic interactions*”, Phys.Lett.B671(2009)356
- PP,R.Roth, “*Large-scale second random-phase approximation calculations with finite-range interactions*”, Phys.Rev.C81(2010)024317
- PP, “*Second random-phase approximation, Thouless’ theorem, and the stability condition re-examined and clarified*”, Phys.Rev.C90(2014)024305

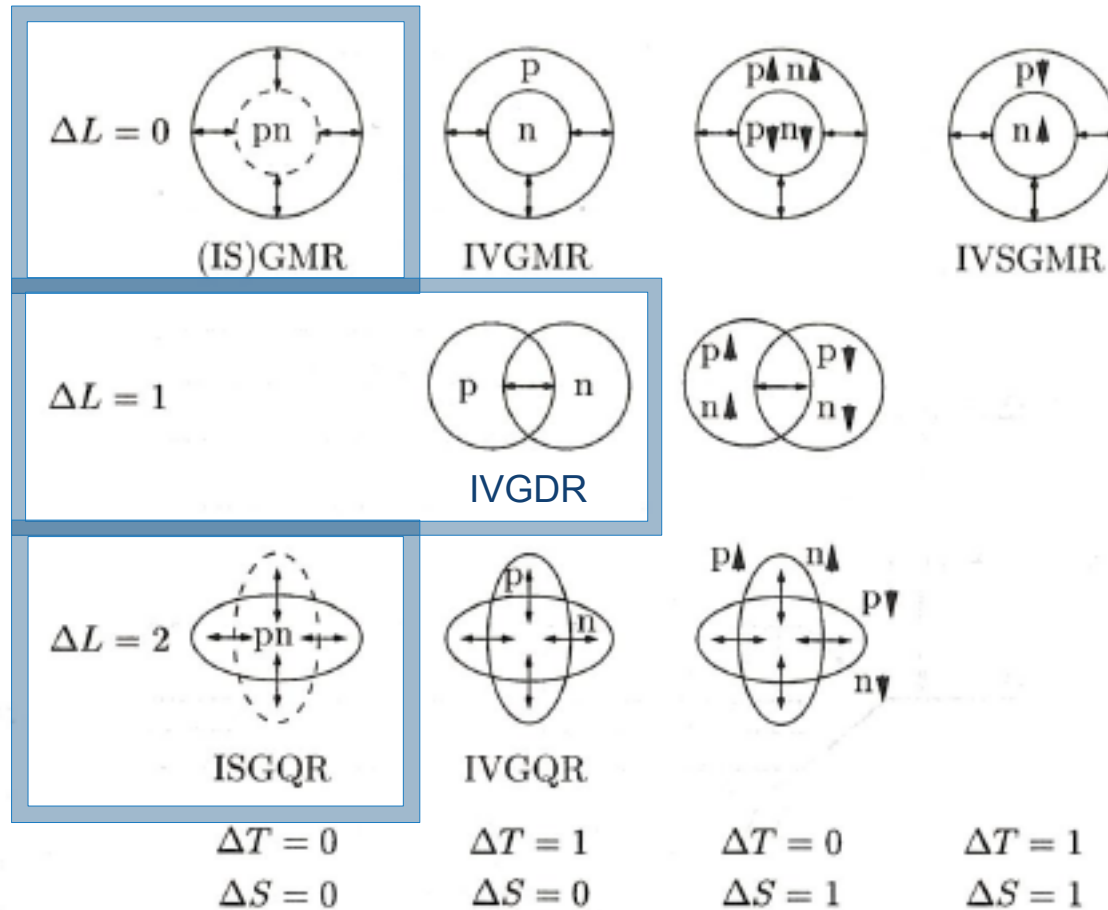
# *INTRODUCTION*

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Nuclear sound

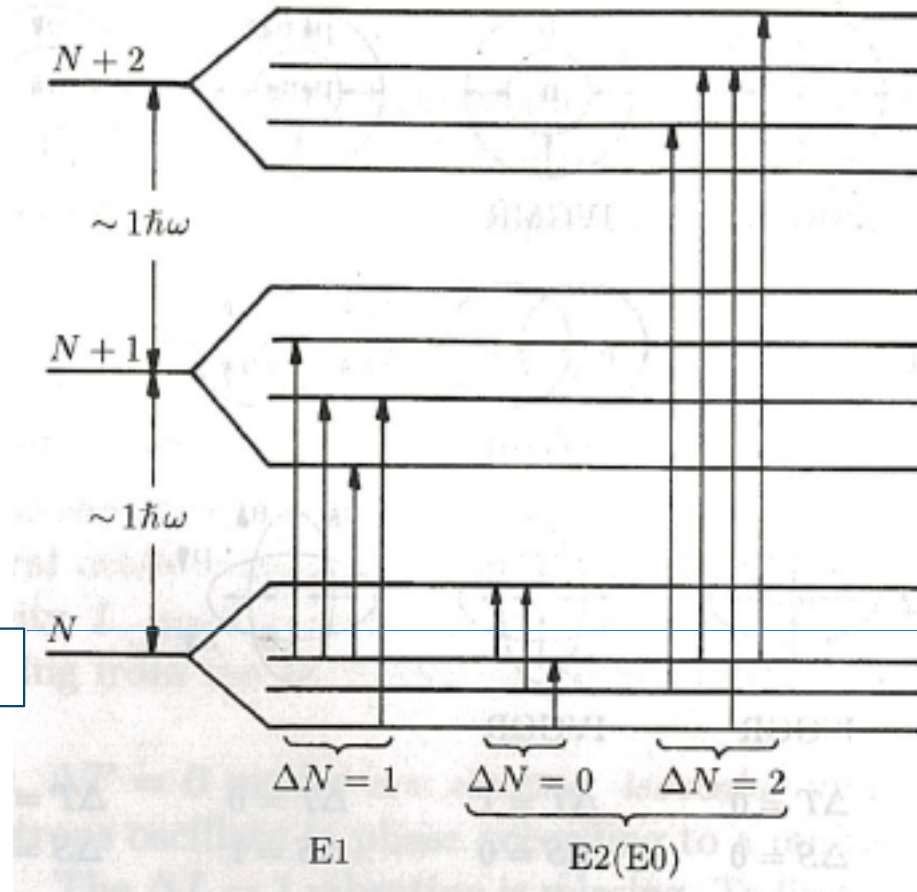
Derivation and properties of (S)RPA

# Nuclear Giant Resonances



[“Giant resonances” book by Harakeh and van der Woude]

# Nuclear Giant Resonances



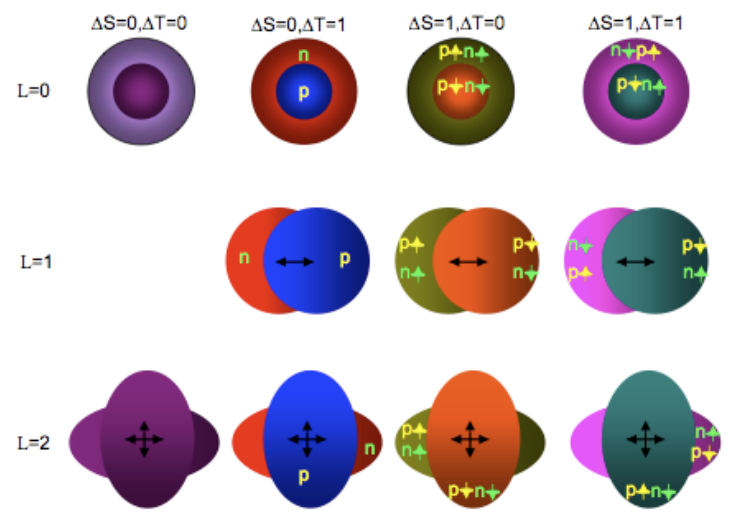
occupied (hole) states:

[“Giant resonances” book by Harakeh and van der Woude]

# Normal modes of vibration

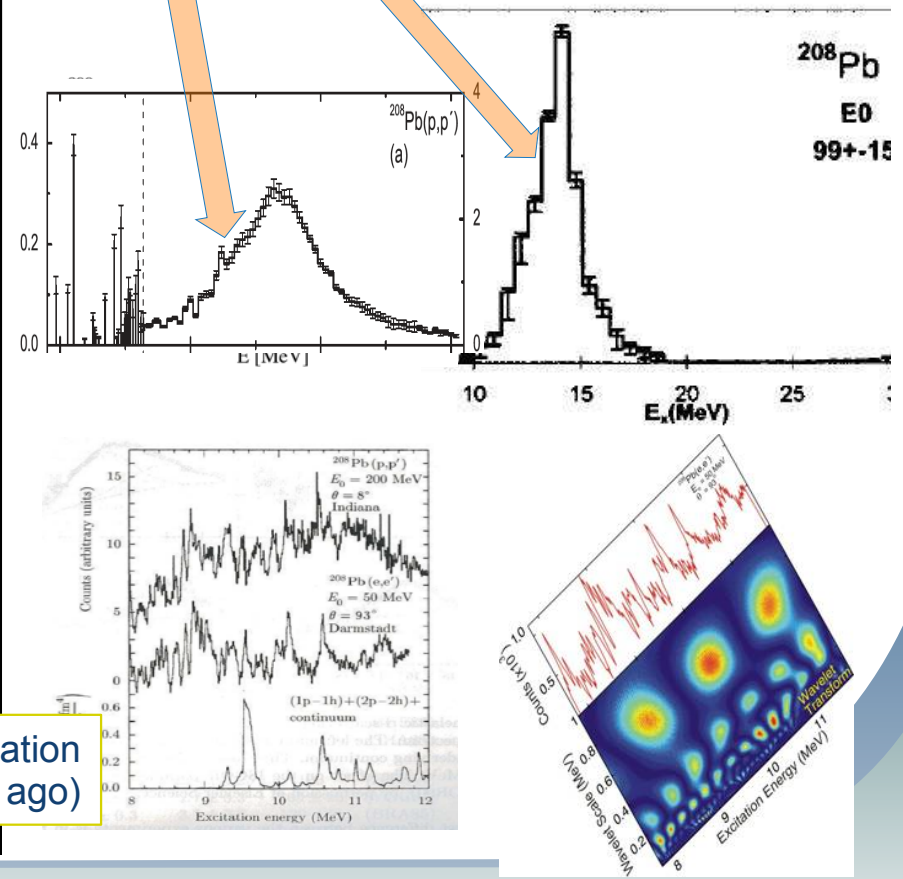
Major part of the EWSR

The simplified picture



SRPA explored to explain attenuation (~30yrs ago)

The reality



- 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  $|0\rangle = |\text{HF}\rangle$ : **HF-RPA**

- Vibration creation operator:

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

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

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

- RPA equations in  $ph$ -space:

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

$$A_{ph,p'h'} = \delta_{pp'}\delta_{hh'}(e_p - e_h) + H_{hp',ph'} \quad ; \quad B_{ph,p'h'} = H_{hh',pp'} \quad ;$$

For some in-medium  
Hamiltonian H

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

- Equivalent to small-amplitude Time-Dependent Hartree-Fock
- Linear Response Theory



- 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:

$$\langle \text{SRPA} | \dots | \text{SRPA} \rangle \rightarrow \langle \text{HF} | \dots | \text{HF} \rangle$$

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

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

$$A_{ph,p'h'} = \delta_{pp'} \delta_{hh'} (e_p - e_h) + H_{hp',ph'} ; \quad B_{ph,p'h'} = H_{hh',pp'}$$

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

$\mathcal{A}_{22}$ :  $\delta_{p_1 p'_1} \delta_{h_1 h'_1} \delta_{p_2 p'_2} \delta_{h_2 h'_2} (e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2})$  + interactions among  $2p2h$  states

For some in-medium Hamiltonian H

- 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:

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$$A_{ph,p'h'} = \delta_{pp'} \delta_{hh'} (e_p - e_h) + H$$

$\mathcal{A}_{12}$ : interactions between  $ph$

$$\mathcal{A}_{22}: \delta_{p_1 p_1'} \delta_{h_1 h_1'} \delta_{p_2 p_2'} \delta_{h_2 h_2'} (e_{p_1} +$$

**linear response with collision term**

$$\rho_{kl}(t) = \langle \psi(t) | a_l^+ a_k | \psi(t) \rangle$$

$$H = \sum_{kl} t_{kl} a_k^+ a_l + \frac{1}{4} \sum_{klpq} \bar{v}_{klpq} a_k^+ a_l^+ a_q a_p$$

$$i\hbar \frac{\partial}{\partial t} \rho_{kl}(t) = \langle \psi(t) | [a_l^+ a_k, H] | \psi(t) \rangle$$

- One-body density matrix
- Hamiltonian
- Equation of motion

$$\rho_{klpq}^{(2)}(t) = \langle \psi(t) | a_p^+ a_q^+ a_l a_k | \psi(t) \rangle$$

$$i\hbar \frac{\partial}{\partial t} \rho_{klpq}^{(2)}(t) = \langle \psi(t) | [a_p^+ a_q^+ a_l a_k, H] | \psi(t) \rangle$$

$$\rho_{klpq}^{(2)} = \rho_{kp} \rho_{lq} - \rho_{kq} \rho_{lp} + g_{klpq}$$

- Two-body density matrix
- Non-trivial part g

- Then EoM takes the form

$$i\hbar \frac{\partial}{\partial t} \rho_{kl}(t) - [h, \rho]_{kl} = I_{kl}$$

- With

$$h_{kl} = t_{kl} + U_{kl} \quad U_{kl} = \sum_{pq} \bar{v}_{kqlp} \rho_{pq}$$

- And a collision term

$$I_{kl} = \frac{1}{2} \sum_{prs} \bar{v}_{kprs} g_{rslp} - \bar{v}_{rslp} g_{kprs}$$

J.Wambach, Rep.Prog.Phys.51(1988)989

- Expand around equilibrium values:

$$\rho = \rho^0 + \delta\rho$$

$$g = g^0 + \delta g.$$

- Assume harmonic dependence:

$$\delta\rho = \delta\rho_{ph} e^{-i\omega t} + \delta\rho_{hp} e^{i\omega t}$$

$$\delta g = \delta g_{pp'hh'} e^{-i\omega t} + \delta g_{hh'pp'} e^{i\omega t}.$$

- Linearization of the EoM yields:

$$\left[ \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{A}^* \end{pmatrix} - \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} x^\nu \\ y^\nu \end{pmatrix} = 0$$

$$\mathcal{A} = \begin{pmatrix} A_{11'} & A_{12'} \\ A_{21'} & A_{22'} \end{pmatrix} \quad \mathcal{B} = \begin{pmatrix} B_{11'} & B_{12'} \\ B_{21'} & B_{22'} \end{pmatrix} \quad x^\nu = \begin{cases} \delta\rho_{ph} = X_{ph}^\nu \\ \delta g_{pp'hh'} = X_{pp'hh'}^\nu \end{cases} \quad y^\nu = \begin{cases} \delta\rho_{hp} = Y_{ph}^\nu \\ \delta g_{hh'pp'} = Y_{pp'hh'}^\nu \end{cases}$$

- Linear response with collision term:

$$i\hbar \frac{\partial}{\partial t} \delta\rho_{kl}(t) = [h^0, \delta\rho]_{kl} + \left[ \frac{\delta h}{\delta\rho} \delta\rho, \rho_0 \right]_{kl} + \left[ \frac{\delta I}{\delta\rho} \delta\rho, \rho_0 \right]_{kl}$$

J.Wambach, Rep.Prog.Phys.51(1988)989

[D.J.Rowe, Rev.Mod.Phys.40(1968)153]  
[D.J.Thouless, Nucl.Phys.22(1961)78]

❖ Solutions appear in adjoint pairs

❖ If the stability condition is satisfied,

$$\langle 0|[F^\dagger, [H, F]]|0\rangle = \sum_{ab} F_a^* M_{ab} F_b \geq 0$$

solutions are real

❖ The EWSR is preserved  $\left( \sum_n (E_n - E_0) |\langle 0|V|n\rangle|^2 = \int d^3r \rho_0(\vec{r}) \frac{(\vec{\nabla}V)^2}{2m} \right)$

$$\sum_{n:N_n=1} |\langle 0|O|n\rangle|^2 E_{n0} = \frac{1}{2} \langle 0|[O, H, O]|0\rangle$$

❖ ... and therefore spurious transitions have zero energy (restoration of symmetries)

*|HF) = vacuum of ph states → stability of RPA for physical states*

# Formal properties of RPA...

[D.J.Rowe, Rev.Mod.Phys.40(1968)153]  
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- ❖ Solutions appear in adjoint pairs
- ❖ If the stability condition is satisfied,

$$\langle 0 | [F^\dagger, [H, F]] | 0 \rangle > 0$$

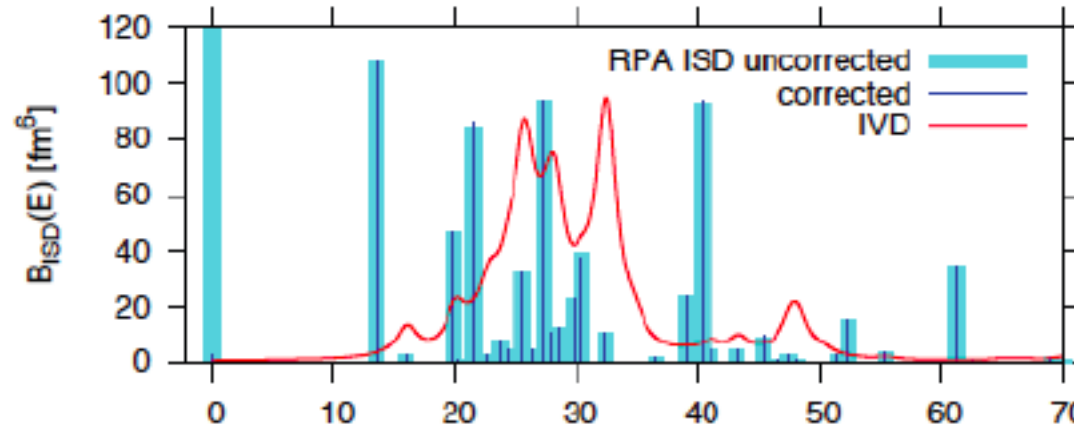
ISD corrected radial operator  $r^3 - \frac{5}{3} \langle r^2 \rangle r$  vs  $r^3$

solution

- ❖ The EV

$$\sum_{n: N_n}$$

- ❖ ... and t (restoration of symmetries)



energy

|HF) = vacuum of ph states → stability of RPA for physical states

As is the case with the simple RPA,<sup>2</sup> the search for formal properties of the second RPA is greatly simplified by the fact that the second RPA excitation operator  $O_v^\dagger$ —which creates a one-phonon state—satisfies the following double-commutator equation:

$$\langle \text{HF} | [R, [H, O_v^\dagger]] | \text{HF} \rangle = \hbar\omega_v \langle \text{HF} | [R, O_v^\dagger] | \text{HF} \rangle, \quad (1)$$

for all  $R$ ,

where  $\hbar\omega_v$  is the excitation energy,  $|\text{HF}\rangle$  is the Hartree-Fock ground state of the nucleus, and  $R$  is any operator in the same space as  $O_v^\dagger$ .  $H$  is the exact many-body Hamiltonian.

$$O_v^\dagger = \sum_{mi} [Y_{mi}(\omega_v) a_m^\dagger a_i - Z_{mi}(\omega_v) a_i^\dagger a_m] + \sum_{m < n, i < j} [Y_{mnij}(\omega_v) a_m^\dagger a_n^\dagger a_j a_i - Z_{mnij}(\omega_v) a_i^\dagger a_j^\dagger a_n a_m]. \quad (2)$$

C.Yannouleas, PRC35(1987)1159

Equipped with Eqs. (1) and (2), one can repeat the steps in Sec. III of Ref. 2 and show that all the formal properties familiar from the simple RPA hold for the zero-temperature second RPA as well. In particular, these formal properties are the following:

- (1) The solutions of the second RPA appear in pairs having symmetric positive and negative eigenvalues.
- (2) The second RPA solutions have real energies when Thouless's stability condition is fulfilled.
- (3) Spurious solutions reflecting the center-of-mass motion separate out and have exactly zero energy.
- (4) The second RPA solutions are orthonormal.
- (5) The nonspurious second RPA solutions form a complete set.
- (6) The matrix elements of any operator  $W$  calculated in the second RPA preserve the energy-weighted sum rule.

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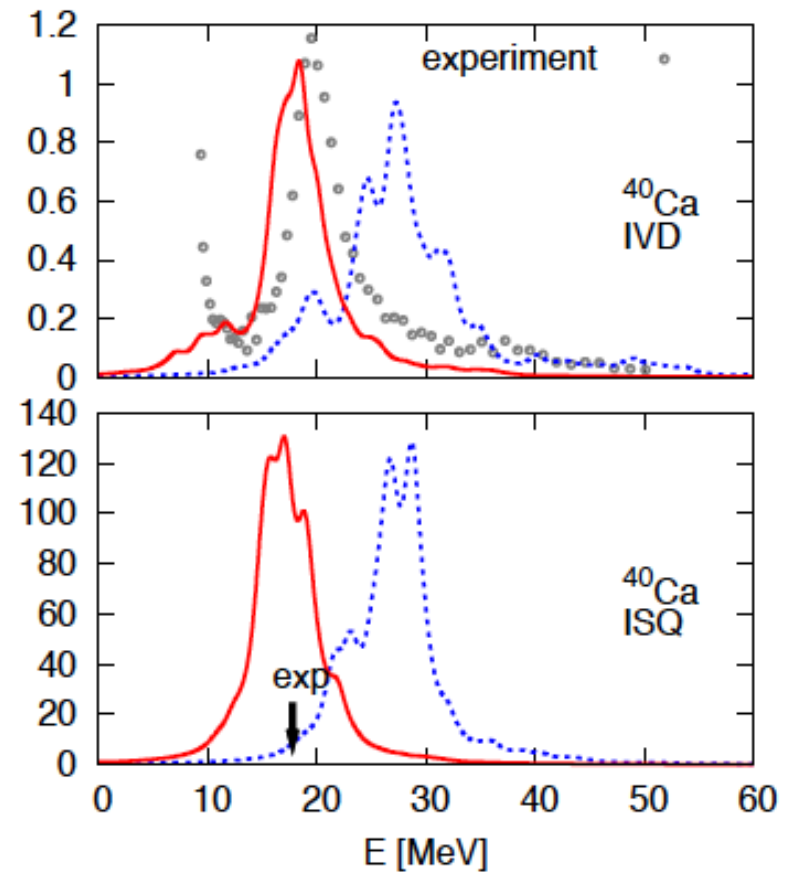
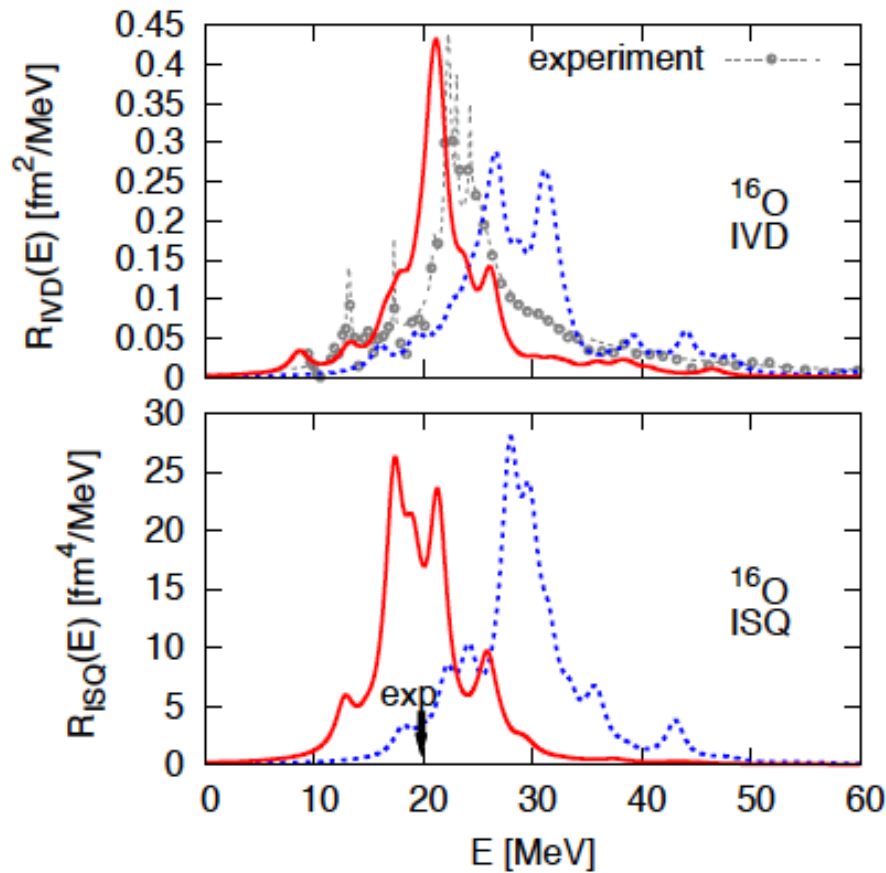
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$|\text{HF}\rangle$  NOT the vacuum of  $2p2h$  states  $\rightarrow ?$



- Softened realistic Hamiltonian (UCOM)
- No arbitrary truncations
- Explored: Energetic shift; EWSR; ph fragmentation; etc.



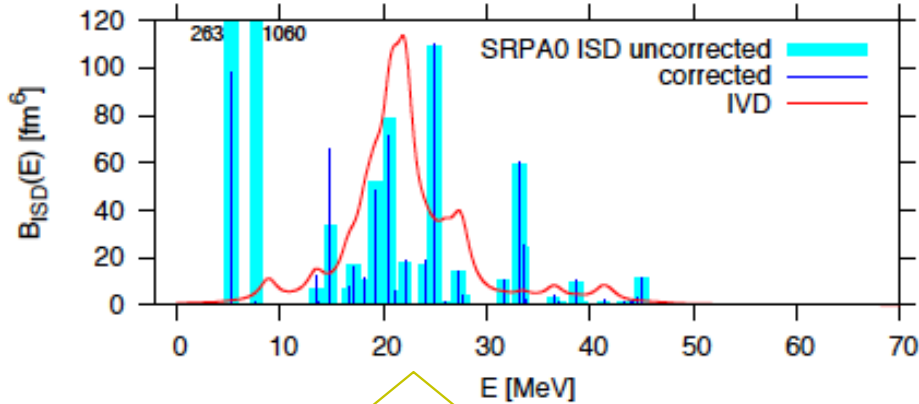
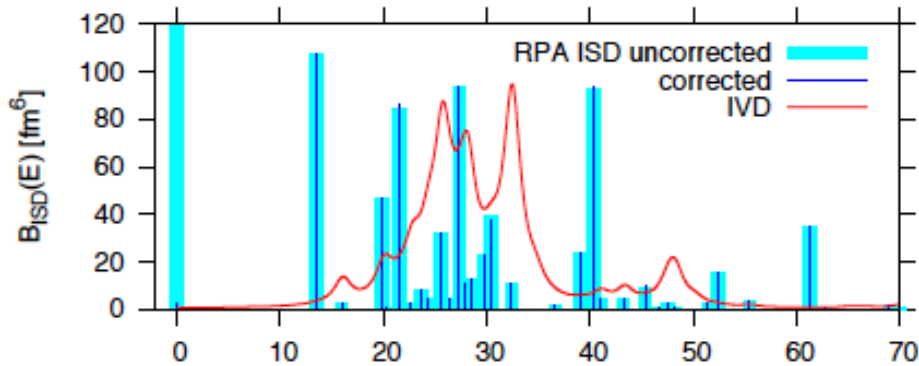
# *VALIDITY OF SRPA*

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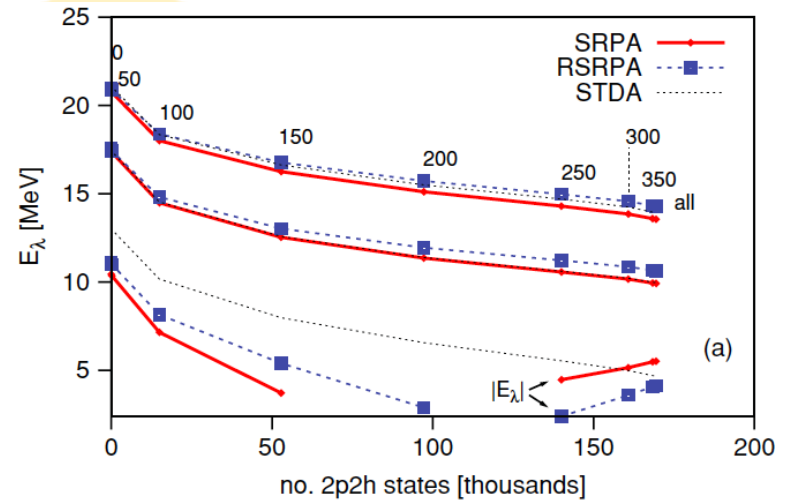
What is at issue?

# Spurious states and instabilities in SRPA

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



spurious admixtures



$R_{VD}(E)$  [ $\text{fm}^2 \text{MeV}$ ]

Instability of low-energy states

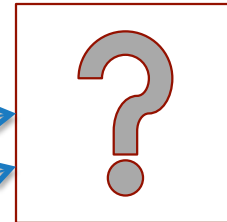


# Formal properties: like RPA?

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C.Yannouleas, PRC35(1987)1159



We found:

- instances of imaginary  $3^-$ ,  $2^+$
- spurious state at finite energy

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C.Yannouleas, PRC35(1987)1159



We found:

- instances of imaginary 3-, 2+
- spurious state at finite energy

**It is not!**

P.P., PRC90(2014)024305

- ❖ **Thouless' theorem still holds:** if all eigenvalues are **real**, the EWSR satisfies

$$\sum_{\nu: N_{\nu}=1} |\langle \nu | O | 0 \rangle|^2 E_{\nu} = \frac{1}{2} \langle 0 | [O, H, O] | 0 \rangle$$

- ❖ For  $H$  commuting with  $O$ , this means that the total EWSR must vanish.

- ❖ **Q: Then how come there is spurious strength at finite energy?**

- ❖ **A: Positive-energy solutions with negative norm may exist:**

- (Their negative-energy counterparts will have positive norm)

- Pairs of « antinormal » solutions:  $N_{\nu} E_{\nu} < 0$

$$|X_{\nu}|^2 - |Y_{\nu}|^2 = N_{\nu} = \pm 1$$

- ❖ **Their contribution to the energy-weighted sum is *negative***

- ❖ **As a result, a spurious state can contribute a finite but negative amount to the total spurious EWSR, such that the total spurious EWSR still vanishes -> Thouless' theorem indeed holds (demonstrated numerically)**

- ❖ **Thouless' theorem still holds:** if all eigenvalues are **real**, the EWSR satisfies

$$\sum_{\nu: E_{\nu} > 0} |\langle \nu | O | 0 \rangle|^2 N_{\nu} E_{\nu} = \frac{1}{2} \langle 0 | [O, H, O] | 0 \rangle$$

- ❖ For  $H$  commuting with  $O$ , this means that the total EWSR must vanish.

- ❖ **Q: Then how come there is spurious strength at finite energy?**

- ❖ **A:** Positive-energy solutions with negative norm may exist:

- (Their negative-energy counterparts will have positive norm)

- Pairs of « antinormal » solutions:  $N_{\nu} E_{\nu} < 0$

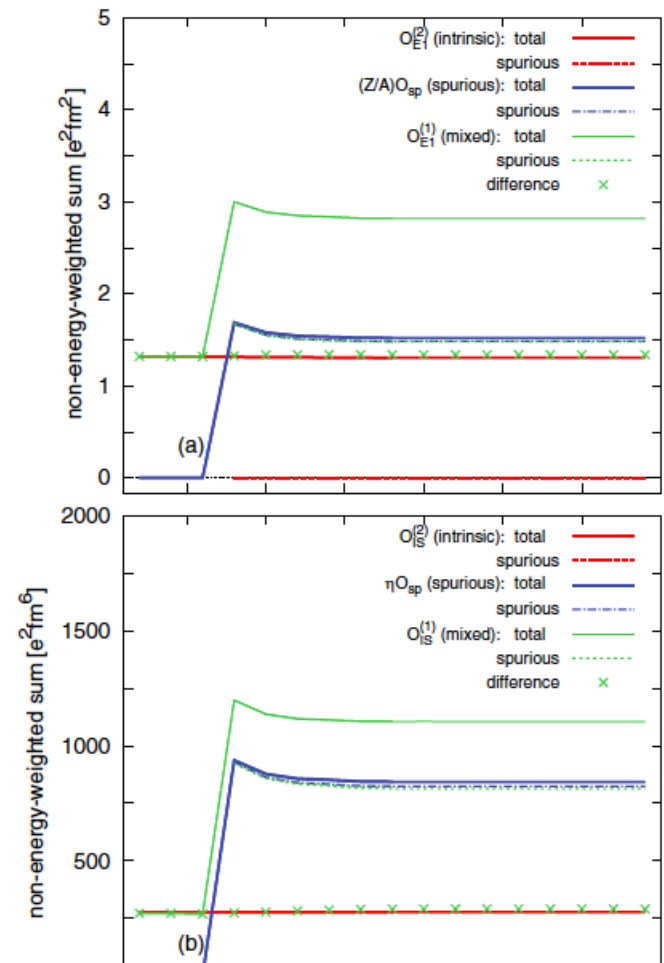
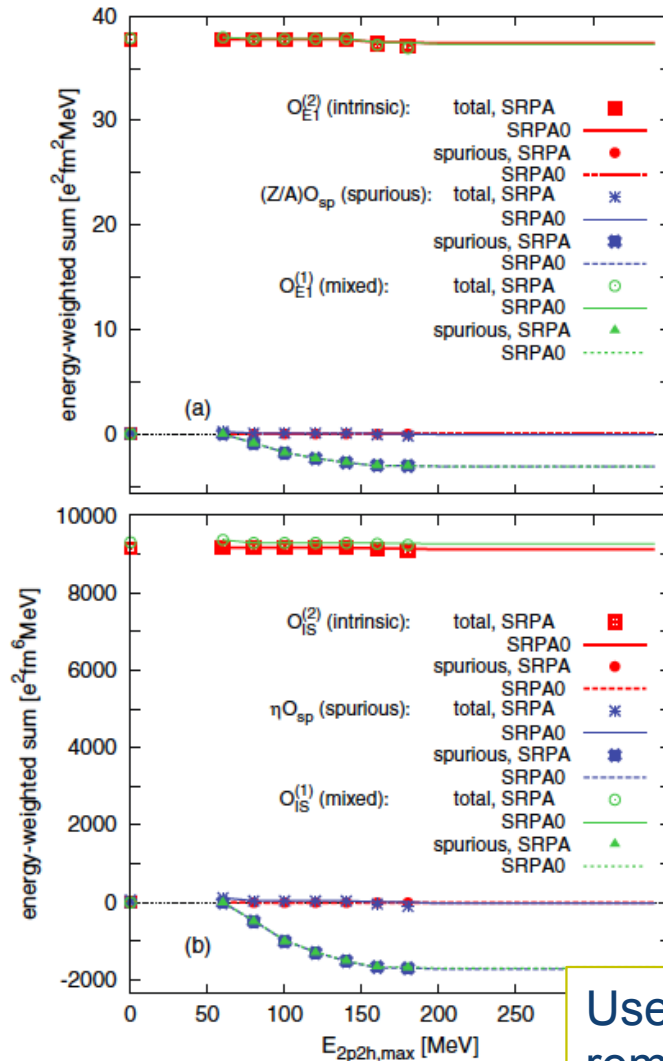
$$|X_{\nu}|^2 - |Y_{\nu}|^2 = N_{\nu} = \pm 1$$

- ❖ **Their contribution to the energy-weighted sum is *negative***

- ❖ As a result, a spurious state can contribute a finite but negative amount to the total spurious EWSR, such that the total spurious EWSR still vanishes -> Thouless' theorem indeed holds (demonstrated numerically)

# Spurious strength in SRPA

PP, PRC90,024305



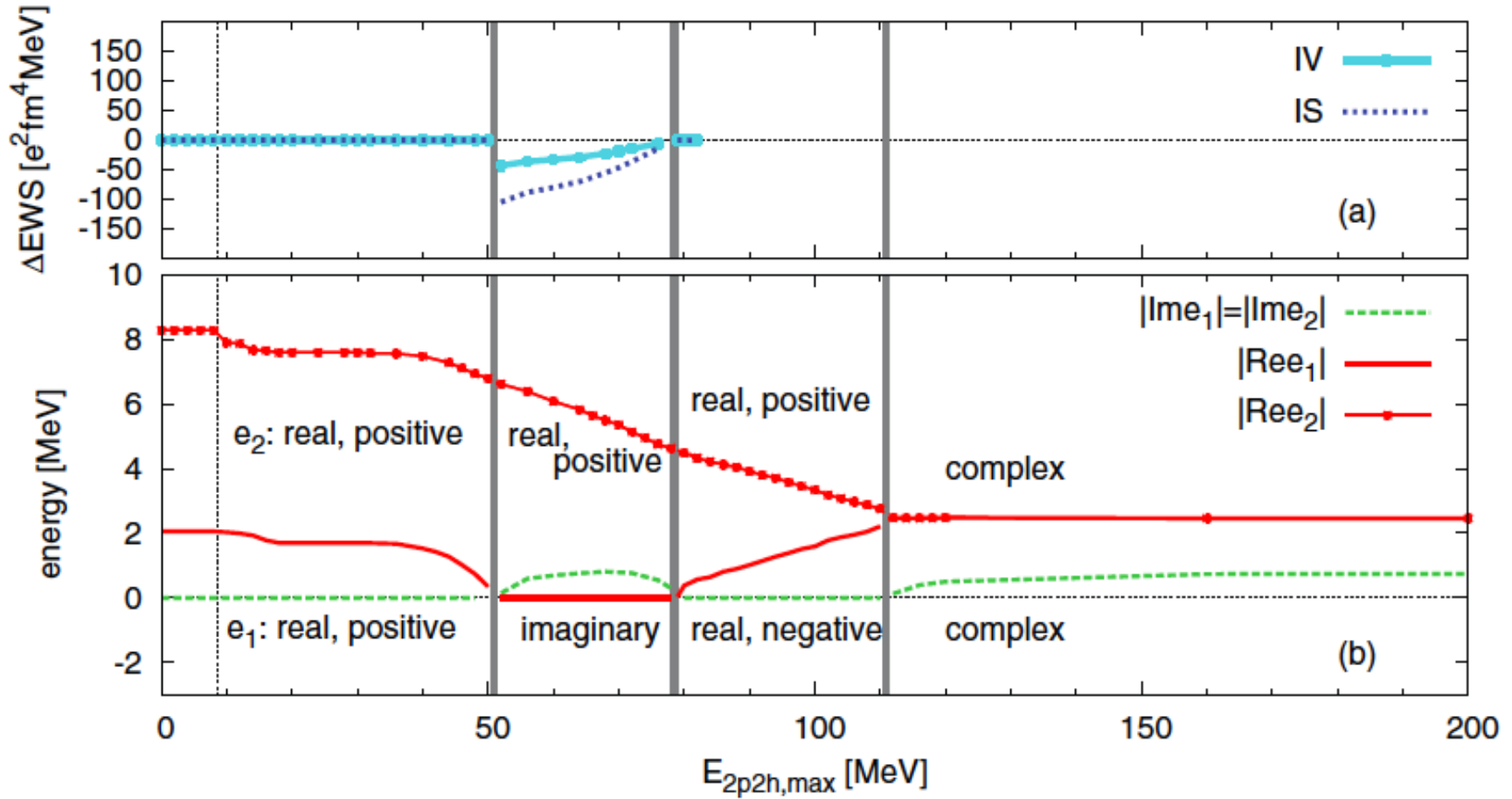
Use of intrinsic (corrected) operators  
remove spurious admixtures efficiently



# Numerical validation of Thouless' theorem

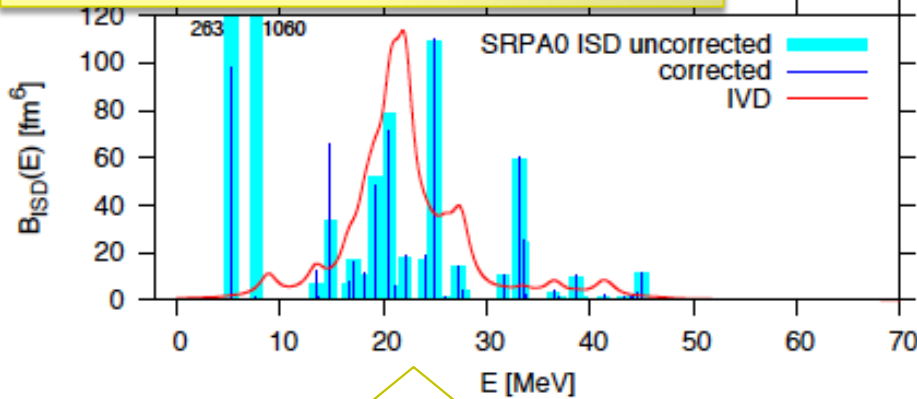
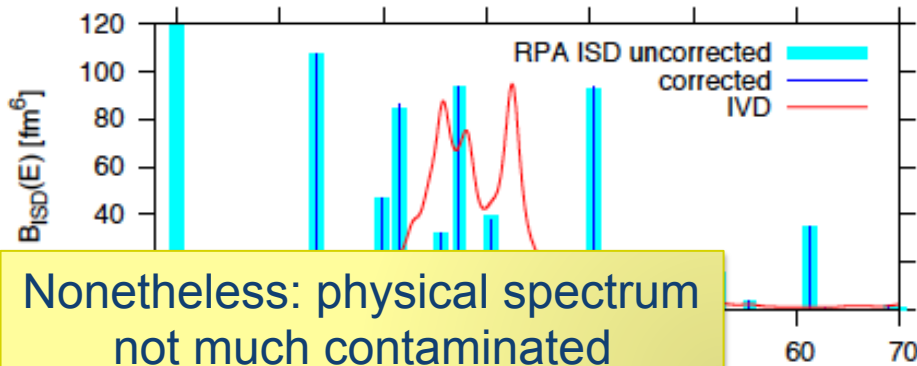
PP, PRC90,024305

$2^+$  of  $^{48}\text{Ca}$ :

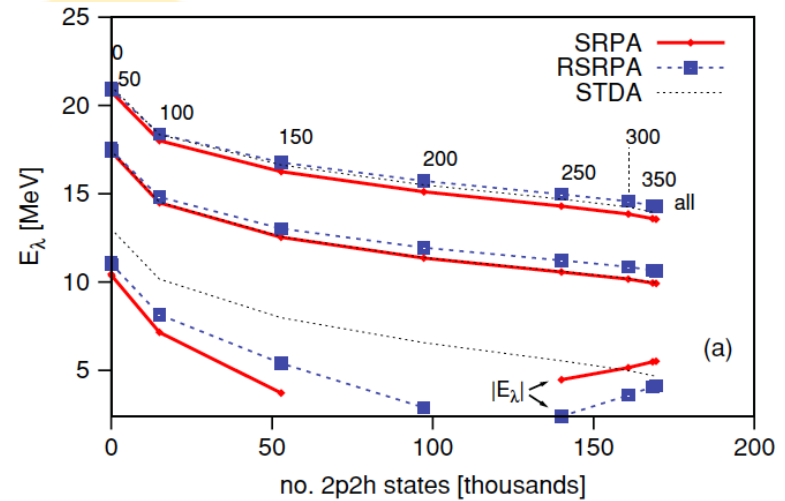


# Spurious states and instabilities in SRPA

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



spurious admixtures

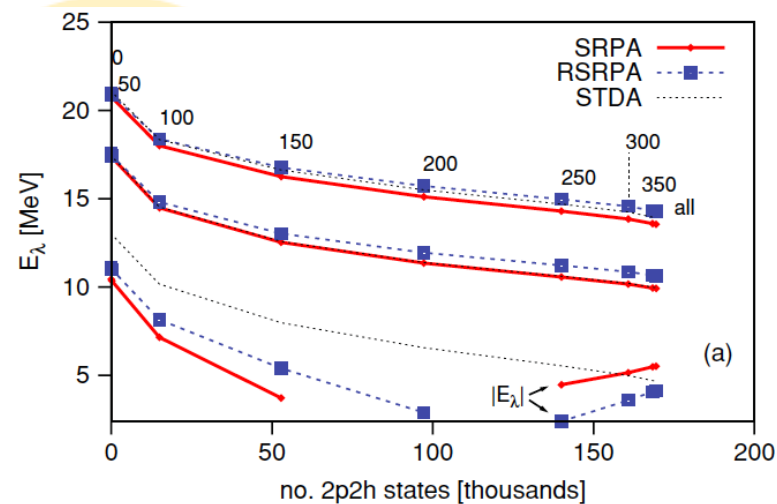
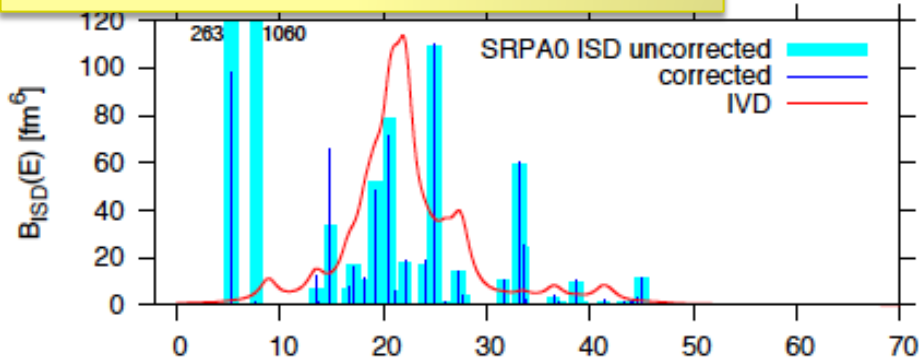
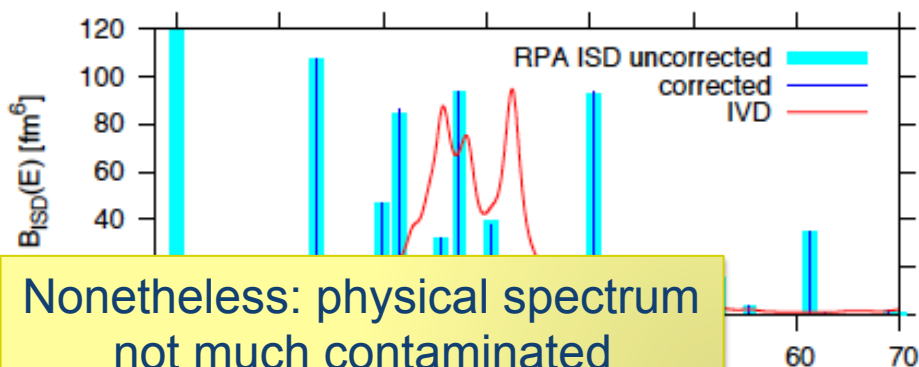


Instability of low-energy states



# Spurious states and instabilities in SRPA

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



$R_{IVD}(E)$  [fm<sup>2</sup>MeV]

Instability of low-

yet to do:  
self-consistent  
second-order  
formalism

- Correlated ground state [P.Tohyama, P.Schuck; N.Pillet et al.]
- Subtraction method [Tselyev, ...]

spurious admixtures

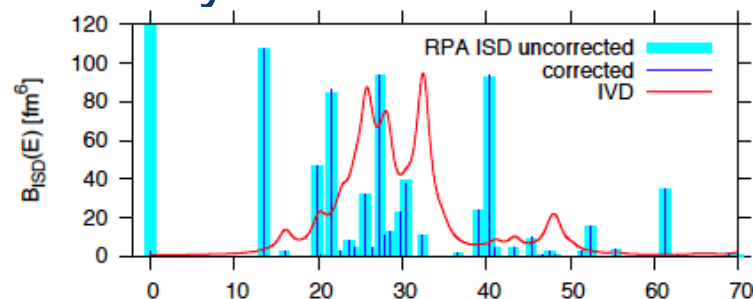
# *SOME THINGS I DON'T UNDERSTAND YET*

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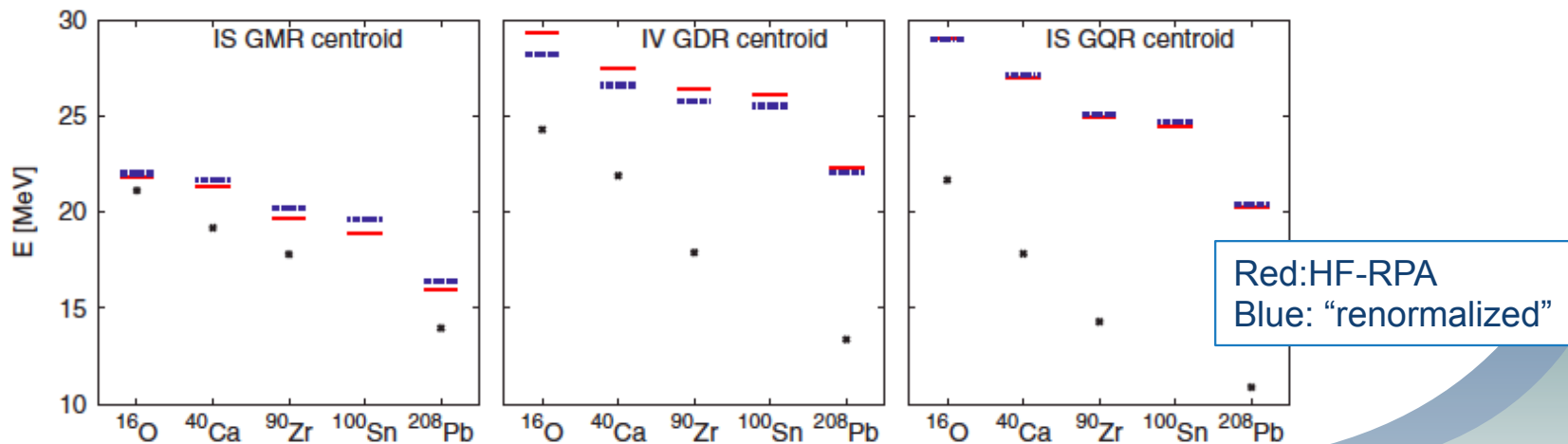
The importance of the reference state

❖ HF reference state ensures consistency and good properties

- |HF) = vacuum of ph states → stability of RPA for physical states
- RPA = small-amplitude TDHF



❖ Quality of quasi-boson approximation



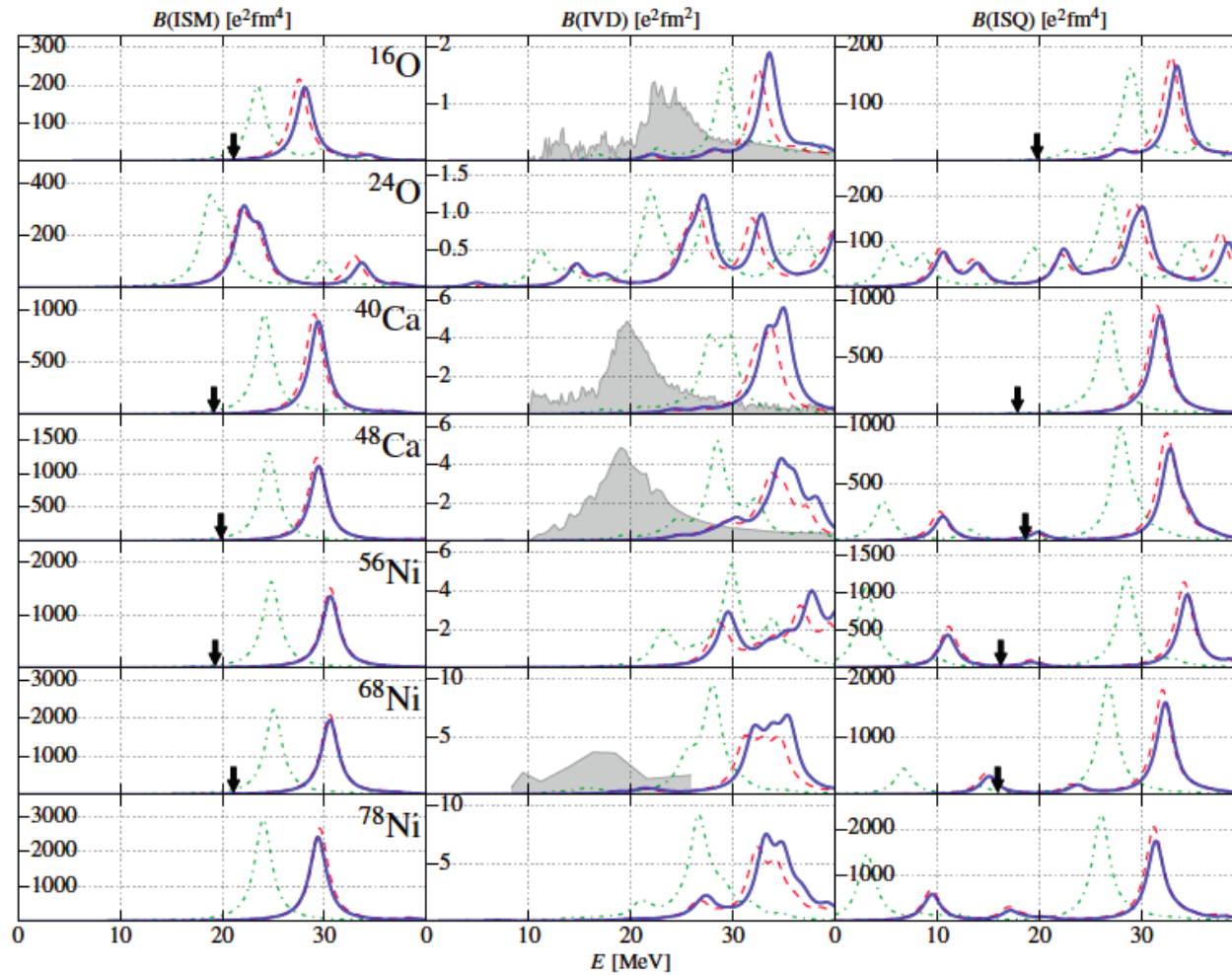


Figure 8.28: Results from HF-RPA (---), CC-RPA (---), IM-RPA (—). Here we use the EM400 interaction ( $\alpha = 0.08 \text{ fm}^4$ ) with  $e\text{Max} = 12$ ,  $E3\text{Max} = 14$  and  $\hbar\Omega = 24 \text{ MeV}$ .

# HF-SRPA vs IM-SRPA (no instabilities?)

R. Trippel, PhD Thesis, TUD, 2016

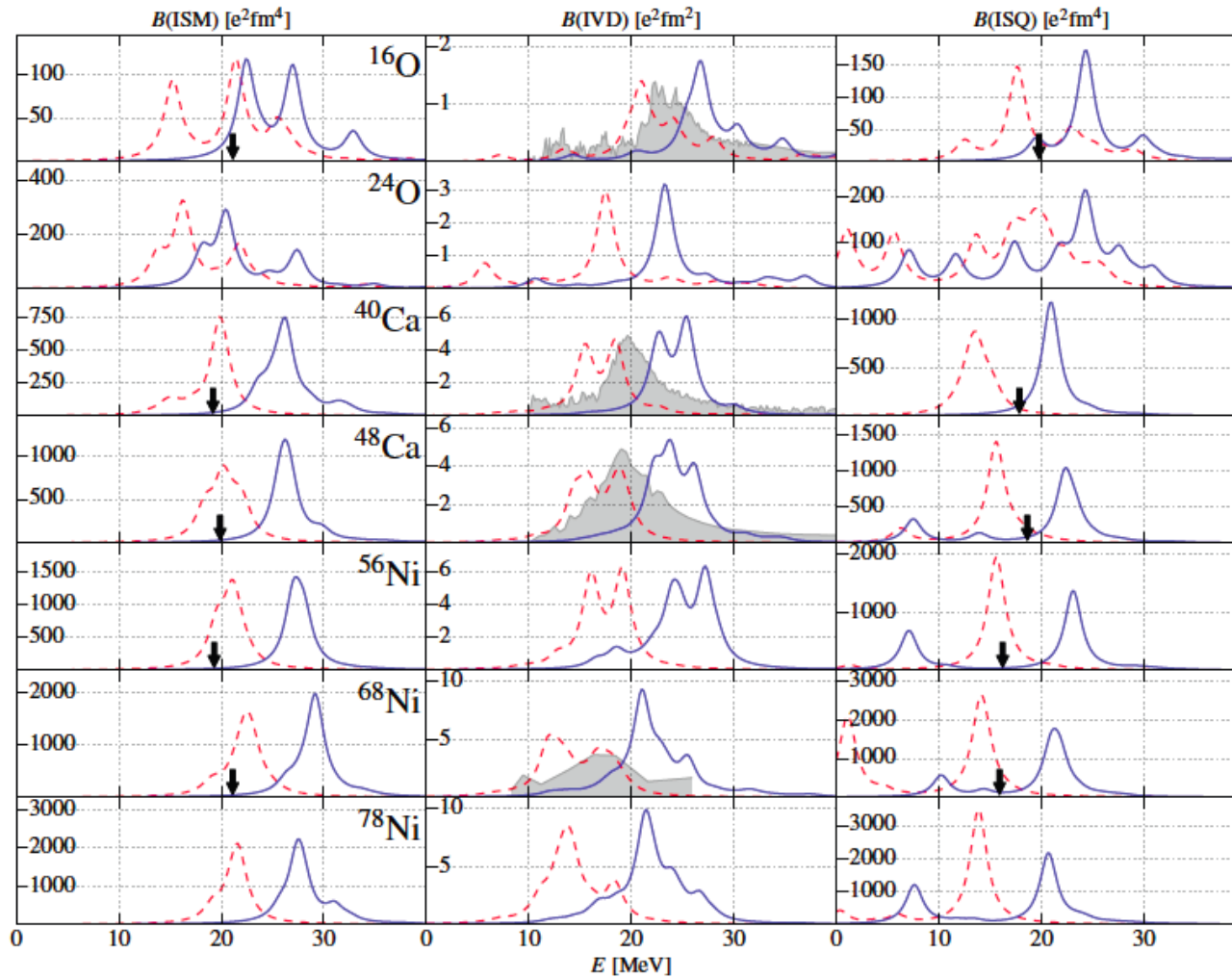


Figure 8.30: Comparison of results from HF-SRPA (---) and IM-SRPA (—). Here we use the SAT interaction ( $\alpha = 0.08 \text{ fm}^4$ ) with  $e\text{Max} = 12$ ,  $E3\text{Max} = 14$  and  $\hbar\Omega = 22 \text{ MeV}$ .

# *CONCEPTUAL ISSUES*

---

RPA or SRPA?



- ❖ The purist
  - Thy shall not use SRPA based on the Hartree-Fock reference state. It suffers from inconsistencies and instabilities.
- ❖ The practitioner
  - If you are interested in [giant resonances / collective phonons, plasmons, ... / excitations exhausting most of the EWSR] it's fine, it will even give you some fine structure and energy corrections
- ❖ The contrarian
  - Then why would I use RPA at all?
  - When should I use what? I'm confused.

- ❖ Interested in one-particle observables only
  - Single-particle density encodes **implicitly** all relevant information.
  - Then:  $E[\rho]$ ; HF, RPA; (SRPA superfluous?)
    - If I determine  $E[\rho]$  indirectly (from fits to data), I do not need to solve the A-particle Schrödinger equation!
    - Density fluctuations:  $E[\rho_0 + \delta\rho] \approx E[\rho_0] + \delta\rho E'[\rho_0]$ : linear response
- ❖ Interested **explicitly** in two-particle observables
  - E.g., 2-phonon states; width of GRs, collisions
  - Two-particle density relevant
  - Then:  $E[\rho, g]$ ; correlated ground state, SRPA

- ❖ Given interaction + many-body method
  - Variational reference state + Equations of Motion
  - To lowest order, HF+RPA
  - Systematic inclusion of correlations / mp-mh until convergence

- *“Wave-function approach” [JT]*
- *Known Hamiltonian*

- ❖ Energy-density functionals + linear-response theory

- *Kohn-Sham EFT [JT]*
- *$E[\rho, \dots]$  known; Hamiltonian not necessarily known*
- *“black box” [AG]*

- The order of truncation depends on the application

- Homogeneous matter -> Ansatz:  $k_F$  powers
- Nuclear EDF by **reverse engineering**
- Success in dilute and dense matter and **nuclear ground states**
- **Poster by Hana Gil!**

❖ KIDS = Korea: IBS - Daegu - Sungkyunkwan

❖ ( ń : Kyungpook - IBS - Daegu - Sungkyunkwan )



## ❖ The purist

- Thy shall not use SRPA based on the Hartree-Fock reference state. It suffers from inconsistencies and instabilities.

## ❖ The practitioner

- If you are interested in [giant resonances / collective phonons, plasmons, ... / excitations exhausting most of the EWSR] it's fine, it will even give you some fine structure and energy corrections

## ❖ The contrarian

- Then why would I use RPA?
- When should I use what?

*RPA:*

- *Kohn-Sham EFT*
- *$E[\rho]$  known somehow*
- *Hamiltonian not necessarily known*
- *"black box"*

## ❖ The purist

- Thy shall not use SRPA based on the Hartree-Fock reference state. It suffers from inconsistencies and instabilities.

## ❖ The practitioner

- If you are interested in [giant resonances / collective phonons, plasmons, ... / excitations exhausting most of the EWSR] it's fine, it will even give you some fine structure and energy corrections

## ❖ The contrarian

- Then why would I use RPA
- When should I use SRPA

*RPA:*

- *Kohn-Sham EFT*
- *$E[p]$  known somehow*

*necessarily known*

*SRPA, etc:*

- *“Wave-function approach”*
- *Known, perturbative Hamiltonian*

## ❖ The purist

- Thy shall not use SRPA based on the Hartree-Fock reference state. It suffers from inconsistencies and instabilities.

## ❖ The practitioner

- If you are interested in [giant resonances / collective phonons, plasmons, ... / excitations exhausting most of the EWSR] it's fine, it will even give you some fine structure and energy corrections

## ❖ The contrarian

- Then why would I use RPA?
- When should I use SRPA, etc:

RPA:

- Kohn-Sham EFT
- *E[p] known somehow*

*necessarily known*

SRPA, etc:

*"Many function approach"*

*In the middle:*

*Good E[p] and RPA; interested in fragmentation: subtraction method?*

Thank you!

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