COLLECTIVE EXCITATIONS IN RANDOM PHASE APPROXIMATION AND BEYOND

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RPA widely used for a microscopic description of collective excitations in many body systems.

Its merits are well known.

Its limitations can be traced back to the use of the

Quasi Boson Approximation (QBA)

Some recent results of our efforts to overcome these limitations.

Quite general approach however up to now

1. Schematic 3 level Lipkin model : comparison with **exact results**

---> clear indications on the improvement with respect to standard RPA

2. Metallic clusters in the jellium approximation.

Very good laboratory since realistic many body system
and the basic interaction is well known

Some results on nuclei within Second RPA (1p-1h + 2p-2h)

---------->> Danilo Gambacurta talk

Delocalized valence electrons moving in the background of positive ions

Existence of magic numbers

Very collective dipole excitation:

c. of m. of electrons against background

Simplest model: Jellium model

Uniformly distributed positive charge + electrons

INTERACTIONS

Jellium-electrons Coulomb from a uniform spherical charge

Derived from energy density functional

Electron-electron = or

Bare Coulomb with exchange

Except for the ionic background (jellium) , like nuclei

BUT MUCH SIMPLER

only one kind of particles

spin-orbit not very important

KNOWN INTERACTION

QBA reasonable if

occupation numbers in the correlated g. s. close to 0 and 1

and generally $|0\rangle$ not very different from $|HF\rangle$

Very often this is not the case

Probability for the presence of 2n p-h excitations in ground state

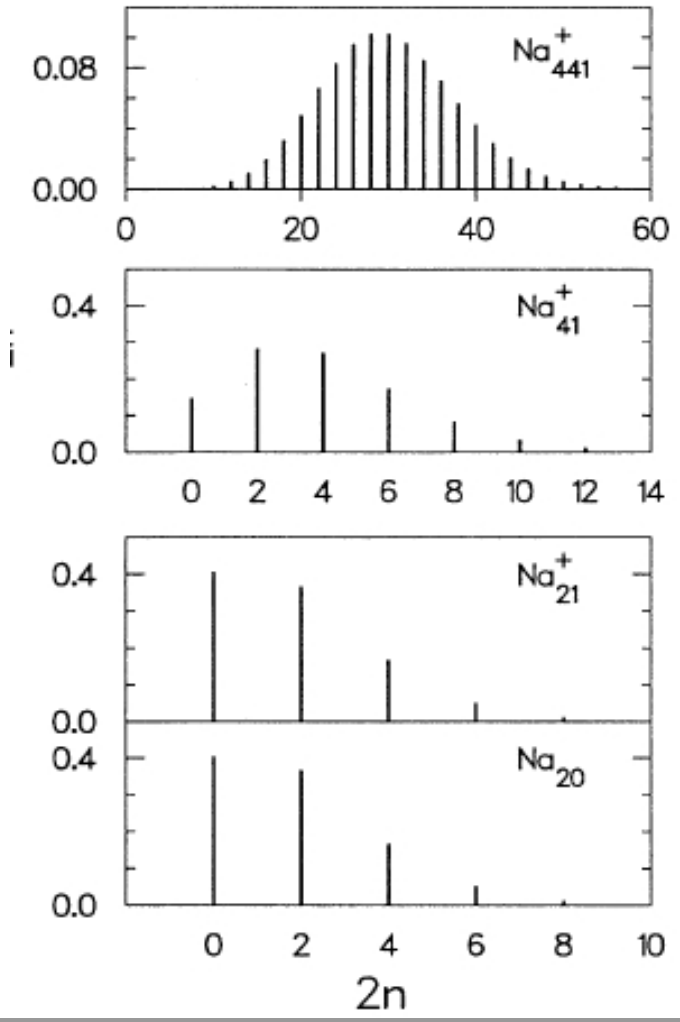
$$P_{2n} = \mathcal{N}_0^2 \frac{1}{n!} \left(\frac{u^2}{2} \right)^n ,$$

$$\mathcal{N}_0^2 = \exp(-u^2/2) ,$$

$$u^2 = \sum_L \sum_{p,h,p',h'} (2L+1)(C^L_{php'h'})^2 .$$

$$P_0 = \mathcal{N}_0^2 ,$$

$$\overline{n} = \sum_{n=1}^{\infty} 2nP_{2n} = u^2 .$$



Necessary to avoid quasi boson approximation

INCONSISTENCY

To derive equations of motion, use is made of correlated |0> as vacuum of Q

BUT

Finally, substituted with | HF >.

Particle-hole excitations within a self consistent RPA

D. Gambacurta and F. Catara, Phys. Rev. B 77, 205434 (2008)

As in RPA, introduce the collective ph operators

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

whose action on the ground state of the system $|0\rangle$ generates the collective states,

$$|\nu\rangle = Q_\nu^\dagger |0\rangle,$$

with $|0\rangle$ defined as the vacuum of the Q_ν's,

$$Q_\nu |0\rangle = 0.$$

Equations of motion method leads to

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix} = \omega_\nu \begin{pmatrix} G & 0 \\ 0 & -G^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix}$$

$$A_{ph,p'h'} = \langle 0|[a_h^\dagger a_p, H, a_{p'}^\dagger a_{h'}]|0\rangle,$$

$$B_{ph,p'h'} = -\langle 0|[a_h^\dagger a_p, H, a_{h'}^\dagger a_{p'}]|0\rangle,$$

$$G_{ph,p'h'} = \langle 0|[a_h^\dagger a_p, a_{p'}^\dagger a_{h'}]|0\rangle,$$

$$[A, B, C] = \tfrac{1}{2}\{[A, [B, C]] + [[A, B], C]\}$$

NOTE: | 0 > correlated

$$\sum_{ph,p'h'} \left(X^\nu_{ph} X^{\nu'}_{p'h'} - Y^\nu_{ph} Y^{\nu'}_{p'h'}\right) G_{ph,p'h'} = \delta_{\nu\nu'}$$

If | 0 >→| HF > standard RPA is obtained

For example

$$G^{(\mathrm{HF})}_{ph,p'h'} = \langle \mathrm{HF}|[a^\dagger_h a_p, a^\dagger_{p'} a_{h'}]|\mathrm{HF}\rangle = \delta_{hh'}\delta_{pp'}$$

Quasi boson approximation

In general one and two-body density matrices appear in the double commutators

Linearization of the equations of motion:

in the commutator

$$[H, a^\dagger_p a_h] \rightarrow a^\dagger a + a^\dagger a^\dagger a a \sim a^\dagger a + \langle \Psi_0 | a^\dagger a | \Psi_0 \rangle a^\dagger a .$$

Contractions in a reference state

Again if contraction in | HF >→standard RPA

If in | 0 >→ ERPA

Problem reduced to one body density matrix

Number operator method (Rowe)

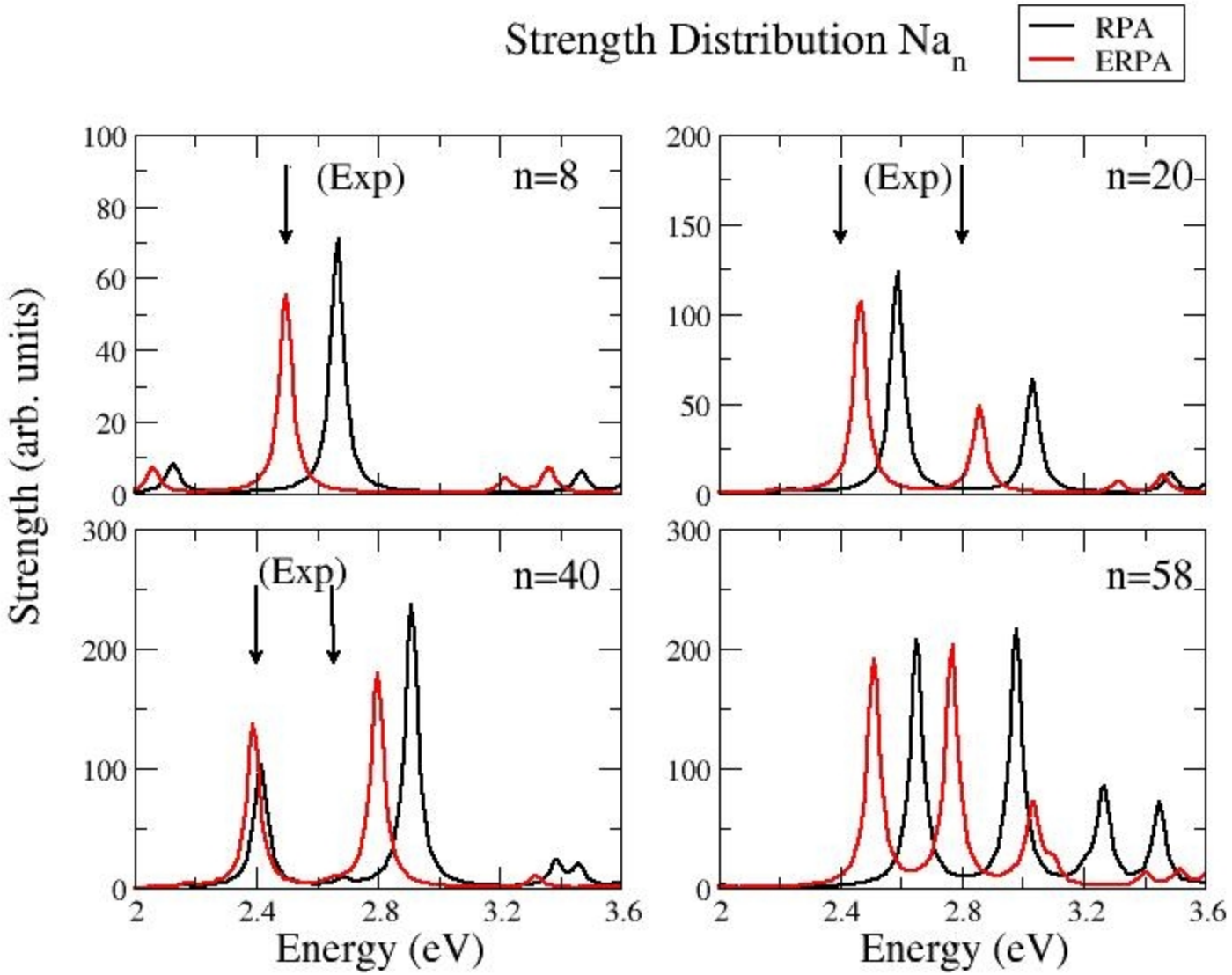
$$\rho(p,h) \equiv \langle 0|a_p^\dagger a_h|0\rangle = 0, \tag{24}$$

$$\rho(p,p') \equiv \langle 0|a_p^\dagger a_{p'}|0\rangle = \sum_{\nu\nu'} S(\nu,\nu') \sum_{p_1h_1} \sum_{p_2h_2} Y^{\nu}_{p_1h_1} Y^{\nu'*}_{p_2h_2} \times \sum_h G(ph,p_1h_1)G^*(p'h,p_2h_2), \tag{25}$$

$$\rho(h,h') \equiv \langle 0|a_h^\dagger a_{h'}|0\rangle = \delta_{hh'} - \sum_{\nu\nu'} S(\nu,\nu') \sum_{p_1h_1} \sum_{p_2h_2} Y^{\nu}_{p_1h_1} Y^{\nu'*}_{p_2h_2} \times \sum_p G(ph,p_1h_1)G^*(ph',p_2h_2), \tag{26}$$

$$S(\nu,\nu') = \delta_{\nu\nu'} - \frac{1}{2} \sum_{p_1h_1,p_2h_2} X^{\nu}_{p_1h_1} X^{\nu'*}_{p_2h_2} \times \sum_{p_3h_3} G(p_3h_3,p_1h_1)G^*(p_3h_3,p_2h_2).$$

NON LINEAR PROBLEM : ITERATIVELY


Strength Distribution Na_n
RPA
ERPA
Strength (arb. units)
(Exp)
n=8
(Exp)
n=20
(Exp)
n=40
n=58
Energy (eV)
Energy (eV)

ENERGY WEIGHTED SUM RULES

$$\sum_{\nu} \omega_{\nu} |\langle \nu | F | 0 \rangle|^2 = \frac{1}{2} \langle 0 | [F,[H,F]] | 0 \rangle,$$

Identity IF eigenstates of H

$$F = \sum_{\alpha,\beta} \langle \alpha | F | \beta \rangle a^{\dagger}_{\alpha} a_{\beta},$$

both particles and holes in general

$$\langle \nu | F | 0 \rangle = \langle 0 | [Q_{\nu}, F] | 0 \rangle.$$

IF | 0 > → | HF > RPA

$$\langle \nu | F | 0 \rangle = \sum_{ph} \{ X^{\nu *}_{ph} \langle p | F | h \rangle + Y^{\nu *}_{ph} \langle h | F | p \rangle \}.$$

BUT in the r.h.s. not only ph components, unless | 0 > → | HF >

Thouless theorem

IN ERPA (only ph components in Q)

$$\langle \nu | F | 0 \rangle = \sum_{php'h'} \{ X^{\nu *}_{ph} \langle p' | F | h' \rangle + Y^{\nu *}_{ph} \langle h' | F | p' \rangle \} G_{ph,p'h'},$$

Exactly satisfied if one takes only ph components of F

and if linearizes the commutator [H,F]

Self consistent in ph space

To have a completely self consistent approach, with the complete F

operator one has to generalize

$$Q_\nu^\dagger = \sum_{\alpha>\beta} \left(X^\nu_{\alpha\beta} a^\dagger_\alpha a_\beta - Y^\nu_{\alpha\beta} a^\dagger_\beta a_\alpha \right),$$

and linearize:

D. Gambacurta, F. Catara and M. Grasso, Phys. Rev. C 80, 014303 (2009)

EWSR exactly preserved

Studied and tested within 3-level Lipkin model

NON PHYSICAL STATE (not corresponding to any exact eigenstate)

It can be isolated looking at

Zero eigenvalues of metrics **G**

and overlap with g.s.

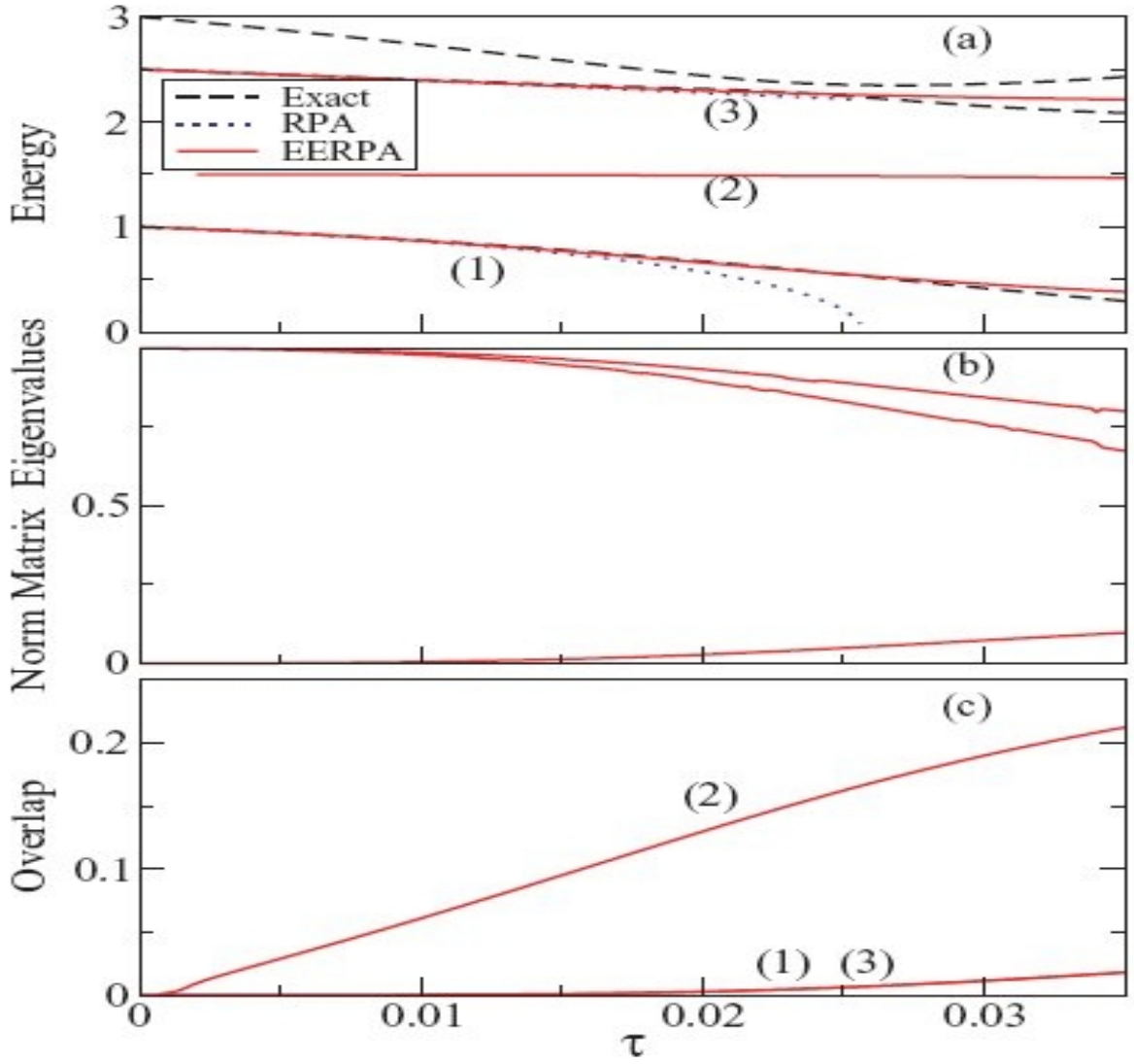


FIG. 1. (Color online) First set of parameters (33). (a): Excitation energies of the states (1), (2), and (3) and the eigenvalues of the norm matrix (b) as a function of the strength parameter $\tau = \chi/\epsilon$. The energies in the Y axis are expressed in units of ϵ. In (c) the corresponding overlaps [Eq. (34)] of the three states with the ground state are shown. See the text for more details.

Another extension of RPA------> **SRPA**

2particle-2hole configurations are considered, in addition to 1p-1h

Also in this case QBA is used

In metallic clusters huge differences with respect to RPA.

Going beyond QBA improves results, not far from RPA

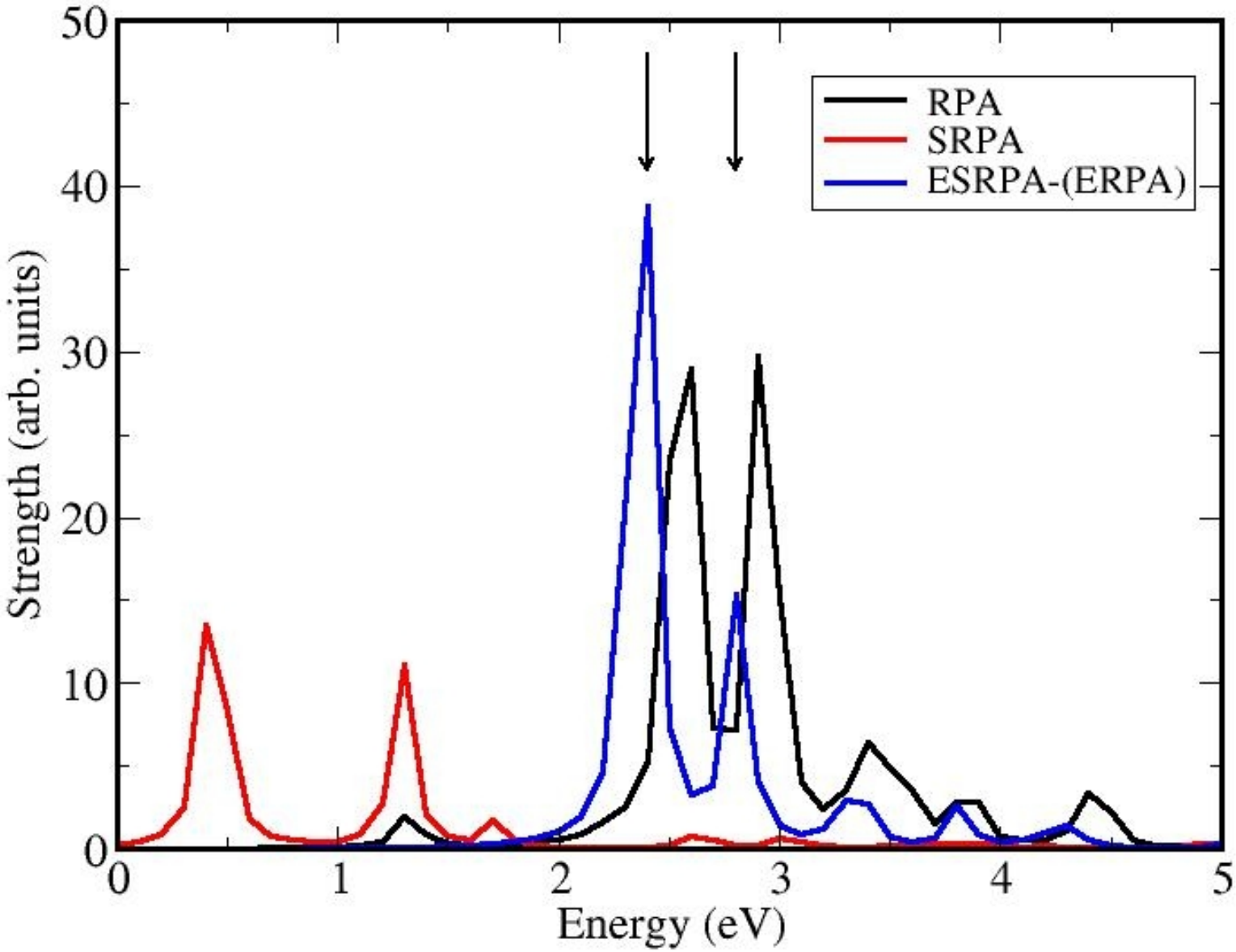
and in better agreement with experiment.

D. Gambacurta and F. Catara, Phys. Rev. B 81, 085418 (2010)

D. Gambacurta and F. Catara Phys. Rev. B 79, 085403 (2009)

D. Gambacurta, M. Grasso, F. Catara and M. Sambataro, Phys. Rev. C 73, 024319 (2006)

Na_{20}


RPA
SRPA
ESRPA-(ERPA)
Strength (arb. units)
Energy (eV)
0
10
20
30
40
50
0
1
2
3
4
5