Effective charges and dipole response function in SCGF with $NNLO_{sat}$

Progress in Ab Initio Techniques in Nuclear Physics

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Background: concept of effective charge in Shell Model calculations

Definition of effective charge

Naive expectation:

in the description of nuclear electromagnetic phenomena **only protons** should appear….

However:

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

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

The most popular "flaws" of the standard SM description

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

- Not all the regions of the nuclear chart are amenable to a SM description yet
- Quadrupole effective charges are needed (But their value is universal and rather well understood)

Purpose: motivations for calculating effective charges from realistic potentials

Open questions

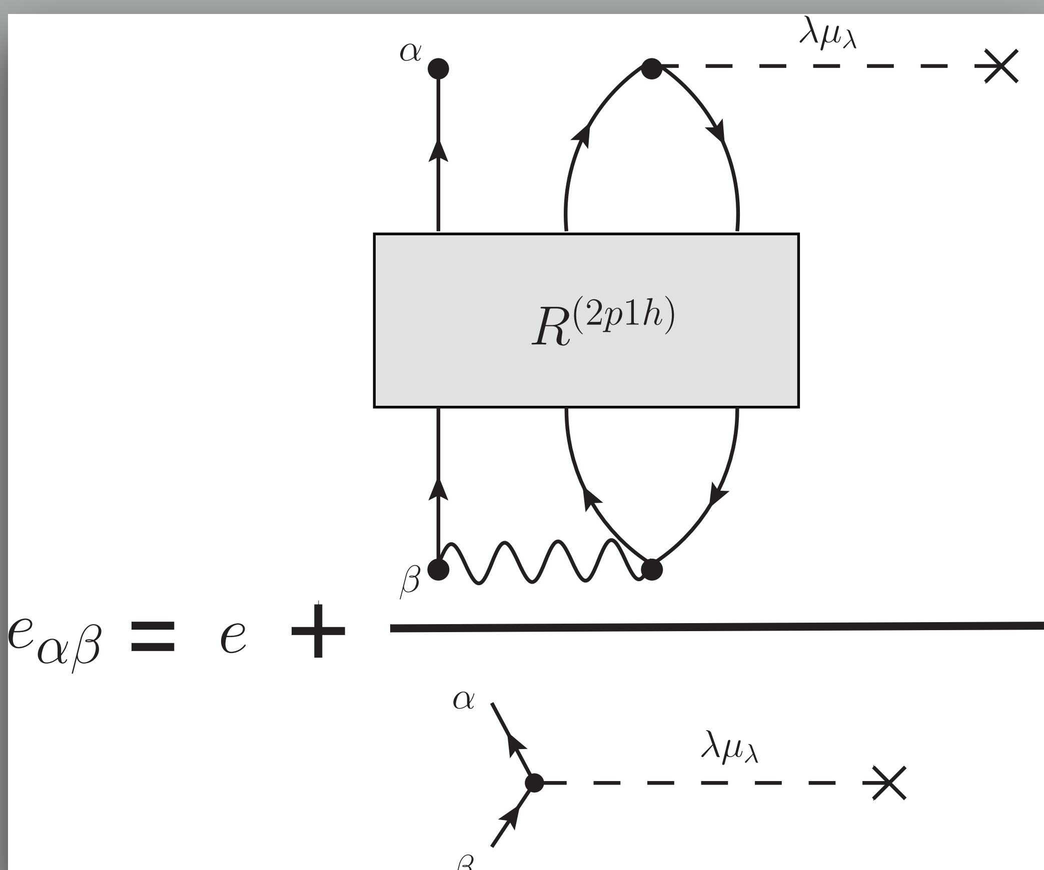
- Universal validity of “standard values” of the effective charges
- Effective charges values for nuclei towards neutron drip line
- Orbital dependence of effective charges
- Physical content of the effective charges in term of modern realistic interactions and correlations described in a many-body approach

Methods: Particle-Vibration coupling in the Self-consistent Green function formalism

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

Results: Theoretical effective charges of Oxygen and Nickel isotopes for E2 operator

Features of the calculation

- Medium-mass isotopes:

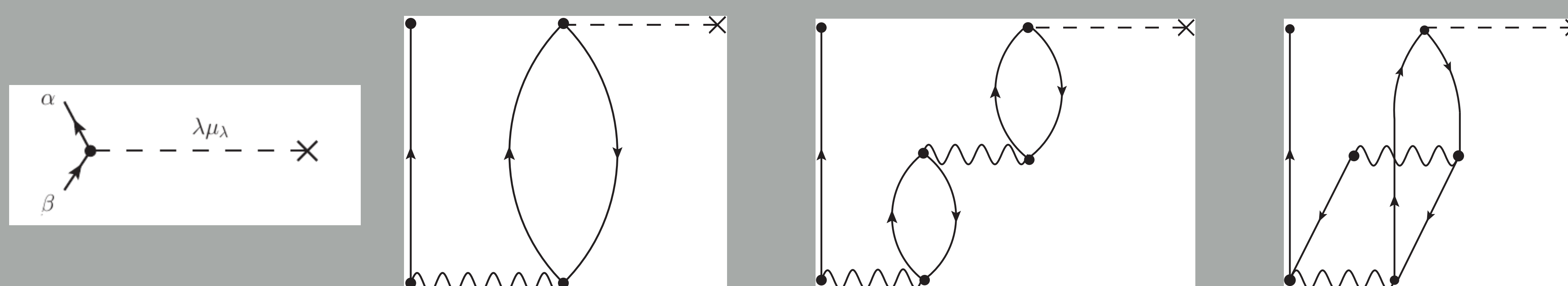
    - Oxygen isotopes in *sd* and *psd* valence space: ^{14}O, ^{16}O, ^{22}O and ^{24}O

    - Nickel isotopes in $0f1p0g_{9/2}$: ^{48}Ni, ^{56}Ni, ^{68}Ni and ^{78}Ni

- NN and 3N nuclear interaction $NNLO_{sat}$ (Phys. Rev. C 91, 051301(R))

- Electric quadrupole operator E2 $\hat{\phi}^{(2\mu)} = \sum_i r_i^2 Y_{2\mu}(\hat{r}_i)$

- Dyson equation solved with self-energy truncated at ADC(3) level:



- Nuclear many-body wave function expanded in HO wave functions with N_{max}=13 and hΩ=20 MeV

Results for Oxygen isotopes

	^{14}O	^{16}O	^{22}O	^{24}O
$\nu s_{\frac{1}{2}}\ \nu d_{\frac{3}{2}}$	0.27	0.19	0.12	0.12
$\nu s_{\frac{1}{2}}\ \nu d_{\frac{5}{2}}$	0.41	0.30 (0.40 ± 0.01)	0.21	0.24
$\nu p_{\frac{1}{2}}\ \nu p_{\frac{3}{2}}$	0.41	0.49 ★	0.41	0.47 ★
$\nu p_{\frac{3}{2}}$	0.48	0.36	0.95 ★	0.32
$\nu d_{\frac{3}{2}}$	0.27	0.19	0.15	0.16
$\nu d_{\frac{3}{2}}\ \nu d_{\frac{5}{2}}$	0.46	0.36	0.24	0.23
$\nu d_{\frac{5}{2}}$	0.44	0.33 (0.37 ± 0.14)	0.31	0.30
	0.3 - 0.5 (0.65)	0.2 - 0.4 (0.53)	0.1 - 0.4 (0.31)	0.1 - 0.3 (0.27)
$\pi s_{\frac{1}{2}}\ \pi d_{\frac{3}{2}}$	0.69	1.07	1.04	1.03
$\pi s_{\frac{1}{2}}\ \pi d_{\frac{5}{2}}$	1.17	1.14 (1.10 ± 0.01)	1.16	1.15
$\pi p_{\frac{1}{2}}\ \pi p_{\frac{3}{2}}$	1.17	1.17	1.21	1.18
$\pi p_{\frac{3}{2}}$	1.03	1.01	1.07	1.05
$\pi d_{\frac{3}{2}}$	0.46	1.03	1.04	1.02
$\pi d_{\frac{3}{2}}\ \pi d_{\frac{5}{2}}$	0.79	1.16	1.22	1.19
$\pi d_{\frac{5}{2}}$	1.13	1.09	1.11	1.09
	0.5 - 1.2 (1.35)	1.0 - 1.2 (1.29)	1.0 - 1.2 (1.15)	1.0 - 1.2 (1.11)

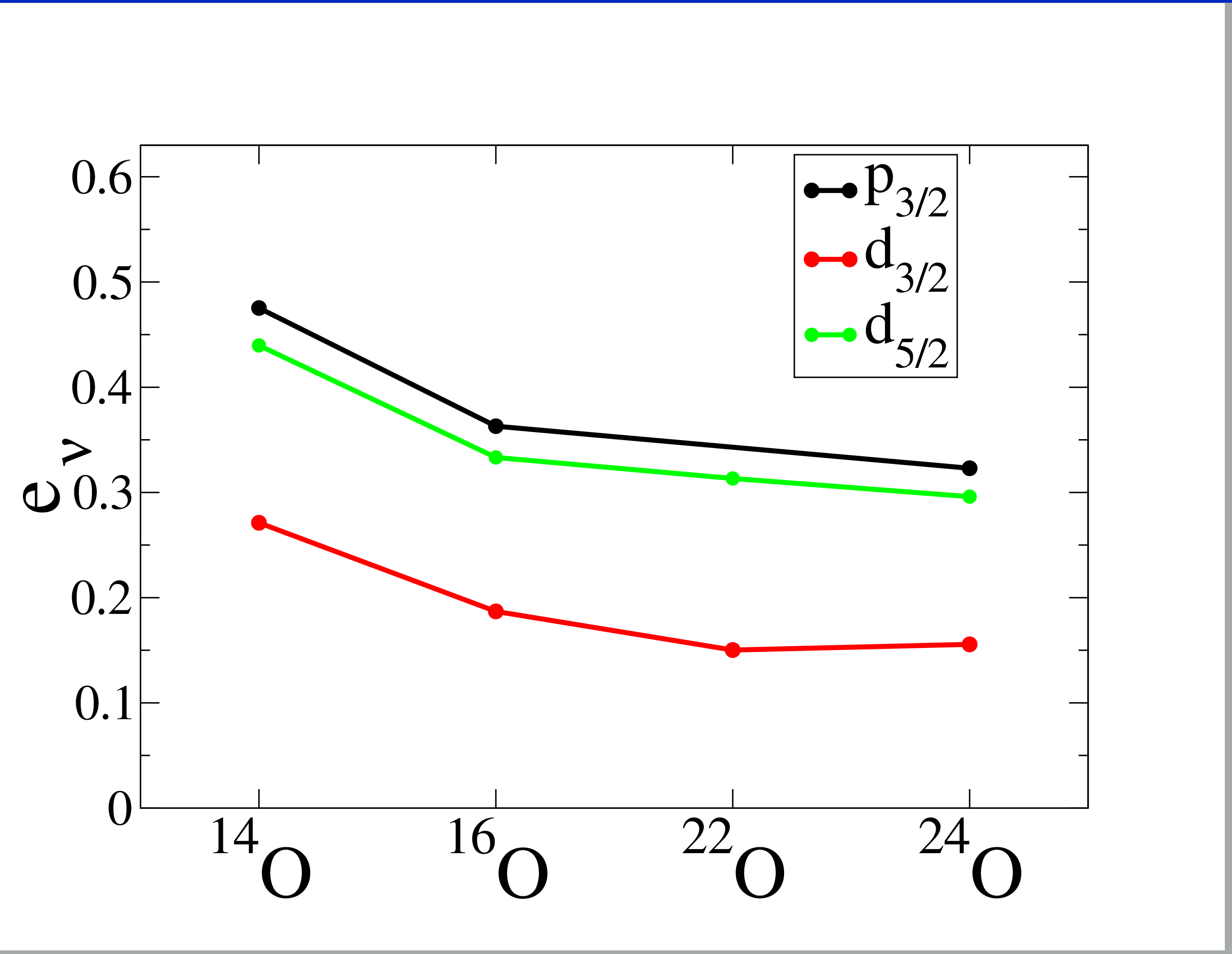
Standard values of experimental effective charges in *psd* nuclei are e_p=1.3 and e_n=0.5

- Neutron-rich nuclei have weaker core polarisation (quench of neutron effective charge)
- Significant isotopic dependence especially for neutrons (compared with Bohr-Mottelson Eq. 6-386b with Sagawa parametrisation of PRC 70, 054316, 200 $e_\pi^{eff} = e + a\frac{Z}{A} + b\frac{N-Z}{A} - \left(c + d\frac{Z}{A}\frac{N-Z}{A}\right)$)

$$e_\nu^{eff} = a\frac{Z}{A} + b\frac{N-Z}{A} + \left(c + d\frac{Z}{A}\frac{N-Z}{A}\right)$$

- Single-particle state dependence also significant (yet to be studied and understood…)

Results for Oxygen isotopes



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Results for Nickel isotopes

TABLE II. Neutron (ν) and proton (π) isoscalar E2 effective charges for static moments and transitions in Nickel isotopes, for shell model calculations performed in $0f\,1p\,0g_{\frac{9}{2}}$ valence space.

	^{48}Ni	^{56}Ni	^{68}Ni	^{78}Ni
$\nu f_{\frac{5}{2}}$	0.58	0.51	0.40	0.44
$\nu f_{\frac{5}{2}}\ \nu f_{\frac{7}{2}}$	0.80	0.55	0.57	0.39
$\nu f_{\frac{5}{2}}\ \nu p_{\frac{1}{2}}$	0.51	0.43	0.33	0.39
$\nu f_{\frac{5}{2}}\ \nu p_{\frac{3}{2}}$	0.52	0.45	0.34	0.45
$\nu f_{\frac{7}{2}}$	0.54	0.44	0.34	0.39
$\nu f_{\frac{7}{2}}\ \nu p_{\frac{3}{2}}$	0.64	0.48	0.43	na
$\nu p_{\frac{1}{2}}\ \nu p_{\frac{3}{2}}$	0.47	0.38	0.29	0.28
$\nu p_{\frac{3}{2}}$	0.45	0.37	0.27	0.29
$\nu g_{\frac{9}{2}}$	0.52	0.43	0.34	0.34
	0.5 - 0.6	0.4 - 0.5	0.3 - 0.4	0.3 - 0.5
$\pi f_{\frac{5}{2}}$	1.14	1.14	1.07	1.13
$\pi f_{\frac{5}{2}}\ \pi f_{\frac{7}{2}}$	1.14	1.17	1.09	1.08
$\pi f_{\frac{5}{2}}\ \pi p_{\frac{1}{2}}$	1.07	1.07	1.02	1.14
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	1.1 - 1.2	1.1 - 1.2	1.0 - 1.1	1.1 - 1.2

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Standard values of experimental effective charges in *pf* nuclei are e_p=1.5 and e_n=0.5

- Recent consensus on smaller values (~ 1.1 - 1.3) of proton effective charges
- Isotopic dependence with quenching of neutron effective charges for neutron-rich nuclei
- No consensus on magnitude of value of neutron effective charges (results consistent with microscopic PVC model with Skyrme interaction in PRC **80**, 014316)

Dipole response function and electric polarisability

Experimental techniques:

- Coulomb excitation
- Photoabsorption

Theoretical methods:

- Nuclear EDF
- Coupled-Cluster/LIT
- SCGF method

Rich nuclear structure phenomena:
GDR, PDR, polarisability

Correlations among observables:
(polarisability , neutron-skin thickness) (polarisability , neutron radius)

Correlations between observables and parameters of a model
(polarisability , symmetry energy in EDF)

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

Dipole response $R(E)$ encodes the excited states of the nuclear system, when "probed" with dipole operator $\hat{D}$

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

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

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

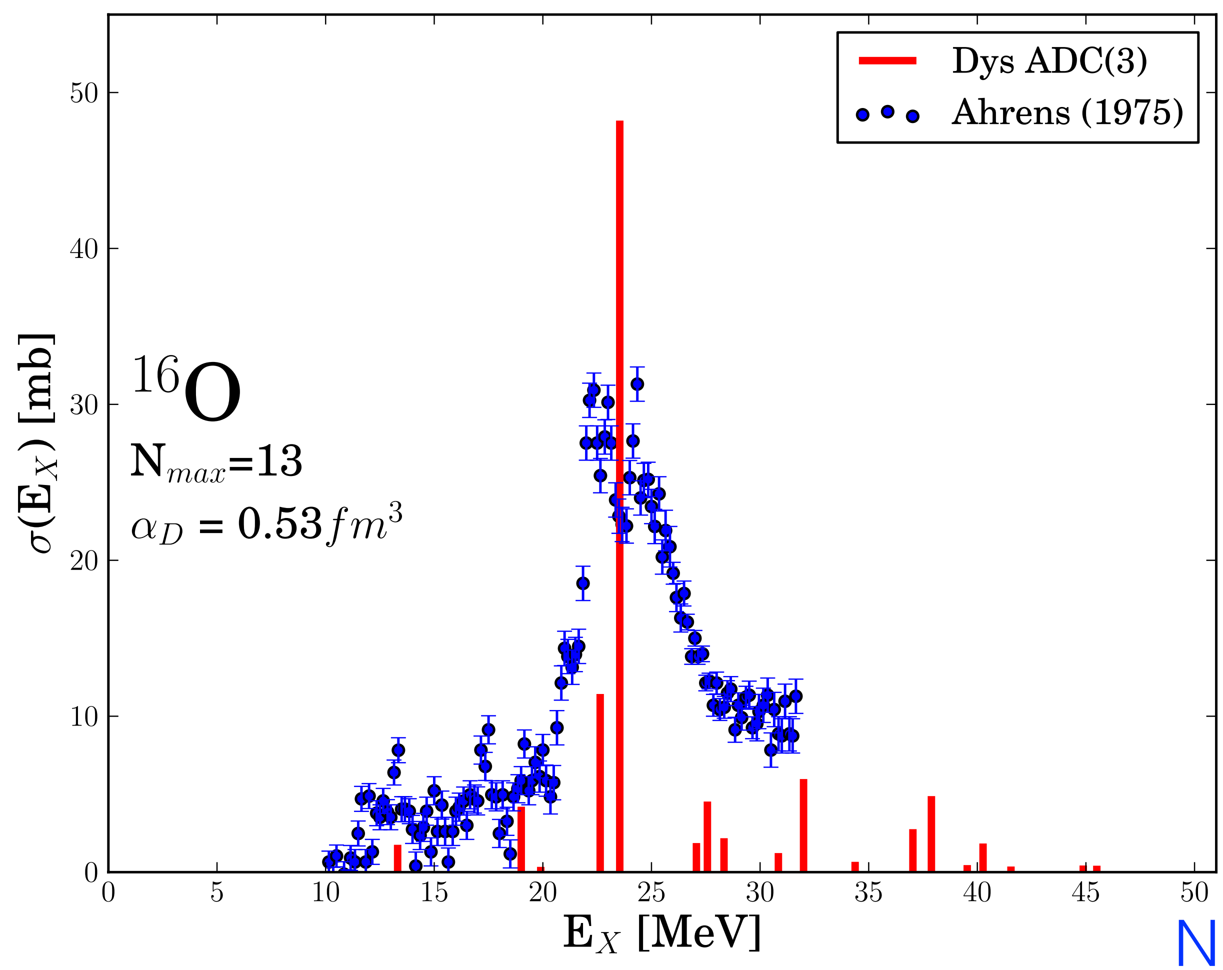
Nuclear structure correlations:
g^{II} RPA level (first order)
g^{I} "dressed" ADC(3)
(Role of 3NF: arXiv:1701.08127)

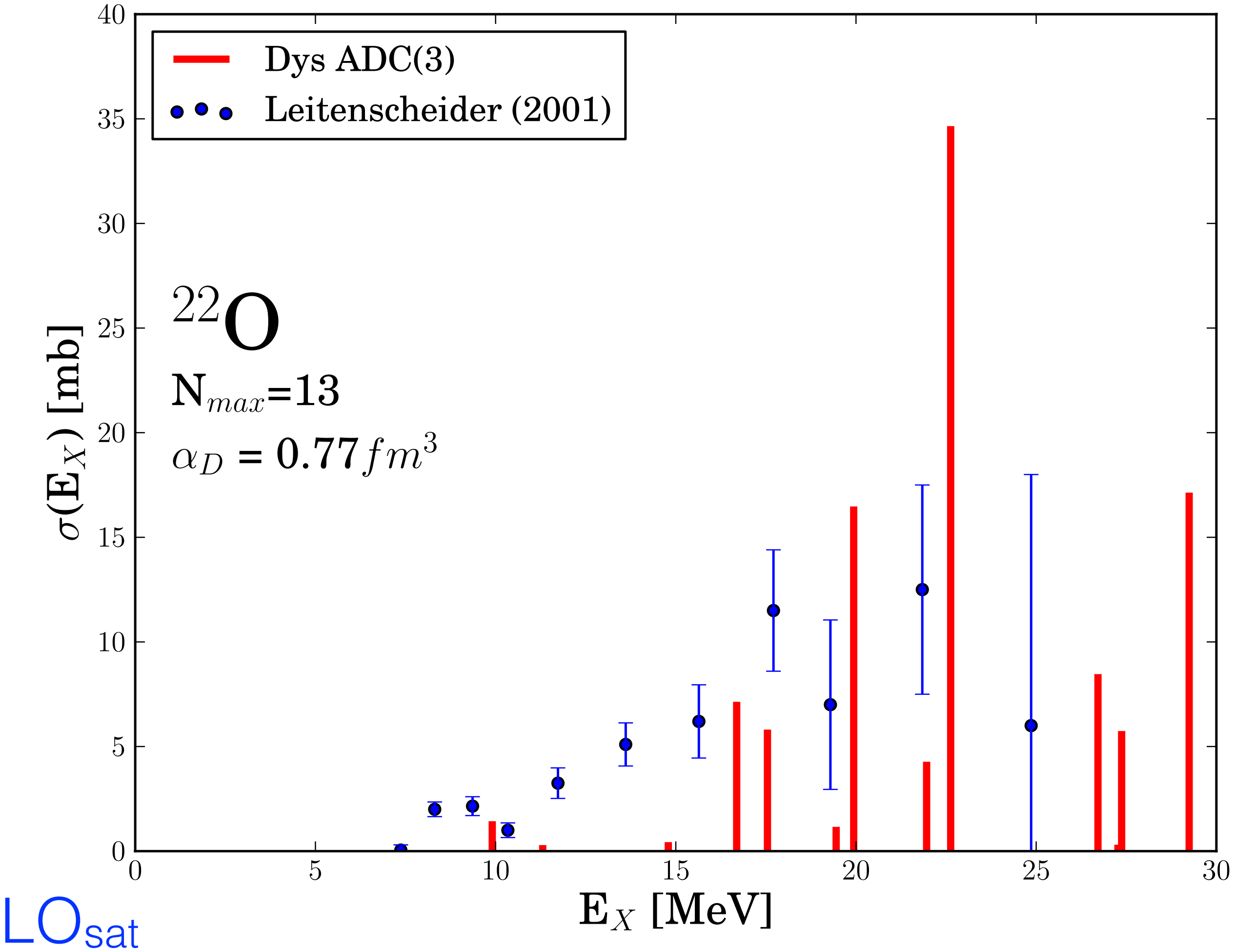
Results: cross section and dipole polarisability

^{16}O ^{22}O ^{40}Ca ^{48}Ca

Results for Oxygen isotopes

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





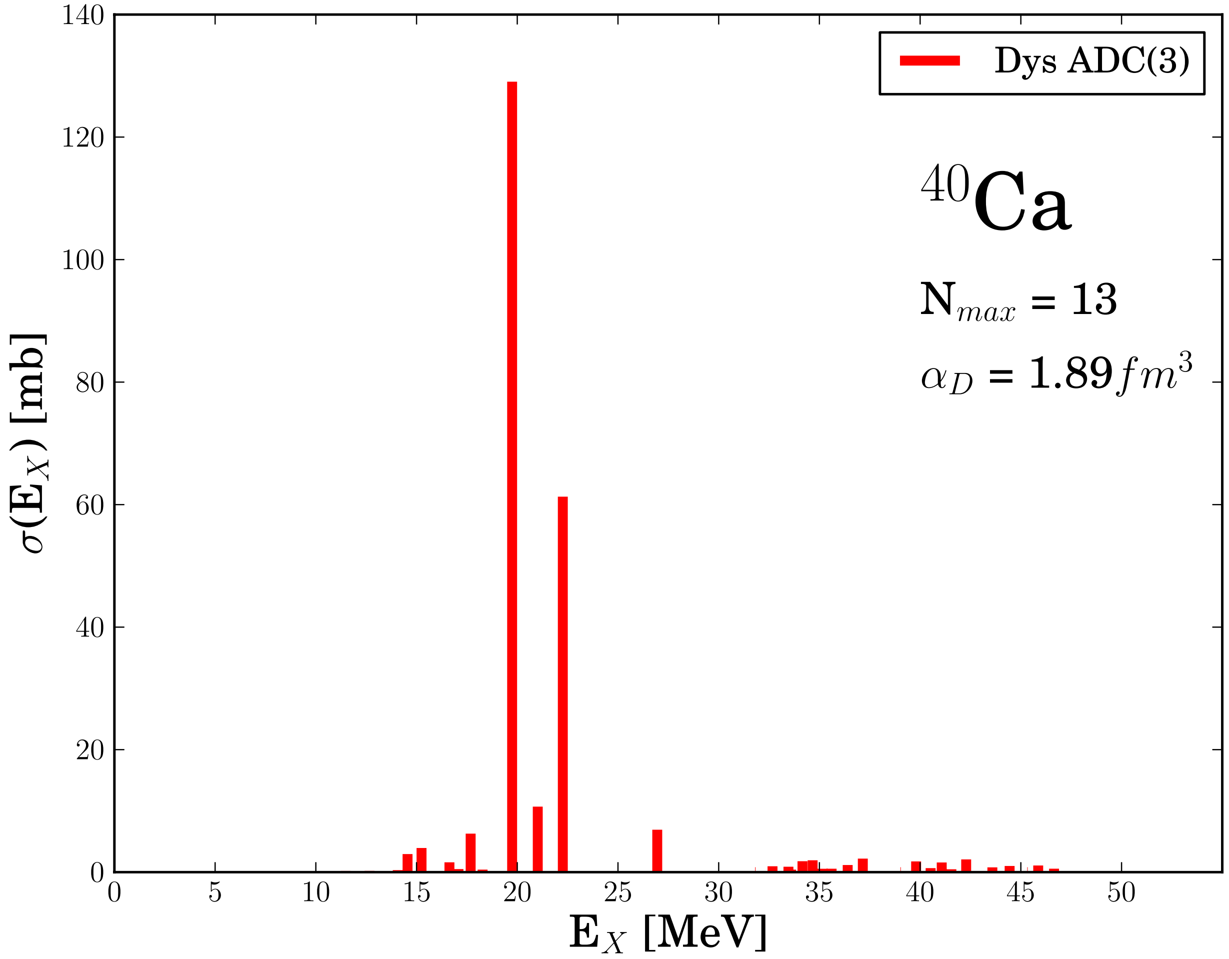
NNLO$_{sat}$

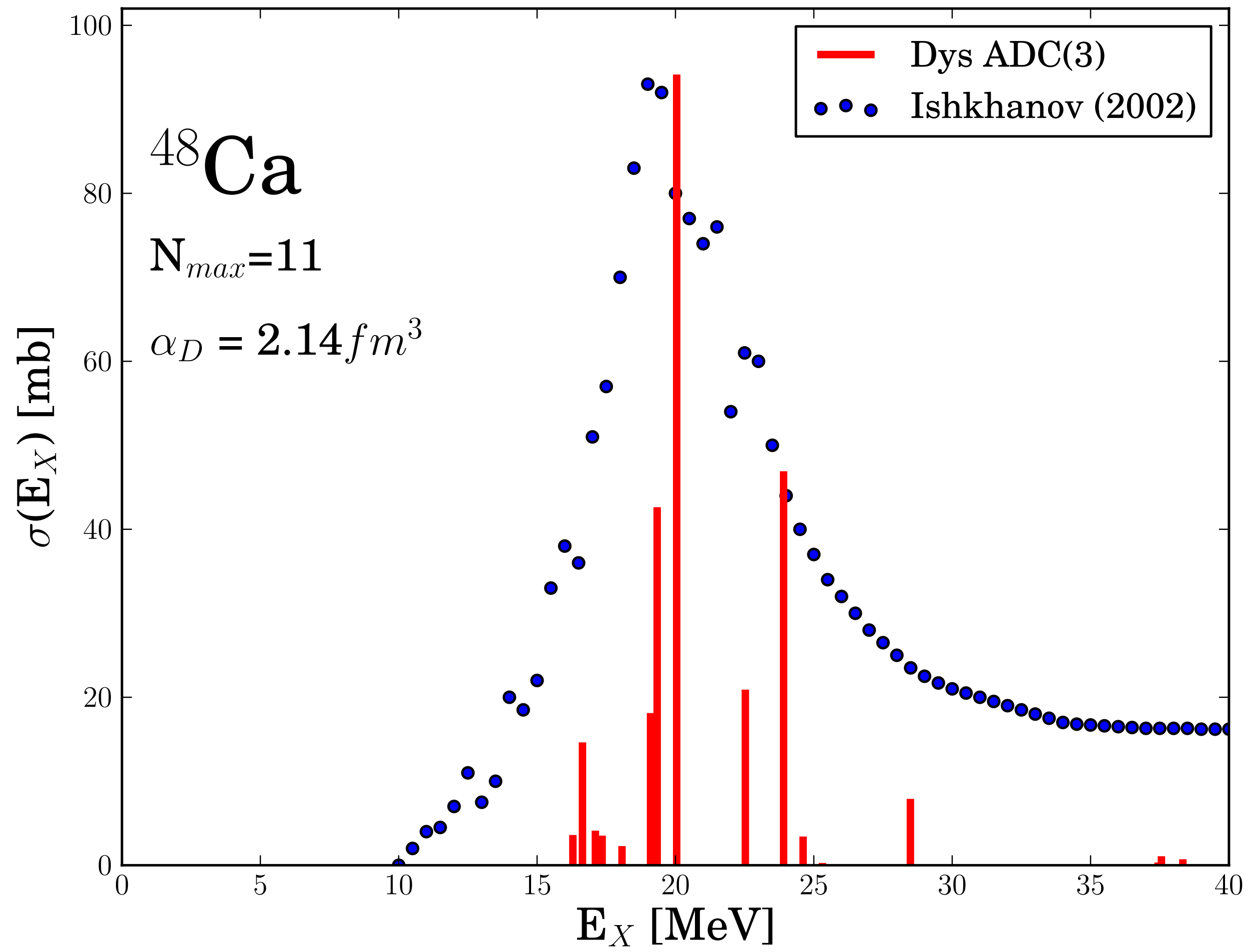
- GDR position of ^{16}O reproduced
- Hint of a soft dipole mode on the neutron-rich isotope

Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{16}O	0.53	0.57(1)	0.585(9)
^{22}O	0.77	0.86(4)	0.43(4)

Results for Calcium isotopes

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





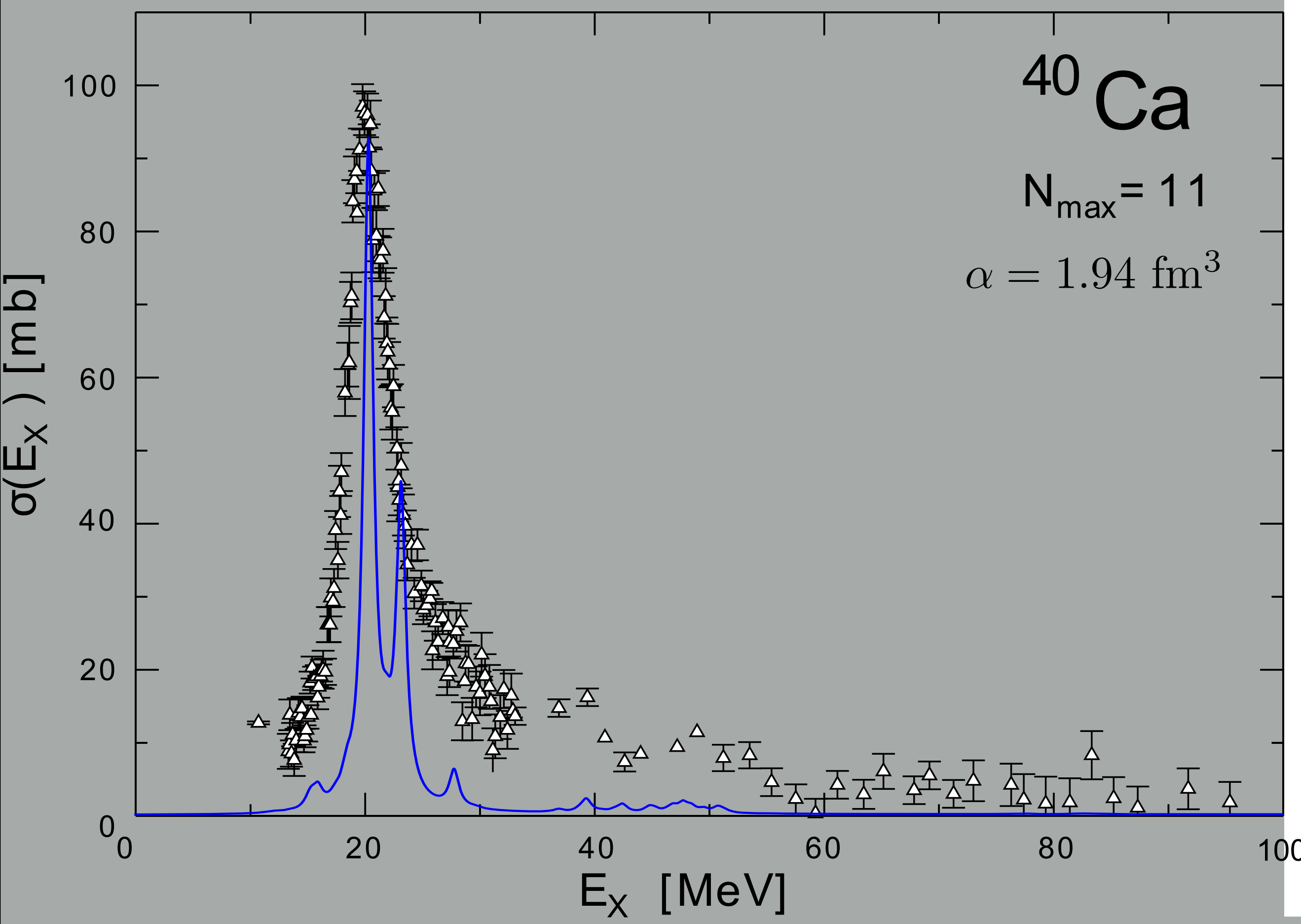
NNLO$_{sat}$

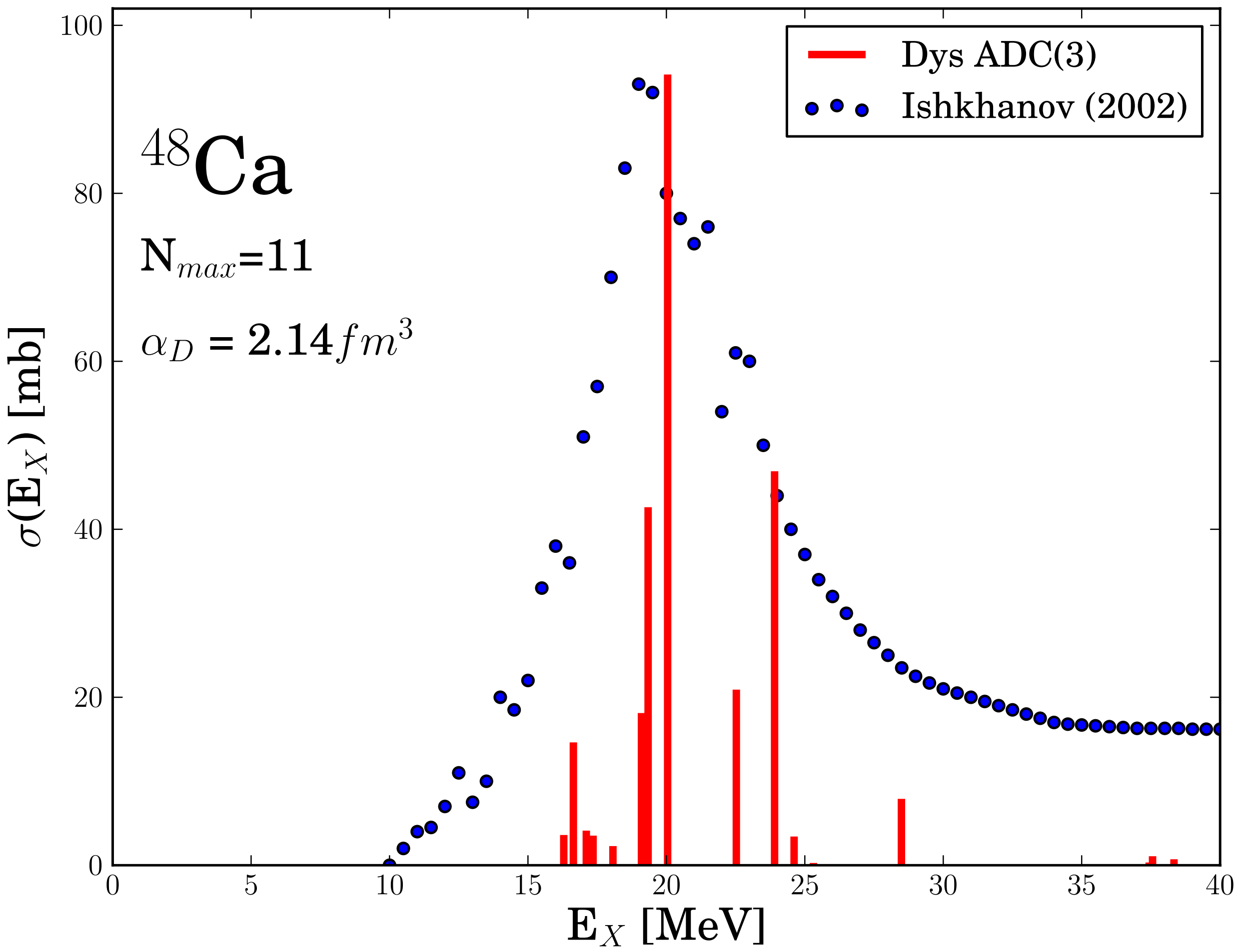
- GDR positions reproduced

Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{40}Ca	1.89	1.47 $(1.87)_{thresh}$	1.87(3)
^{48}Ca	2.14	2.45	2.07(22)

Results for Calcium isotopes

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





NNLO$_{sat}$

- Width = 1 MeV (Lorentzian convolution)

Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{40}Ca	1.89	1.47 $(1.87)_{thresh}$	1.87(3)
^{48}Ca	2.14	2.45	2.07(22)

Conclusions 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

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- 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?

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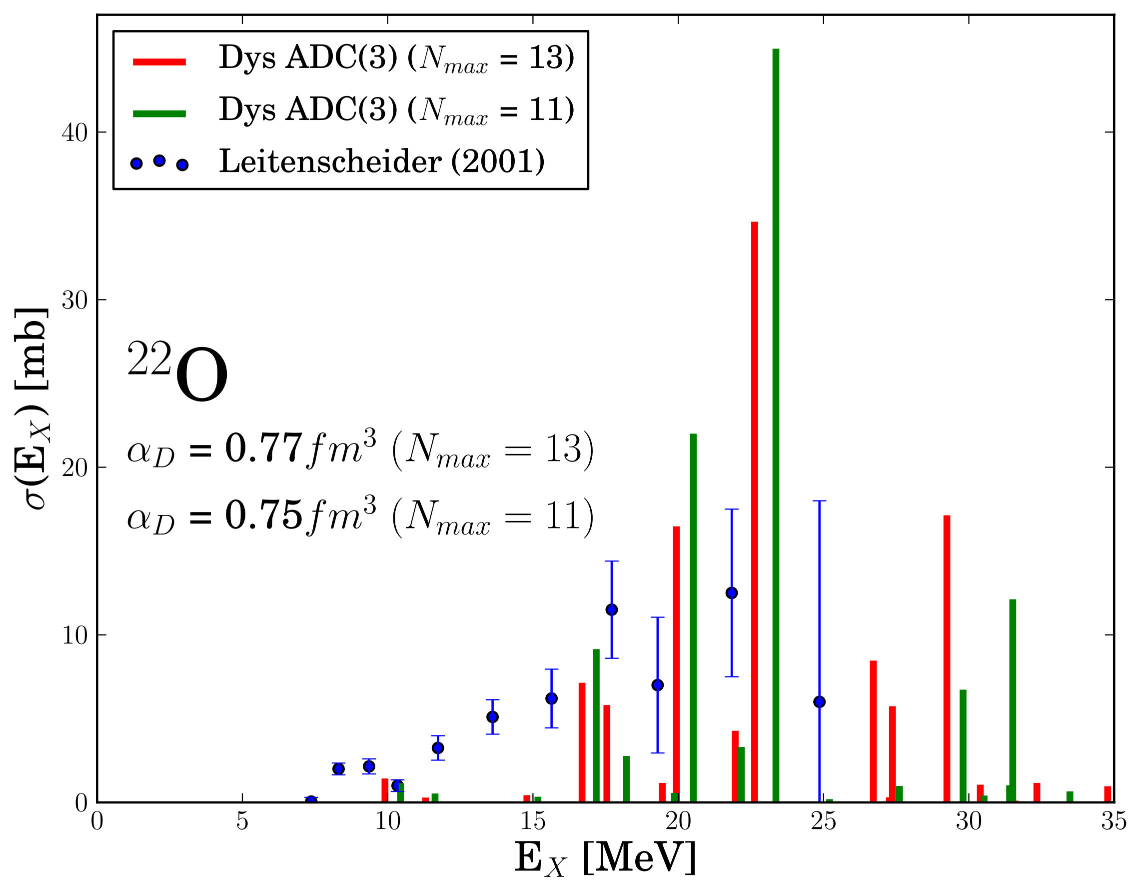
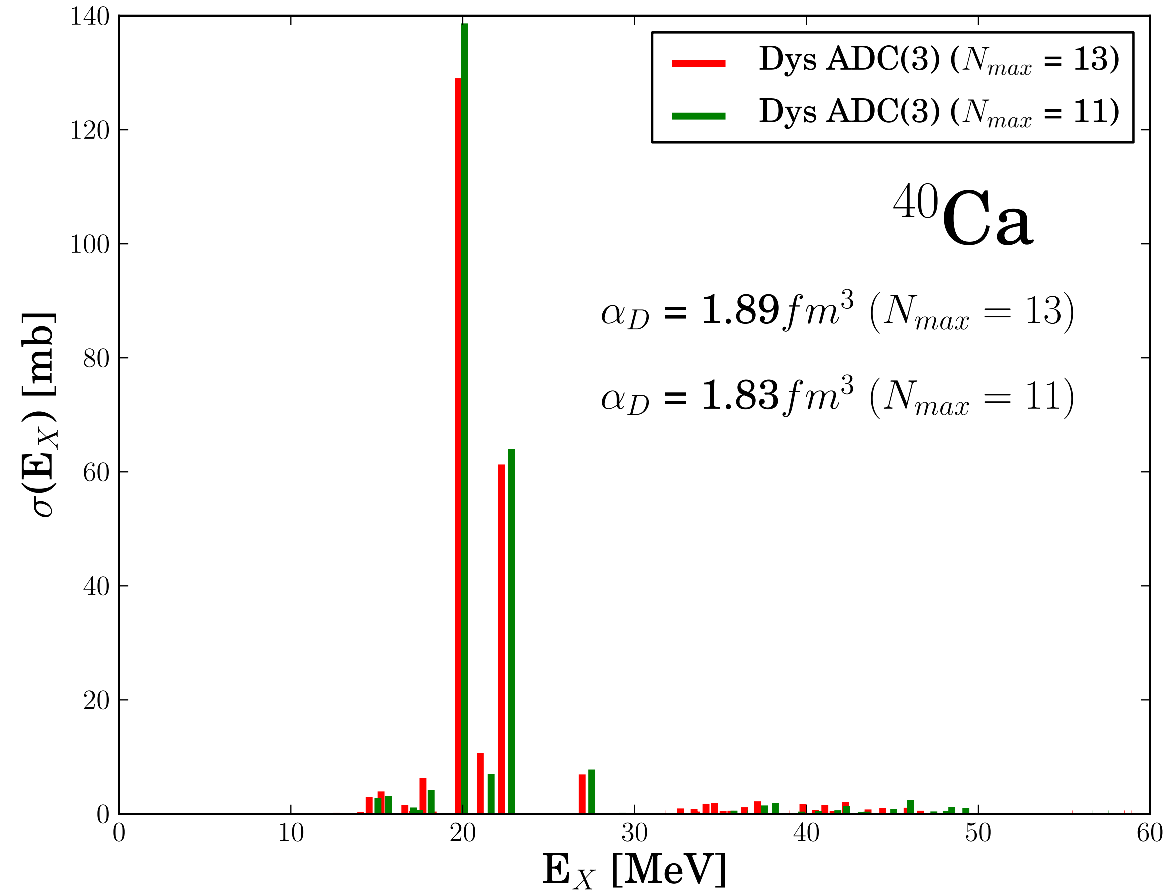
Thank you!

Backup slides

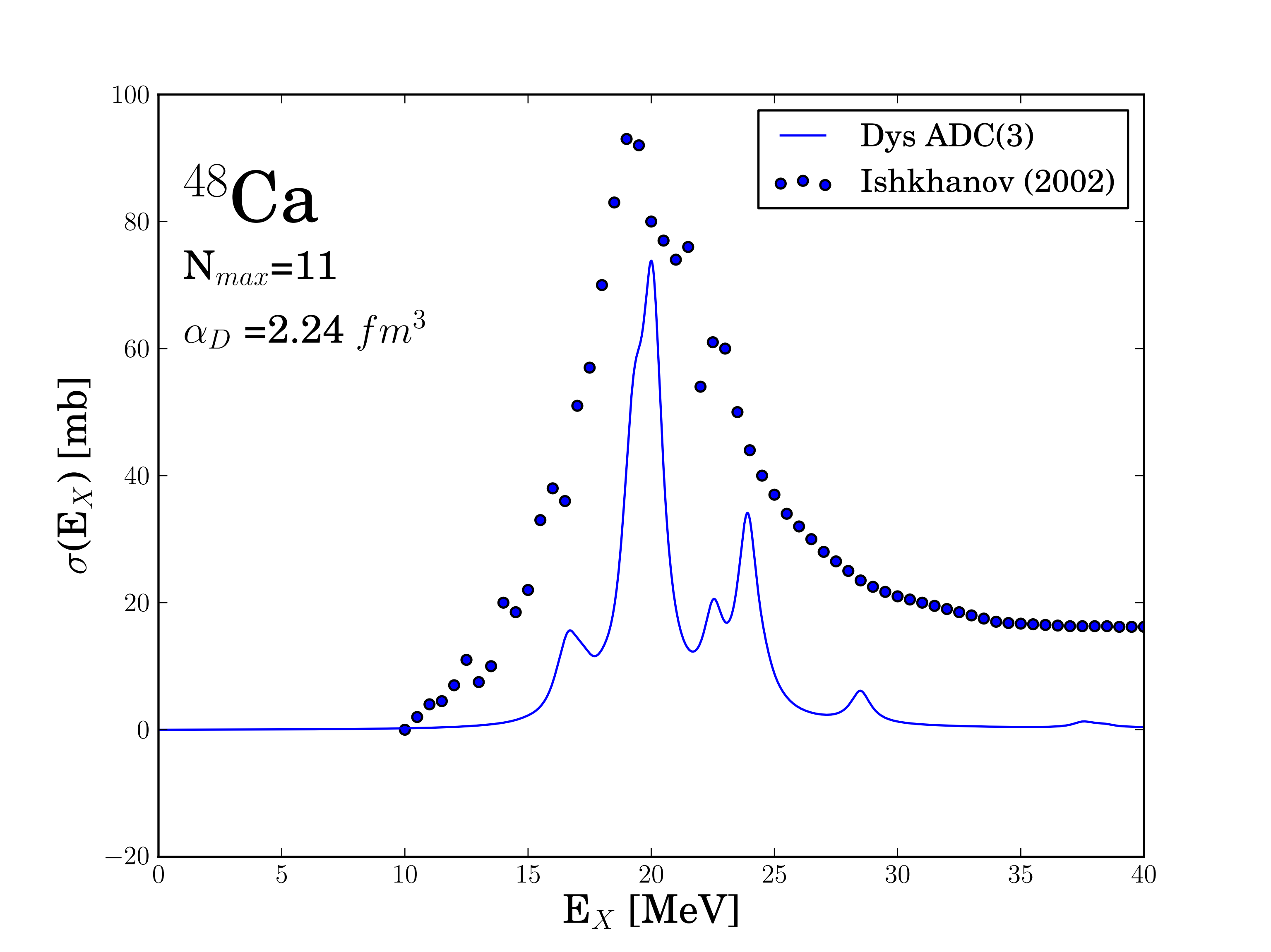
Size of the model space (N_{max} = 11, 13)





$NNLO_{sat}$

Convoluted Response (Γ = 1 MeV)

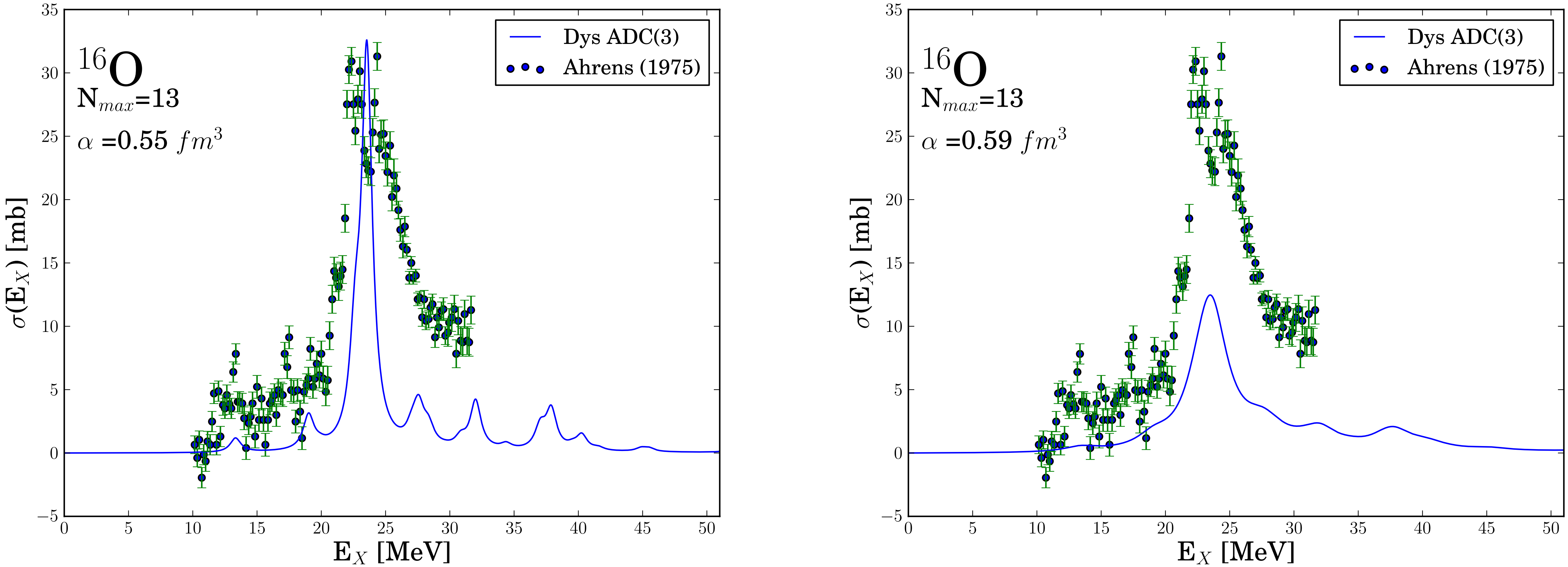


NNLO$_{sat}$

α_D (conv) = 2.24 fm^3
α_D (discr) = 2.14 fm^3

Difference within experimental uncertainty

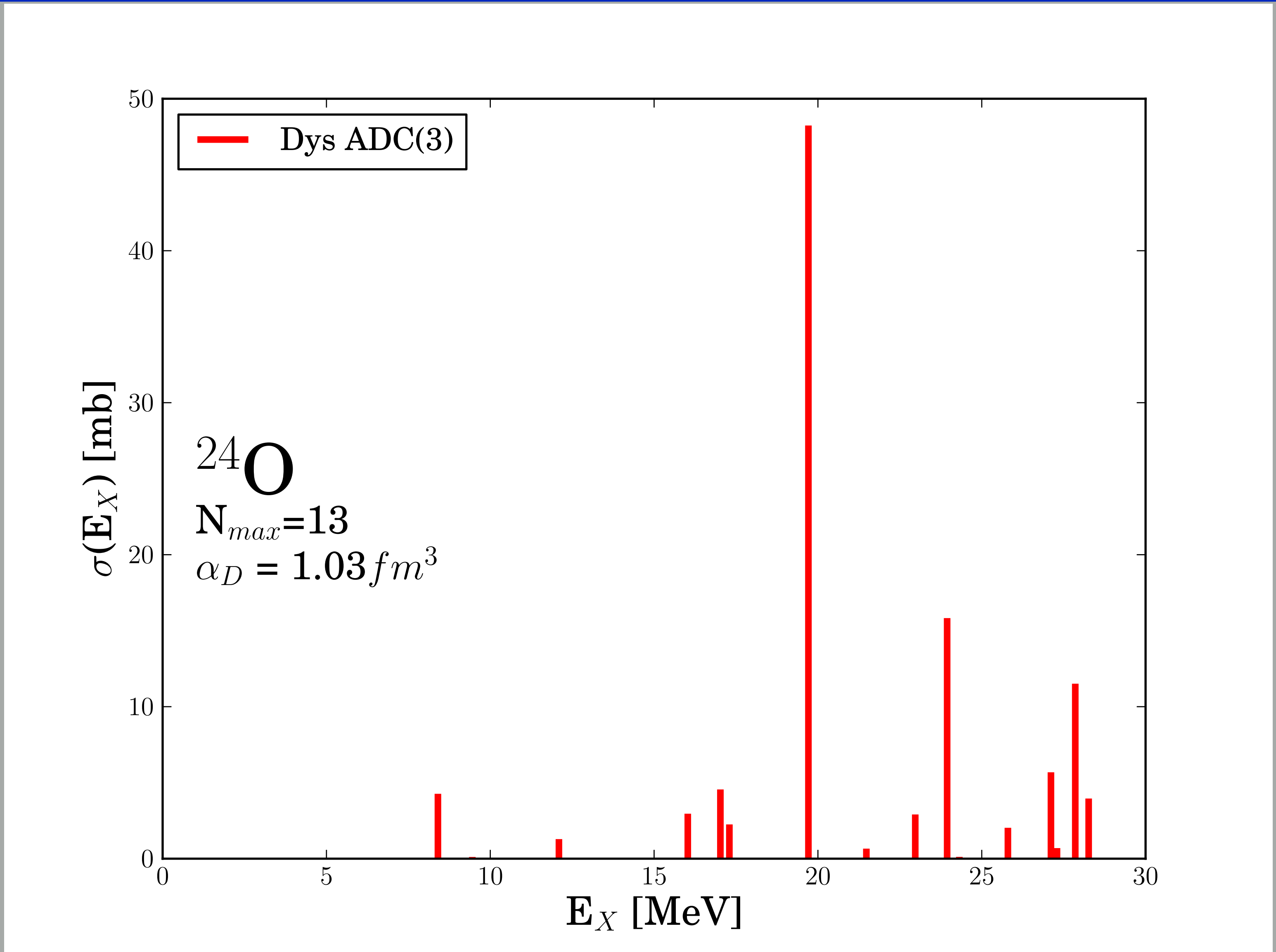
^{16}O convoluted Response (Lorentzian)



Γ = 1.0 MeV

Γ = 3.0 MeV

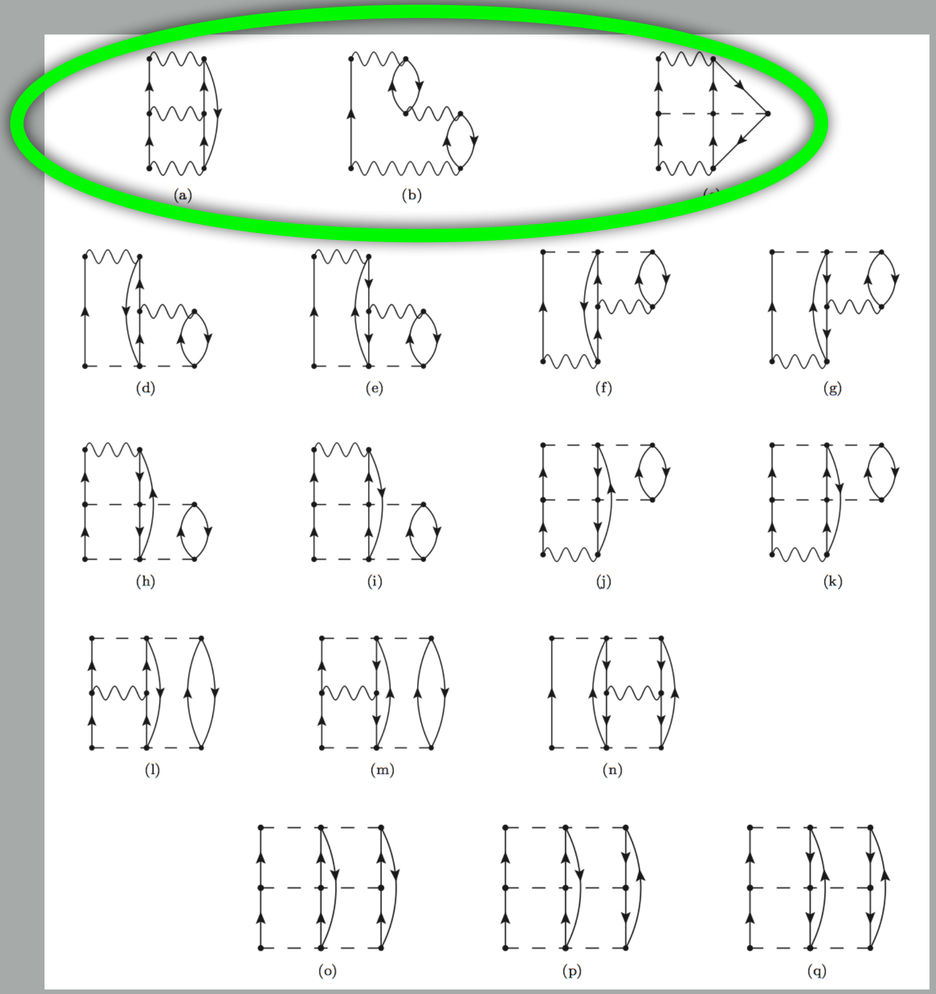
^{24}O dipole response



NNLO$_{sat}$

ADC(3) formalism

Extension of the Algebraic Diagrammatic Construction (ADC) method in the Self-Consistent Green Function formalism to 3N interactions



Third order perturbation expansion diagrams of the self energy with 3N forces

Status:

- Derivation of the formulas for all irreducible self-energy diagrams at third-order
- Organisation of the self-energy formulas according to the ADC(3) scheme
- Dominant diagram with bare 3N force implemented

What's next:

- Publish the equations
- Assess the importance of this diagram through computation of binding energies and radii with realistic interaction

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 charge

Naive expectation for low-energy nuclear structure:
in the description of nuclear electromagnetic phenomena **only protons** should appear….

However:

- 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:
Effective charge in the nuclear dipole moment: $\mathbf{q^{eff} = q - (Ze)/A}$

Green functions for nuclear physics

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

Schrödinger equation with microscopic nuclear Hamiltonian

$$\hat{H} = \sum_{\alpha\beta} T_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{4} \sum_{\substack{\alpha\gamma \\ \beta\delta}} V_{\alpha\gamma,\beta\delta}\, a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta + \frac{1}{36} \sum_{\substack{\alpha\gamma\epsilon \\ \beta\delta\eta}} W_{\alpha\gamma\epsilon,\beta\delta\eta}\, a^\dagger_\alpha a^\dagger_\gamma a^\dagger_\epsilon a_\eta a_\delta a_\beta$$

Green function (Lehmann representation)

$$G_{\alpha\beta}(\omega) \;=\; \sum_n \frac{\langle \Psi_0^A | a_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | a^\dagger_\beta | \Psi_0^A \rangle}{\omega - \varepsilon_n^+ + \mathrm{i}\eta} \;+\; \sum_k \frac{\langle \Psi_0^A | a^\dagger_\beta | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | a_\alpha | \Psi_0^A \rangle}{\omega - \varepsilon_k^- - \mathrm{i}\eta}$$

Dyson equation

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

Green functions for nuclear physics

In the presence of an external potential

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 function (Lehmann representation)

$$\tilde{G}_{\alpha\beta}(\omega) = \sum_{n} \frac{\langle \Psi_0^A | a_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | a^{\dagger}_{\beta} | \Psi_0^A \rangle}{\omega - \varepsilon_n^{+} + \mathrm{i}\eta} + \sum_{k} \frac{\langle \Psi_0^A | a^{\dagger}_{\beta} | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | a_\alpha | \Psi_0^A \rangle}{\omega - \varepsilon_k^{-} - \mathrm{i}\eta}$$

Dyson equation

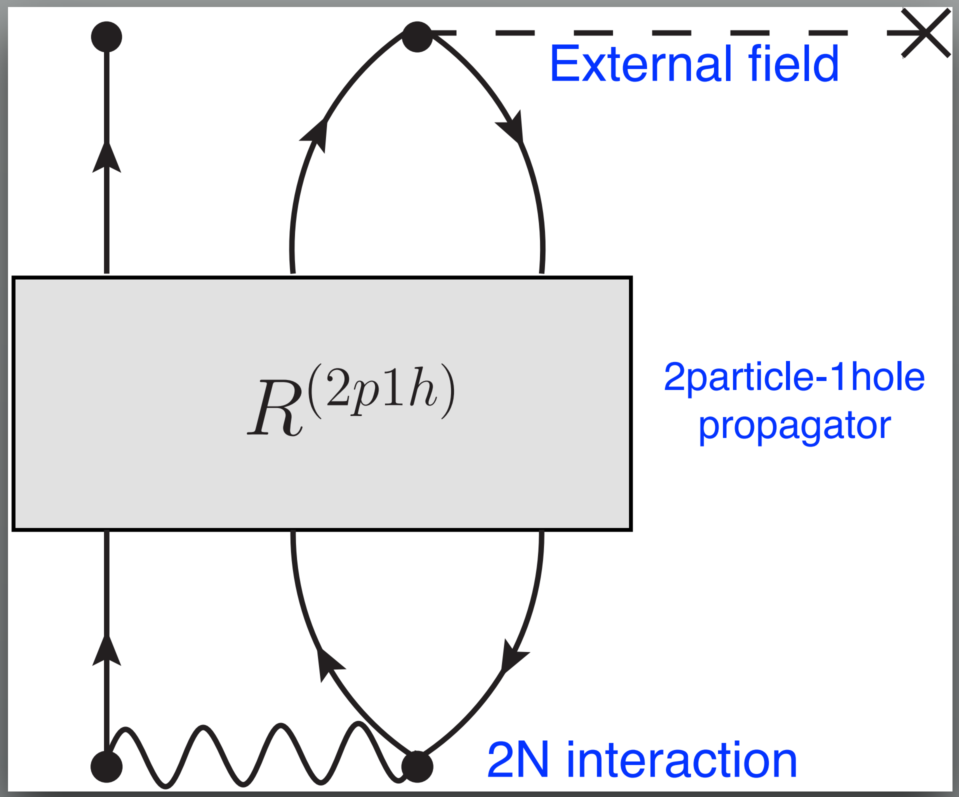
$$\begin{aligned}\tilde{G}_{\alpha\beta}(t-t') = {} & G^{(0)}_{\alpha\beta}(t-t') + G^{(0)}_{\alpha\gamma}(t-t_1)\phi^{(\lambda\mu_\lambda)}_{\gamma\delta}(t_1)\tilde{G}_{\delta\beta}(t_1-t') \\ & + G^{(0)}_{\alpha\gamma}(t-t_1)\tilde{\Sigma}^{(\lambda\mu_\lambda)}_{\gamma\delta}(t_1-t_2)\tilde{G}_{\delta\beta}(t_2-t')\end{aligned}$$

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

- Defined through the Dyson equation
- Written as perturbative expansion in the 2N interaction and external potential
- Organised in an approximate truncated scheme (Algebraic Diagrammatic Construction ADC)

Particle-vibration coupling (PVC)

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ELEMENTARY MODES OF EXCITATION IN THE NUCLEUS

Nobel Lecture, December 11, 1975

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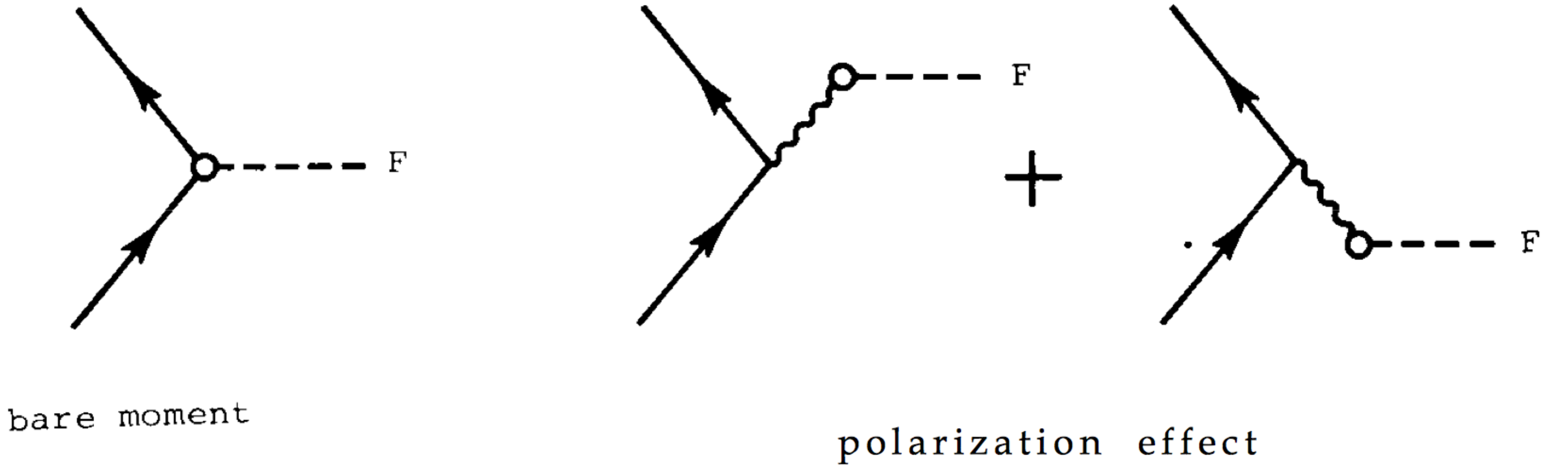


Fig. 11. Renormalization of the matrix elements of a single-particle moment resulting from particle-vibration coupling. The moment F may be any operator that acts on the degrees of freedom of a single particle, such as an electric or magnetic moment, β-decay transition moment, etc.

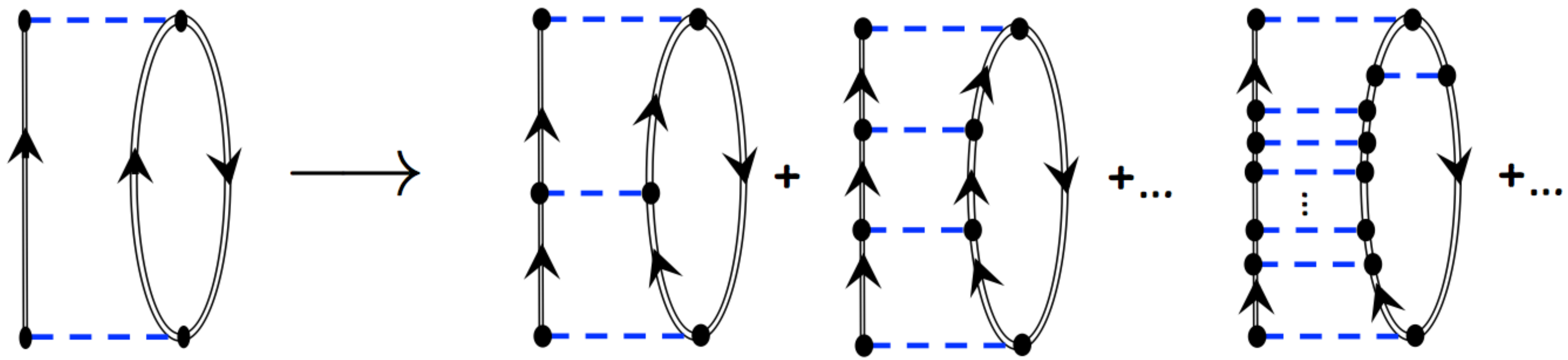
Coupling of a s.p. fermion with a collective boson

- Collective variables for excitation modes
- RPA phonons
- SCGF self-energy with external field

Dyson-ADC(n)

A technique to solve the Dyson equation:

1) At a given order n in the perturbative expansion w.r.t. the interaction, it allows a straightforward inclusion of higher-order diagrams (the so-called ladder and ring diagrams)



2) The Dyson equation attains a form in which the poles and transition amplitudes of the Green functions are found as eigenvalues and eigenvectors of an Hermitian matrix

Equivalence of the Dyson equation to an eigenvalue problem

Dyson equation

$$g_{\alpha\beta}(\omega) = g^0_{\alpha\beta}(\omega) + \sum_{\gamma\delta} g^0_{\alpha\gamma}(\omega)\Sigma^\star_{\gamma\delta}(\omega) g_{\delta\beta}(\omega)$$

$$g_{\alpha\beta}(\omega) = \sum_i \frac{\mathcal{Z}^{i\dagger}\mathcal{Z}^i}{\omega - \varepsilon_i^\pm \pm \mathrm{i}\eta}$$

ε_i and $\mathcal{Z}^i$ are the unknown

$$\Updownarrow$$

Self-consistent eigenvalue problem

$$\epsilon_i \begin{pmatrix} \mathcal{Z}^i \\ \\ \mathcal{W}^i \end{pmatrix} = \begin{pmatrix} diag\{\epsilon^{(0)}\} + \Sigma^\infty & \mathcal{M}^{(r)} & \mathcal{M}^{(q)} \\ \mathcal{M}^{(r)\dagger} & diag\{E^{(r)}\} & \\ \mathcal{M}^{(q)\dagger} & & diag\{E^{(q)}\} \end{pmatrix} \begin{pmatrix} \mathcal{Z}^i \\ \\ \mathcal{W}^i \end{pmatrix}$$

$$\mathcal{W}^i \equiv \left[\frac{1}{\omega - diag(E)}\mathcal{M}\right]_{\omega=\epsilon_i} \mathcal{Z}^i$$

$\mathcal{M}$ are matrices coupling the single-particle propagator to more complex intermediate configurations

How does ADC(n) work practically (I)

General form of the irreducible self-energy

$$\Sigma^{\star}_{\alpha,\beta}(\omega) = \Sigma^{\infty}_{\alpha,\beta} + \sum_{i\,j} \mathbf{M}^{\dagger}_{\alpha i} \left[\frac{1}{\omega - (\underbrace{\mathbf{E}^{fw}}_{\varepsilon_{2p1h},\ \varepsilon_{3p2h},\ \dots} + \underbrace{\mathbf{C}}_{\text{First order in the interaction}}) + i\eta} \right]_{i\,j} \mathbf{M}_{j\beta}$$

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

$$\mathbf{M} = \mathbf{M}^1(v^1) + \mathbf{M}^2(v^2) + \mathbf{M}^3(v^3) + \dots$$

$$\begin{aligned}
\mathbf{M}^{\dagger}\frac{1}{\omega-(E+\mathbf{C})}\mathbf{M} \quad \longrightarrow \quad & \mathbf{M}^{1\dagger}\frac{1}{\omega-E}\mathbf{M}^1 \\
& + \mathbf{M}^{2\dagger}\frac{1}{\omega-E}\mathbf{M}^1 + \mathbf{M}^{1\dagger}\frac{1}{\omega-E}\mathbf{M}^2 + \mathbf{M}^{1\dagger}\frac{1}{\omega-E}\mathbf{C}\frac{1}{\omega-E}\mathbf{M}^1 \\
& + \mathbf{M}^{3\dagger}\frac{1}{\omega-E}\mathbf{M}^1 + \mathbf{M}^{2\dagger}\frac{1}{\omega-E}\mathbf{M}^2 + \mathbf{M}^{1\dagger}\frac{1}{\omega-E}\mathbf{C}\frac{1}{\omega-E}\mathbf{C}\frac{1}{\omega-E}\mathbf{M}^1 +
\end{aligned}$$

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