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Nuclear structure with beyond-mean-field models

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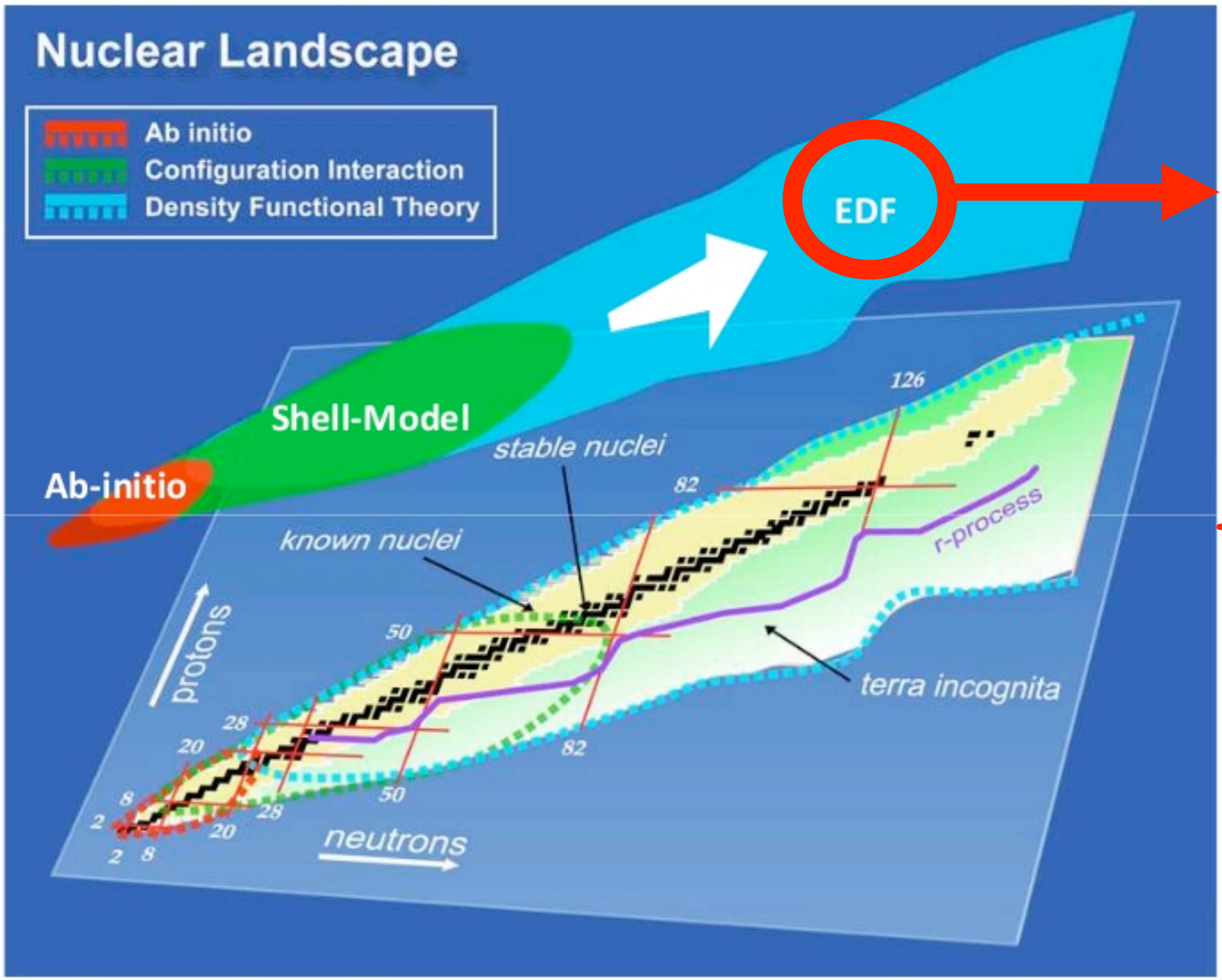
A unified theory for nuclear structure, reactions and stars

The Energy Density Functional (EDF) Concept



http://unedf.org/

- ***Mean field for ground-state nuclear structure (HF, HFB,..)***
- ***RPA and QRPA for small-amplitude oscillations***
- ***Beyond small-amplitude oscillations: time-dependent mean field for dynamics (TDHF, TDHFB,…)***
- ***Beyond-mean - field models (correlations).***

- Describing complex phenomena

- Improving the predictive power

Beyond-mean-field models.
Some examples

- **Single-particle and collective degrees of freedom are coupled** (generator-coordinate method, particle-vibration coupling,…)

- **Single-particle and multi-particle degrees of freedom are coupled** (variational multiparticle-multihole configuration mixing, second RPA, …)

- **Correlations are explicitly included in the ground state** (extensions of RPA, generator-coordinate method, variational multiparticle-multihole configuration mixing,…)

Going **beyond mean-field models** with

second random-phase approximation (SRPA): coupling with 2 particle - 2 hole configurations

Catania-Orsay collaboration

Content

- A natural extension of RPA. Second RPA (SRPA): richer form of the excitation operators (formal aspects)
- Residual interaction in the case of SRPA with density-dependent interactions
- First applications: ^{16}O and ^{48}Ca
- Conclusions and Perspectives

SRPA equations. The formal scheme is well established since many years

- Equations of motion method (Yannouleas, PRC 35, 1159 (1986))
- Small amplitude limit of Time Dependent Density Matrix (Tohyama and Gong, Z. Phys. A 332, 269 (1989); Lacroix et al., Prog. Part. Nucl. Phys. 52, 497 (2004))
- Variational procedure (Providencia, Nucl. Phys. 61, 87 (1965))

Currently employed approximations

- Second Tamm-Dancoff

- Diagonal approximation

RECENTLY:

- Closed-shell nuclei with a realistic interaction derived from the Argonne V18 potential (Unitary Correlation Operator Method) (Papakonstantinou and Roth, Phys. Lett. B 671, 356 (2009))

- Small metallic clusters (Gambacurta and Catara, Phys. Rev. B 79, 085403 (2009))

Formal scheme

$$Q_\nu^\dagger = \sum_{ph} (X_{ph}^\nu a_p^\dagger a_h - Y_{ph}^\nu a_h^\dagger a_p)$$

$$+ \sum_{p<p',h<h'} (X_{php'h'}^\nu a_p^\dagger a_h a_{p'}^\dagger a_{h'} - Y_{php'h'}^\nu a_h^\dagger a_p a_{h'}^\dagger a_{p'}).$$

Excitation operators

The X's and Y's are solutions of the equations,

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

where:

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

1 and 2: short-hand notation for 1p1h and 2p2h

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

1p1h and 2p2h configurations are mixed

The SRPA ground state is: $|\Psi\rangle = e^{\hat{S}}|\Phi\rangle$,

where |Φ> is the HF ground state

RPA $\hat{S} = \sum_{ph} C_{ph}(t) a_p^\dagger a_h$

SRPA $S = \sum_{ph} C_{ph} a_p^\dagger a_h + \frac{1}{2} \sum_{pp'hh'} C_{pp'hh'} a_p^\dagger a_{p'}^\dagger a_{h'} a_h$

The quasiboson approximation is used also in SRPA

Some technical details. Calculations for ^{16}O

- HF in coordinate space (20 fm box)
- First n = 7 states for each l (up to 6)
- s.p. wave functions are expressed as superposition of square well ones
- In principle, EWSR are satisfied in SRPA (Yannouleas 1986). Coulomb and spin-orbit are not taken into account in the residual interaction. Violations: 5%
- 1p1h configurations fixed in order to have stable EWSR (100-150 configurations); cutoff for 2p2h configurations: unperturbed energy lower than 120 MeV (2 - 3 10^4 configurations)
- Diagonalization of matrices of the order of 5 - 6 10^4
- 50 - 70 hours of CPU for each calculation (looking at energies up to 50 MeV)
- Skyrme interaction. Contact interaction: ultraviolet divergence. Numerical check of the stability of the results

SRPA with density-dependent forces (Skyrme or Gogny). Rearrangement terms in the residual interaction **(derivative with respect to the density of the mean-field hamiltonian)**

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

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

Two approximations:

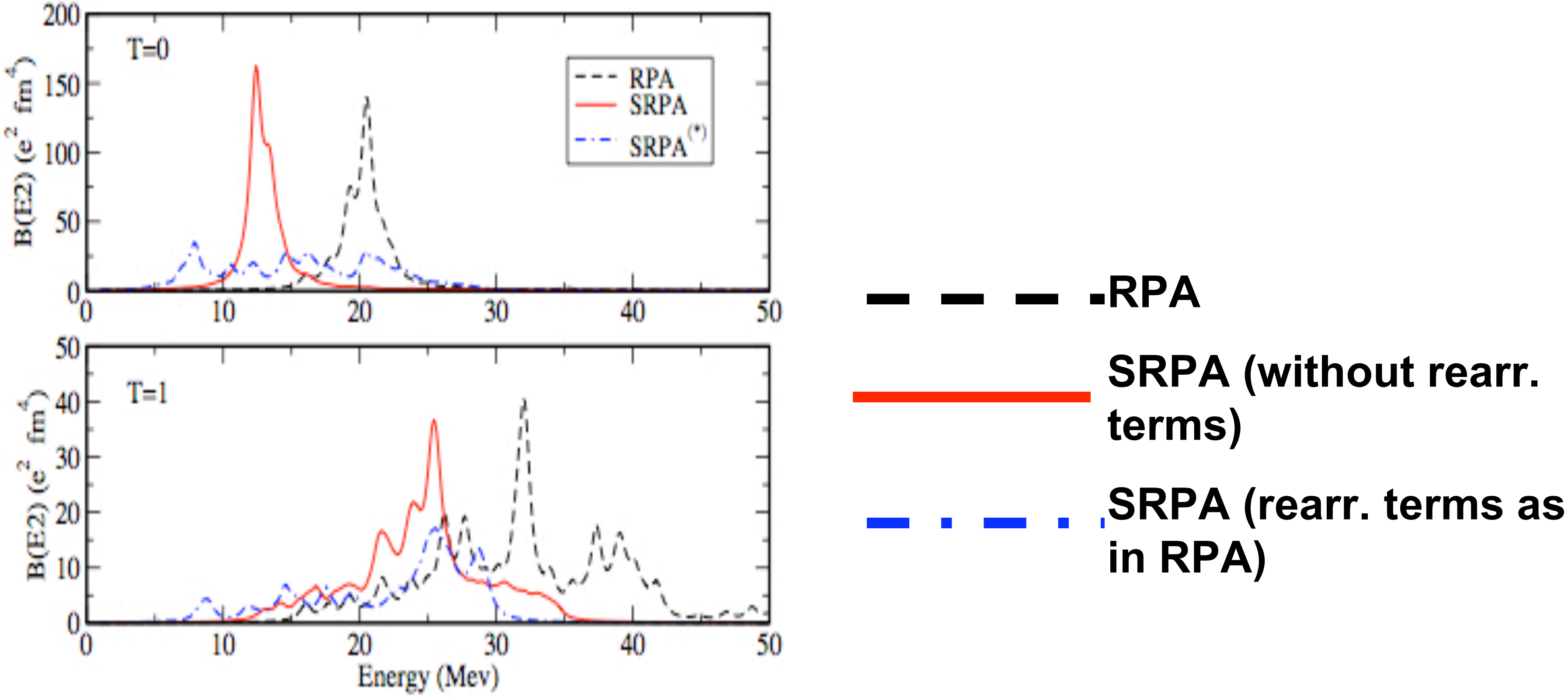
- **Neglecting the new rearrangement terms**

- **Treating them as in RPA**

Quadrupole response

Gambacurta, Grasso, Catara, PRC 81, 054312 (2010)

SGII ^{16}O



Low-lying 0^+ and 2^+ states

Low Lying 0^+ energy (MeV)					
Exp	RPA	SRPA	SRPA-D	SRPA*	SRPA*-D
~6	16.19	6.43	11.23	5.29	Imm.

SGII

^{16}O

Low Lying 2^+ energy (MeV)					
Exp	RPA	SRPA	SRPA-D	SRPA*	SRPA*-D
~7	16.03	7.16	12.44	4.70	Imm.

Gambacurta, Grasso, Catara, PRC 81, 054312 (2010)

Residual interaction. Rearrangement terms for SRPA matrix elements (variational procedure as in Providencia's work)

Density-dependent interaction expanded around the HF density ρ_0 up to quadratic order

$$\hat{V}_{\alpha\beta\gamma\delta}(\rho) \sim \hat{V}_{\alpha\beta\gamma\delta}(\rho_0) + \sum_{ab} \left[\frac{\delta \hat{V}_{\alpha\beta\gamma\delta}}{\delta \rho_{ab}} \right]_{\rho=\rho_0} \delta \rho_{ab}$$

$$+ \frac{1}{2} \sum_{abcd} \left[\frac{\delta^2 \hat{V}_{\alpha\beta\gamma\delta}}{\delta \rho_{ab} \delta \rho_{cd}} \right]_{\rho=\rho_0} \delta \rho_{ab} \delta \rho_{cd} \; ;$$

$\delta \rho_{ab}$ is the variation of the density around ρ_0:

$$\rho_{\alpha\beta} = \rho_{0,\alpha\beta} + \delta\rho_{\alpha\beta} =< \Psi | a^\dagger_\beta a_\alpha | \Psi > =< \Phi | e^{S^\dagger} a^\dagger_\beta a_\alpha e^S | \Phi >$$

$$=< \Phi | (1 + S^\dagger + \frac{1}{2} S^{\dagger 2} + ...) a^\dagger_\beta a_\alpha (1 + S^2 + \frac{1}{2} S^2 + ...) | \Phi >$$

$$\sim \rho_{0,\alpha\beta} + < \Phi | a^\dagger_\beta a_\alpha S + S^\dagger a^\dagger_\beta a_\alpha | \Phi > +$$

$$< \Phi | \frac{1}{2} a^\dagger_\beta a_\alpha S^2 + S^\dagger a^\dagger_\beta a_\alpha S + \frac{1}{2} S^{\dagger 2} a^\dagger_\beta a_\alpha | \Phi > \; ,$$

Gambacurta, Grasso, Catara, submitted J. Phys. G

$$\delta\rho^{(1)}_{ph} = C_{ph} \; ;$$

$$\delta\rho^{(1)}_{hp} = C^*_{ph} \; ;$$

linear

$$\delta\rho^{(2)}_{ph} = \sum_{mi} C^*_{mi}\hat{C}_{pmhi} \; ;$$

$$\delta\rho^{(2)}_{hp} = \sum_{mi} C_{mi}\hat{C}^*_{pmhi} \; ;$$

$$\delta\rho^{(2)}_{hh'} = -\sum_{m} C^*_{mh}C_{mh'} + \frac{1}{2}\sum_{mni} \hat{C}^*_{mnih}\hat{C}_{mnh'i} \; ;$$

$$\delta\rho^{(2)}_{pp'} = \sum_{i} C^*_{p'i}C_{pi} + \frac{1}{2}\sum_{mij} \hat{C}^*_{p'mij}\hat{C}_{pmij} \; .$$

quadratic

The mean value of the Hamiltoninan in $|\Psi>$, $<H>$, can be written as

$<H>=<\Phi|H|\Phi> +$ **linear and quadratic terms in C and C***

The usual RPA rearrangement terms are found for the RPA sub-matrices A_{11} and B_{11} by calculating

$$A_{mi,pk} = \left[\frac{\delta^2 < H >}{\delta C^*_{mi}\delta C_{pk}}\right]_{C=C^*=0} \qquad B_{mi,pk} = \left[\frac{\delta^2 < H >}{\delta C^*_{mi}\delta C^*_{pk}}\right]_{C=C^*=0}$$

For example the matrix A_{12} . By calculating

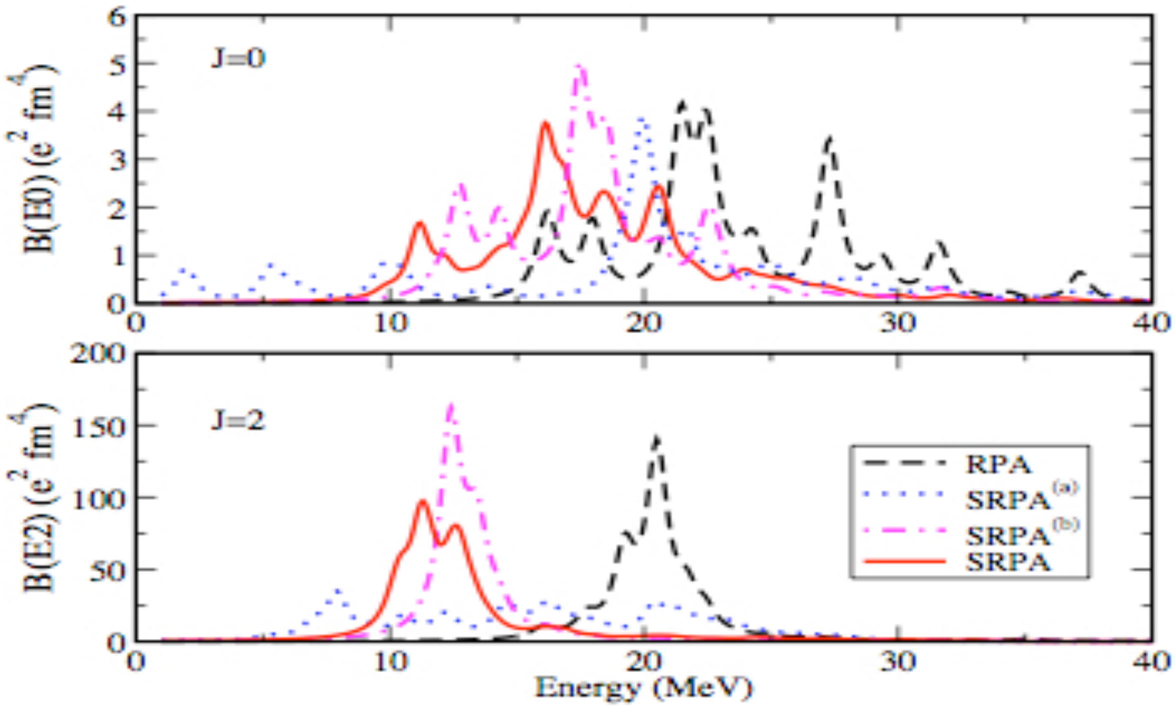
$$A_{mi,pqkl} = \left[\frac{\delta^2 < H >}{\delta C^*_{mi}\delta \hat{C}_{pqkl}}\right]_{C=C^*=0}$$

one obtains a rearrangement term of the type:

$$< kl| \left[\frac{\delta \hat{V}(\rho)}{\delta \rho_{im}}\right]_{\rho=\rho_0} \rho_{im}|pq >$$

Rearrangement terms in SRPA

Isoscalar monopole (top) and quadrupole (bottom) strength distributions for ^{16}O. DIFFERENT FRAGMENTATION



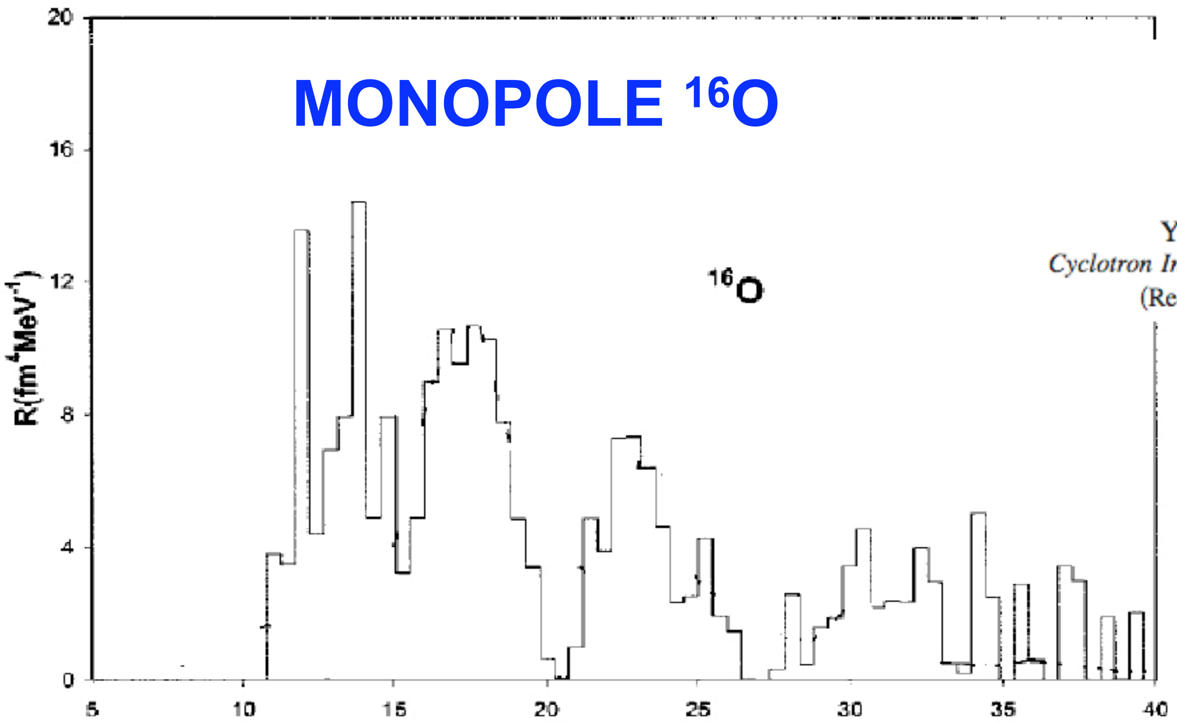
Gambacurta, Grasso, Catara, submitted J. Phys.

RPA

SRPA (correct rearrangement terms)

SRPA (neglecting new rearrangement terms)

SRPA (treating all rearrangement terms like in RPA)

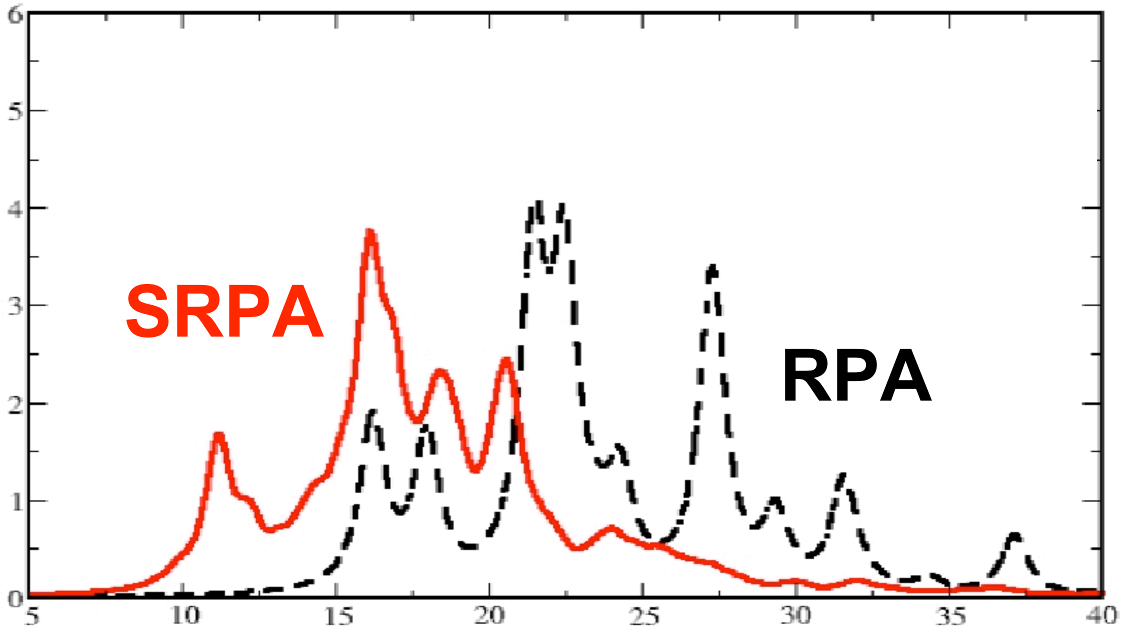


PHYSICAL REVIEW C, VOLUME 64, 064308

Giant resonances in ^{16}O

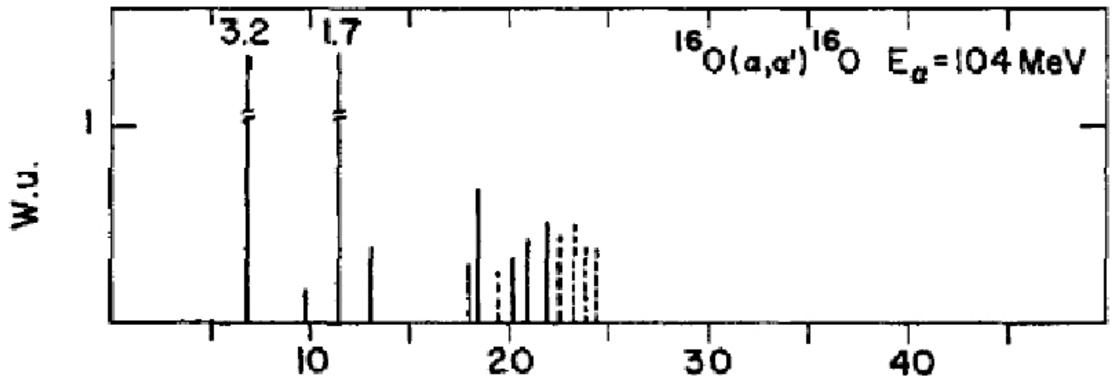
Y.-W. Lui, H. L. Clark, and D. H. Youngblood
Cyclotron Institute, Texas A&M University, College Station, Texas 77843
(Received 31 May 2001; published 16 November 2001)

Inelastic scattering of 240 MeV alpha particles



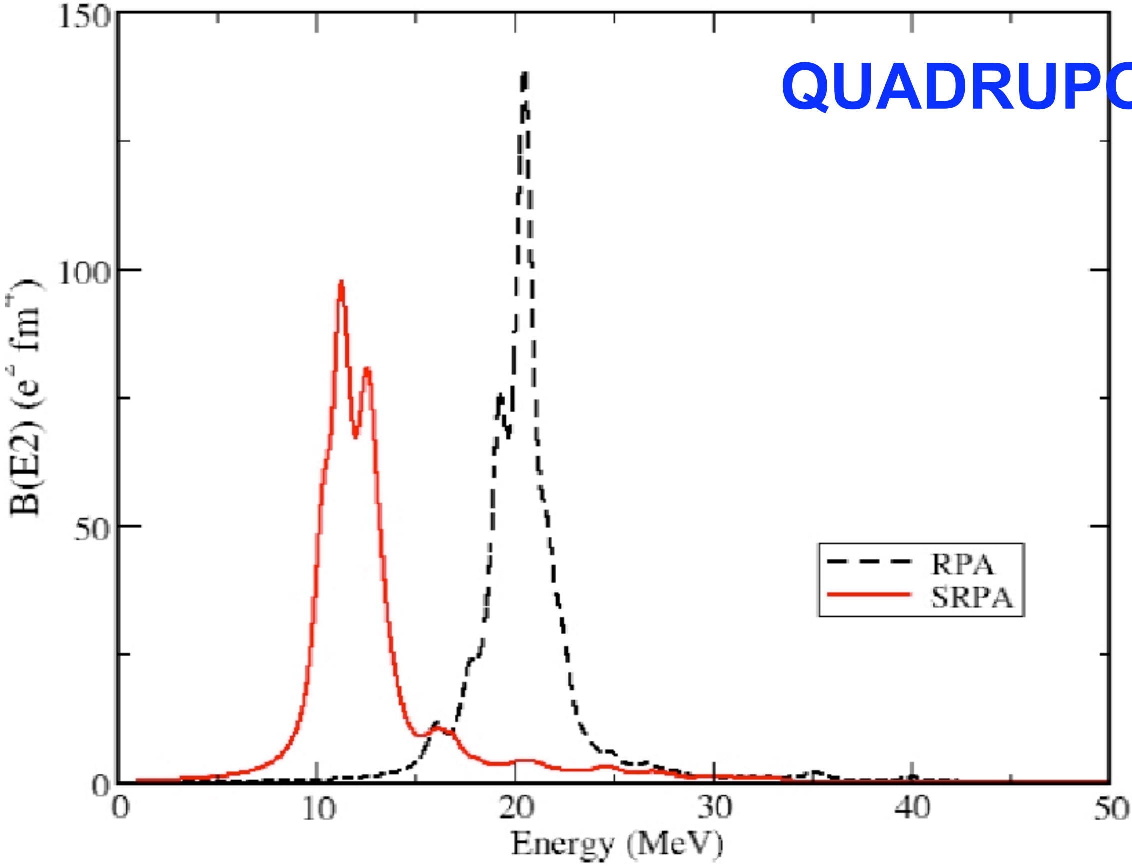
Gambacurta, Grasso, in preparation

B(E0) (e^2 fm^4)



Harakeh et al., NPA 265, 189 (1976)

QUADRUPOLE ^{16}O



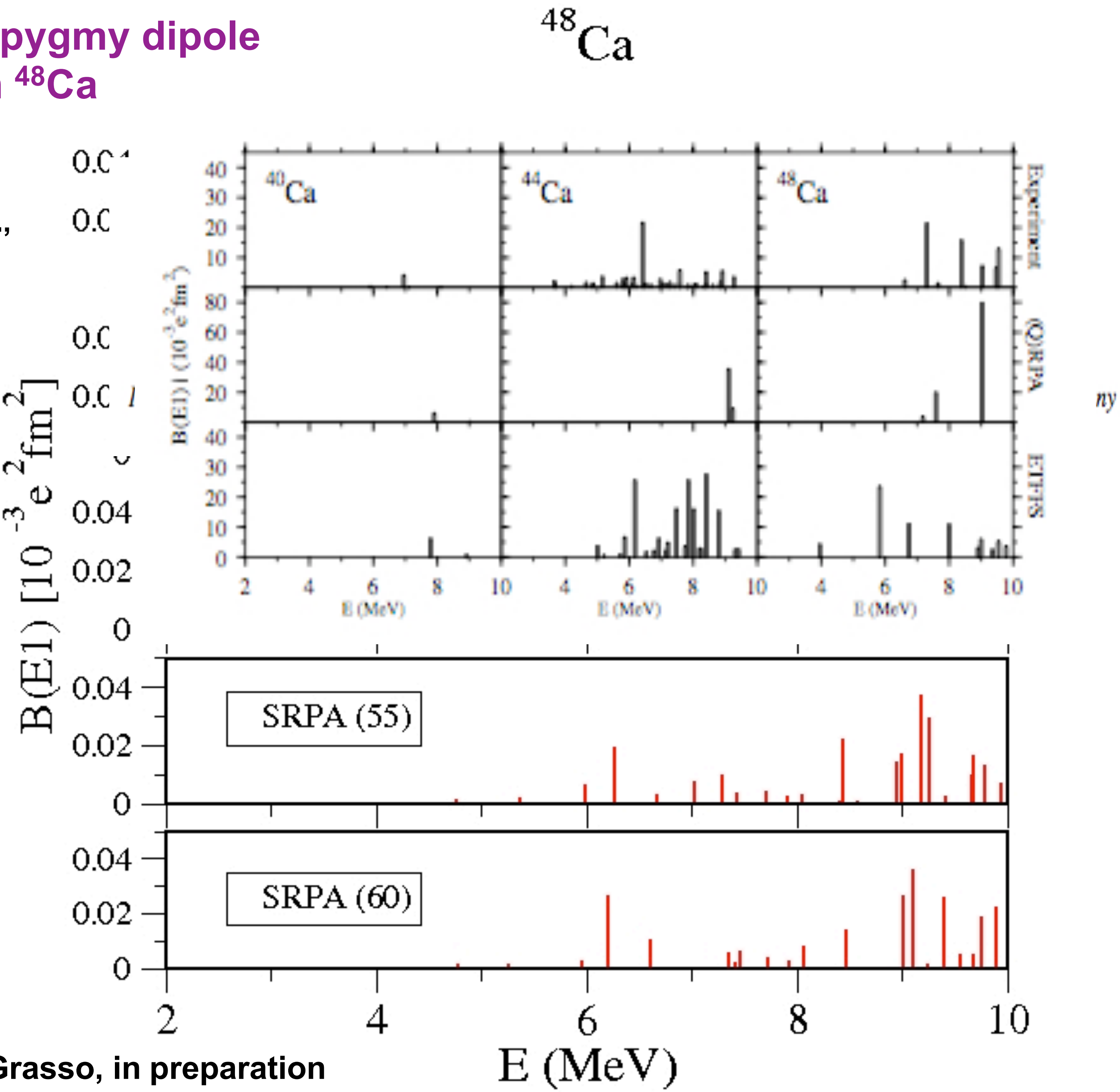
Gambacurta, Grasso, in preparation

Preliminary: pygmy dipole resonance in ^{48}Ca

Hartmann, et al.,

PRL 93, 192501

(2004)



Gambacurta, Grasso, in preparation

Conclusions and perspectives

- General conclusions: 1) width of the modes; 2) shift of the strength to lower energies by several MeV with respect to RPA.

PERSPECTIVES

- 1) Interaction fitted for this kind of calculations (also pppp and hhhh matrix elements are present)
- 2) QBA is a serious problem (violations of Pauli principle)… using renormalized SRPA to better treat correlations?
- 3) Ultraviolet divergence (exploratory study: Moghrabi, Grasso, Colò, Van Giai, in preparation)