Shapes and Symmetries in Nuclei: from Experiment to Theory

6-10 November 2017, Gif-sur-Yvette

Marcella Grasso

A beyond-mean-field description for nuclear excitation spectra: Second RPA (including 2 particle-2 hole configurations in the energy-density-functional approach)

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Collaborators
(work on beyond mean-field)

- F. Catara (Catania Univ.), G. Co' (Lecce univ.), V. De Donno (Lecce Univ.),D. Gambacurta (ELI, Bucharest), J. Engel (North Carolina), O. Vasseur (IPN Orsay)

SRPA with zero-range and finite-range effective interactions and Implementation with a subtraction procedure

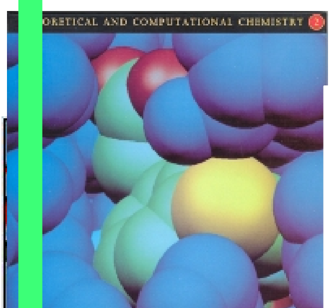
SRPA

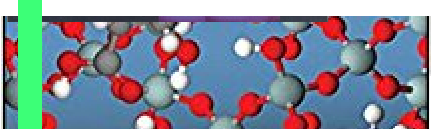
- J. Bonnard (IPN Orsay), G. Colo' (Milano Univ.), U. van Kolck (IPN Orsay), D. Lacroix, (IPN Orsay), X. Roca-Maza (Milano Univ.), J. Yang (IPN Orsay)

Nuclear interaction designed for beyond mean field

Work on the density functional

Density Functional Theory in chemistry and solid state physics

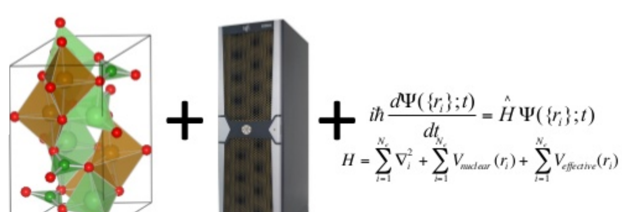




EDF as a DFT for decades … but in practice …

Nuclear many-body problem with effective interactions

Energy Density Functional (EDF) theory (functionals derived in most cases from effective phenomenological interactions adjusted at the mean-field level)

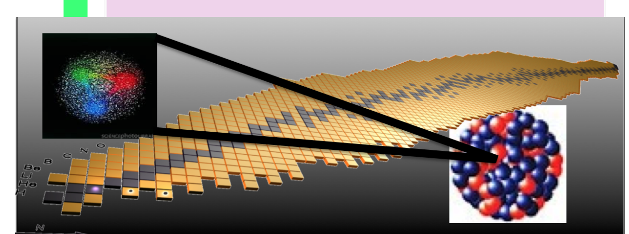


Beyond mean field

Necessary to go beyond a DFT-like strategy.
Double counting, divergences …

-Models

-Functionals/Interaction (Bridging with EFT/ ab initio)



Outline

- Beyond RPA with the second RPA (SRPA) model employing effective phenomenological interactions such as Skyrme or Gogny interactions
- Implementation of the SRPA model. Application of a subtraction method to handle double counting, instabilities and ultraviolet divergences
- Some results for nuclear excitations. Dipole excitations in ^{48}Ca
- Conclusions and perspectives

SRPA model : formally established since several decades

$$Q_\nu^\dagger = \sum_{ph} \left(X^\nu_{ph} a^\dagger_p a_h - Y^\nu_{ph} a^\dagger_h a_p \right) + \sum_{p<p',h<h'} \left(X^\nu_{php'h'} a^\dagger_p a_h a^\dagger_{p'} a_{h'} - Y^\nu_{php'h'} a^\dagger_h a_p a^\dagger_{h'} a_{p'} \right)$$

Excitation operators: 2p2h configurations are included, together with the RPA 1p1h configurations

- Hoshino and Arima, Phys. Rev. Lett. 37, 266 (1976)
- Knupfer and Huber, Z. Phys. A 276, 99 (1976)
- Adachi and Yoshida, Nucl. Phys. A 306, 53 (1978)
- Tohyama, Gong, Z. Phys.A 332, 269 (1989)
- Lacroix, Ayik, Chomaz, Prog. Part. Nucl. Phys. 52, 497 (2004)
- Schwesinger, Wambach, Phys. Lett. B 134, 29 (1984)
- Schwesinger, Wambach, Nucl. Phys. A 426, 253 (1984)
- Wambach, Rep. Prog. Phys. 51, 989 (1988)
- Drozdz, Nishizaki, Speth, Wambach, Phys. Rep. 197, 1 (1990)
- Nishizaki and Wambach, Phys. Lett. B 349, 7 (1995)
- Nishizaki and Wambach, Phys. Rev. C 57, 1515 (1998)

Examples of first applications for the calculation of fragmentation and spreading widths (strong cuts in the 2p2h space, Second Tamm-Dancoff, truncations and approximations in the 2p2h sector of the matrix)

No approximations in 2p2h matrix elements and large 2p2h cutoff values

- Papakonstantinou and Roth, Phys. Lett. B 671, 356 (2009)
- Papakonstantinou and Roth, Phys. Rev. C 81, 024317 (2010)

Microscopic interaction (derived from Argonne V18)

- Gambacurta, Grasso, and Catara, Phys. Rev. C 81, 054312 (2010)
- Gambacurta, Grasso, and Catara, J. Phys. G 38, 035103 (2011)
- Gambacurta, Grasso, and Catara, Phys. Rev. C 84, 034301 (2011)
- Gambacurta, Grasso, De Donno, Co, and Catara, Phys. Rev. C 86 021304(R) (2012)

Phenomen. Skyrme and Gogny interactions

SRPA model

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

Schematically: same form as RPA equations

$$\mathcal{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

$$\mathcal{X}^\nu = \begin{pmatrix} X_1^\nu \\ X_2^\nu \end{pmatrix}, \quad \mathcal{Y}^\nu = \begin{pmatrix} Y_1^\nu \\ Y_2^\nu \end{pmatrix}.$$

1 and 2:

short-hand notation for 1p1h and 2p2h

A_{11} and B_{11}: standard RPA matrices

A_{12}, A_{21}, B_{12}, and B_{21}: coupling between 1p1h and 2p2h

A_{22} and B_{22}: 2p2h sector

SRPA with density-dependent forces

New rearrangement terms with respect to RPA

(Waroquier et al., Phys. Rep. 148, 249 (1987), Adachi and Yoshida, Phys. Lett. B 81, 98 (1979))

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

where:

$$\mathcal{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \mathcal{B} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},$$

Through a variational derivation of SRPA with density-dependent forces:

Gambacurta, Grasso, Catara, J. Phys. G: Nucl. and Part. Phys. 38, 035103 (2011)

Variational procedure to derive the SRPA equation, formulated it in the case of a density-dependent interaction

$$|\Psi\rangle = e^{\hat{S}}|\Phi\rangle$$

HF state

$$\hat{S} = \sum_{ph} C_{ph}(t) a_p^\dagger a_h + \frac{1}{2} \sum_{php'h'} \hat{C}_{pp'hh'}(t) a_p^\dagger a_{p'}^\dagger a_h a_{h'}.$$

$$\hat{C}_{\alpha\beta\gamma\delta} = C_{\alpha\beta\gamma\delta} - C_{\alpha\beta\delta\gamma}$$

-The coefficients C are used as variational parameters (minimization of the expectation value of the Hamiltonian)

-The coefficients C are assumed very small => expansion of the expectation values of 1- and 2-body operators truncated at the second order in C

Gambacurta, Grasso, Catara, J. Phys. G: Nucl. and Part. Phys. 38, 035103 (2011)

For cases where the interaction is density independent and with A_{22} diagonal:

$$\Omega^{SRPA} \begin{bmatrix} A_{11'}(\omega) & B_{11'} \\ -B^*_{11'} & -A^*_{11'}(\omega) \end{bmatrix} \qquad \Omega^{RPA} \begin{bmatrix} A_{11'} & B_{11'} \\ -B^*_{11'} & -A^*_{11'} \end{bmatrix}$$

where the energy-dependent matrix elements are

$$A_{11'}(\omega) = A_{11'} + \sum_{2} A_{12}(\omega + i\eta - A_{22})^{-1} A_{2\,1'}$$

↑

Second-order self-energy insertion -> leads to a beyond mean-field model and provides the description of spreading widths and fragmentation (in addition to the single-particle Landau damping) through de coupling with 2p2h

Drawbacks of the SRPA model (two are general and two are associated with the choice of specific interactions)

- (Too) strong shift to lower energies with respect to the RPA spectrum

- Instabilities (Thouless theorem)

Recent studies about instabilities and double counting:

- Tselyaev, Phys. Rev. C 88, 054301 (2013)
- Papakonstantinou, Phys. Rev. C 90, 024305 (2014)

EDF and double counting for extensions of RPA (Tselyaev)

- **Correlations implicitly included in the functional (because of the adjustment of the parameters at mean-field level to reproduce some observables). In the spirit of DFT: 'universal exact functional for a mean-field-like calculation'**

- **Thus, this functional must produce a static RPA response function which is the 'exact' zero-energy response function.**

- **Any modification of the response function (to go beyond the mean field) should be zero in the static limit to avoid double counting of correlations**

Response function in RPA and SRPA

RPA derived as small-amplitude limit of TDHF equations

$$i\hbar\dot{\rho} = [\, h[\rho] + f(t), \rho \,]$$

h -> 1-body HF Hamiltonian
f -> external field

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} \rho^{(1)ph} \\ \rho^{(1)hp} \end{pmatrix} = - \begin{pmatrix} f^{ph} \\ f^{hp} \end{pmatrix}$$

$$\rho^{(1)ph}(\Omega_\nu) =< 0|a_p^\dagger a_h|\nu >$$

Transition density

By inverting these equations one defines the response function or polarization operator R,

$$\rho^{(1)kl} = \sum_{pq} R_{klpq}(\omega) f^{pq}$$

and the dynamic polarizability

$$\Pi(\omega) = \sum_{pqp'q'} f^{pq*} R_{pqp'q'}(\omega) f^{p'q'}$$

Response function in RPA and SRPA

RPA

$$R^{RPA}(E) = \begin{pmatrix} E - A & -B \\ -B & -E - A \end{pmatrix}^{-1}$$

SRPA

$$R^{SRPA}(E) = \frac{1}{\begin{pmatrix} E - A & -B \\ -B & -E - A \end{pmatrix} - \begin{pmatrix} \Sigma(E) & 0 \\ 0 & \Sigma(E) \end{pmatrix}}$$

Density-independent interaction

Σ(E) -> energy-dependent second-order self-energy

We require that

$$R^{SRPA}(0) = R^{RPA}(0)$$

This may be guaranteed by following the subtraction procedure by Tselyaev (the zero-energy second-order self-energy is subtracted)

$$A^S_{11'}(\omega) = A_{11'}(\omega) - E_{11'}(0)$$

Subtraction:

$$B^S_{11'}(\omega) = B_{11'}(\omega) - F_{11'}(0)$$

$$E_{11'}(\omega) = \sum_{2,2'} A_{12}(\omega + i\eta - A_{22'})^{-1} A_{2'1'} - \sum_{2,2'} B_{12}(\omega + i\eta + A_{22'})^{-1} B_{2'1'}$$

$$F_{11'}(\omega) = \sum_{2,2'} A_{12}(\omega + i\eta - A_{22'})^{-1} B_{2'1'} - \sum_{2,2'} B_{12}(\omega + i\eta + A_{22'})^{-1} A_{2'1'}$$

This also leads to the equality of the static polarizability in RPA and SRPA:

$$\Pi^{SRPA}(0) = \Pi^{RPA}(0) = -2m^{RPA}_{-1}$$

$$\alpha^{RPA} = -\Pi(0) = 2\sum_{\nu} \frac{|<\nu|F|0>|^2}{E_\nu - E_0} = 2m^{RPA}_{-1}$$

Adachi, Lipparini, Nucl. Phys. A 489, 445 (1988)

Stability condition in RPA (Thouless theorem, Nucl. Phys. 21, 225 (1960), Nucl. Phys. 22, 78 (1961))

If the HF state minimizes the expectation value of the Hamiltonian -> the RPA stability matrix is positive semi-definite **(real eigenvalues and eigenvectors with positive eigenvalues have positive norm)**

- **Double counting**

- **Instabilities (Thouless theorem)**

- **Strong shift downwards of energies (with respect to RPA) and divergences (with zero-range forces) ?**

Σ(E) - Σ(0)

The second-order self-energy is responsible for the divergence. The subtraction removes it: the self-energy has the same divergence at finite E and at E=0.

By following Tselayev 2013 ->

It is possible to rewrite the equations (after subtraction) in a non energy dependent SRPA form:

$$\mathcal{A}_F^S = \begin{pmatrix} A_{11'} + \sum_2 A_{12}(A_{22'})^{-1}A_{21'} + \sum_2 B_{12}(A_{22'})^{-1}B_{21'} & A_{12} \\ A_{21} & A_{22'} \end{pmatrix}$$

$$\mathcal{B}_F^S = \begin{pmatrix} B_{11'} + \sum_2 A_{12}(A_{22'})^{-1}B_{21'} + \sum_2 B_{12}(A_{22'})^{-1}A_{21'} & B_{12} \\ B_{21} & B_{22'} \end{pmatrix}$$

S -> subtracted
F -> full scheme (inversion of the matrix $A_{22'}$)

Gambacurta, Grasso, Engel, PRC 92, 034303 (2015)

SOME APPLICATIONS

SRPA including the subtraction procedure

Gambacurta, Grasso, Engel, PRC 92, 034303 (2015)

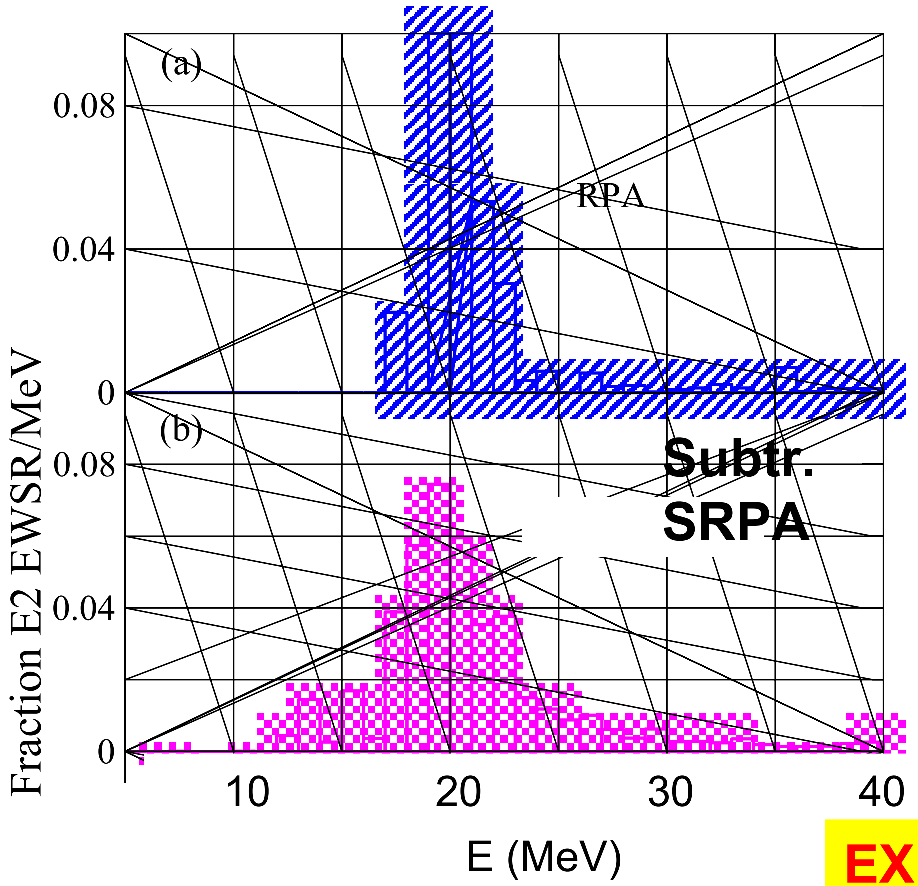
Gambacurta, Grasso Eur. Phys. J A 52 7, 198 (2016)

Gambacurta, Grasso, Vasseur, arXiv:1708.07083

Vasseur, Gambacurta, Grasso, in preparation

Quadrupole excitations. Spreading width

^{16}O



Centroid: 20.73 MeV
Width: 2.42 MeV

Centroid: 20.21 MeV
Width: 4.05 MeV

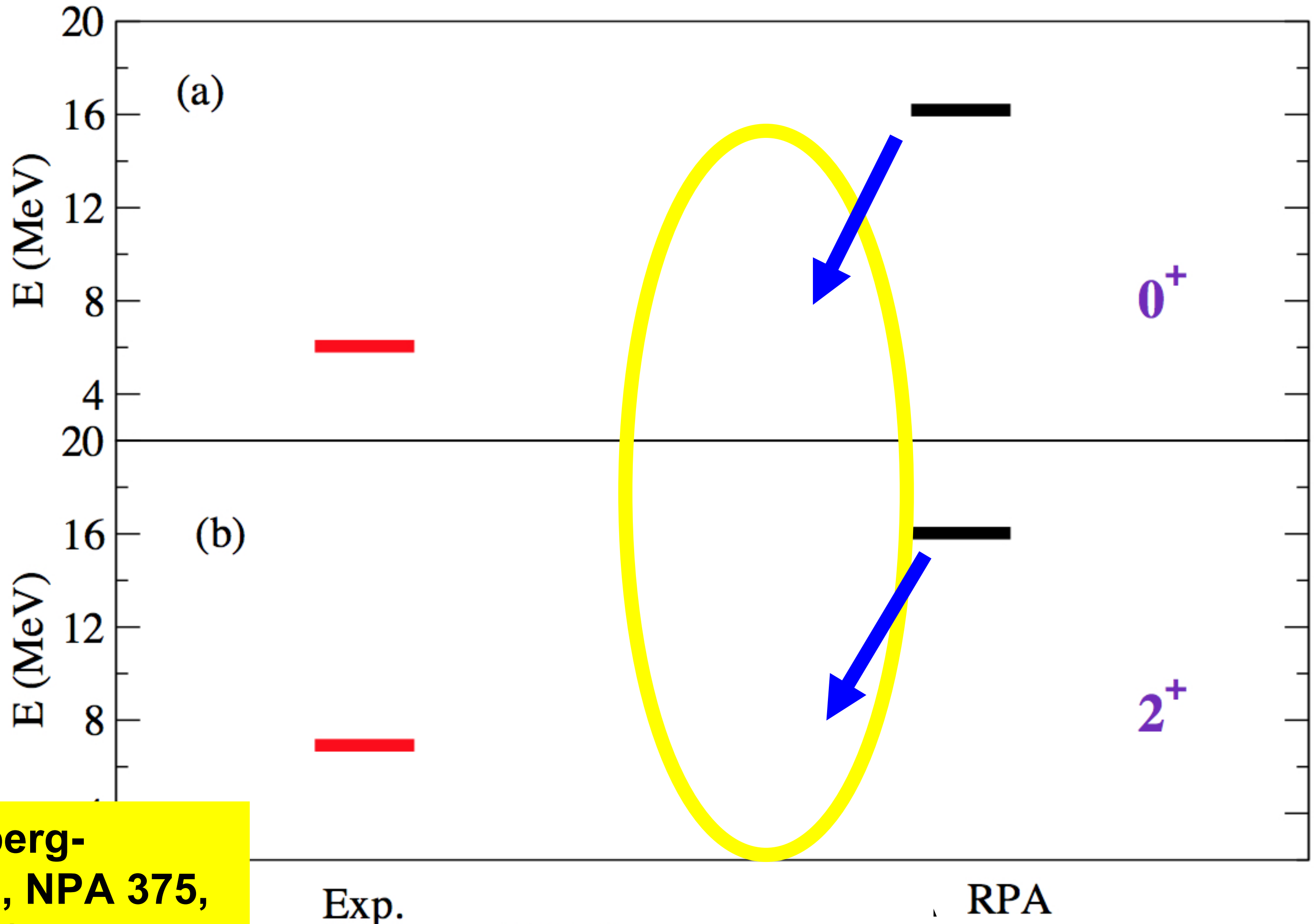
EXP: Lui, Clark, Youngblood, PRC 64, 064308 (2001)

Centroid: 19.76 MeV
Width: 5.11 MeV

Gambacurta, Grasso, Engel, PRC 92, 034303 (2015)

Low-lying states. Two-particle/two-hole states

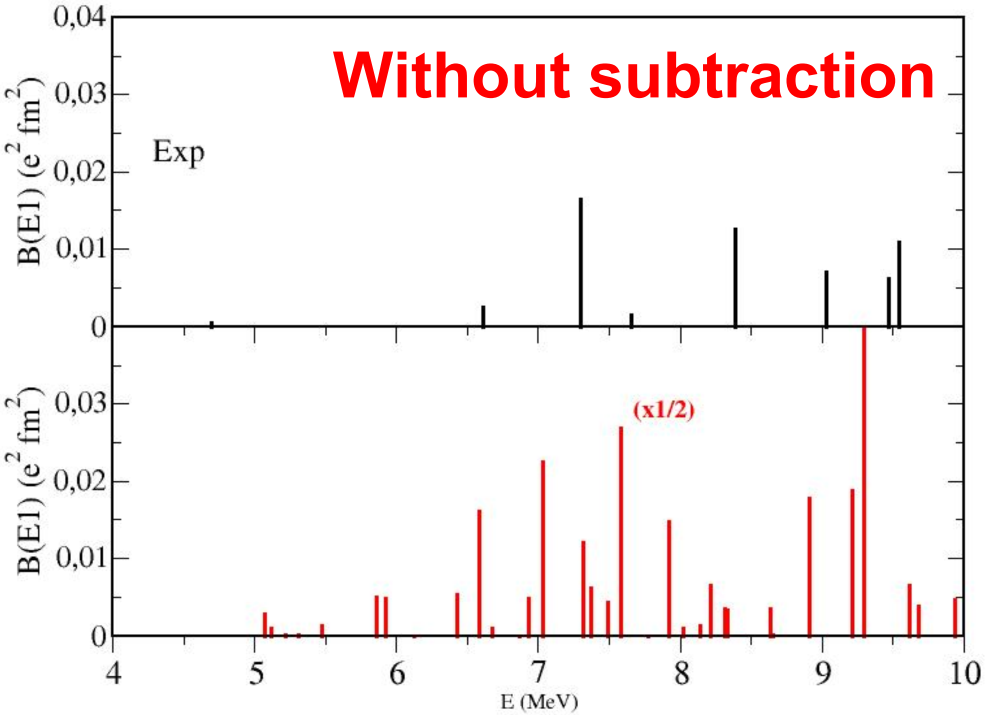
^{16}O



Ajzenberg-Selove, NPA 375, 1 (1985)

Gambacurta, Grasso, Engel, PRC 92, 034303 (2015)

Dipole low-lying response in ^{48}Ca



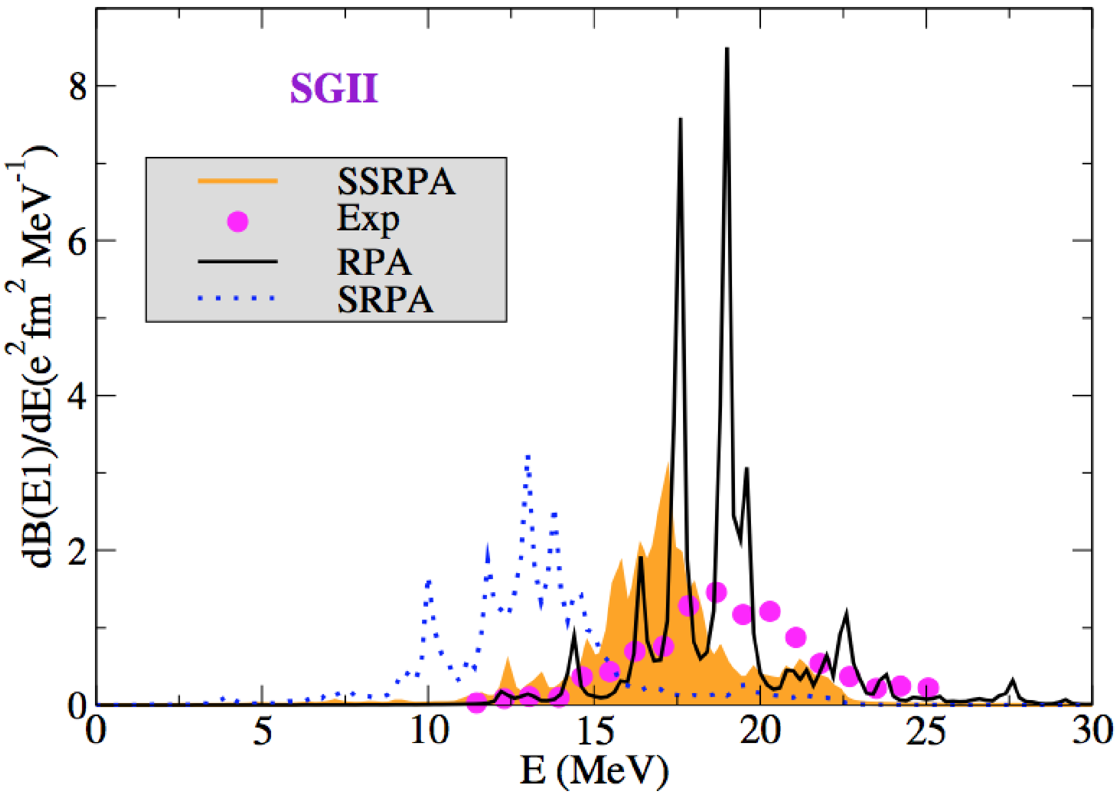
Exp: Hartmann et al., PRL 93, 192501 (2004)

(γ,γ') data at Darmstadt

Gambacurta, Grasso, Vasseur, arXiv:1708.07083

	Exp	SRPA SGII	SSRPA SGII	SRPA SLy4	SSRPA SLy4
Centroid					
$\sum B(E1)$	0.068 $\pm$ 0.008	0.563	0.078	1.012	0.126
$\sum_i E_i B_i(E1)$	0.570 $\pm$ 0.062	4.618	0.621	8.795	1.062

GDR in ^{48}Ca



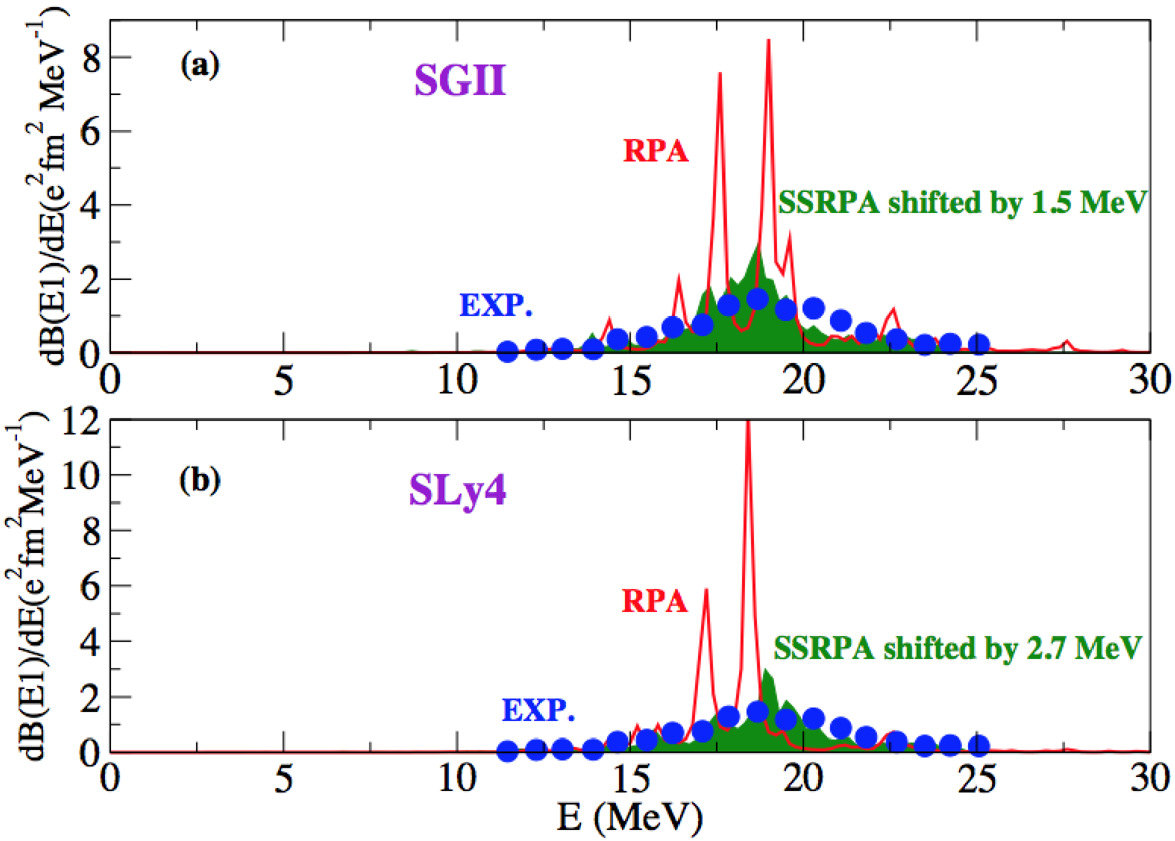
Exp centroid: 18.9 MeV
Exp width: 3.9 MeV

Exp: Birkhan et al., PRL 118, 252501 (2017)

(p,p') data at RCNP,Osaka

Gambacurta, Grasso, Vasseur, arXiv:1708.07083

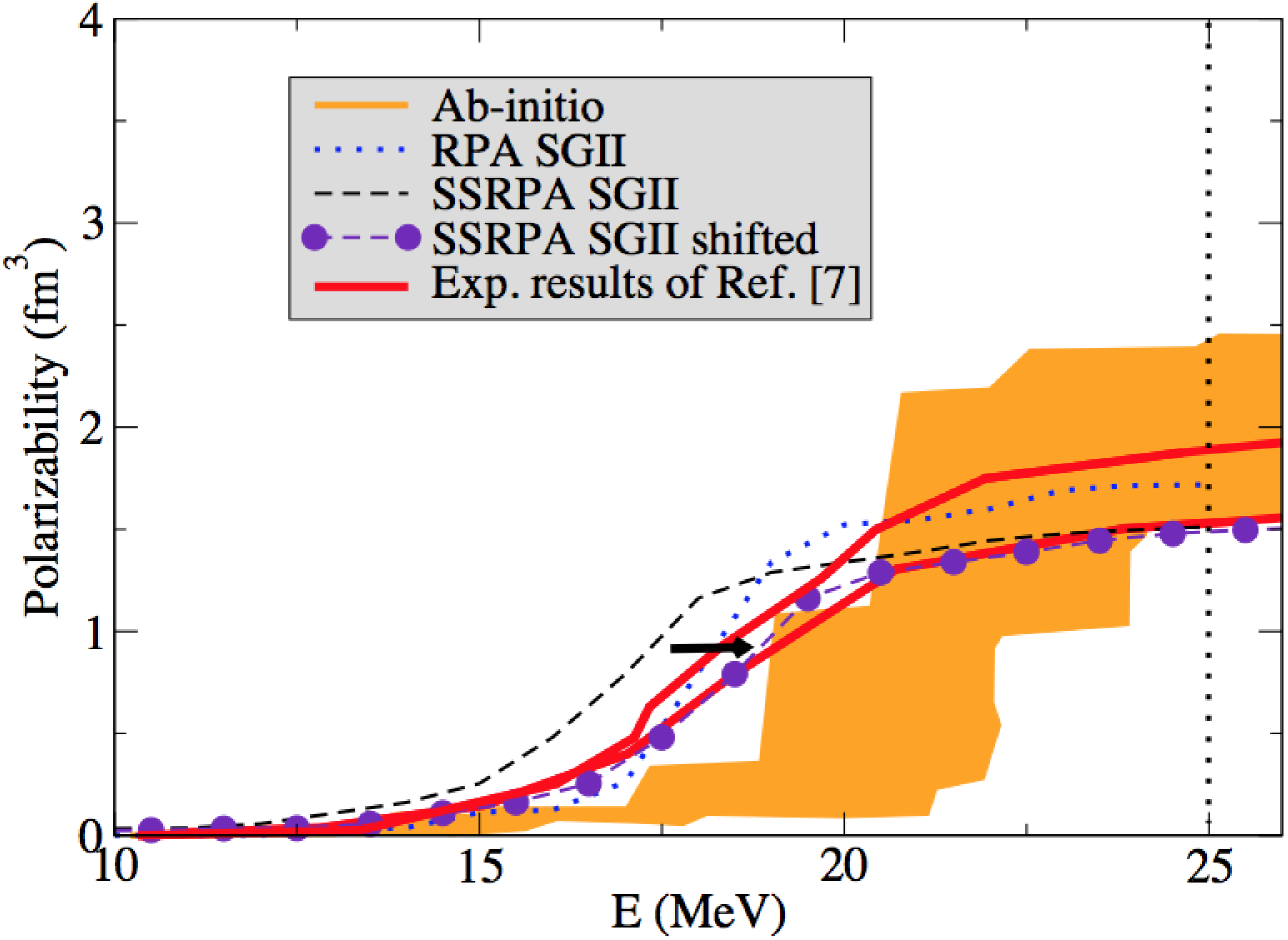
GDR in ^{48}Ca



Exp: Birkhan et al., PRL 118, 252501 (2017)

Gambacurta, Grasso, Vasseur, arXiv:1708.07083

Electric dipole polarizability (important for constraining the symmetry energy -> key ingredient for predictions of neutron skin thickness, radius and proton fraction in neutron stars, …)



$$\alpha_D = \frac{8\pi}{9}\int \frac{B(E1, E_x)}{E_x} dE_x.$$

Exp: Birkhan et al., PRL 118, 252501 (2017)

Gambacurta, Grasso, Vasseur, arXiv:1708.07083

Summary

- Implementation of the SRPA model by a subtraction procedure:
- Double counting
- Stability condition (correction of the shift with respect to the RPA)
- Convergence with respect to the cutoff

- Applications. Dipole response in ^{48}Ca
- Perspectives (SRPA with a correlated ground state -> PhD thesis of Olivier Vasseur) (the inclusion of correlations produces a subtractive term in the self-energy -> Takayanagi et al. Nucl. Phys. A477, 205 (1988))