May 18-22, 2015

ICNT: Theory for open-shell nuclei near the limits of stability

NCSL/MSU

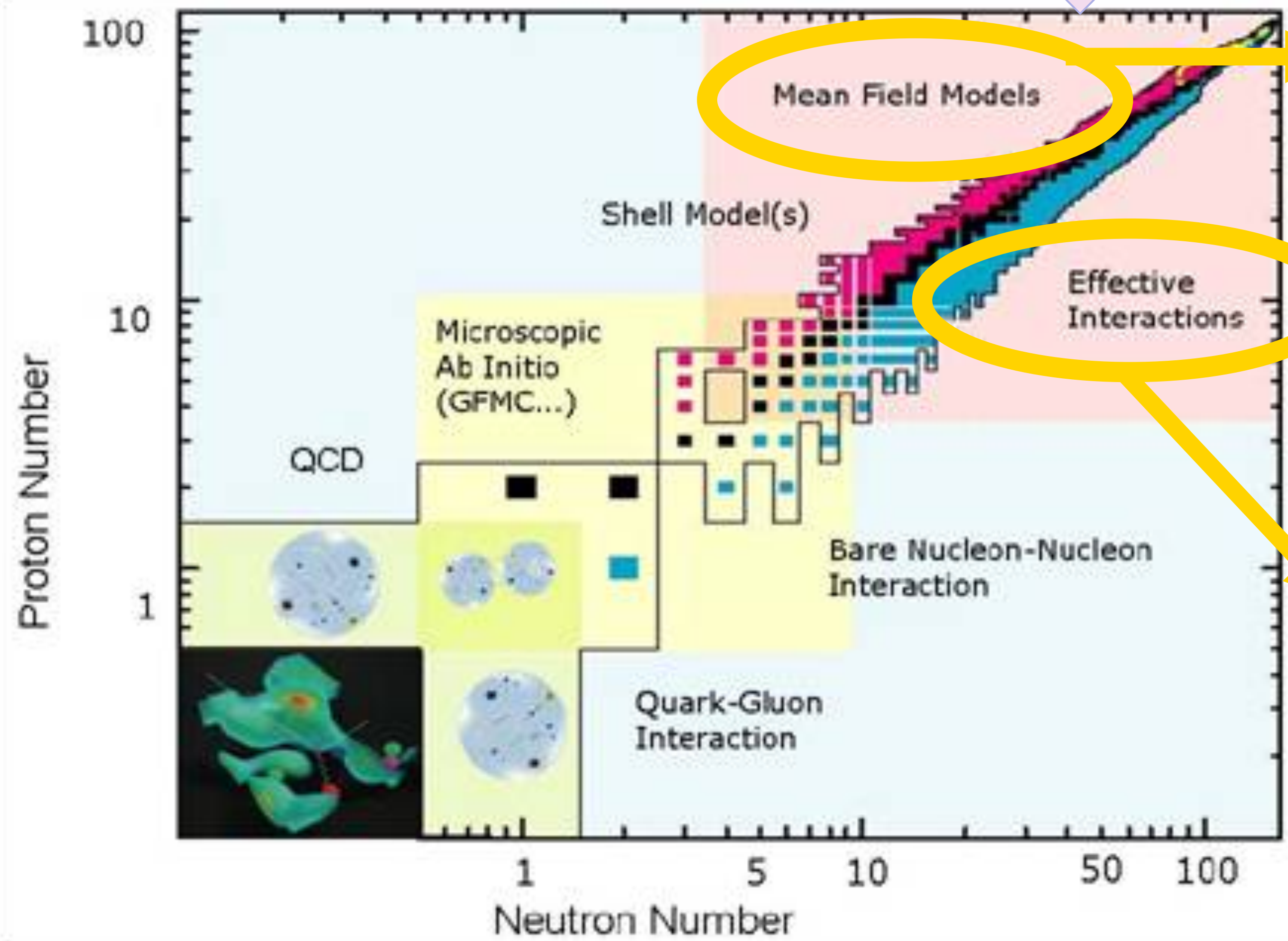
Beyond mean-field corrections in the nuclear many-body problem

Marcella Grasso

INSTITUT DE PHYSIQUE NUCLÉAIRE ORSAY

Nuclear structure, reactions and stars

Energy Density Functional (EDF) models



Beyond-mean -field models (correlations).

- Describing complex phenomena

- Improving predictive power of models

- *NUMERICAL COMPLEXITY*
- *DIVERGENCES*
- *INTERACTION ? Phenomenological effective interactions adjusted at the mean-field level*

Outline

- **Danilo Gambacurta**, **Francesco Catara**

  Catania (funding by the LIA COLL-AGAIN)

- **Jon Engel**

  North Carolina

- **Bira van Kolck, Jerry Yang**

  IPN Orsay

- **Gianluca Colo', Xavi Roca-Maza**

  Milano University

Full calculations (no cut in the matrix elements and large cutoff)

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

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

Problems difficult to cure, up to very recently:

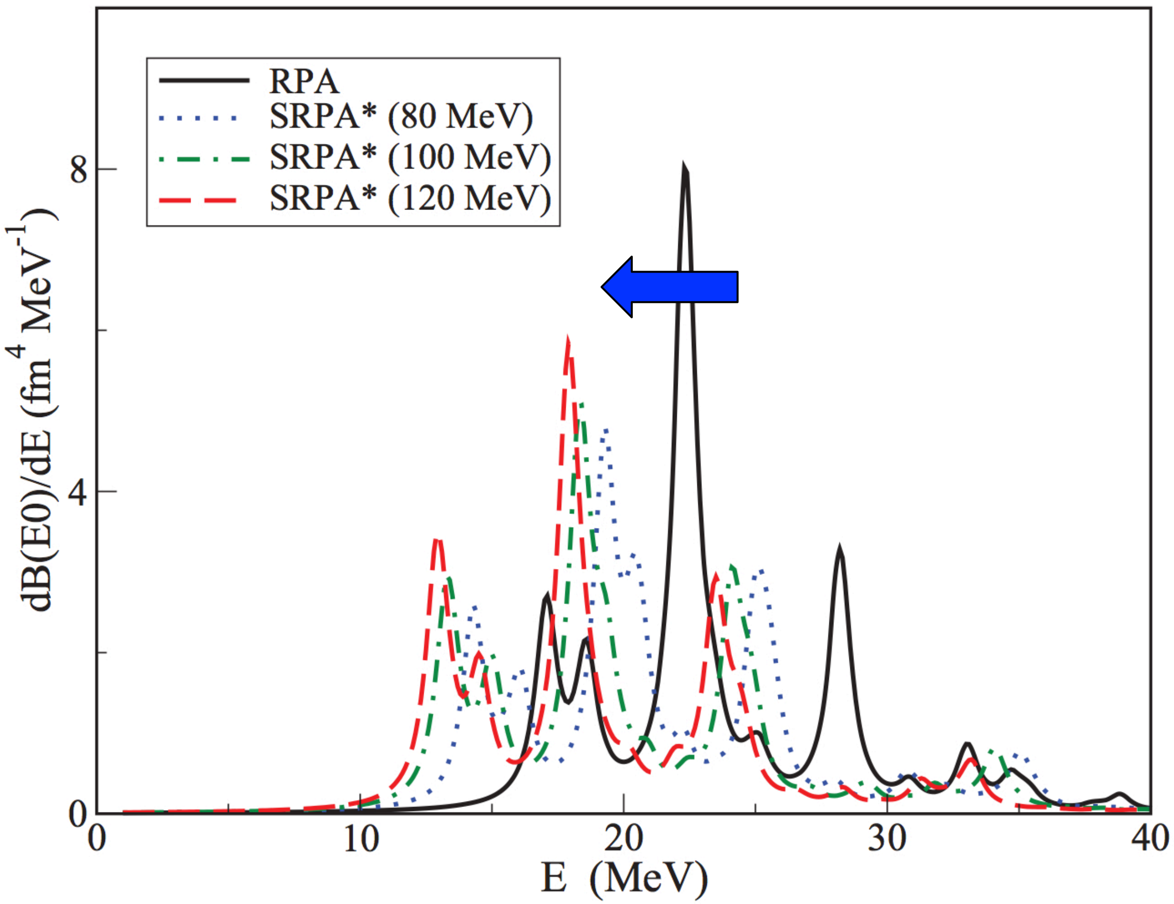
- (Too) strong shift to lower energies with respect to the RPA spectrum (even in those cases where RPA works well)

- Strong dependence on the cutoff (ultraviolet divergence in the case of zero-range interactions)

- In some cases (for some values of the cutoff): imaginary solutions and/or states with positive energy and negative norm

With the Gogny force (density-dependent contact term in the construction of the residual interaction) - ^{16}O

Isoscalar monopole response. The cutoff is in 2p2h configurations (in parentheses)



Gambacurta, Grasso, et al., Phys. Rev. C 86, 021304 (R) (2012)

The SRPA model

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

Excitation operators

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

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

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

1 and 2:

short-hand notation for 1p1h and 2p2h

Yannouleas, Phys. Rev. C 35, 1159 (1987)

- If the interaction does not depend on the density:
- $B_{12} = B_{21} = B_{22} = 0$ (when the QBA is used)
- The beyond-RPA matrix elements for the matrix A are:

Coupling 1p1h with 2p2h (matrix elements of the interaction: hppp, phhh)

$$
\begin{aligned}
A_{12} &= A_{ph,p_1p_2h_1h_2} \\
&= \langle \mathrm{HF}|\left[a_h^\dagger a_p, \left[H, a_{p_1}^\dagger a_{p_2}^\dagger a_{h_2} a_{h_1}\right]\right]|\mathrm{HF}\rangle \\
&= \chi(h_1, h_2)\underline{\bar{V}_{h_1pp_1p_2}}\delta_{hh_2} - \chi(p_1, p_2)\underline{\bar{V}_{h_1h_1p_1h}}\delta_{pp_2},
\end{aligned}
$$

Antisymmetrizer

Coupling 2p2h with 2p2h (matrix elements of the interaction: pppp, hhhh, phhp)

$$
\begin{aligned}
A_{22} &= A_{p_1h_1p_2h_2,p_1'h_1'p_2'h_2'} \\
&= \langle \mathrm{HF}|\left[a_{h_1}^\dagger a_{h_2}^\dagger a_{p_1} a_{p_2}, \left[H, a_{p_2'}^\dagger a_{p_1'}^\dagger a_{h_2'} a_{h_1'}\right]\right]|\mathrm{HF}\rangle \\
&= \left(\epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_1} - \epsilon_{h_2}\right)\chi(p_1, p_2)\chi(h_1, h_2) \\
&\quad \times \delta_{h_1h_1'}\delta_{p_1p_1'}\delta_{h_2h_2'}\delta_{p_2p_2'} + \chi(h_1, h_2)\underline{\bar{V}_{p_1p_2p_1'p_2'}}\delta_{h_1h_1'}\delta_{h_2h_2'} \\
&\quad + \chi(p_1, p_2)\underline{\bar{V}_{h_1h_2h_1'h_2'}}\delta_{p_1p_1'}\delta_{p_2p_2'} \\
&\quad + \chi(p_1, p_2)\chi(h_1, h_2)\chi(p_1', p_2')\chi(h_1', h_2') \\
&\quad \times \underline{\bar{V}_{p_1h_1'h_1p_1'}}\delta_{h_2h_2'}\delta_{p_2p_2'},
\end{aligned}
$$

SRPA with density-dependent forces (Skyrme or Gogny)

New rearrangement terms derived for the residual interaction

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

where:

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

Inspired by the variational derivation of SRPA equations by da Providencia, Nucl. Phys. 61, 87 (1965)

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

Residual interaction. Rearrangement terms for SRPA matrix elements when the interaction is density dependent

Some works in beyond-RPA frameworks:

- Shell model

Waroquier et al., Phys. Rep. 148, 249 (1987)

- Some matrix elements beyond standard RPA (however the procedure does not allow one to obtain the standard RPA rearrangement terms)

Adachi and Yoshida, Phys. Lett. B 81, 98 (1979)

Variational procedure to derive the SRPA equation:, da Providencia Nucl. Phys. 61, 87 (1965)

$$|\Psi\rangle = e^{\hat{S}}\boxed{|\Phi\rangle} \longrightarrow \text{HF state}$$

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

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

-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

Expansion of the one-body density around the HF density

$$\delta\rho^{(1)}_{hh'} = \delta\rho^{(1)}_{pp'} = 0; \qquad \delta\rho^{(1)}_{ph} = C_{ph}; \qquad \delta\rho^{(1)}_{hp} = C^*_{ph};$$

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

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

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

Mean value of the Hamiltonian in the ground state:

$$\langle H\rangle = \langle\Phi|H|\Phi\rangle + \sum_{mi}(C^*_{mi}\lambda_{mi}(\rho) + C_{mi}\lambda_{im}(\rho))$$
$$+ \sum_{i<j,m<n}(\hat{C}^*_{mnij}\hat{V}_{mnij}(\rho) + \hat{C}_{mnij}\hat{V}_{ijmn}(\rho)) + F^{(2)}$$

Examples of RPA and beyond-RPA matrices:

$$A_{mi,pk} = \left[\frac{\delta^2\langle H\rangle}{\delta C^*_{mi}\delta C_{pk}}\right]_{C=C^*=0} \equiv A_{11},$$

$$A_{mi,pqkl} = \left[\frac{\delta^2\langle H\rangle}{\delta C^*_{mi}\delta \hat{C}_{pqkl}}\right]_{C=C^*=0} \equiv A_{12},$$

Sum of quadratic terms

Expansion of the density-dependent interaction around the HF density:

$$\hat{V}_{\alpha\beta\gamma\delta}(\rho) \sim \hat{V}_{\alpha\beta\gamma\delta}(\rho^{(0)}) + \sum_{ab}\left[\frac{\delta\hat{V}_{\alpha\beta\gamma\delta}}{\delta\rho_{ab}}\right]_{\rho=\rho^{(0)}} \delta\rho_{ab} + \frac{1}{2}\sum_{abcd}\left[\frac{\delta^2\hat{V}_{\alpha\beta\gamma\delta}}{\delta\rho_{ab}\delta\rho_{cd}}\right]_{\rho=\rho^{(0)}} \delta\rho_{ab}\delta\rho_{cd},$$

where

$$\delta\rho_{\alpha\beta} = \delta\rho^{(1)}_{\alpha\beta} + \delta\rho^{(2)}_{\alpha\beta}.$$

Examples of rearrangement terms:

$$A^{(\mathrm{rearr})}_{mi,pqkl} = \left[\frac{\delta\hat{V}_{klpq}}{\delta\rho_{im}}\right]_{\rho=\rho^{(0)}} \rho_{im}$$

Double counting (interaction adjusted at the mean-field level) and instabilities. Recent analyses:

- **Papakonstantinou, Phys. Rev. C 90, 024305 (2014)***

- **Tselyaev, Phys. Rev. C 88, 054301 (2013) (subtraction method)**

* Suggestion of using a correlated ground state. This has been implemented only in the case of metallic clusters: Gambacurta, Catara, Phys. Rev. B 81, 085418 (2010)

Subtraction method

- Tselyaev, Phys. Rev. C 75, 024306 (2007).

Applied first to models that include particle-vibration coupling

- Tselyaev, Phys. Rev. C 88, 054301 (2013) (for extensions of the RPA model)

Main objective of the method: Eliminating double counting

What is developed in Tselyaev 2013:

- stability of extended RPA results (real solutions) guaranteed
- 'Though the problem of the convergence is not generally resolved…., one can see that its use at least improves the situation'

SRPA equations may be written as RPA-type equations with energy dependent RPA matrices

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

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

SRPA and RPA matrices to be diagonalized:

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

Subtraction to eliminate double counting

The used energy density functional 'already contains a part of the contributions of those complex configurations which are explicitly included' in SRPA: static contributions (the dynamic contributions will lead to the formation of the spreading width of the resonances).

Static contributions should be eliminated. This is done by imposing that the two matrices are equal at zero energy.

$\Omega^{SRPA}(0) = \Omega^{RPA}$

One can show that this is equivalent to impose the equality of the static polarizability (related to the inverse energy-weighted moment of the strength distribution) calculated in the two models

The energy dependent parts of the matrices are

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

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

Subtraction:

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

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

By following Tselayev 2013 and Shirmer and Angonoa, J. Chem. Phys. 91, 1754 (1989) ->

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 $A_{22'}$)

A diagonal approximation in the calculation of the corrective term will be also tested:

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

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

Stability condition in RPA (Thouless theorem)

A necessary condition for the HF state to minimize the expectation value of the Hamiltonian is that the RPA stability matrix be positive semi-definite (it can be shown that this leads to real eigenvalues)

Stability RPA matrix

$$\begin{bmatrix} A_{11'} & B_{11'} \\ B^{*}_{11'} & A_{11'} \end{bmatrix}$$

This does not imply that the SRPA stability matrix is also positive semi-definite.

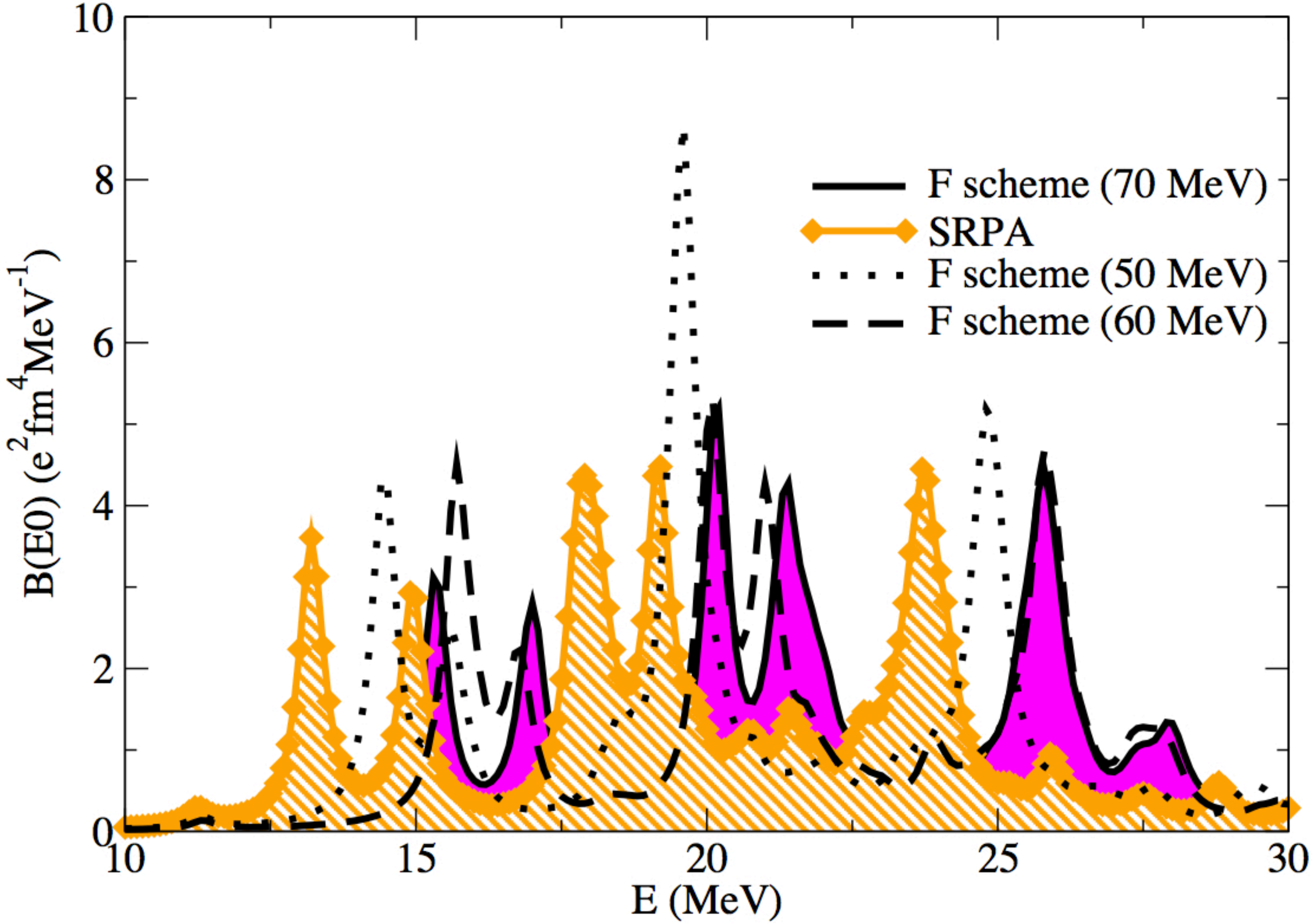
The theorem can be extended to SRPA either by using a correlated ground state instead of HF (Papakonstaninou 2014) or by applying the subtraction procedure (Tselyaev 2013)

APPLICATIONS

(Skyrme SGII)

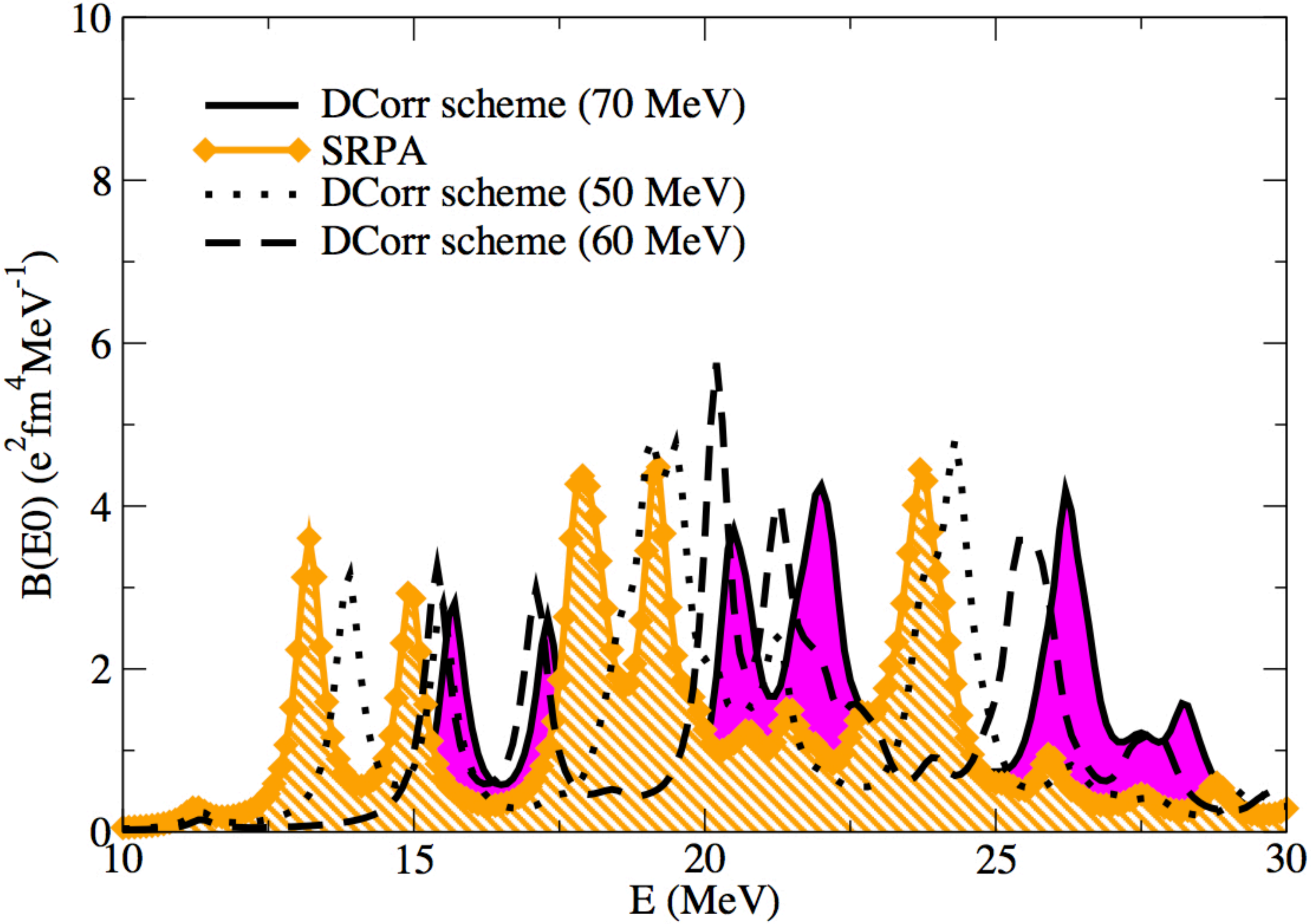
Effect of the subtraction
Monopole as an illustration

Isoscalar monopole response. Effect of the subtraction on the SRPA spectra. Full calculation



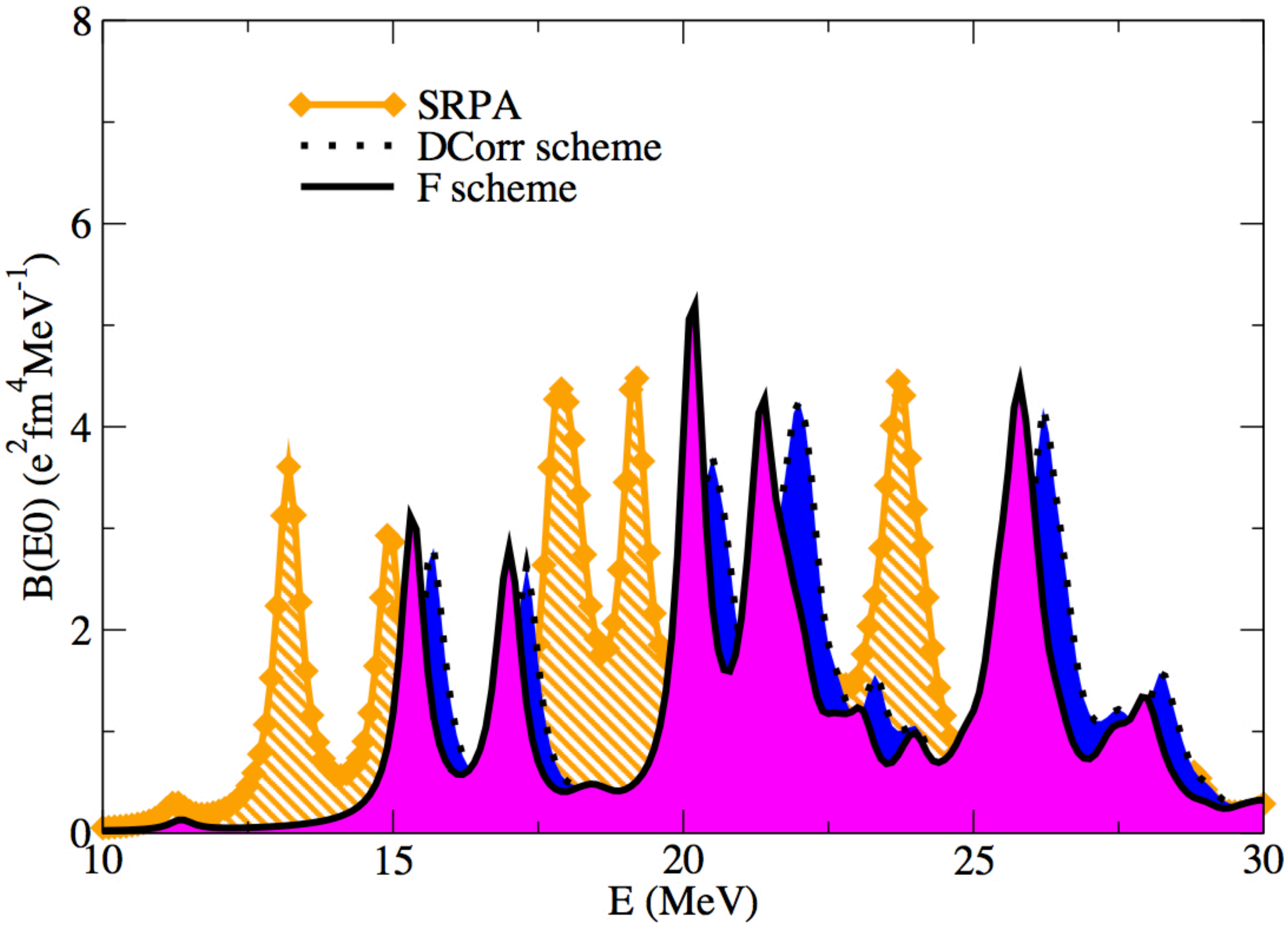
Gambacurta, Grasso, Engel, in preparation

Isoscalar monopole response. Effect of the subtraction on the SRPA spectra. Diagonal approximation in the corrective term



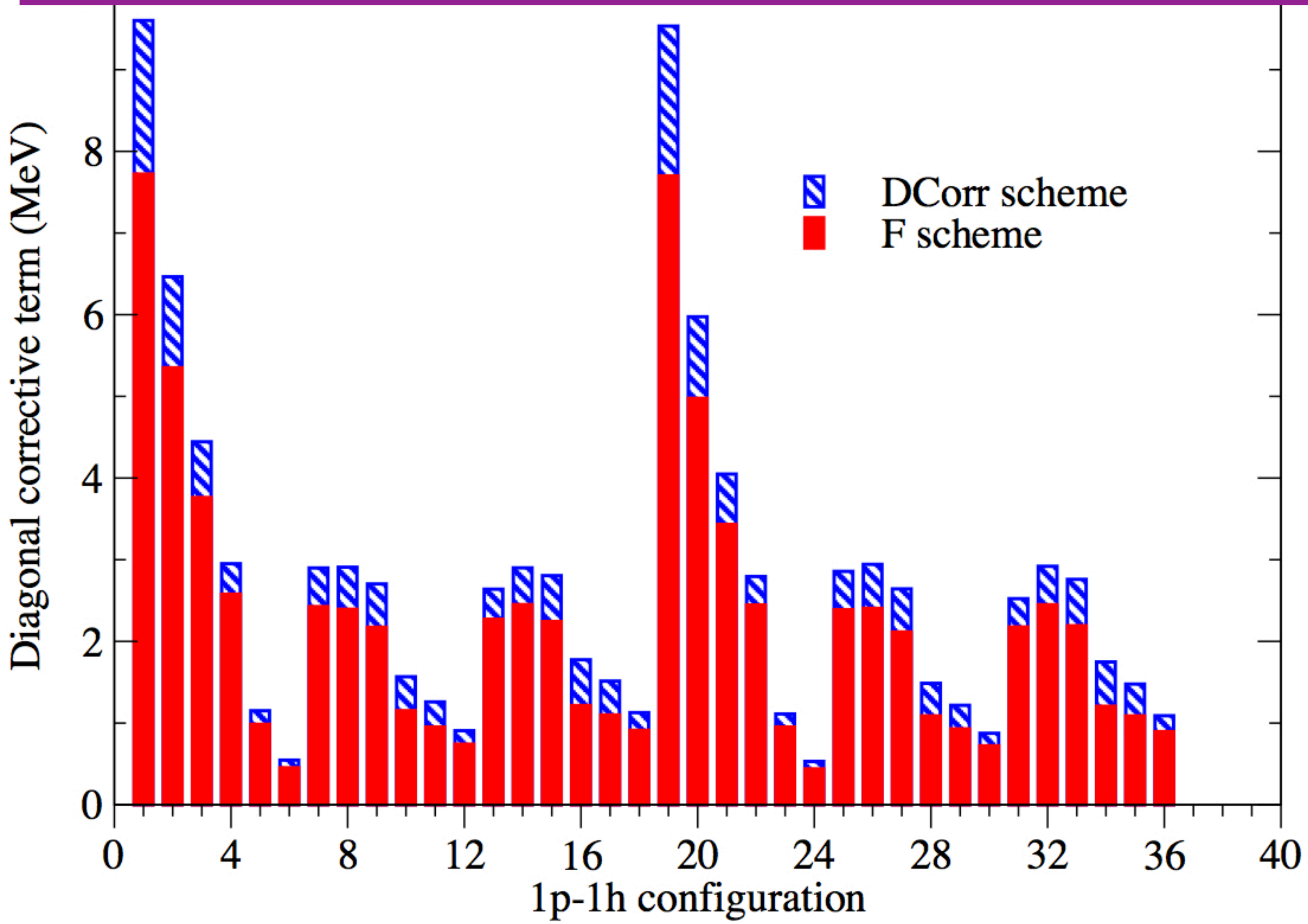
Gambacurta, Grasso, Engel, in preparation

Full calculation versus diagonal approximation



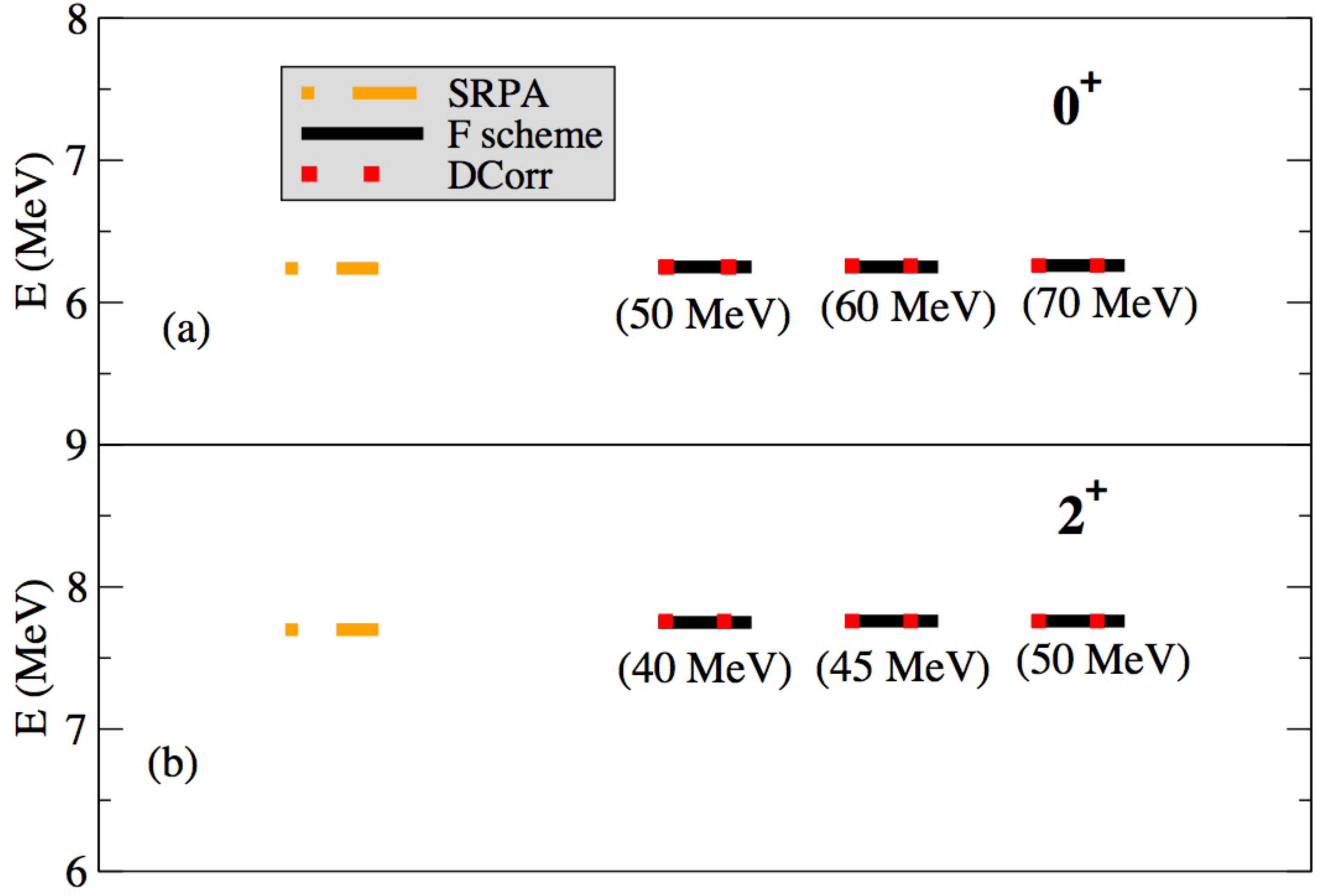
Gambacurta, Grasso, Engel, in preparation

Plot of the diagonal part of the corrective term: it can be viewed as a correction on the particle-hole excitation energies. This provides the shift to higher energies with respect to SRPA



Gambacurta, Grasso, Engel, in preparation

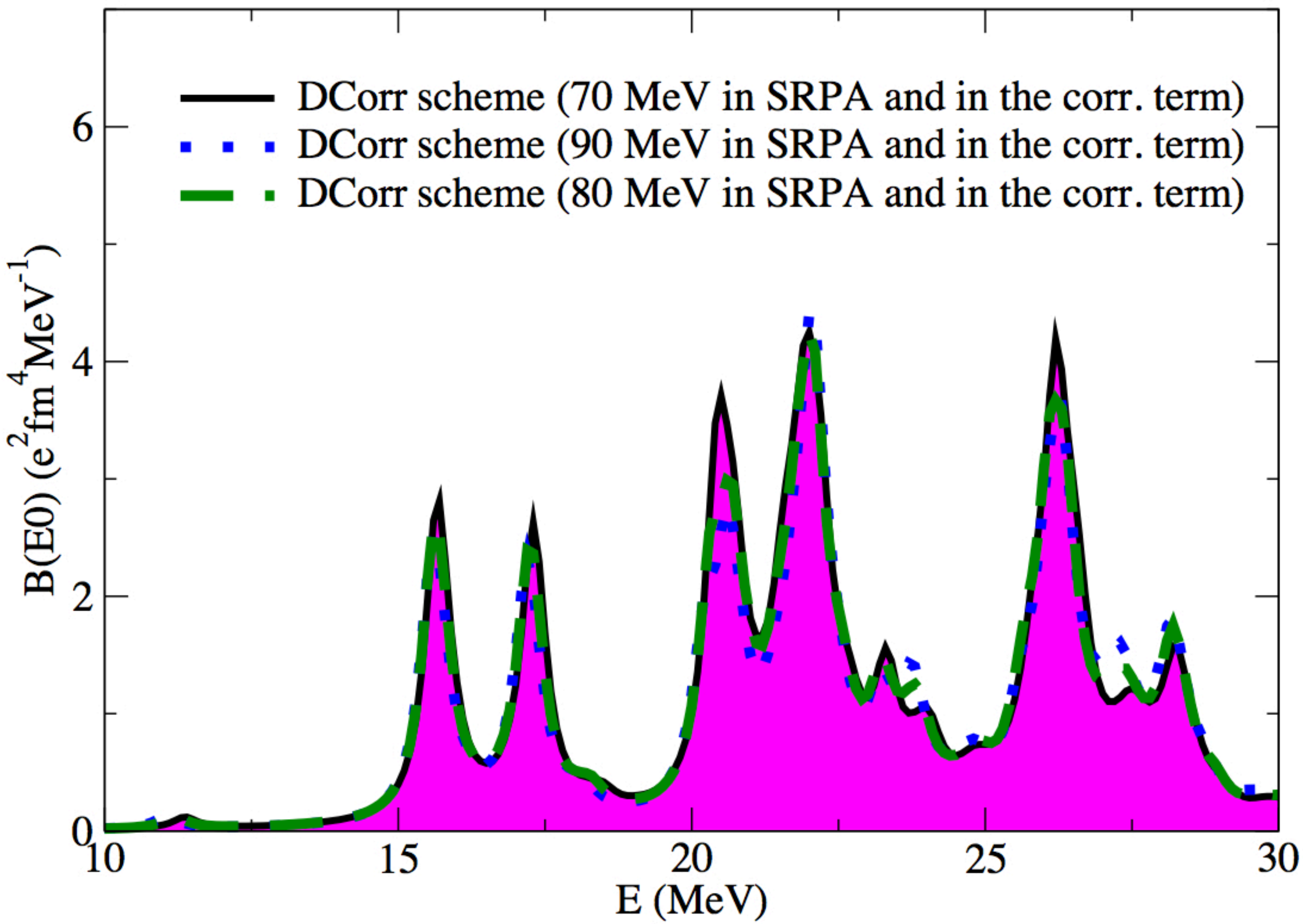
Different behavior for the low-lying states that have mostly a multiparticle-multihole nature



Gambacurta, Grasso, Engel, in preparation

Cutoff dependence?
Robust predictions?

Robustness of the predictions. Dependence on the cutoff?



Gambacurta, Grasso, Engel, in preparation

Comparison with RPA and experimental results

To compute centroids and widths we will make use of the moments of the strength function,

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

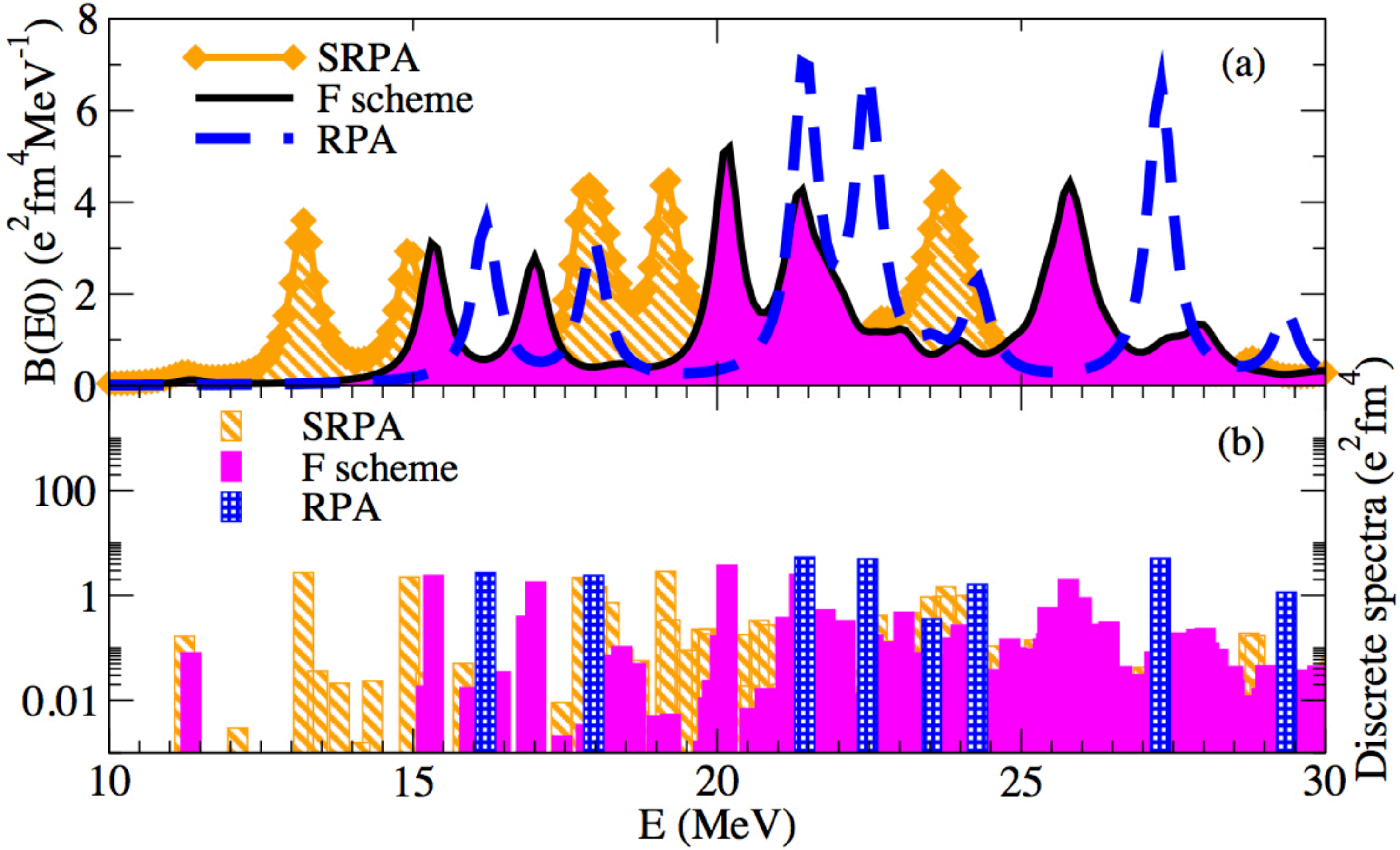
where the strength function is

$$S(E) = \sum_n |\langle n|Q|0\rangle|^2 \delta(E_n - E)$$

Centroid energy: $\dfrac{m_1}{m_0}$

Width: $\sigma^2 = \dfrac{m_2}{m_0} - \left(\dfrac{m_1}{m_0}\right)^2$

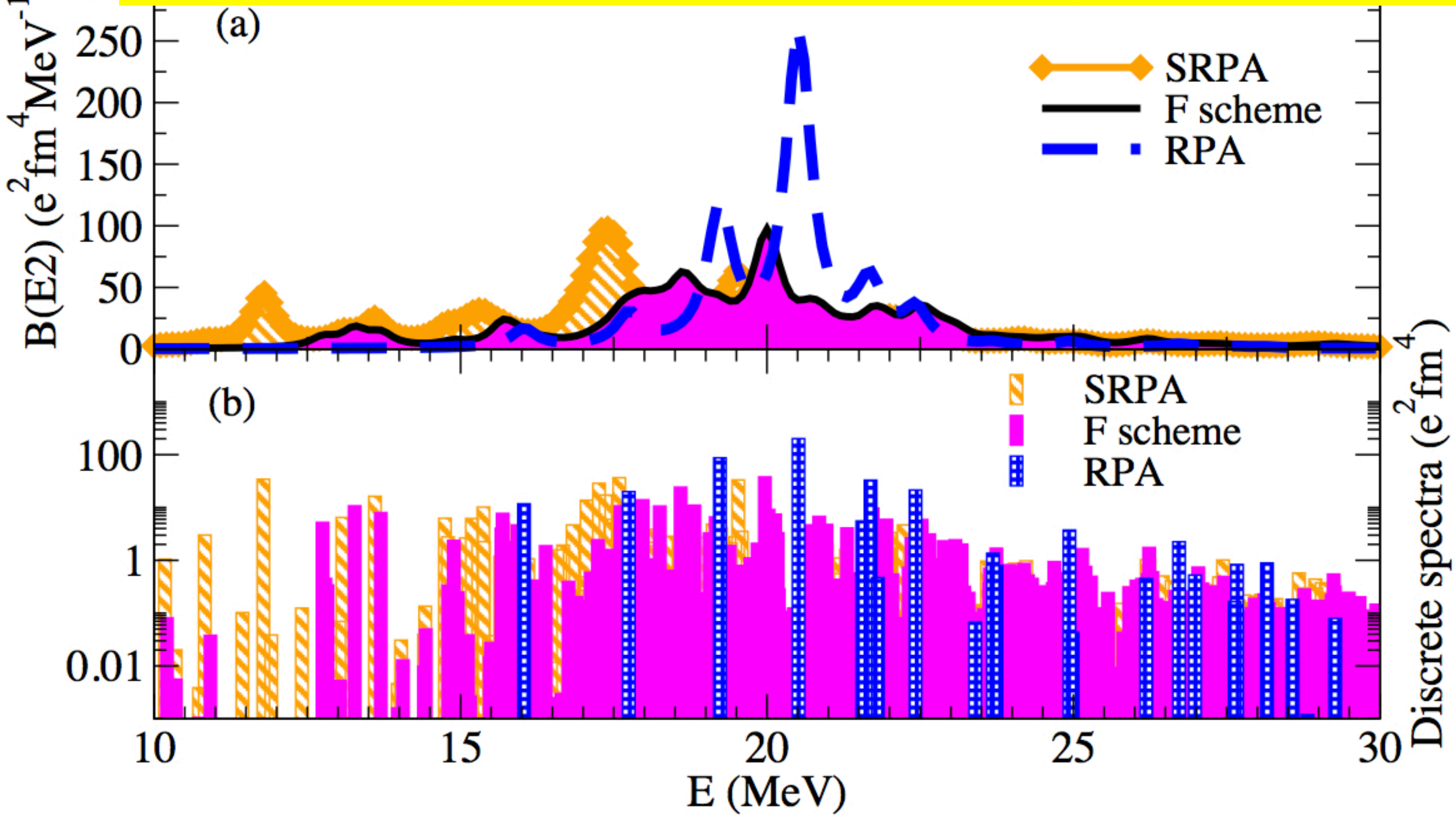
Let us compare now with RPA. The F scheme as an illustration. Monopole



Gambacurta, Grasso, Engel, in preparation

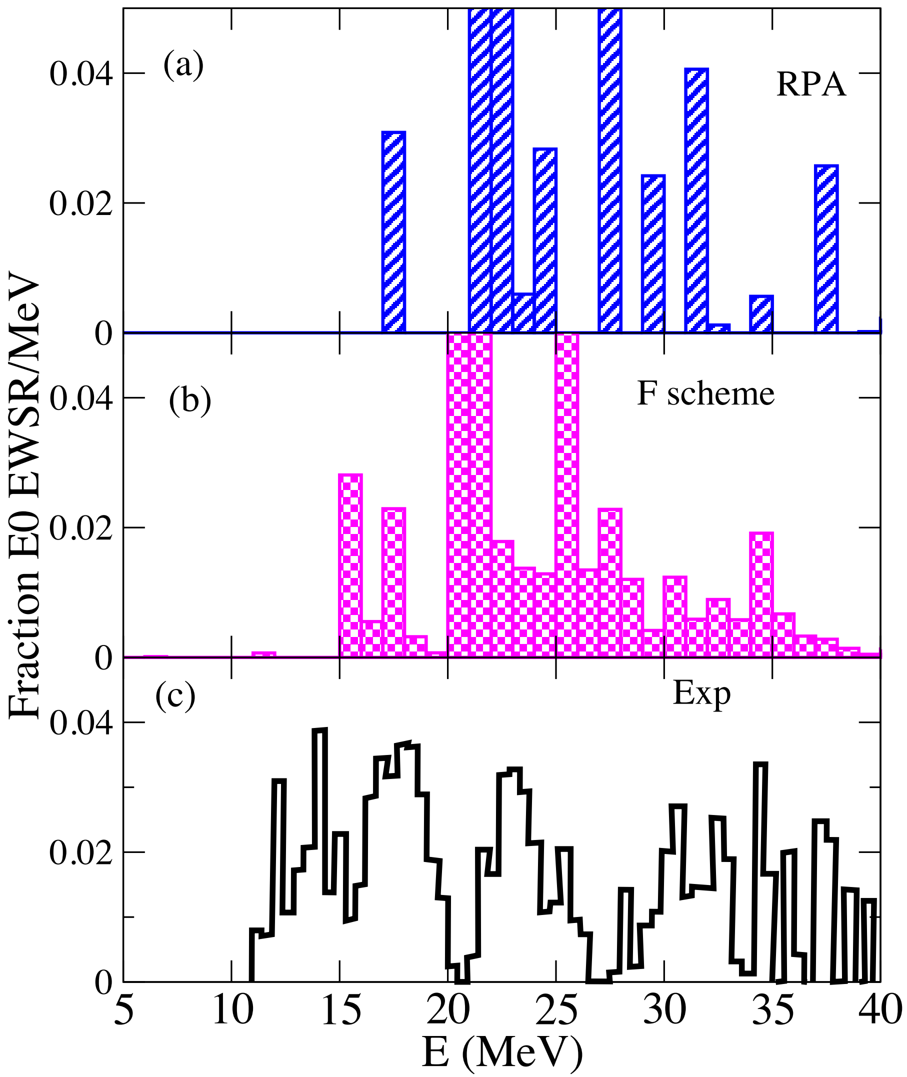
Quadrupole

Centroid and width RPA: 20.73 MeV, 2.42 MeV
Centroid and width F scheme: 20.21 MeV, 4.05 MeV



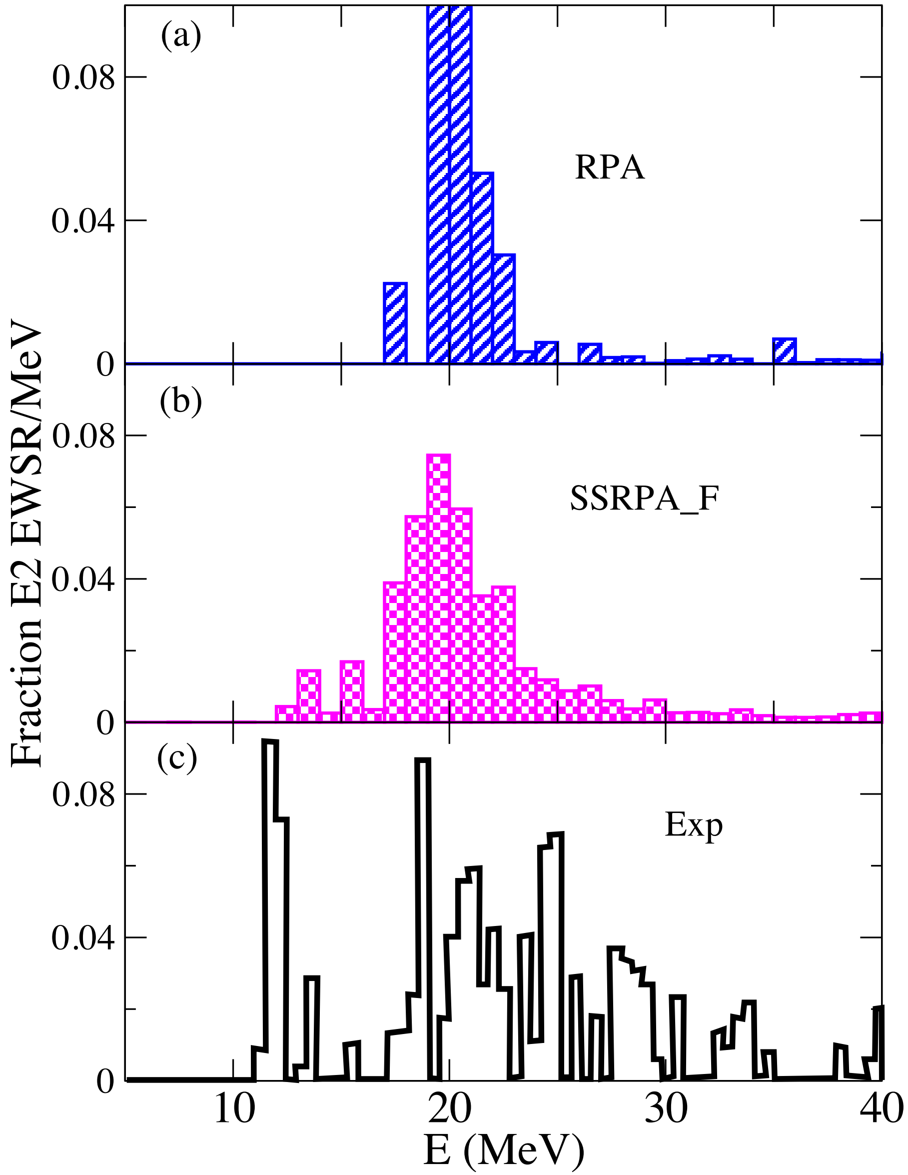
Gambacurta, Grasso, Engel, in preparation

Comparison with experiment. Monopole



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

Quadrupole



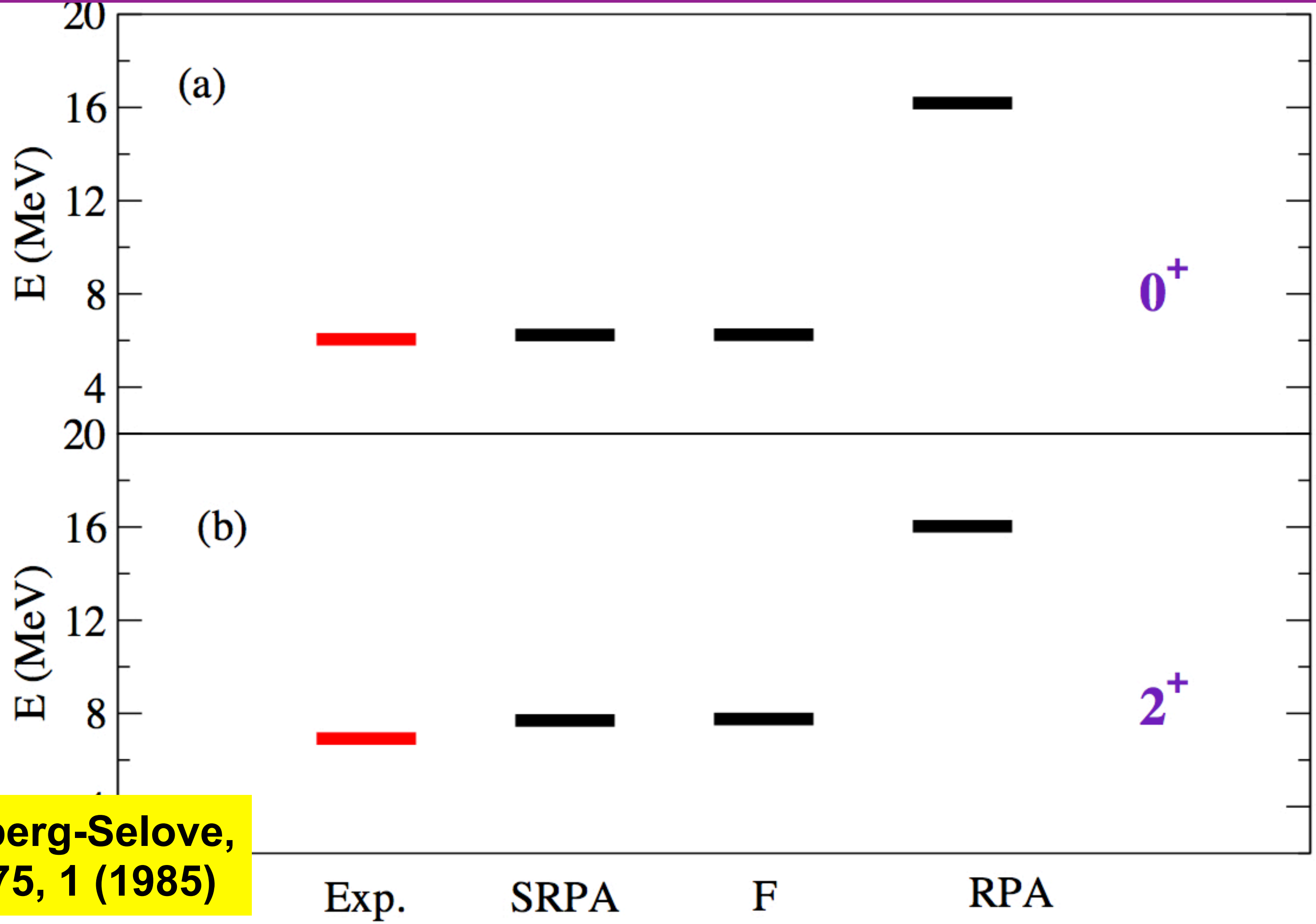
Centroid: 20.73 MeV
Width: 2.42 MeV

Centroid: 20.21 MeV
Width: 4.05 MeV

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

Centroid: 19.76 MeV
Width: 5.11 MeV

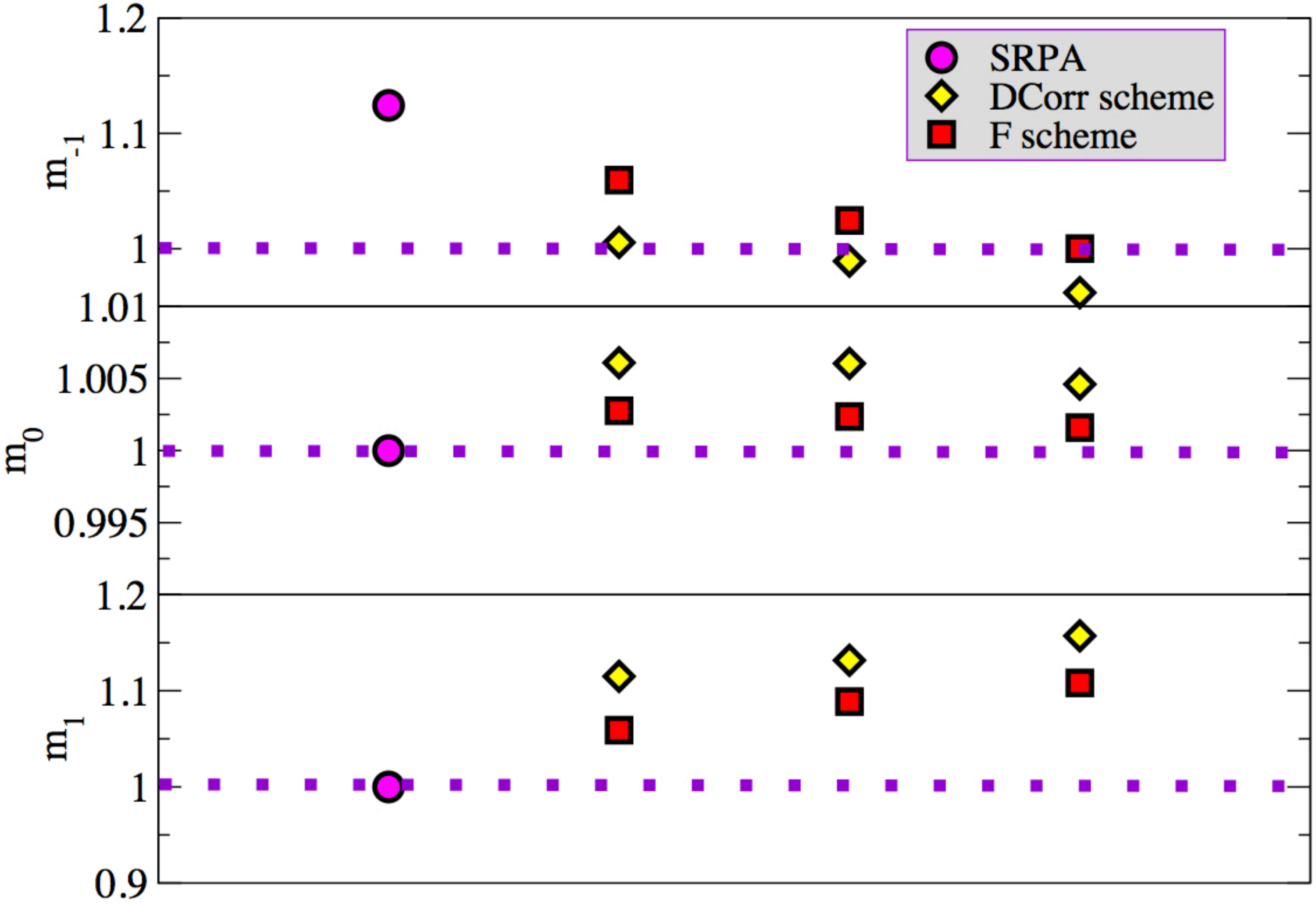
Low-lying states. Two-particle/two-hole states



Ajzenberg-Selove, NPA 375, 1 (1985)

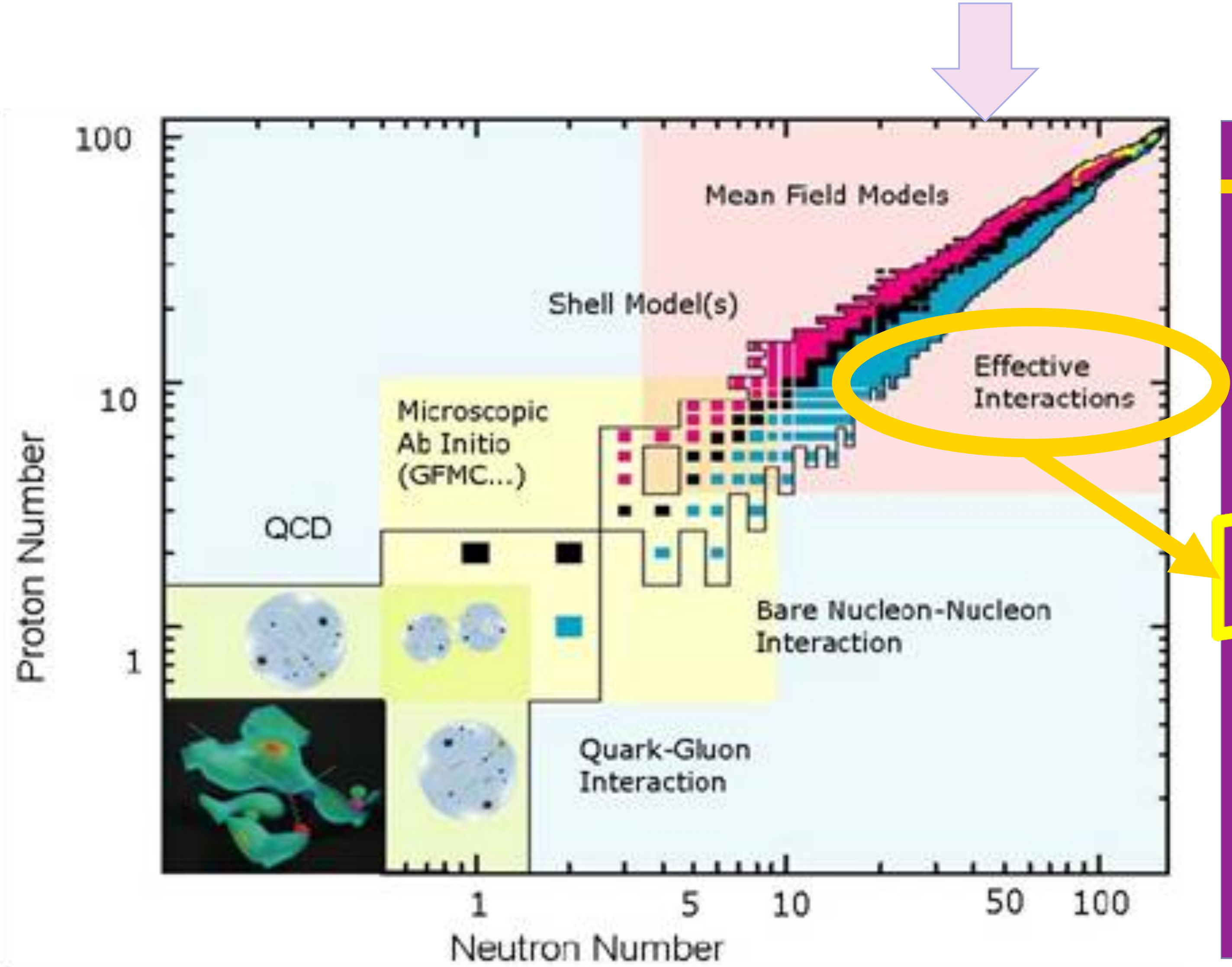
Gambacurta, Grasso, Engel, in preparation

Ratios with respect to RPA



Gambacurta, Grasso, Engel, in preparation

Energy Density Functional (EDF) models



Beyond-mean -field models (correlations).

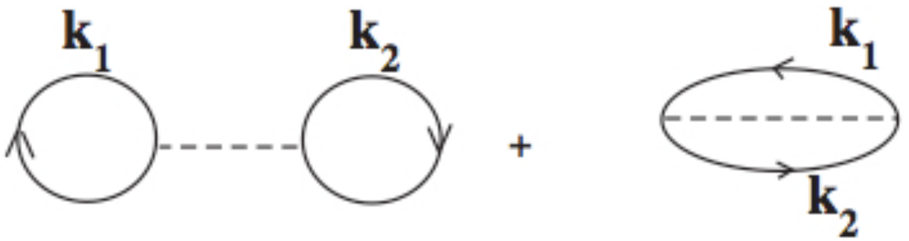
- Describing complex phenomena

- Improving predictive power of models

- INTERACTION ?

The mean-field approximation represents the leading order of the perturbative many-body problem.

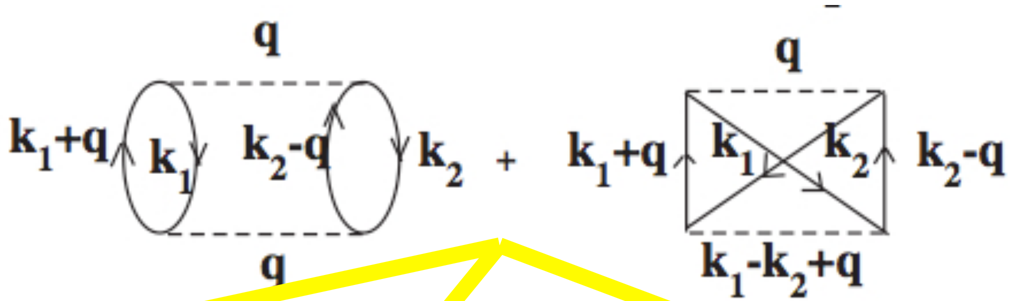
Total energy at first order



1st order equation of state of matter

What happens if one goes beyond the mean-field level within the EDF framework?

2nd order for the equation of state of nuclear matter:



1

Commonly used interactions (Skyrme) are adjusted at the mean-field level. <u>Double counting</u> problems when one uses them beyond

2

Zero-range terms in conventional forces -> <u>ultraviolet divergences</u> when one goes beyond the mean field

3

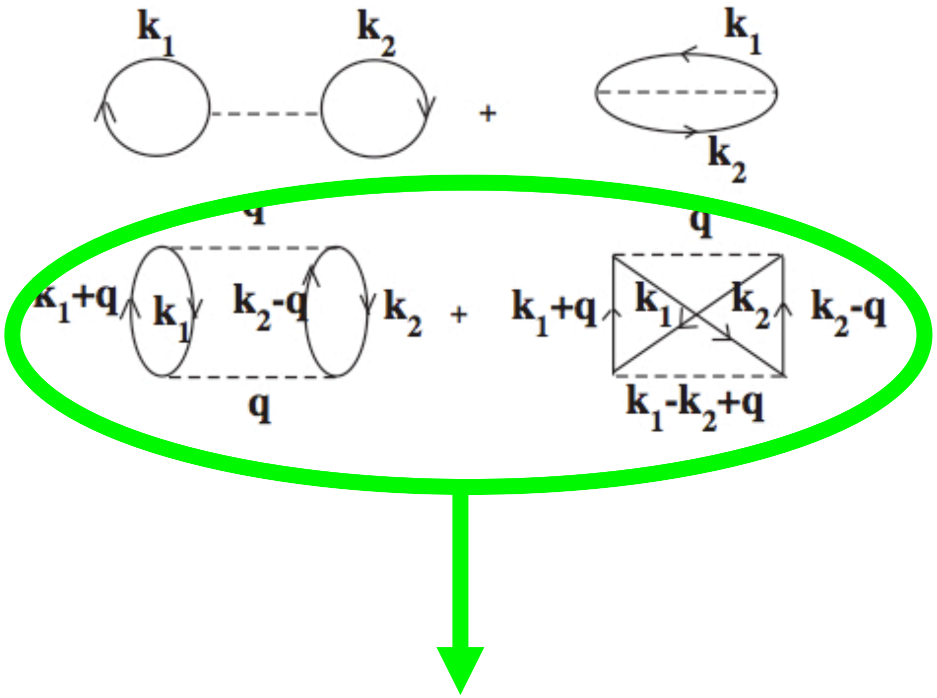
Is our problem really <u>perturbative</u> when conventional forces are used?

Regularization techniques

Power counting analysis

Moghrabi, Grasso, Colo', and Van Giai, PRL 105, 262501 (2010)

Equation of state of nuclear matter with a Skyrme-type interaction



This second-order contribution diverges with a Skyrme-type interaction

Asymptotic behavior: linear divergence (with respect to the cutoff). The second-order correction is proportional to:

$$\frac{-11+2\ln 2}{105}+\frac{\Lambda}{9k_F}-\frac{2k_F}{45\Lambda}+\mathcal{O}\left(\frac{k_F^2}{\Lambda^2}\right)$$

Coherent with the Lee-Yang expression (ground state energy of a low-density Fermi gas). Expansion as a power series in the scattering length a:

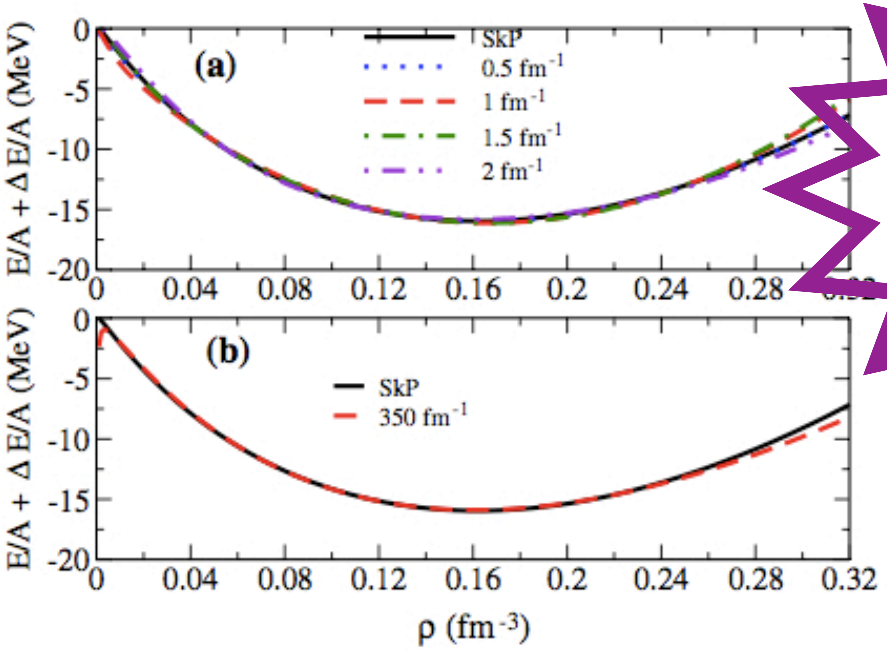
$$\frac{E}{N}=\frac{\hbar^2k_F^2}{2m}\left(\frac{3}{5}+\frac{2}{3\pi}ak_F+\frac{4}{35\pi^2}(11-2\ln 2)(ak_F)^2\right),$$

Lee and Yang, Phys. Rev. 105, 1119 (1957)

How the equation of state looks like:

Two problems: divergence and double counting

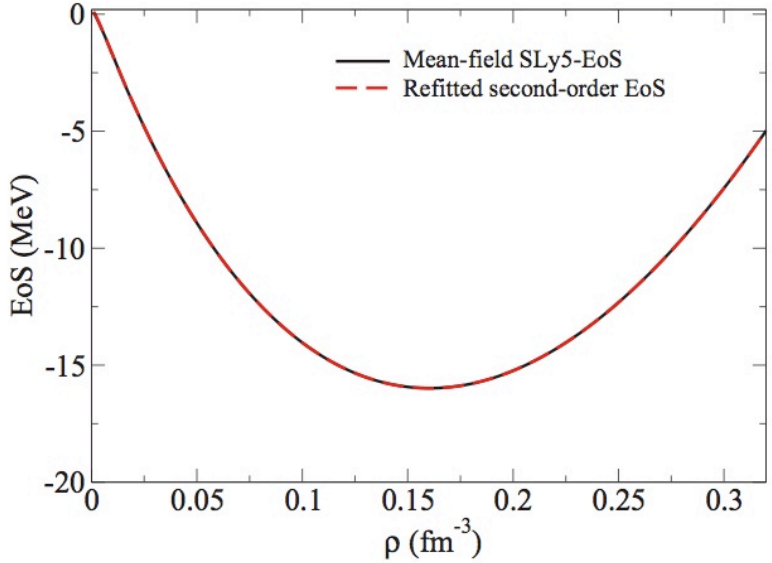
Cutoff regularization



FIT: for each cutoff value

FIG. 4 (color online). (a) Second-order-corrected equations of state compared with the reference equation of state (SkP at mean-field level). (b) Extreme case of $\Lambda = 350\ \mathrm{fm}^{-1}$.

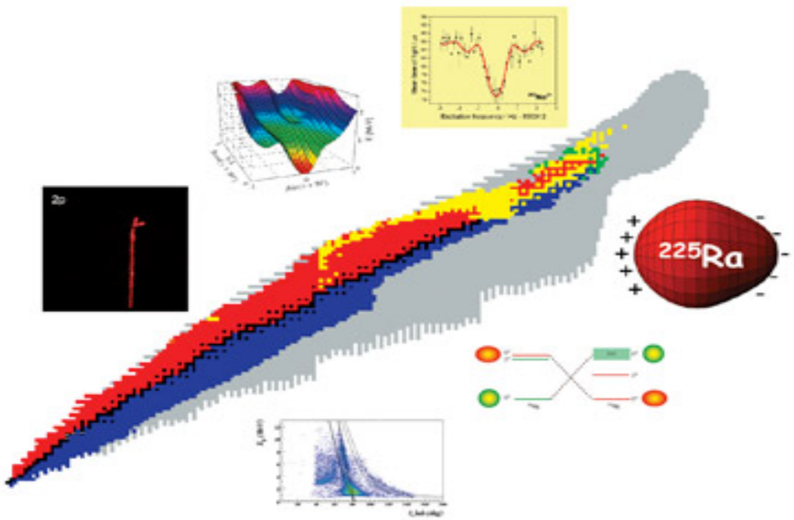
Recently done



Going from matter …

… to finite nuclei with beyond-mean-field models. First attempt:

Brenna, Colo, Roca-Maza, PRC 90, 044316 (2014)



Summary

- Implementation of the SRPA model by a subtraction procedure:
  - Double counting
  - Stability condition (real solutions)
  - We have verified that results are stable with respect to the cutoff.

- Many systematic applications to low-lying and giant resonances (physical width) are foreseen

- Interaction in beyond mean field models (second order in matter). Parameters are refitted