Electromagnetic response in finite nuclei with the self-consistent Green's function formalism

(CEA, 15 June 2018)

Francesco Raimondi

(University of Surrey)

Outline

- Extension of the Algebraic Diagrammatic Construction (ADC) method with three-nucleon interactions
- Effective charges in Oxygen and Nickel isotopes from realistic nuclear interactions
- Dipole Response Function and Polarisability in Oxygen and Calcium isotopes

Outline

- Extension of the Algebraic Diagrammatic Construction (ADC) method with three-nucleon interactions
- Effective charges in Oxygen and Nickel isotopes from realistic nuclear interactions
- Dipole Response Function and Polarisability in Oxygen and Calcium isotopes

Correlations: a historical remark

GREEK ATOMISM

Leucippus
Democritus
("fathers of science")

"The principles of everything are atoms and void,
and everything else is conventional...
The atoms are infinite in size and number,
and they are carried about in the whole in a swirl,
and in that way they generate all the compounds"

Atoms

- Uncuttable, simple, eternal
- Moving in the empty space
- (geometrical shape)
- Moved by chaos/necessity

Ancient Atomism (5th c BC) ..... Birth of modern science (16th c AD)

Green's function (propagator)

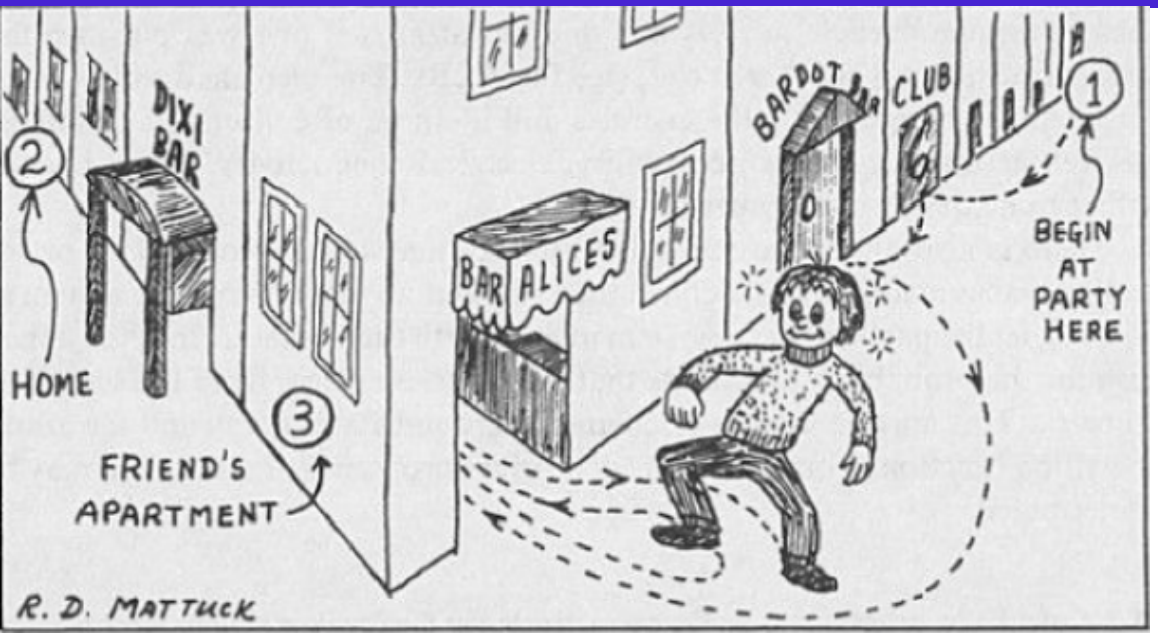
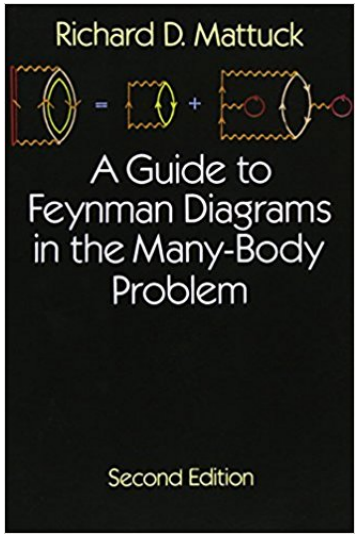


Fig. 1.1 Propagation of Drunken Man



$$g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A | a_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | a_\beta^\dagger | \Psi_0^A \rangle}{\omega - \varepsilon_n^+ + i\eta}$$

Particle propagation
(Lehmann representation)

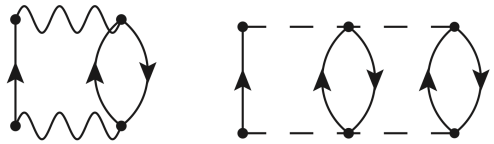
Self-energy and Dyson equation

$$G_{\alpha\beta}(\omega) = G^{(0)}_{\alpha\beta}(\omega) + \sum_{\gamma\delta} G^{(0)}_{\alpha\gamma}(\omega)\,\Sigma^{\star}_{\gamma\delta}(\omega)\,G_{\delta\beta}(\omega)$$

Self-energy: effective potential affecting the s.p. propagation in the nuclear medium

- Post-Hartree-Fock method based on self-consistency
- Based on realistic 2N and 3N forces
- Expansion of self-energy in Feynman diagrams
- Non-perturbative resummation of the correlations

Second Order diagrams

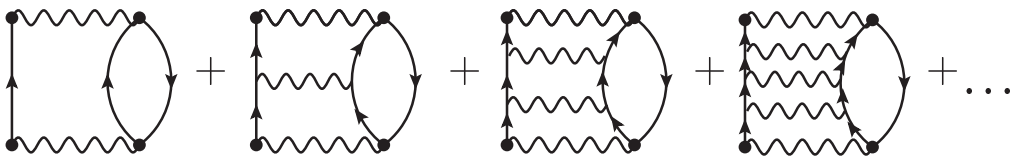


Correlations resummed non-perturbatively

$$G_{\alpha\beta}(\omega) = G^{(0)}_{\alpha\beta}(\omega) + \sum_{\gamma\delta} G^{(0)}_{\alpha\gamma}(\omega)\,\Sigma^{\star}_{\gamma\delta}(\omega)\,G_{\delta\beta}(\omega)$$

Self-energy: effective potential affecting the s.p. propagation in the nuclear medium

Entire classes of self-energy diagrams (ladder and ring) are summed at infinite order by means of a geometric series



2p1h correlations involved

Formalism to include 3p2h correlations already developed

Impact depending on computing capabilities and accuracy of next-generation realistic interaction

F.R., C. Barbieri:

- Proceeding of NTSE (2016)
- PRC**97**, 054308 (2018)

Algebraic Diagrammatic Construction method at order 3

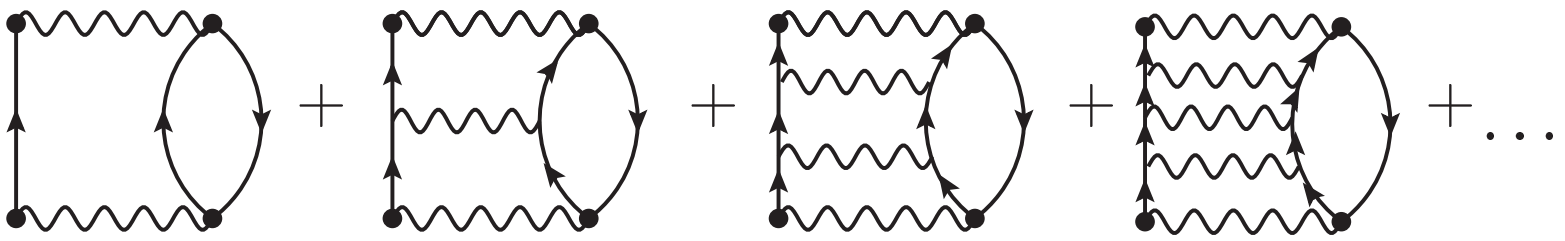
J. Schirmer and collaborators:

Phys. Rev. A26, 2395 (1982)
Phys. Rev. A28, 1237 (1983)

Dyson ADC(n)

Self-energy expansion is treated NON-perturbatively:

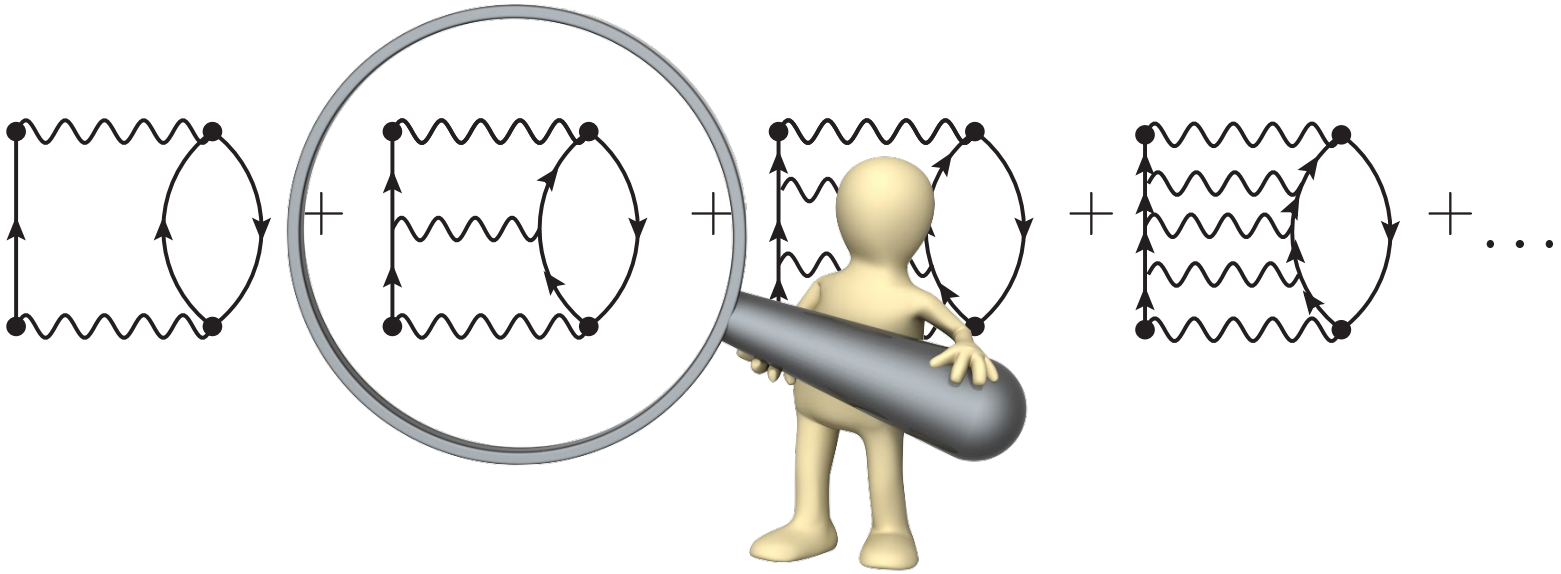
Entire classes of self-energy diagrams (ladder and ring) are summed at infinite order by means of a geometric series



Dyson ADC(3)

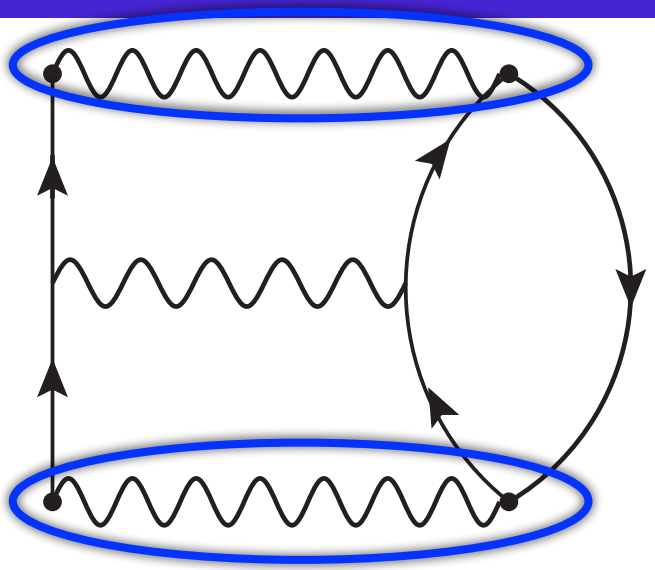
Self-energy expansion is treated NON-perturbatively:

Entire classes of self-energy diagrams (ladder and ring) are summed at infinite order by means of a geometric series



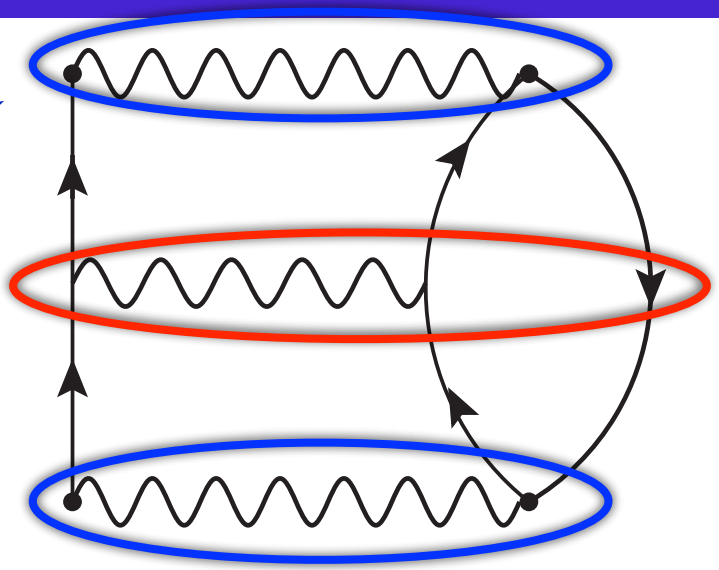
Dyson ADC(3)

M: matrices coupling the single-particle propagator to more complex intermediate configurations



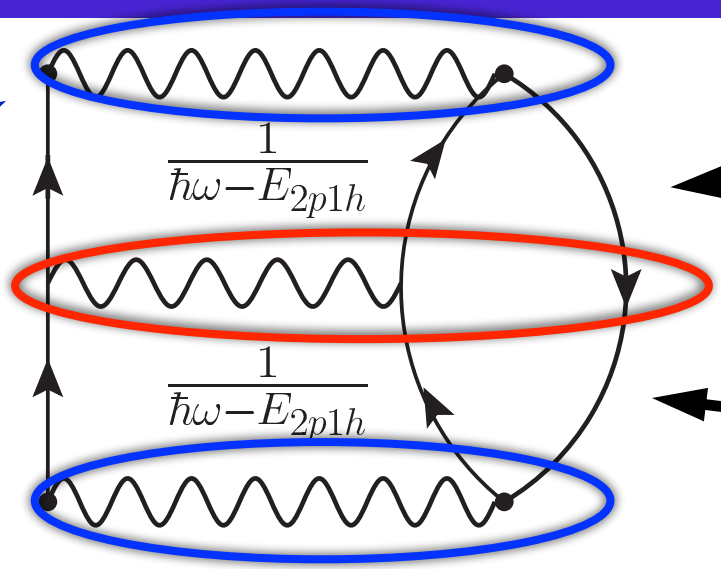
Dyson ADC(3)

M: matrices coupling the single-particle propagator to more complex intermediate configurations



C: interaction matrix linked only to internal fermion lines

Dyson ADC(3)



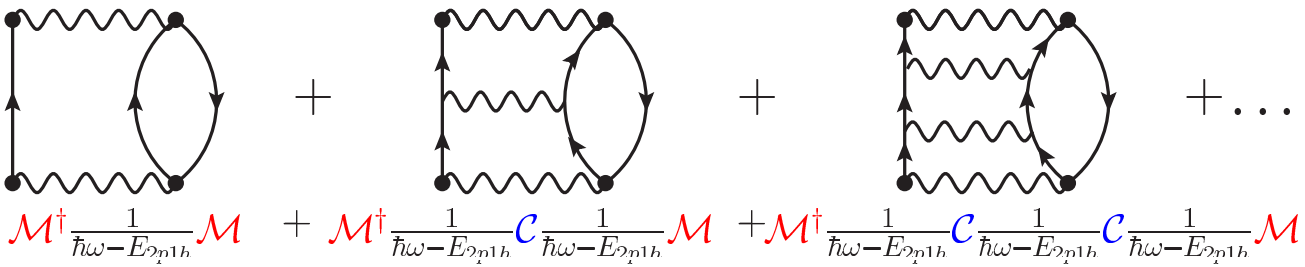
M: matrices coupling the single-particle propagator to more complex intermediate configurations

Propagator
(intermediate state configurations)

C: interaction matrix linked only to internal fermion lines

Propagator
(intermediate state configurations)

The set of ladder diagrams is a geometric series



Sum

$$\mathcal{M}^\dagger \frac{1}{\hbar\omega - E_{2p1h} - \mathcal{C}} \mathcal{M}$$

How does ADC(n) work practically

General form of the irreducible self-energy

$$\Sigma_{\alpha\beta}(\omega) = \mathcal{M}^{\dagger} \frac{1}{\hbar\omega - E_{ph} - \mathcal{C}} \mathcal{M}$$

ε_{2p1h}, ε_{3p2h}, ...

First order in the interaction

Formal expansion of **M** in powers of interactions

$$\mathcal{M} = \mathcal{M}^{(I)} + \mathcal{M}^{(II)} + \mathcal{M}^{(III)} + \ldots$$

How does ADC(n) work practically

General form of the irreducible self-energy

$$\Sigma_{\alpha\beta}(\omega) = \mathcal{M}^{\dagger} \frac{1}{\hbar\omega - E_{ph} - \mathcal{C}} \mathcal{M}$$

$\mathcal{C}$: ε_{2p1h}, ε_{3p2h}, ...

$\mathcal{M}$: First order in the interaction

Formal expansion of **M** in powers of interactions

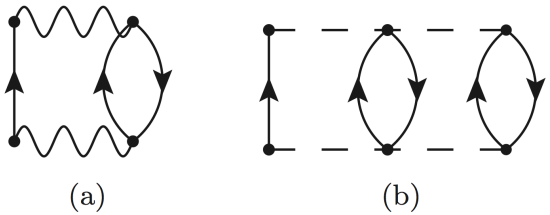
$$\mathcal{M} = \mathcal{M}^{(I)} + \mathcal{M}^{(II)} + \mathcal{M}^{(III)} + \ldots$$

Explicit expressions for **M** and **C** are found by comparing with derived expressions of self-energy Goldstone diagrams up to the same order

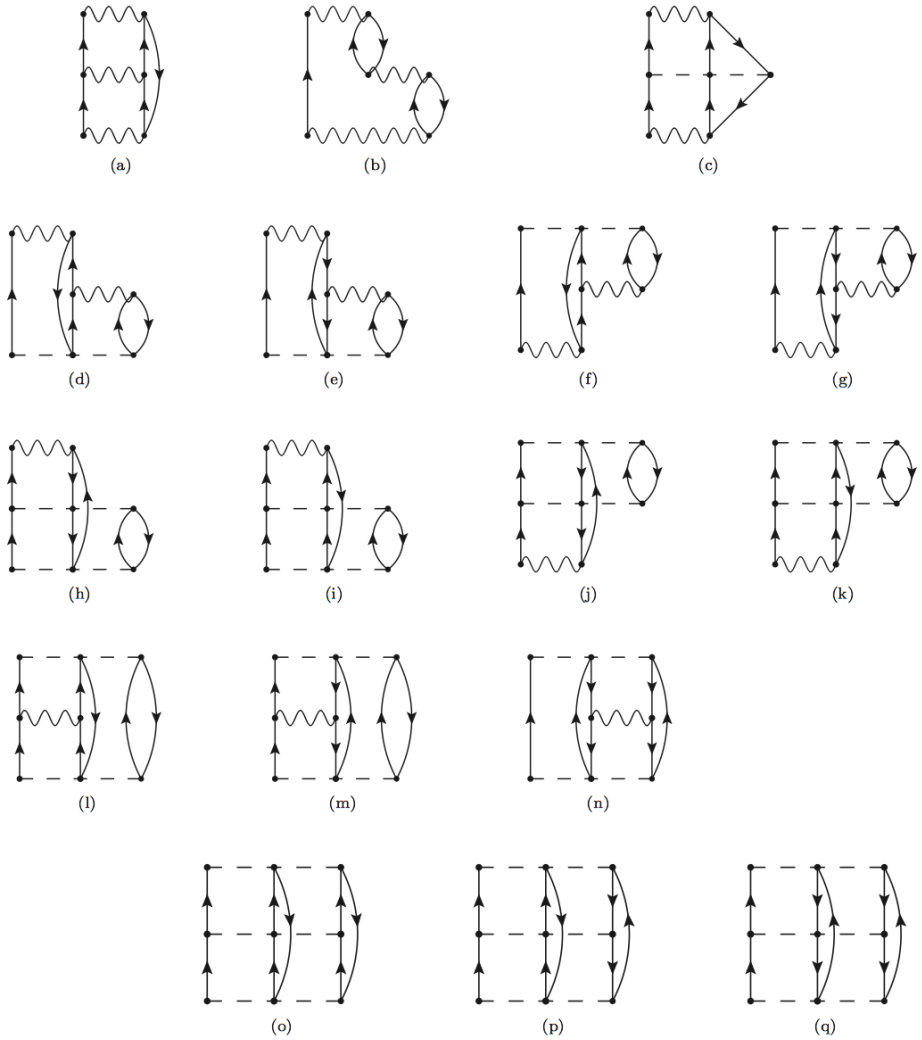
$$\mathcal{M}^{\dagger} \frac{1}{\hbar\omega - E_{ph} - \mathcal{C}} \mathcal{M} = \mathcal{M}^{(I)\dagger} \frac{1}{\hbar\omega - E_{ph}} \mathcal{M}^{(I)} + \mathcal{M}^{(II)\dagger} \frac{1}{\hbar\omega - E_{ph}} \mathcal{M}^{(I)} + \mathcal{M}^{(I)\dagger} \frac{1}{\hbar\omega - E_{ph}} \mathcal{M}^{(II)} + \mathcal{M}^{(I)\dagger} \frac{1}{\hbar\omega - E_{ph}} \mathcal{C} \frac{1}{\hbar\omega - E_{ph}} \mathcal{M}^{(I)} + \text{fourth order} + \ldots$$

Interaction-irreducible Self-Energy with NN and 3NFs

Second order diagrams with NN and 3N forces



Third order diagrams with NN and 3N forces



Complete set of ADC(3) working equations in Phys Rev C **97**, 054308 (2018)

Outline

- Extension of the Algebraic Diagrammatic Construction (ADC) method with three-nucleon interactions

- Effective charges in Oxygen and Nickel isotopes from realistic nuclear interactions

- Dipole Response Function and Polarisability in Oxygen and Calcium isotopes

Effective charges in shell model approach

In the shell model approach, based on the distinction between a valence space and an inert-core space, the effects of the polarization of the inert core are taken into account by the renormalization of the electromagnetic charge

Isolde Shell Model Course for Non Practitioners

E. Caurier, G. Martinez-Pinedo,
F. Nowacki, A. Poves and K. Sieja

Isolde Shell Model Course for Non Practitioners
CERN, October 14^{th}-18^{th}-2013

Effective charges in shell model approach

In the shell model approach, based on the distinction between a valence space and an inert-core space, the effects of the polarization of the inert core are taken into account by the renormalization of the electromagnetic charge

Basic notions

Isolde Shell Model Course for Non Practitioners

Starting with a regularized interaction, the exact solution of the secular problem, in the (infinite) Hilbert space built on the mean field orbits, is approximated in the large scale shell model calculations by the solution of the Schrödinger equation in the valence space, using an effective interaction such that:

$$H\Psi = E\Psi \longrightarrow \mathcal{H}_{eff.}\Psi_{eff.} = E\Psi_{eff.}$$

In general, effective operators have to be introduced to account for the restrictions of the Hilbert space

$$\langle\Psi|\mathcal{O}|\Psi\rangle = \langle\Psi_{eff.}|\mathcal{O}_{eff.}|\Psi_{eff.}\rangle$$

Definition of Effective charges

- nucleons have internal structure (form factor, polarizabilities,…)
- exchange currents
- many-body correlations couple neutrons and protons:

  - center-of-mass conservation
  - core-polarization effects
  - particle-vibration coupling

Mechanism of coupling of the single particle with collective nuclear excitations dressing the charge

Coupling of neutrons and protons via center-of-mass conservation:

E1 (dipole) effective charge: $q^{eff} = q - (Ze)/A$

↓

Isospin dependence

Green's function with external field

Tools of choice for the Green functions practitioners in many-body nuclear physics:

Schrödinger equation with microscopic nuclear Hamiltonian

$$\hat{H}^{\phi}(t) = \sum_{\alpha\beta} T_{\alpha\beta}\, a^{\dagger}_{\alpha} a_{\beta} + \frac{1}{4} \sum_{\substack{\alpha\gamma \\ \beta\delta}} V_{\alpha\gamma,\beta\delta}\, a^{\dagger}_{\alpha} a^{\dagger}_{\gamma} a_{\delta} a_{\beta} + \frac{1}{36} \sum_{\substack{\alpha\gamma\epsilon \\ \beta\delta\eta}} W_{\alpha\gamma\epsilon,\beta\delta\eta}\, a^{\dagger}_{\alpha} a^{\dagger}_{\gamma} a^{\dagger}_{\epsilon} a_{\eta} a_{\delta} a_{\beta} + \sum_{\alpha\beta} \phi_{\alpha\beta}(t)\, a^{\dagger}_{\alpha} a_{\beta}$$

External Field

Green's function (Lehmann representation)

$$\tilde{G}_{\alpha\beta}(\omega) = \sum_{n} \frac{\langle \Psi^{A}_{0} | a_{\alpha} | \Psi^{A+1}_{n} \rangle \langle \Psi^{A+1}_{n} | a^{\dagger}_{\beta} | \Psi^{A}_{0} \rangle}{\omega - \varepsilon^{+}_{n} + \mathrm{i}\eta} + \sum_{k} \frac{\langle \Psi^{A}_{0} | a^{\dagger}_{\beta} | \Psi^{A-1}_{k} \rangle \langle \Psi^{A-1}_{k} | a_{\alpha} | \Psi^{A}_{0} \rangle}{\omega - \varepsilon^{-}_{k} - \mathrm{i}\eta}$$

Dyson equation

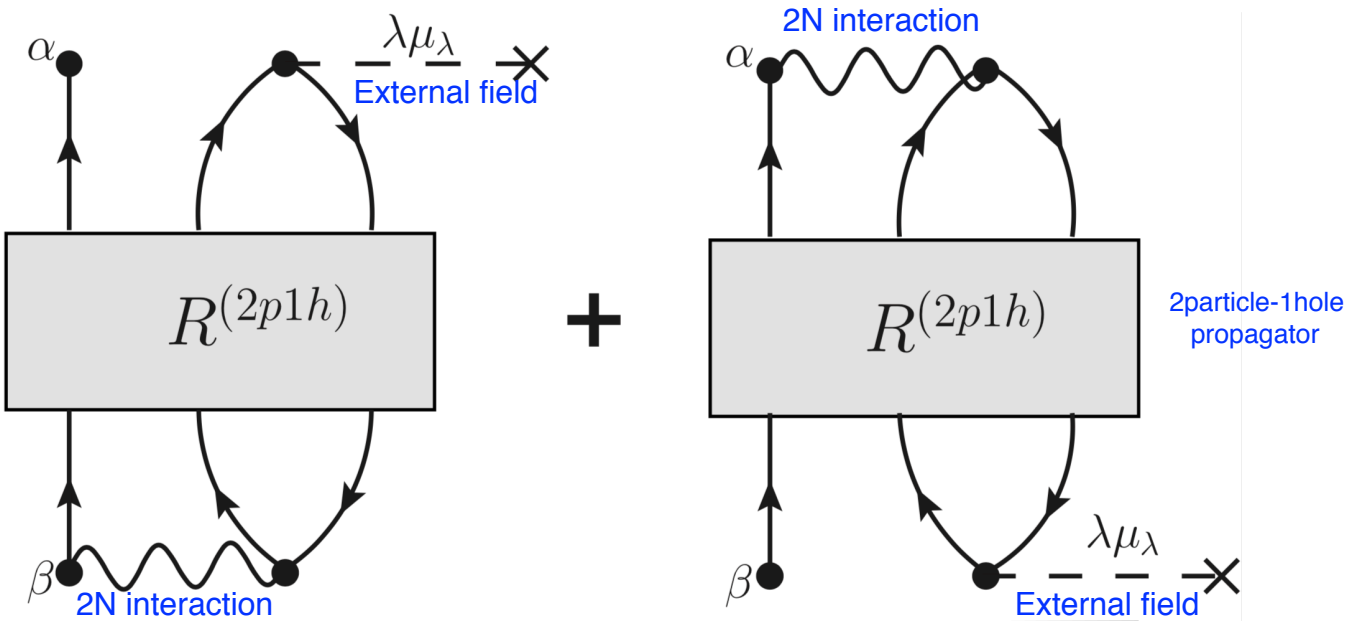
$$\begin{aligned} \tilde{G}_{\alpha\beta}(t-t') = G^{(0)}_{\alpha\beta}(t-t') &+ G^{(0)}_{\alpha\gamma}(t-t_1) \phi^{(\lambda\mu_\lambda)}_{\gamma\delta}(t_1) \tilde{G}_{\delta\beta}(t_1-t') \\ &+ G^{(0)}_{\alpha\gamma}(t-t_1) \tilde{\Sigma}^{(\lambda\mu_\lambda)}_{\gamma\delta}(t_1-t_2) \tilde{G}_{\delta\beta}(t_2-t') \end{aligned}$$

Irreducible Self-Energy

Irreducible self-energy : $\tilde{\Sigma}^{(\lambda\mu_\lambda)}_{\alpha\beta}$

In the presence of an external field, the energy-dependent part of the self-energy dynamic is

$$\tilde{\Sigma}^{(\lambda\mu_\lambda)}_{\alpha\beta}(\tau) =$$



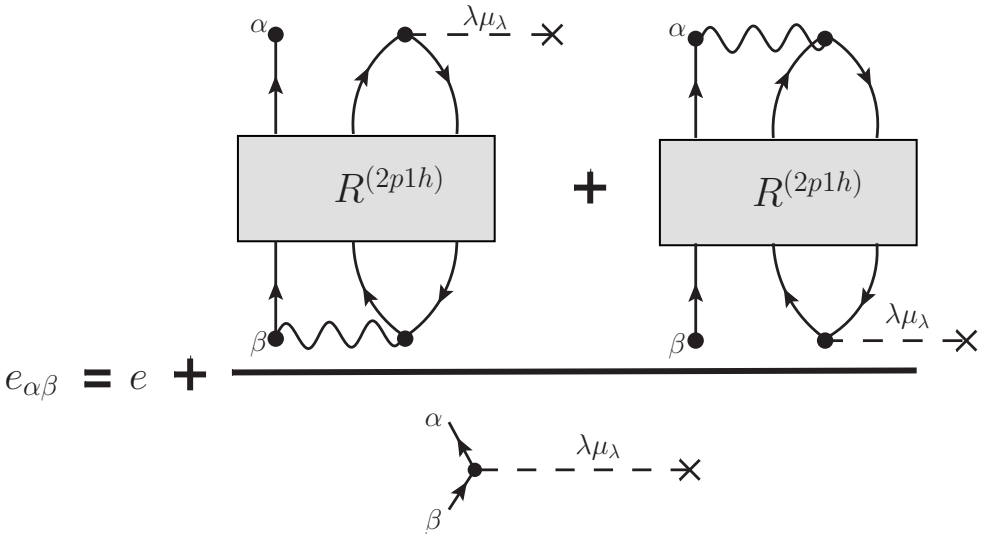
Effective potential including the correlations of the interacting nuclear medium AND the effects of the presence of the external field

Theoretical effective charges

(as opposed to the ones extracted from experiment)

Our purpose is to calculate effective charges without resorting to any measurement of electromagnetic observables

Basic idea: calculate the core-polarization effect felt by the single-particle orbital of interest because of the energy-dependent effective potential, calculated at ADC(3) level

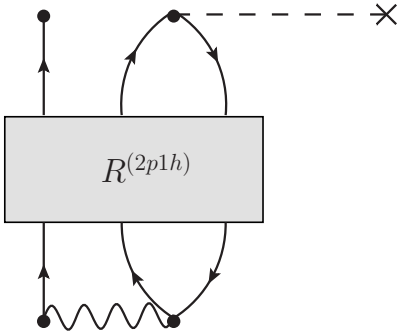


Effective charge as the ratio between the transition strengths (with and without the core-polarization) of a given multipole field:

$$\frac{\langle\tilde{\alpha}|\hat{\phi}^{(\lambda\mu_\lambda)}|\tilde{\beta}\rangle}{\langle\alpha|\hat{\phi}^{(\lambda\mu_\lambda)}|\beta\rangle} = 1 + \frac{\tilde{\Sigma}^{(\lambda\mu)}_{\alpha\beta}}{\langle\alpha|\hat{\phi}^{(\lambda\mu_\lambda)}|\beta\rangle}$$

$|\tilde{\alpha}\rangle \equiv$ s.p. state with correlations induced by the nuclear interaction and electromagnetic operator

Inputs for the 2p1h propagator



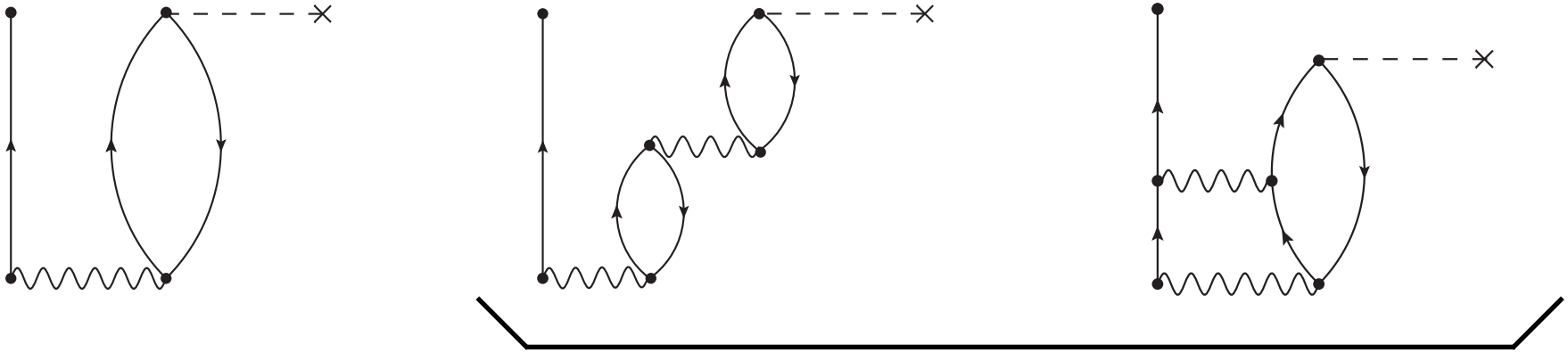
ADC(3) Propagator reduced to an optimal mean-field-like propagator

NN and 3N nuclear interaction $NNLO_{sat}$

(A. Ekström et al.
Phys. Rev. C 91, 051301(R))

$$\hat{\phi}^{(2\mu)} = \sum_i r_i^2 \, Y_{2\mu}(\hat{r}_i)$$

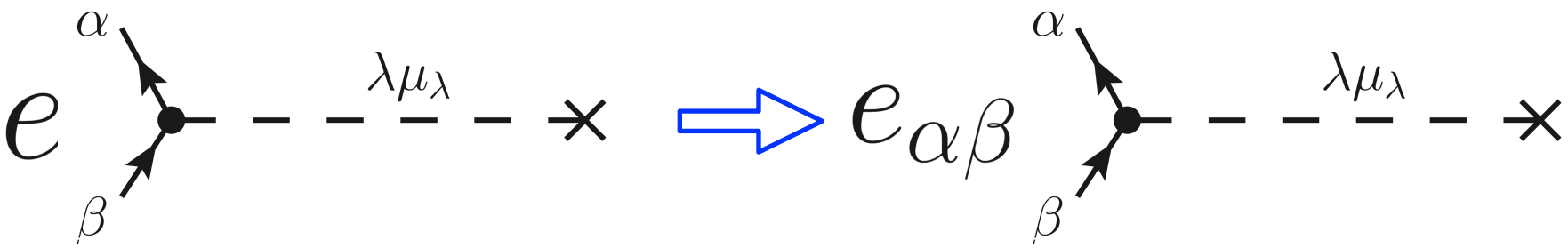
Topologies in the self-energy diagrams:



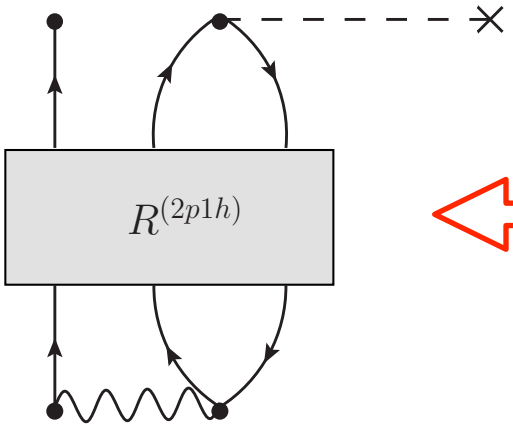
Resummation in FTDA and FRPA

(C.Barbieri et al Phys. Rev. C 63, 034313 (2001))

Effective coupling of an operator



Renormalization of the EM operator
(tailored to the considered model space)



Internal excitations (phonons)
made s.p. orbitals in the valence space
are removed from 2p1h propagator

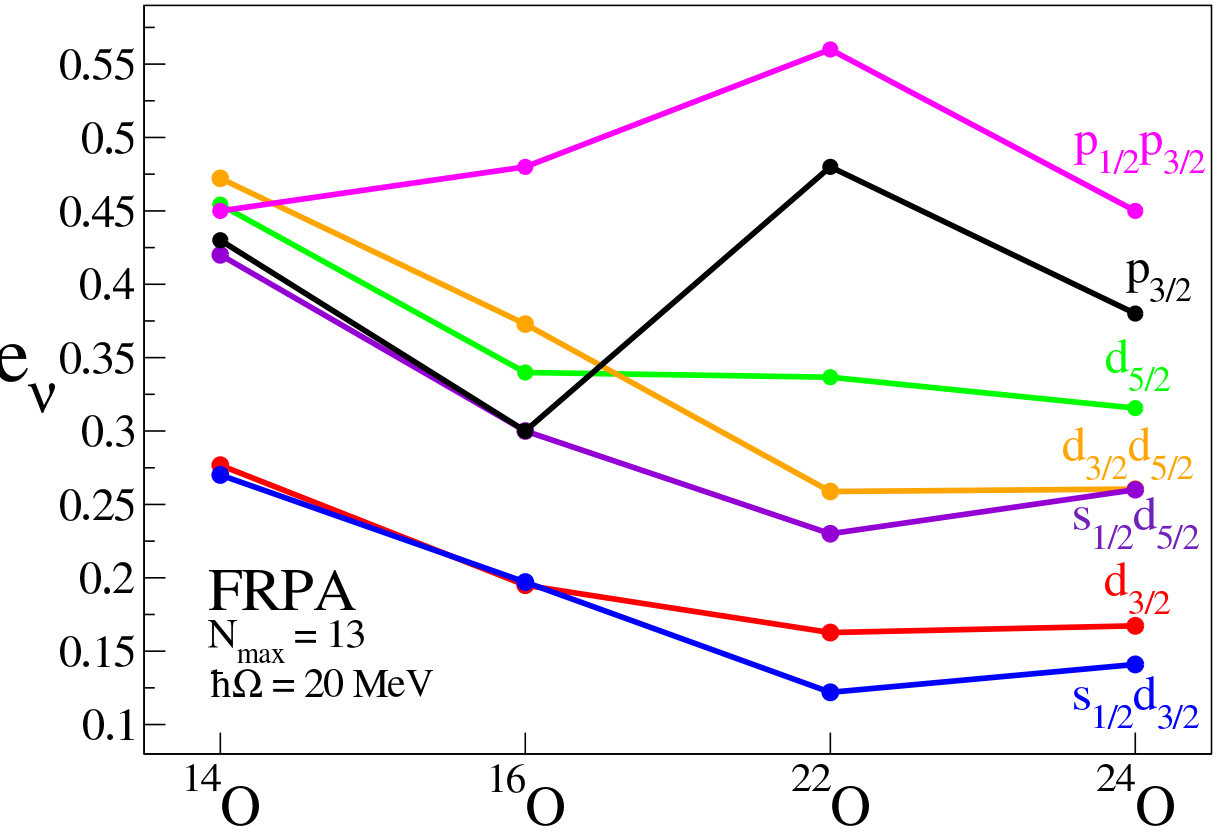
0p0d1s valence space: ^{14}O, ^{16}O, ^{22}O and ^{24}O

0f1p0g$_{9/2}$ valence space: ^{48}Ni, ^{56}Ni, ^{68}Ni and ^{78}Ni

Oxygen effective charges

0p0d1s valence space

Neutrons



	^{14}O	^{16}O	^{22}O	^{24}O
$\langle r_\nu^2 \rangle^{1/2}$	2.37	2.62	2.93	3.11
$\langle r_\pi^2 \rangle^{1/2}$	2.57	2.64	2.67	2.71

Orbital dependence:
0.14 - 0.45 (^{24}O)

Isotopic trend:
quench of polarisation effect

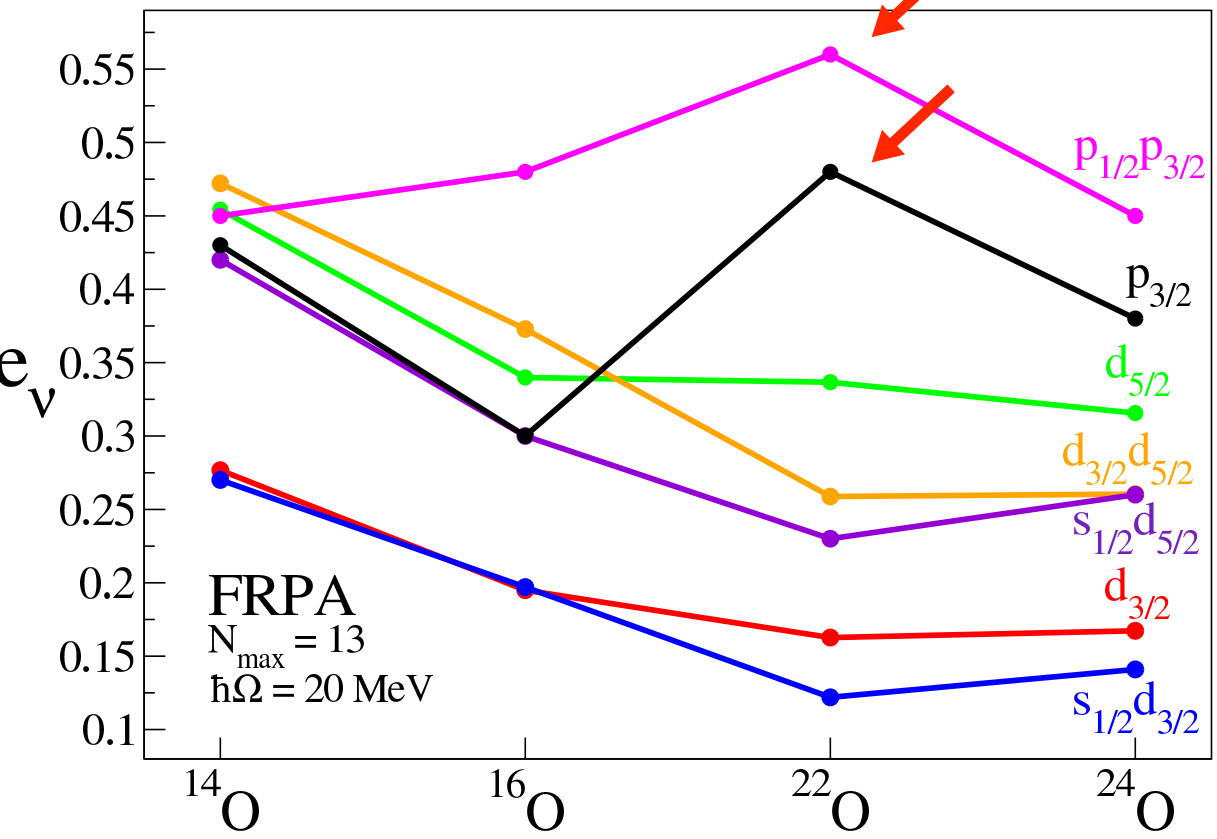
Most of values within 10%
w.r.t. FTDA

Oxygen effective charges

0p0d1s valence space

Neutrons

Erratic value of $p_{3/2}$ in ^{22}O



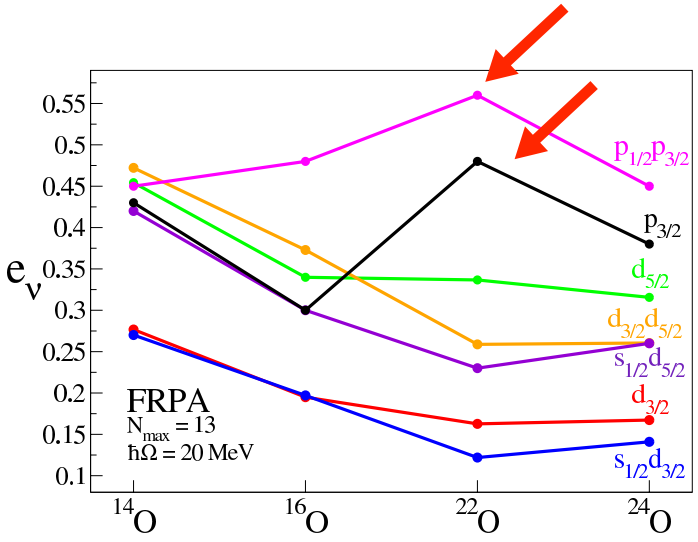
	^{14}O	^{16}O	^{22}O	^{24}O
$\langle r_\nu^2 \rangle^{1/2}$	2.37	2.62	2.93	3.11
$\langle r_\pi^2 \rangle^{1/2}$	2.57	2.64	2.67	2.71

Orbital dependence:
0.14 - 0.45 (^{24}O)

Isotopic trend:
quench of polarisation effect

Most of values within 10%
w.r.t. FTDA

Divergencies and erratic values of the effective charges



$$\frac{\langle\tilde{\alpha}|\hat{\phi}^{(\lambda\mu_\lambda)}|\tilde{\beta}\rangle}{\langle\alpha|\hat{\phi}^{(\lambda\mu_\lambda)}|\beta\rangle} = 1 + \frac{\tilde{\Sigma}^{(\lambda\mu)}_{\alpha\beta}}{\langle\alpha|\hat{\phi}^{(\lambda\mu_\lambda)}|\beta\rangle}$$

$$|\tilde{\alpha}\rangle = |\alpha\rangle_{\mathrm{OpRS}} + \sum_r \frac{\langle r|\hat{H}_1|\alpha\rangle_{\mathrm{OpRS}}}{\varepsilon_\alpha - \varepsilon_r}|r\rangle$$

$$= |\alpha\rangle_{\mathrm{OpRS}} + \sum_n \frac{1}{\varepsilon_\alpha - [\mathbf{E}^{>} + \mathbf{C}]_n}\mathbf{M}_{n\alpha}|n\rangle$$

$$\langle\tilde{\alpha}|\hat{\phi}^{(\lambda\mu_\lambda)}|\tilde{\beta}\rangle = \langle\alpha|\hat{\phi}^{(\lambda\mu_\lambda)}|\beta\rangle_{\mathrm{OpRS}} + \sum_n \left({}^1\phi^{(\lambda\mu_\lambda),n}_\alpha\right)^* \frac{1}{\varepsilon_\beta - [\mathbf{E}^{>} + \mathbf{C}]_n}\mathbf{M}_{n\beta} + \sum_k {}^1\phi^{(\lambda\mu_\lambda),k}_\alpha \frac{1}{\varepsilon_\beta - [\mathbf{E}^{<} + \mathbf{D}]_k}(\mathbf{N}_{\beta k})^*$$

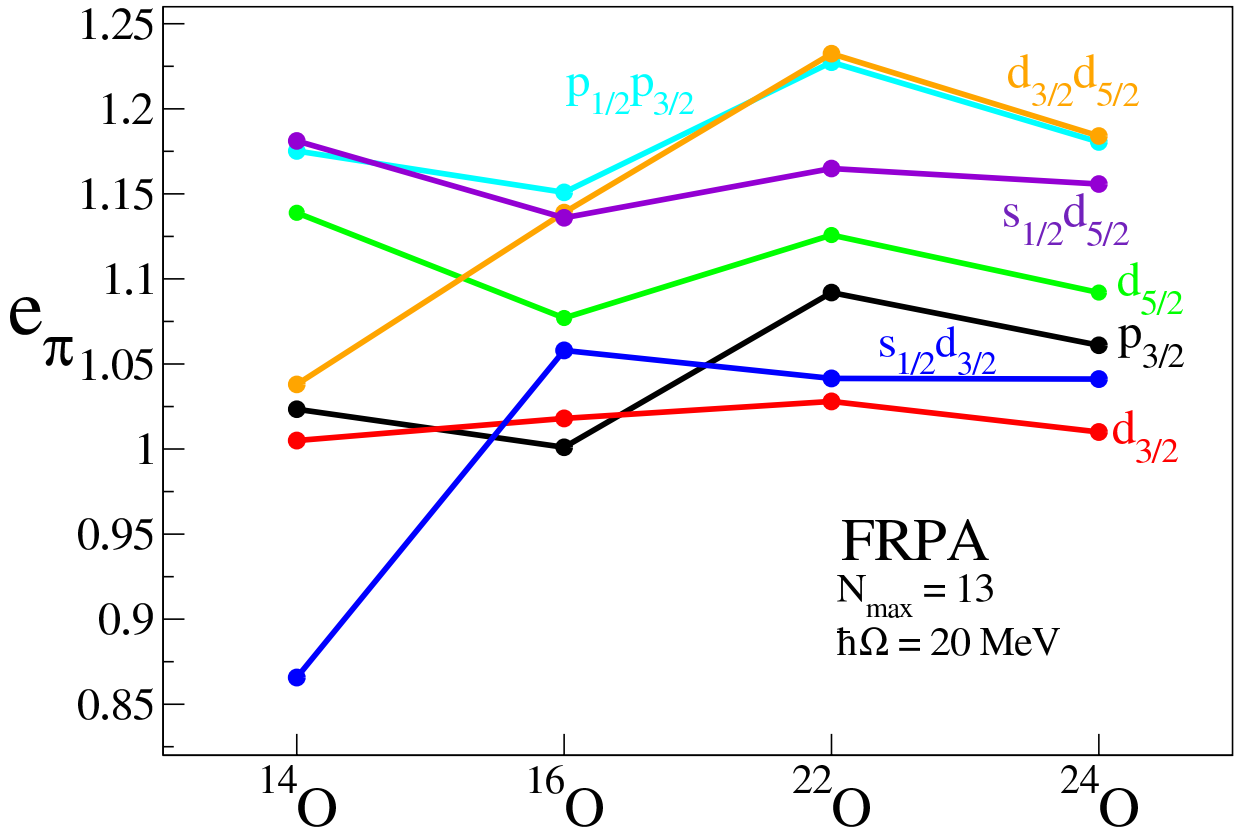
$$= \langle\alpha|\hat{\phi}^{(\lambda\mu_\lambda)}|\beta\rangle_{\mathrm{OpRS}} + \Sigma^{\mathrm{L}(\lambda\mu)}_{\alpha\beta}(\omega = \varepsilon_\beta) + \Sigma^{\mathrm{R}(\lambda\mu)}_{\alpha\beta}(\omega = \varepsilon_\alpha)$$

< 50 KeV

Oxygen effective charges

0p0d1s valence space

Protons



Flat isotopic trend

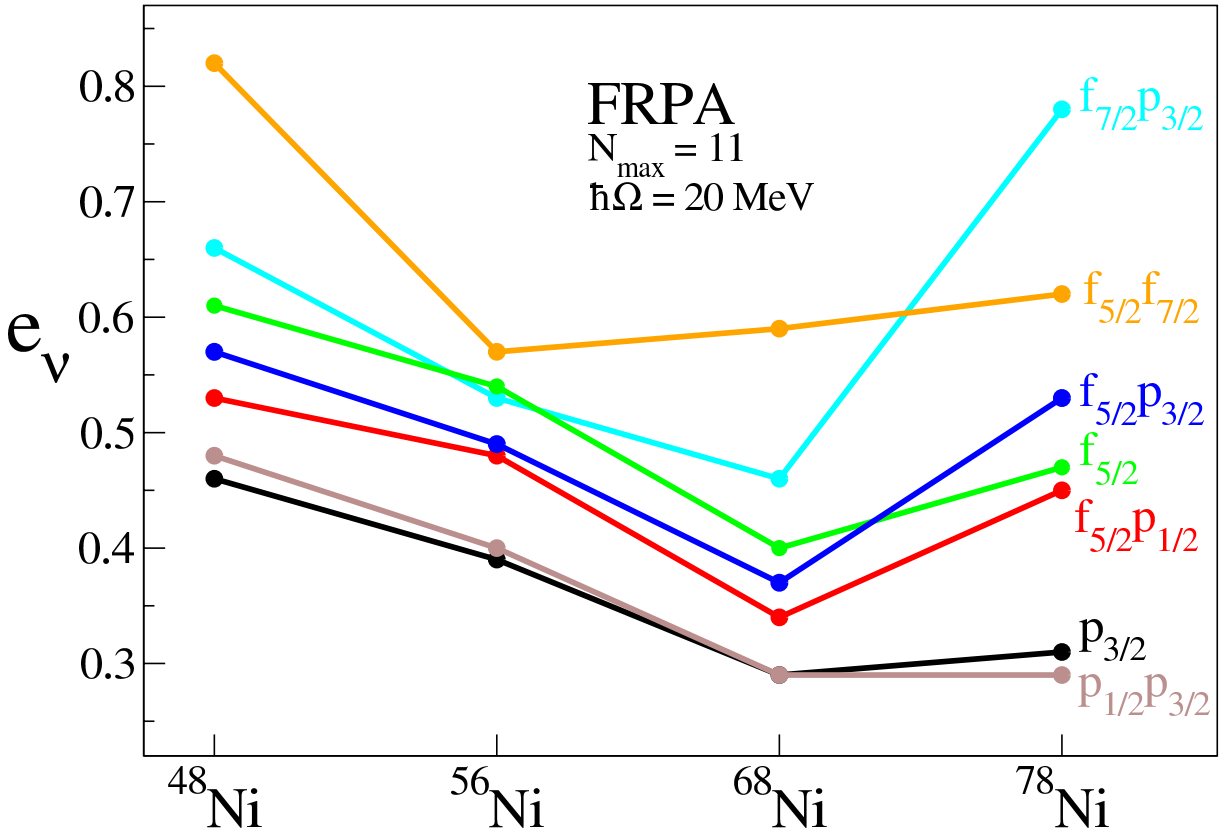
Orbital dependence:
1.0 - 1.2

Significant difference w.r.t.
Standard e_π values (~1.5)

Nickel effective charges

0f1p0g$_{9/2}$ valence space

Neutrons



Orbital dependence significant: 0.46 - 0.82 (^{48}Ni)

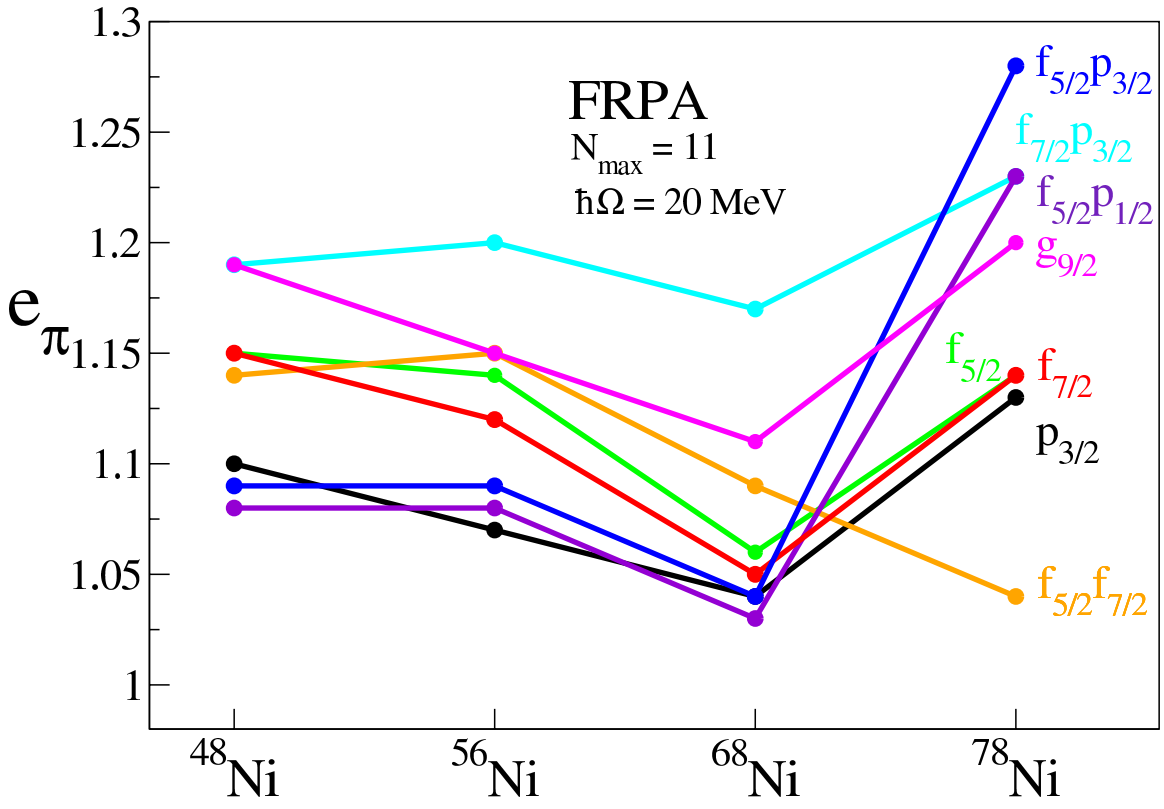
Isotopic trend: quench of polarisation effect up to ^{68}Ni

Systematic inversion of the trend in ^{78}Ni (Poor convergence?)

Nickel effective charges

0f1p0g$_{9/2}$ valence space

Protons



Orbital dependence:
1.0 - 1.2

Flat isotopic trend
(Up to ^{68}Ni)

Confirmed systematic inversion
of the trend in ^{78}Ni
(Poor convergence?)

Outline

- Extension of the Algebraic Diagrammatic Construction (ADC) method with three-nucleon interactions

- Effective charges in Oxygen and Nickel isotopes from realistic nuclear interactions

- Dipole Response Function and Polarisability in Oxygen and Calcium isotopes

Electromagnetic response in SCGF

OBSERVABLES

$$\sigma_\gamma(E) = 4\pi^2 \alpha E \, R(E)$$ PHOTOABSORPTION CROSS SECTION

$$\alpha_D = 2\alpha \int dE \, \frac{R(E)}{E}$$ ELECTRIC DIPOLE POLARIZABILITY

Response $R(E)$ depends on excited states of the nuclear system, when "probed" with dipole operator $\hat{D}$

$$R(E) = \sum_\nu |<\psi_\nu^A|\hat{D}|\psi_0^A>|^2 \, \delta_{E_\nu, E}$$

Electromagnetic response in SCGF

OBSERVABLES

$$\sigma_\gamma(E) = 4\pi^2 \alpha E\, R(E)$$ PHOTOABSORPTION CROSS SECTION

$$\alpha_D = 2\alpha \int dE\, \frac{R(E)}{E}$$ ELECTRIC DIPOLE POLARIZABILITY

Response $R(E)$ depends on excited states of the nuclear system, when "probed" with dipole operator $\hat{D}$

$$R(E) = \sum_\nu |<\psi_\nu^A|\hat{D}|\psi_0^A>|^2\, \delta_{E_\nu,E}$$

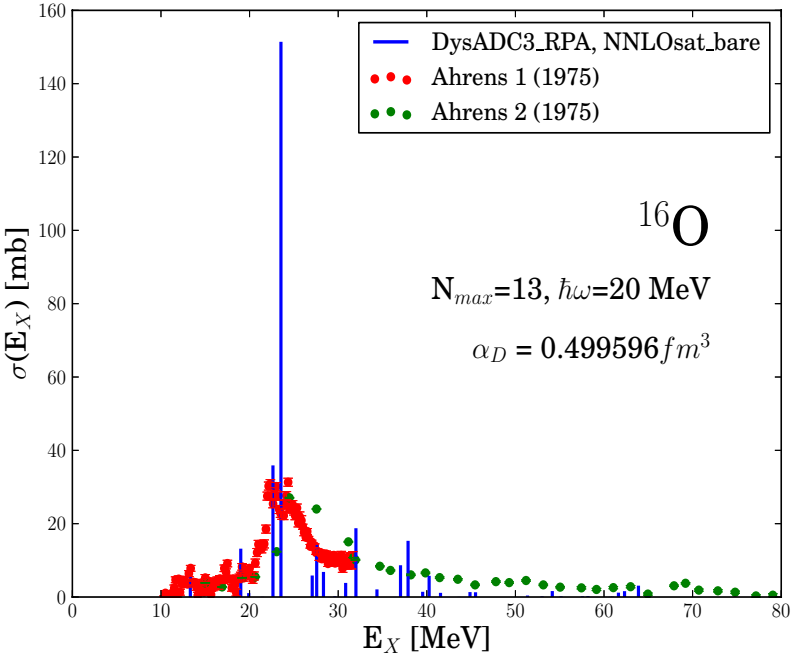
$$\sum_{ab} <a|\hat{D}|b> <\psi_\nu^A|c_a^\dagger c_b|\psi_0^A>$$

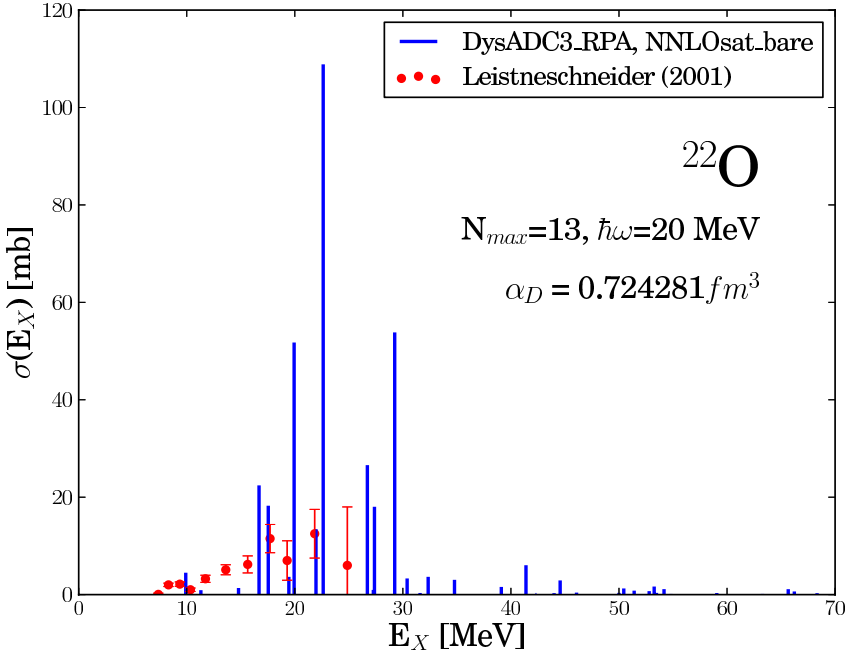
S.p. matrix element of the dipole one-body operator

Nuclear structure correlations:
g^{II} RPA level (first order)
g^{I} "dressed" ADC(3)

Results for Oxygen isotopes

σ from RPA response (discretized spectrum) vs σ from photoabsorption and Coulomb excitation





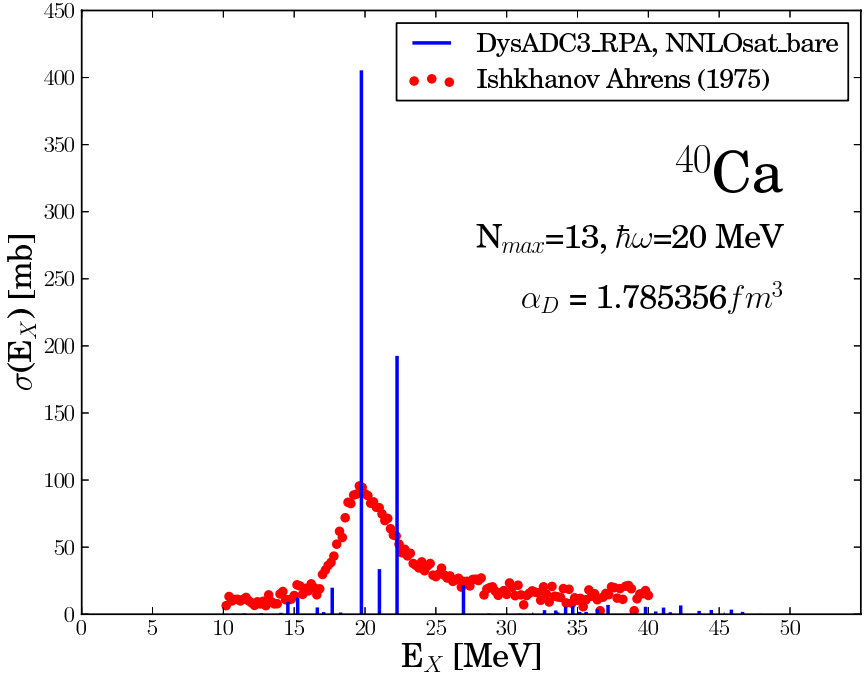
NNLO$_{sat}$

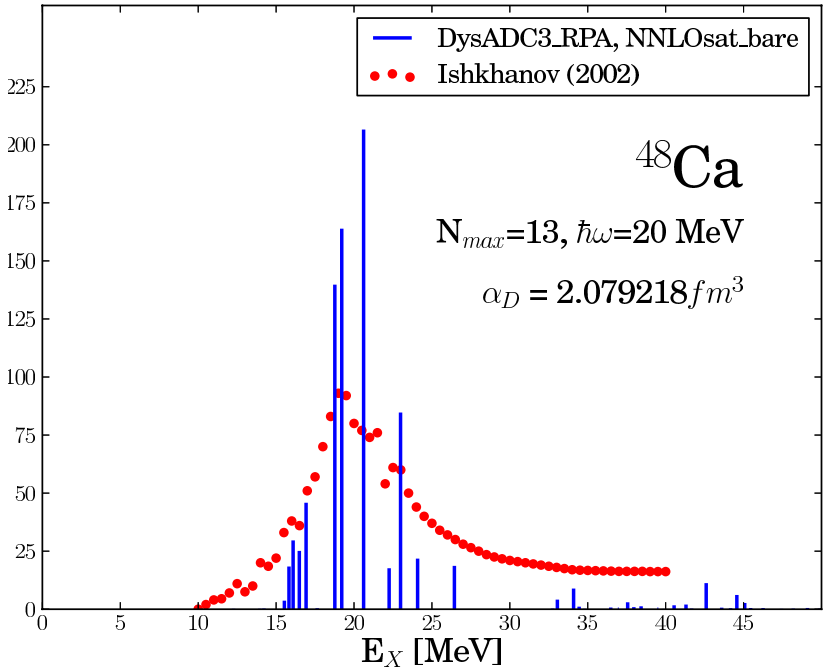
- GDR position of ^{16}O reproduced
- Hint of a soft dipole mode on the neutron-rich isotope

Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{16}O	0.50	0.57(1)	0.585(9)
^{22}O	0.72	0.86(4)	0.43(4)

Results for Calcium isotopes

σ from RPA response (discretized spectrum) vs σ from photoabsorption and Coulomb excitation





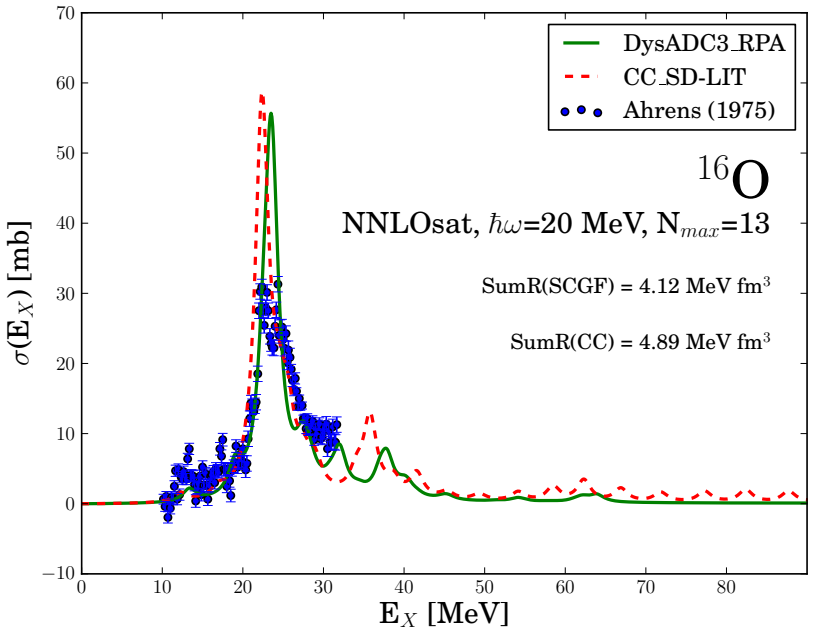
NNLO$_{sat}$

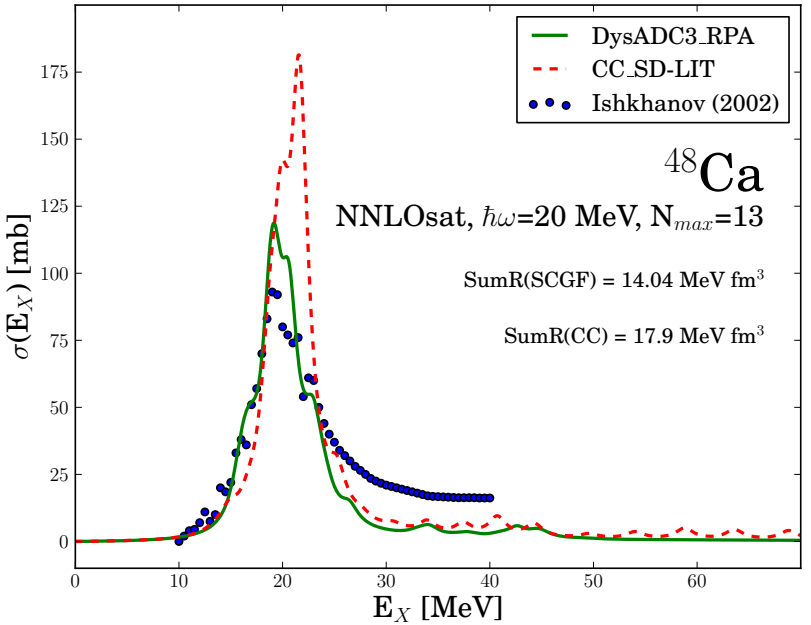
- GDR positions reproduced
- Total sum rule reproduced but poor strength distribution (Lack of correlations)

Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{40}Ca	1.79	1.47 $(1.87)_{thresh}$	1.87(3)
^{48}Ca	2.08	2.45	2.07(22)

Comparison with CC-LIT
(Couple Cluster- Lorentz Integral Transform method)

In collaboration with M. Miorelli and S. Bacca (TRIUMF, University of Mainz)





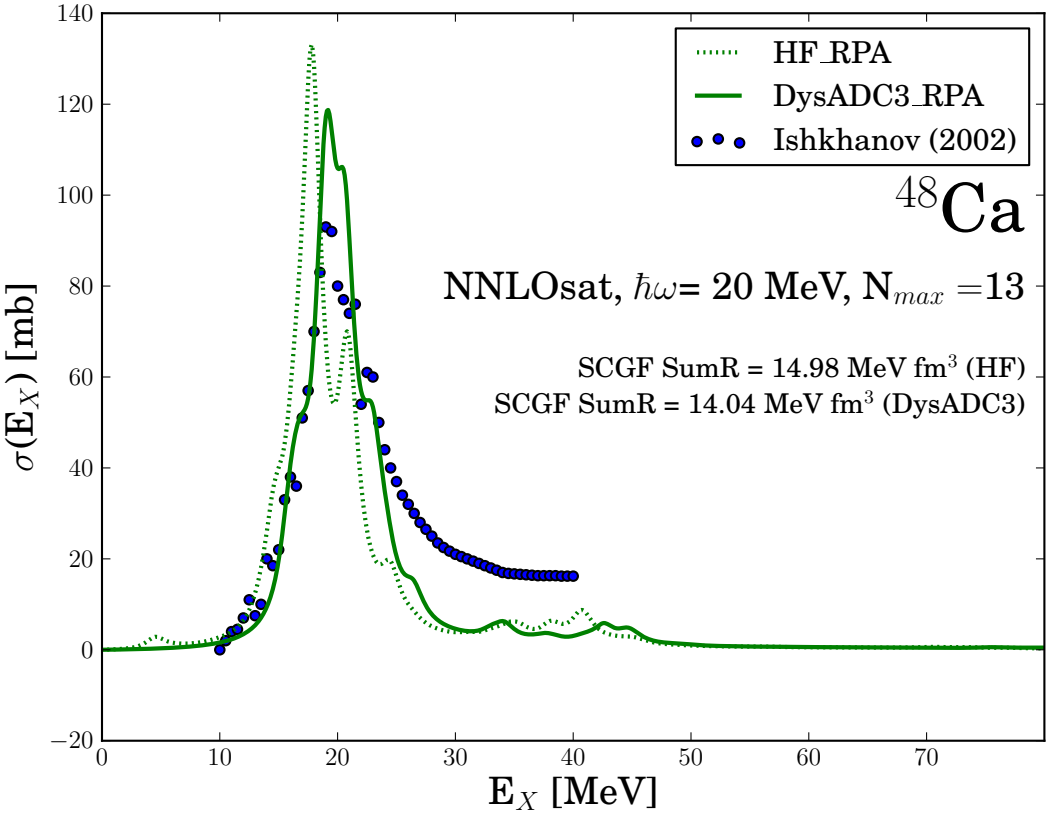
- CC-Singles-Doubles (analogous to 2nd RPA)
- LIT reduces a continuum state problem to a bound-state-like problem

Different treatment of the correlations:

SCGF
Reference state correlated
RPA (first-order two-body correlator)

CC-SD-LIT
HF Reference state
Singles-Doubles

Role of the correlations included in the reference state



Role of correlations beyond Hartree-Fock expected to be important for other observables

Conclusion and perspectives

- Set of effective charges for Oxygen and Nickel isotopes calculated from realistic potential (ready to be used as input in Shell Model calculations)
- Expected isospin-dependence of neutron effective charges is found
- Dipole response and polarisability calculated from first principles
- Continuum to be included, but dipole polarisability seems quite insensitive to it
- Correlations: going beyond 1st order RPA approximations?

Convergence trend

Neutrons