Self-Consistent Green's Function calculations of nuclear structure and dipole responses

Neutrini and nuclei, challenges and opportunities for nuclear theory
(27-31 may 2019, ECT* - Trento)

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Outline

- Self-consistent Green's function (SCGF) method
  Recent pedagogical review: A. Carbone, C. Barbieri *Lect. Notes Phys.* 936 (2017)
- Testing nuclear Hamiltonians with SCGF
  V. Somà, FR, C. Barbieri, P. Navrátil,T. Duguet, *to be published*
  - Comparison among different models of χEFT interactions
  - Systematics of medium-mass nuclei with $\mathbf{N3LO_{lnl}}$
    "local-nonlocal"
- Dipole Response Function and Polarisability in medium mass nuclei
  FR, C. Barbieri,
  Phys. Rev. C **99** 054327 (2019)
  - ^{14}O, ^{16}O, ^{22}O and ^{24}O
  - ^{36}Ca, ^{40}Ca, ^{48}Ca and ^{54}Ca
  - ^{68}Ni

Ab initio methods based on many-body expansion

A-body Schrödinger equation

$$\mathcal{H}\,|\Psi_n^A\rangle = E_n^A\,|\Psi_n^A\rangle$$

A-body Hamiltonian

$$\mathcal{H} = T + V^{2N} + V^{3N} + V^{4N} + \cdots + V^{AN}$$

A-body wave function

$$|\Psi_n^A\rangle, \quad \langle\Psi_n^A|\mathcal{O}|\Psi_n^A\rangle$$

Realistic interaction:

- Truncated at 3N level
- QCD-based
- Main source of theoretical error in nuclei computation

Expansion around a reference state:

- Uncorrelated mean-field reference state
- Include correlations through *np-nh* excitations
- Truncated but systematically improvable
- Resummed beyond perturbative regime

SCGF

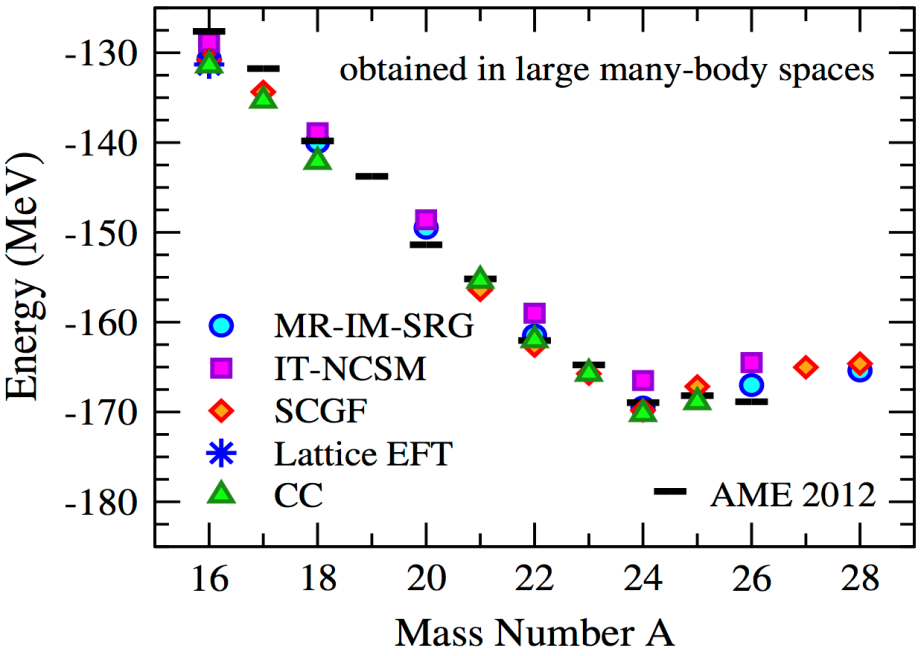
Coupled cluster theory

MBPT

In-medium SRG theory

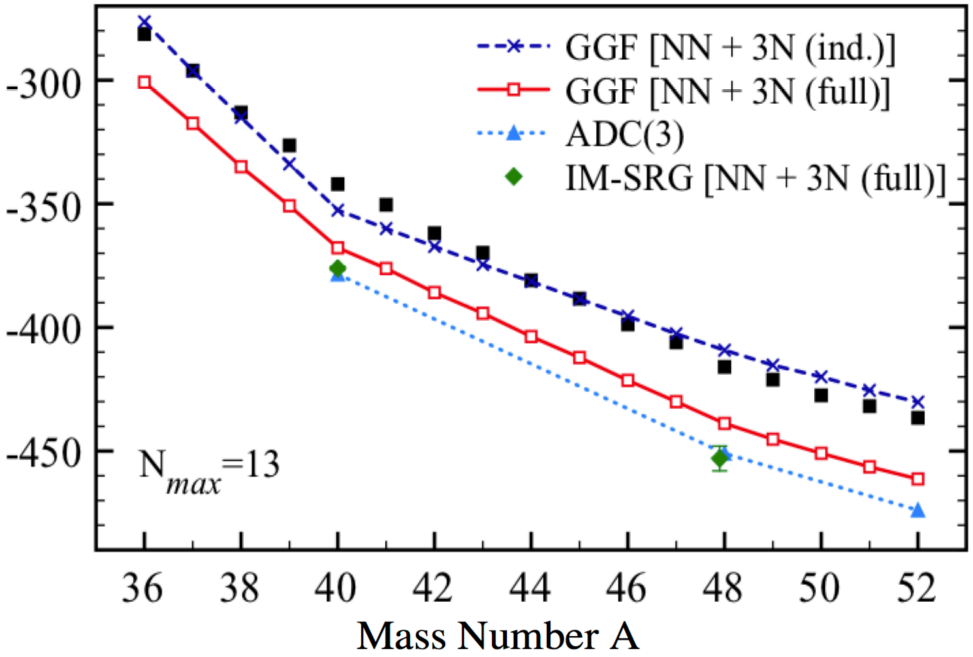
Comparison within a family of many-body methods

Oxygen isotopic chain



[Hebeler *et al.* 2015]

Calcium isotopic chain



[Somà *et al.* 2014]

- Medium-mass nuclei
- Ground and excited states properties of closed/open shell nuclei
- Extension to heavier isotopic chains

Self-consistent Green's function formalism

A-body Schrödinger equation

$$\mathcal{H}\,|\Psi_n^A\rangle = E_n^A\,|\Psi_n^A\rangle$$

Introduce 1-body, 2-body, … A-body quantities (Green's functions)

$$i\,\mathcal{G}^{1b}_{ab}(t,t') \equiv \langle\Psi_0^A|T\left\{a_a(t)a_b^\dagger(t')\right\}|\Psi_0^A\rangle$$

Energy and one-body observables

Expansion around a reference state

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

$$|\Phi_0^A\rangle \qquad |\Psi_0^A\rangle = \hat{\Omega}\,|\Phi_0^A\rangle$$

Wave operator

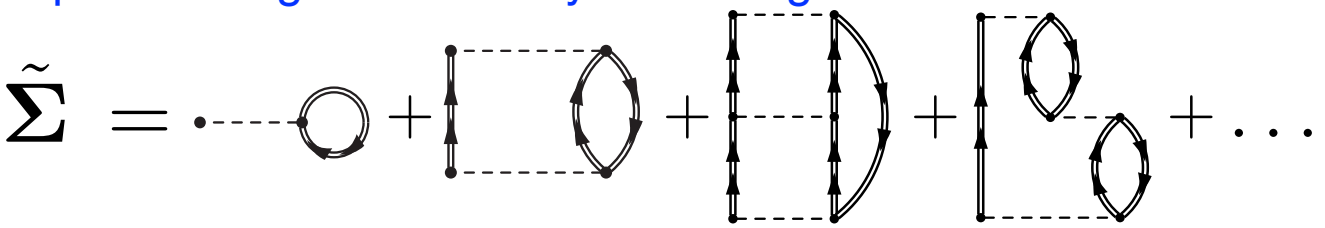
Dyson equation

$$\mathcal{G}_{ab}(\omega) = \mathcal{G}^{(0)}_{ab}(\omega) + \sum_{cd}\mathcal{G}^{(0)}_{ac}(\omega)\,\tilde{\mathbf{\Sigma}}_{cd}(\omega)\,\mathcal{G}_{db}(\omega)$$

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

Self-energy expansion and resummation

Expansion organised in Feynman diagrams

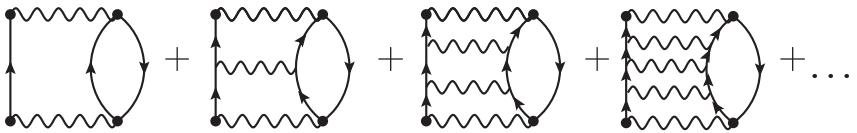


Nonperturbative resummation

Algebraic Diagrammatic Construction ADC(N)

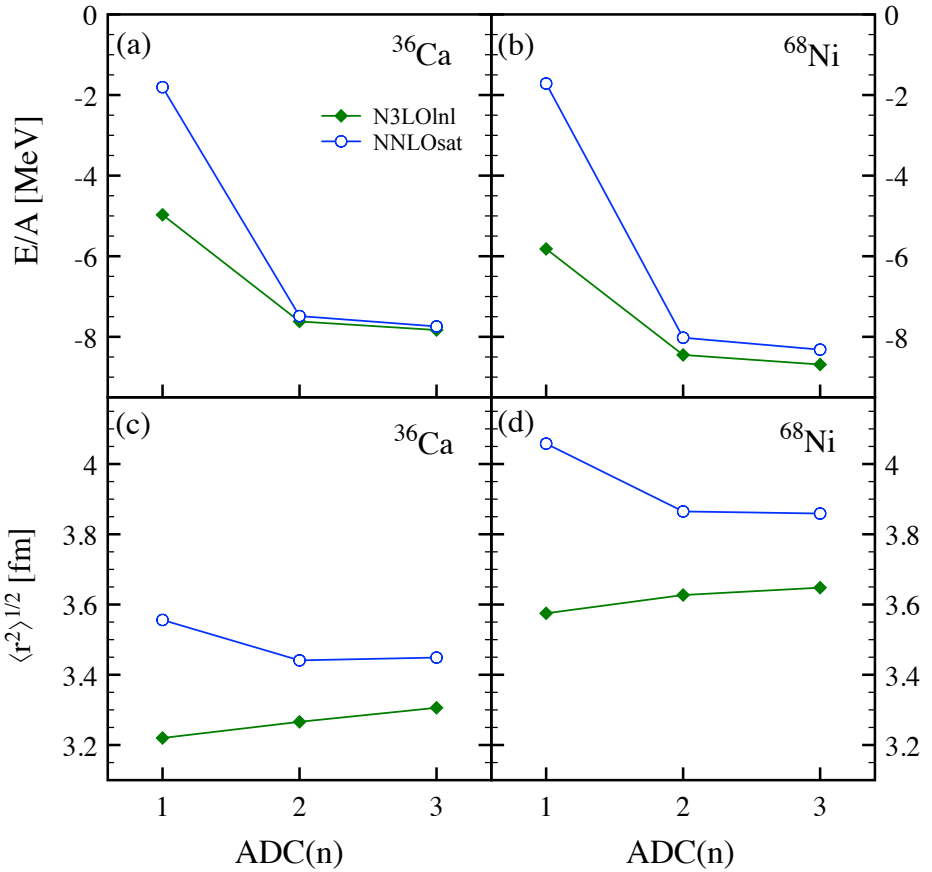
J. Schirmer
Phys. Rev. A26, 2395 (1982)
Phys. Rev. A28, 1237 (1983)

Classes of diagrams (ladder and ring) summed at infinite order by means of a geometric series



ADC(3) with 2N and 3N interactions to include 2p1h and 3p2h correlations already developed

A. Carbone, C. Barbieri Lect. Notes Phys. 936 (2017)
F.R., C. Barbieri PRC**97**, 054308 (2018)



Gorkov-Green's functions for open-shell systems

Open-shell systems:
zero-order degeneracies

$$\mathcal{H}\,|\Psi_n^{\cancel{A}}\rangle = E_n^{\cancel{A}}|\Psi_n^{\cancel{A}}\rangle$$

Breakdown of many-body perturbation theory
(no account of superfluidity)

$$|\Psi_0\rangle \equiv \sum_A^{\text{even}} c_A\,|\psi_0^A\rangle$$

U(1) symmetry broken
(particle number)

$$\Omega = \mathcal{H} - \lambda A$$

Grand potential
(λ chemical potential)

Gorkov diagrammatic for SCGF [Somà, Duguet & Barbieri 2011]

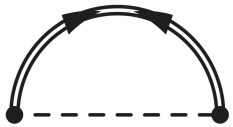
$$i\,G_{ab}^{11}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a_b^\dagger(t')\right\}|\Psi_0\rangle$$

$$i\,G_{ab}^{22}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}_a^\dagger(t)\bar{a}_b(t')\right\}|\Psi_0\rangle$$

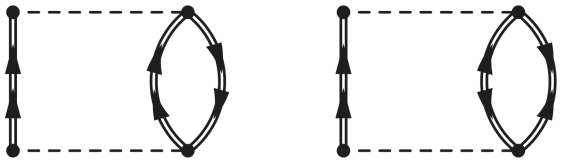
$$i\,G_{ab}^{12}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle$$

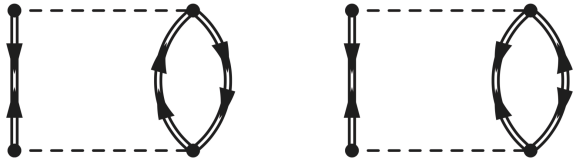
$$i\,G_{ab}^{21}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}_a^\dagger(t)a_b^\dagger(t')\right\}|\Psi_0\rangle$$

$\Sigma^{11(1)}$ 

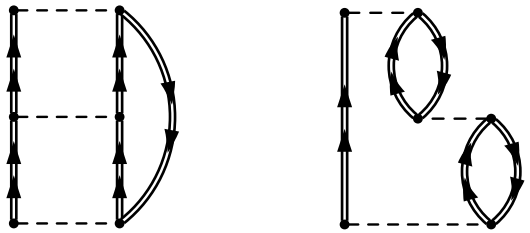
$\Sigma^{12(1)}$ 

G-ADC(1)=HFB

$\Sigma^{11(2)}$ 

$\Sigma^{12(2)}$ 

G-ADC(2)

$\Sigma^{11(3)}$ 

$\cdots$

G-ADC(3) in progress

Energy and one-body operators

Lehmann representation of the one-body Green's function

$$\mathcal{G}^{1b}_{\alpha\beta}(\omega) = \sum_n \frac{\langle\Psi_0^A|a_\alpha|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|a_\beta^\dagger|\Psi_0^A\rangle}{\hbar\omega-(E_n^{A+1}-E_0^A)+i\eta} + \sum_k \frac{\langle\Psi_0^A|a_\beta^\dagger|\Psi_k^{A-1}\rangle\langle\Psi_k^{A-1}|a_\alpha|\Psi_0^A\rangle}{\hbar\omega-(E_0^A-E_k^{A-1})-i\eta}$$

$$\equiv \sum_n \frac{(\mathcal{X}_\alpha^n)^*\mathcal{X}_\beta^n}{\hbar\omega-\varepsilon_n^+ +i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k(\mathcal{Y}_\beta^k)^*}{\hbar\omega-\varepsilon_k^- -i\eta}\,,$$

Spectroscopic factors

$$SF_k^- = \sum_\alpha |\mathcal{Y}_\alpha^k|^2$$

$$SF_n^+ = \sum_\alpha |\mathcal{X}_\alpha^n|^2$$

One-nucleon addition separation energies

One-nucleon removal separation energies

Spectral functions

$$S(\omega) = \sum_\alpha S^p_{\alpha\alpha}(\omega) + \sum_\alpha S^h_{\alpha\alpha}(\omega)$$

$$= \sum_n SF_n^+\,\delta(\omega-E_n^{A+1}+E_0^A) + \sum_n SF_k^-\,\delta(\omega-E_0^A+E_k^{A-1})$$

- Ground-state Energy (Koltun sum rule)

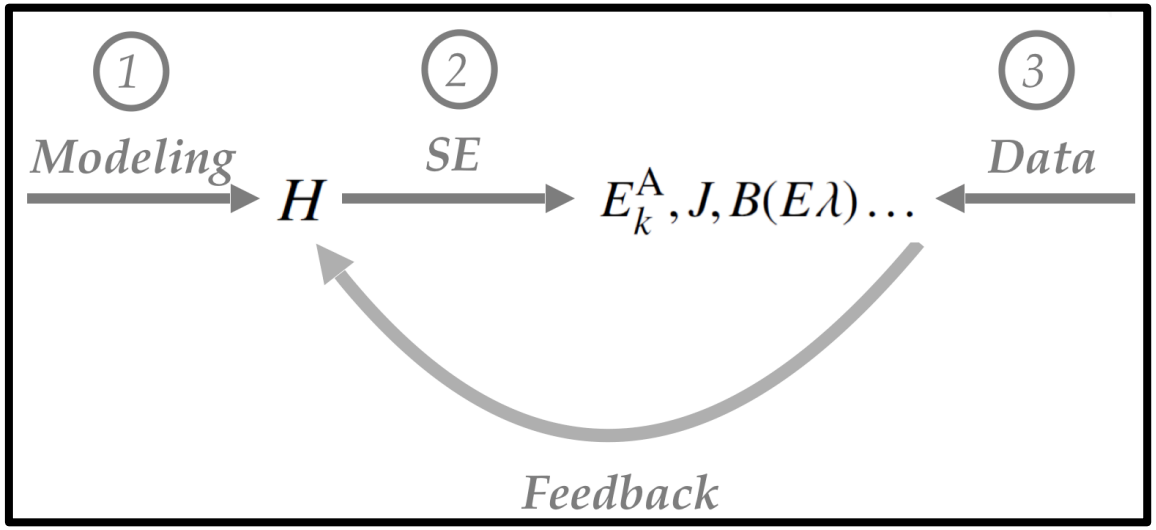
$$E_0^A = \sum_{\alpha\beta}\frac{1}{2}\int_{-\infty}^{\varepsilon_0^-}[T_{\alpha\beta}+\omega\,\delta_{\alpha\beta}]\,S^h_{\beta\alpha}(\omega)\,d\omega - \frac{1}{2}\langle\widehat{W}\rangle$$

- One-body density matrix / observables

$$\rho_{\alpha\beta} \equiv \langle\Psi_0^A|a_\beta^\dagger a_\alpha|\Psi_0^A\rangle = \int_{-\infty}^{\varepsilon_0^-} S^h_{\alpha\beta}(\omega)\,d\omega \longrightarrow \langle\widehat{O}^{1B}\rangle = \sum_{\alpha\beta} O^{1B}_{\alpha\beta}\,\rho_{\beta\alpha}$$

Testing Hamiltonians with SCGF

Slide courtesy from V. Somà and T. Duguet



2 Gorkov ADC(2) SCGF
Dyson ADC(3) SCGF

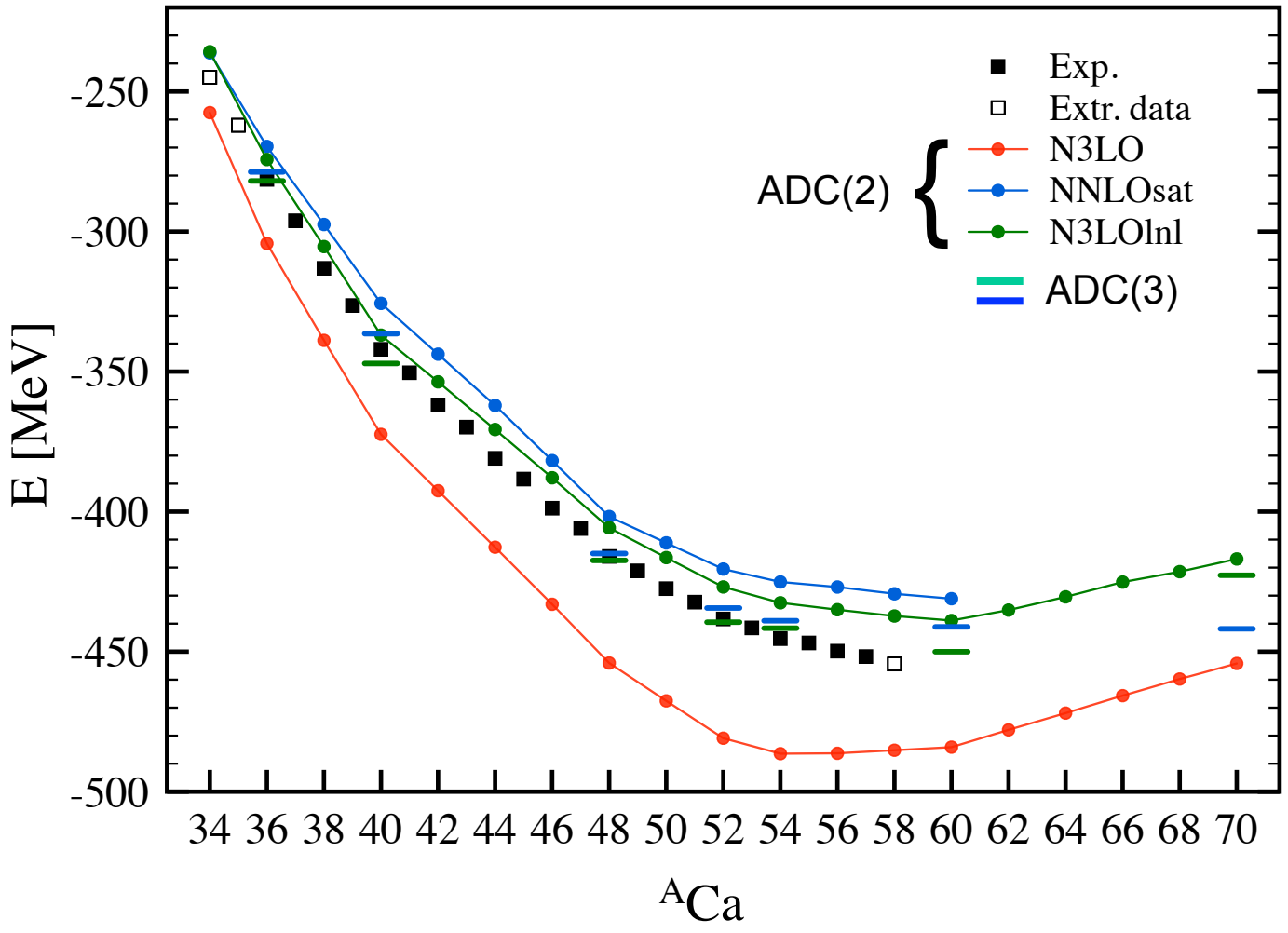
3 BE, Charge Radii, S_{2N}

1a **N3LO (~2010)** [Entem & Machleidt 2003, Navrátil 2007, Roth et al. 2012]
First generation of ChEFT interactions (N^3LO *NN* + N^2LO *3N*)
SRG λ=2.0 fm^{-1}
Follows traditional ab initio strategy (fit *X*-body sector on *X*-body data)
Successful for light nuclei, but overbinding and too small radii for heavier systems

1b **$NNLO_{sat}$ (2015)** [Ekström *et al.* 2015]
Development prompted by inability to reproduce radii beyond light nuclei
Data from not-so-light nuclei (*A*=14-25) included in fit
Description of two- and few-few-body systems slightly deteriorated

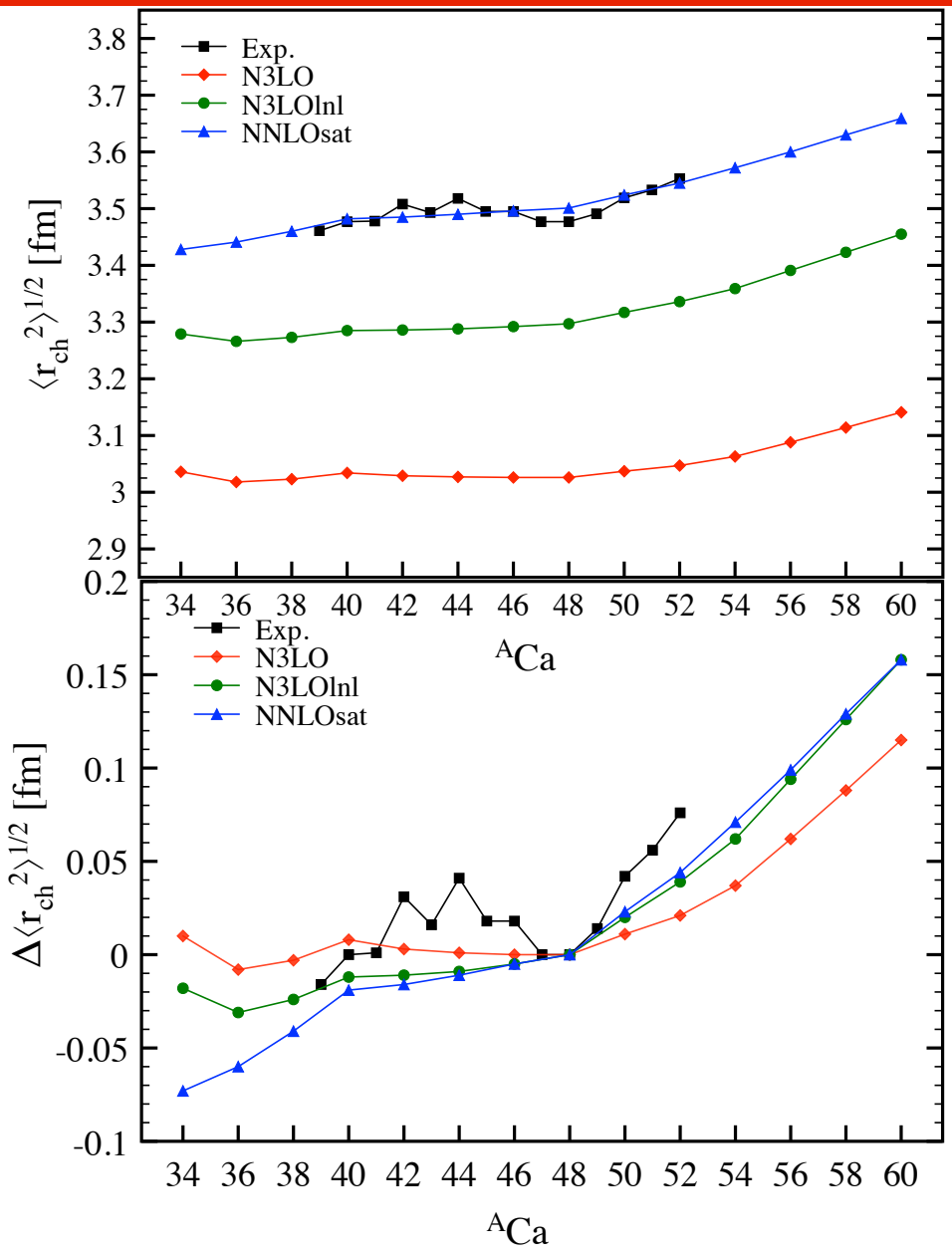
1c **$N3LO_{lnl}$ (2018)** [Entem & Machleidt 2003, Navrátil 2018]
Back to standard ab initio strategy but with non-local regulators
SRG λ=2.0 fm^{-1}
Mid-mass and heavy systems? Radii?

Binding energies in Ca isotopes



- **N3LO$_{lnl}$** corrects for overbinding
- ADC(3) crucial for accurate description of binding energies

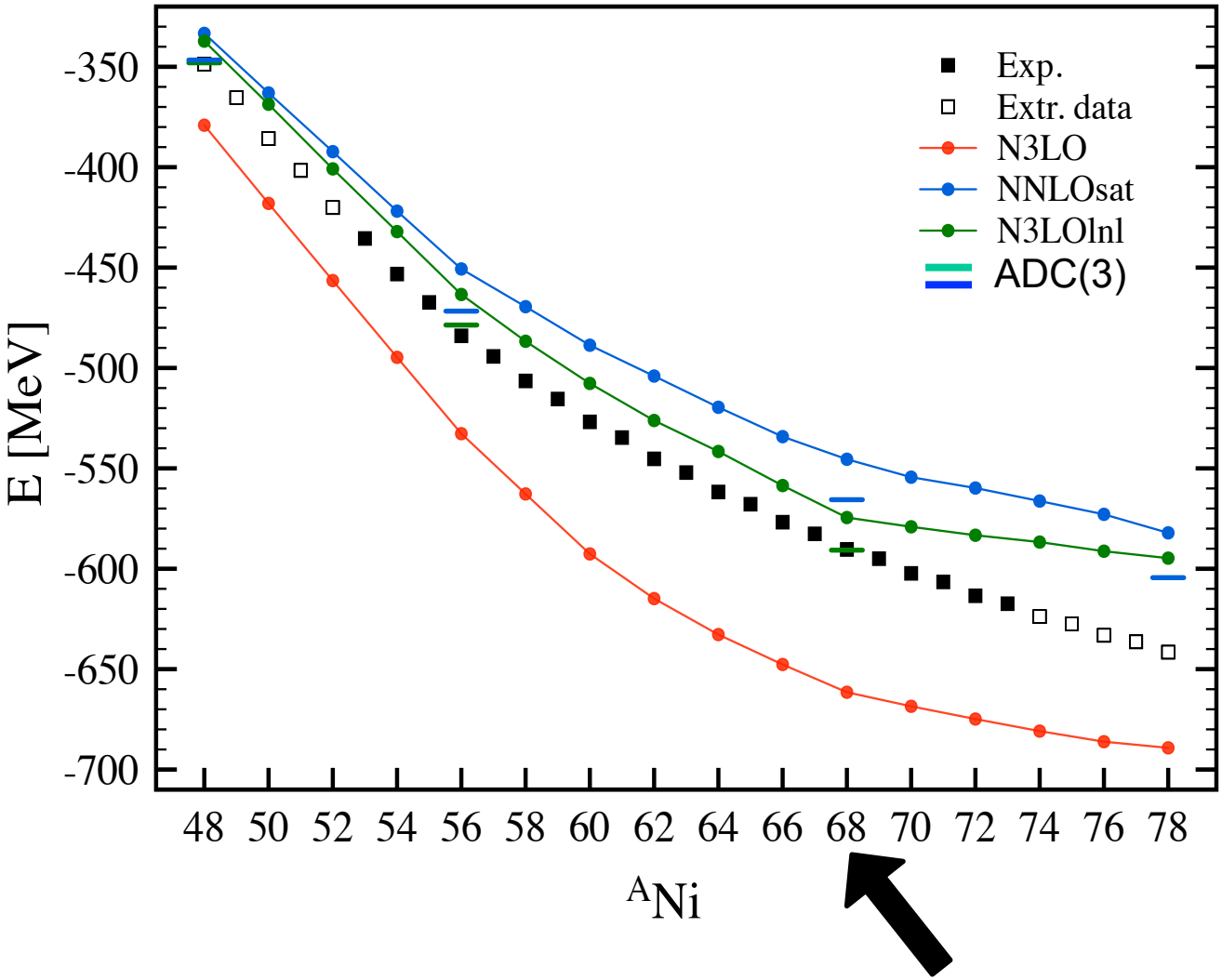
Charge radii in Ca isotopes



- **N3LO$_{lnl}$** improves significantly with respect to **N3LO**
- **N3LO$_{lnl}$**: 5-6% underestimation of experimental values
- Current chiral interaction cannot reproduce radii (unless fitted)

- Isotope shift may correct systematic errors (inconsistent SRG evolution)
- No account of parabolic trend ^{40}Ca-^{48}Ca (missing high-order *mp-mh* excitations)

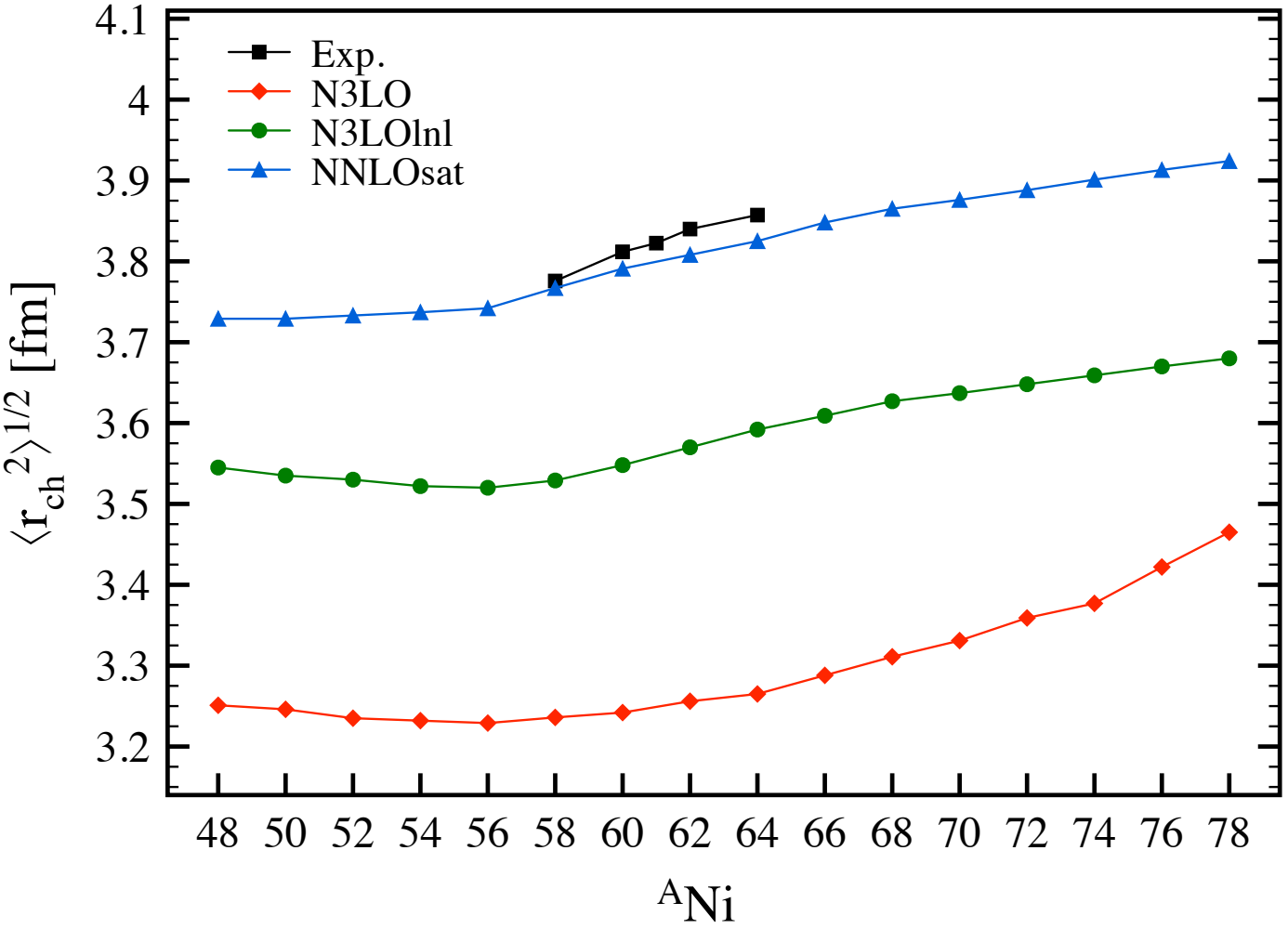
Binding energies in Ni isotopes



Over/underbinding wrt to experiment

^{68}Ni	ΔBE(%)
N3LO	-10.9
$NNLO_{sat}$	7.6
ADC(3)	4.2
$N3LO_{lnl}$	2.6
ADC(3)	0.05

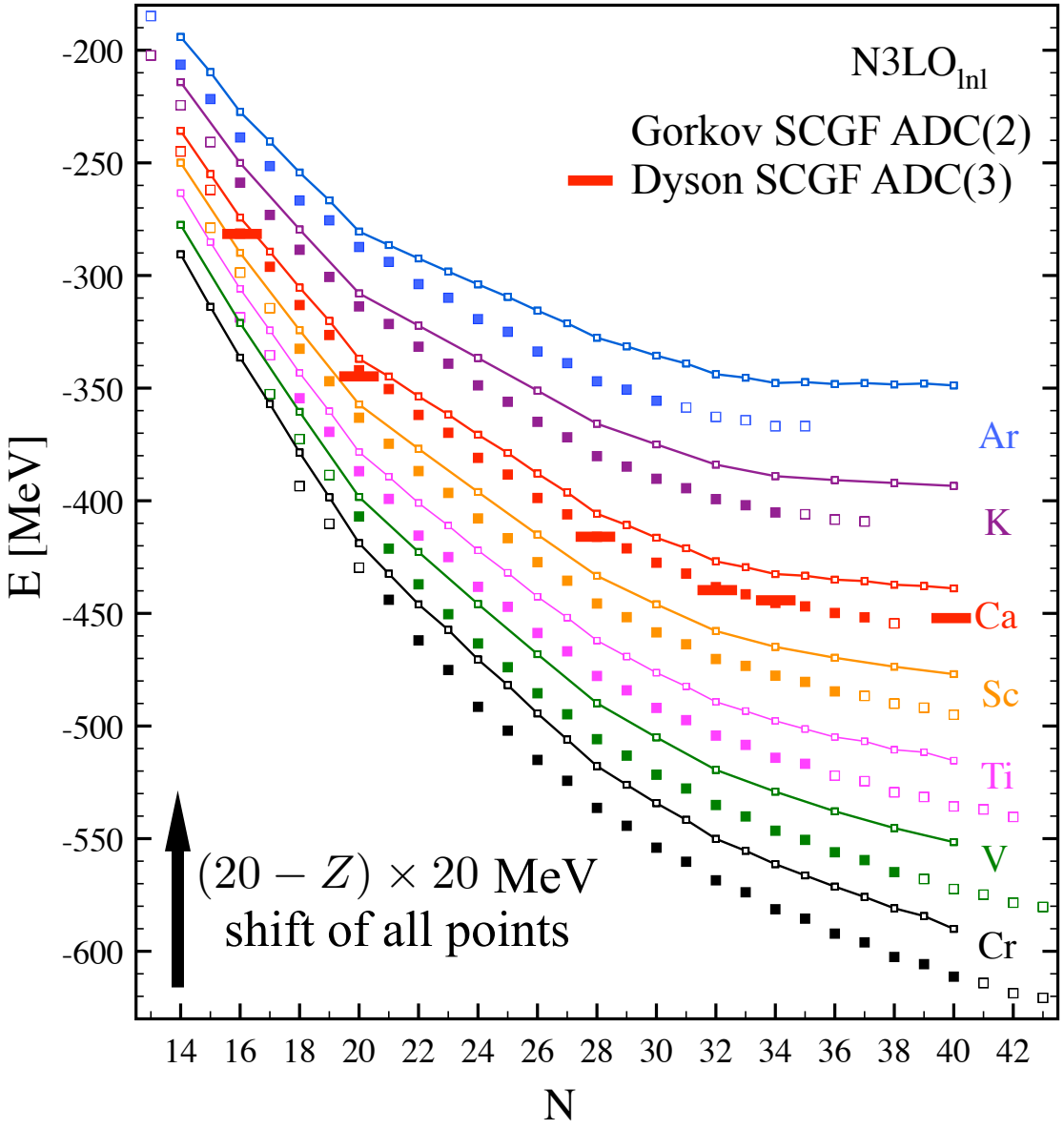
Charge radii in Ni isotopes



- **NNLO$_{sat}$** preserves good reproduction of charge radii in **A**~60 region
- Kink at ^{56}Ni (closed shell)
- Trend of experimental data reproduced

Systematics of medium-mass nuclei: BE

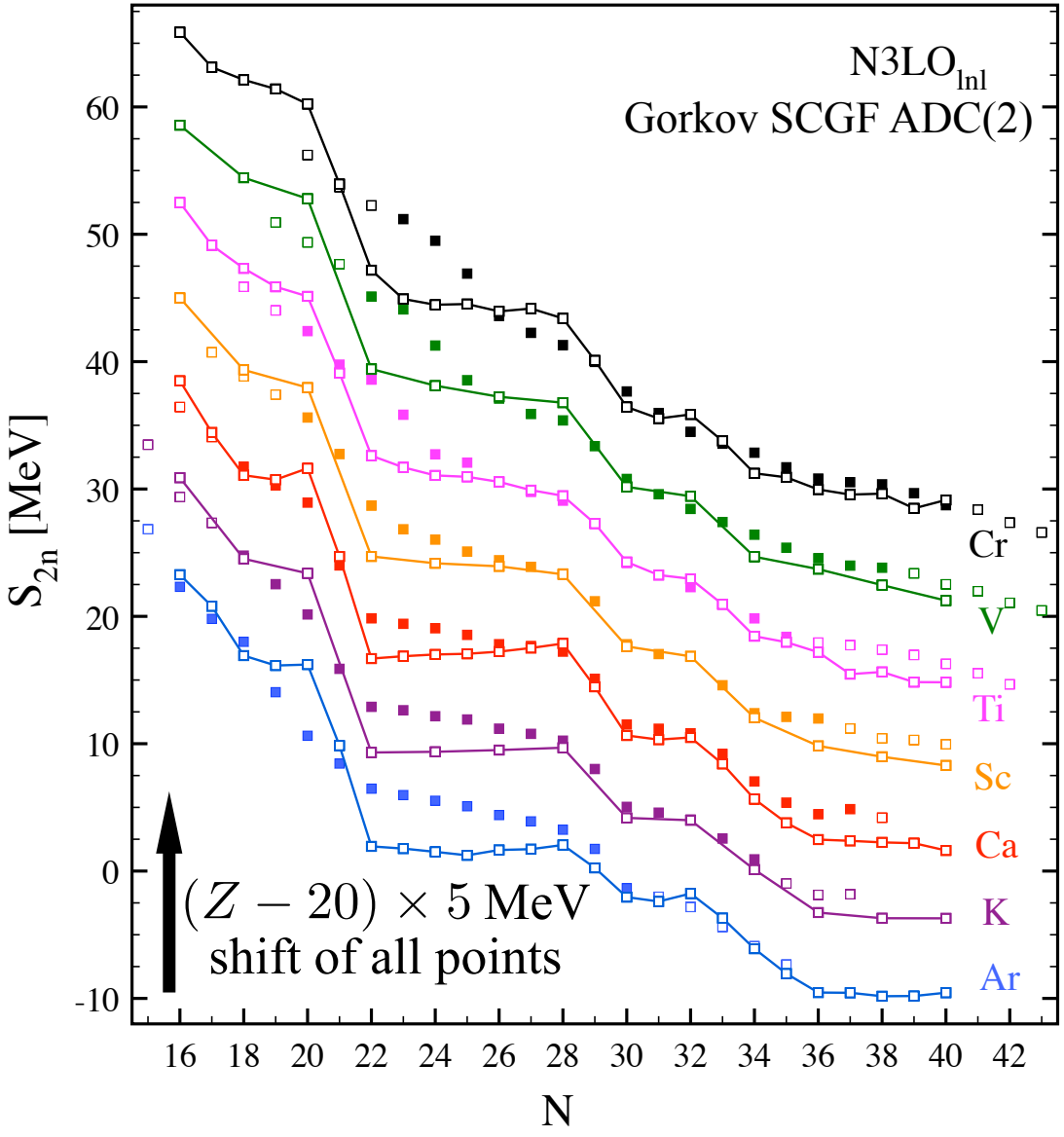
Total binding energies Z = 18 - 24 isotopic chains



- Global trend described
- Systematic underbinding (worsen with mass number)
- Closed-subshell Calcii:
  ΔE(ADC(2)) ≲ 3%
  ΔE(ADC(3)) ≲ 1%

Systematics of medium-mass nuclei: S_{2n}

Two-neutron separation energies $\mathbf{Z}$ = 18 - 24 isotopic chains



$$S_{2n}(N,Z) \equiv |E(N,Z)| - |E(N-2,Z)|$$

- Main gap at $\mathbf{N}$ = 20 reproduced but overestimated
- Main gap at $\mathbf{N}$ = 28 reproduced
- Description worsens in doubly open-shell nuclei

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 component: Transition density matrix

Polarization propagator and Bethe-Salpeter equation

$$\Pi_{\gamma\delta,\alpha\beta}(\omega) = \sum_n \frac{< \Psi_0^A | a_\delta^\dagger a_\gamma | \Psi_n^A > < \Psi_n^A | a_\alpha^\dagger a_\beta | \Psi_0^A >}{\hbar\omega - (E_n^A - E_0^A) + i\eta}$$

Two-body Propagator

$$\epsilon_n^\pi \equiv E_n^A - E_0^A$$

Energies of the excited states of the A-nucleon system

Equation for the polarization propagator

$$\Pi_{\gamma\delta,\alpha\beta}(\omega) = \Pi^f_{\gamma\delta,\alpha\beta}(\omega) + \Pi^f_{\gamma\delta,\mu\rho}(\omega) K^{(p-h)}_{\mu\sigma,\rho\nu}(\omega) \Pi_{\nu\sigma,\alpha\beta}(\omega)$$

Free polarization Propagator

p-h kernel

Approximated solution of the Bethe-Salpeter equation

$$\Pi_{\gamma\delta,\alpha\beta}(\omega) = \Pi^{f}_{\gamma\delta,\alpha\beta}(\omega) + \Pi^{f}_{\gamma\delta,\mu\rho}(\omega) K^{(p-h)}_{\mu\sigma,\rho\nu}(\omega) \Pi_{\nu\sigma,\alpha\beta}(\omega)$$

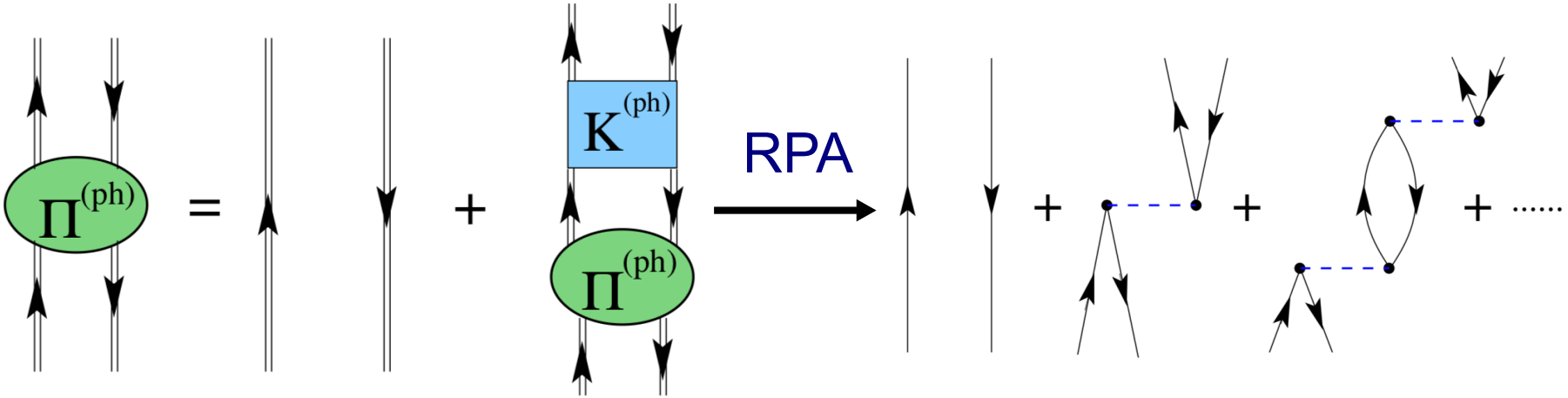


Fig. from PRC 68, 014311 (2003)

Extension of the RPA: 1) Fully-dressed (correlated) single-particle propagator in the RPA diagrams

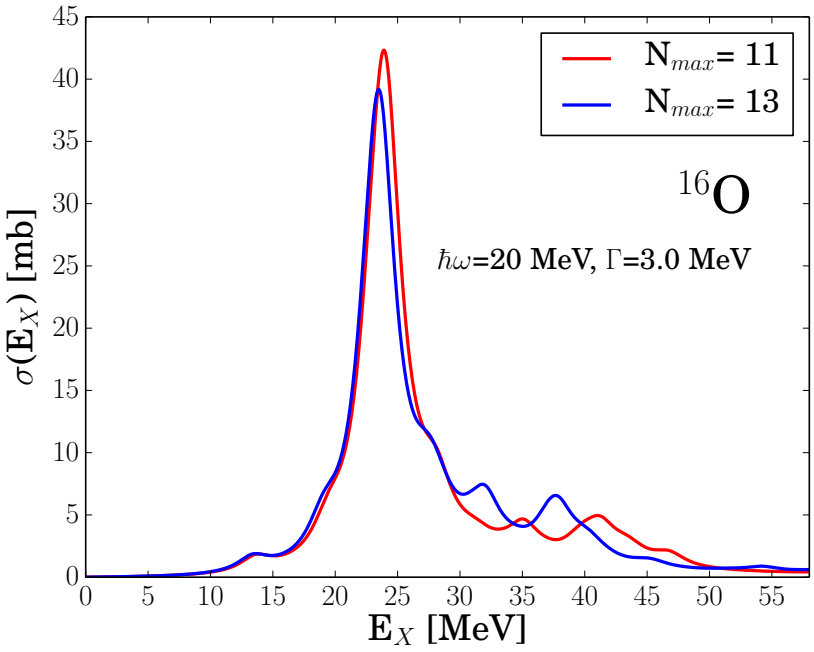
C. Barbieri, W. Dickhoff PRC 68, 014311 (2003)

2) Reduction of the number of poles of the dressed propagator

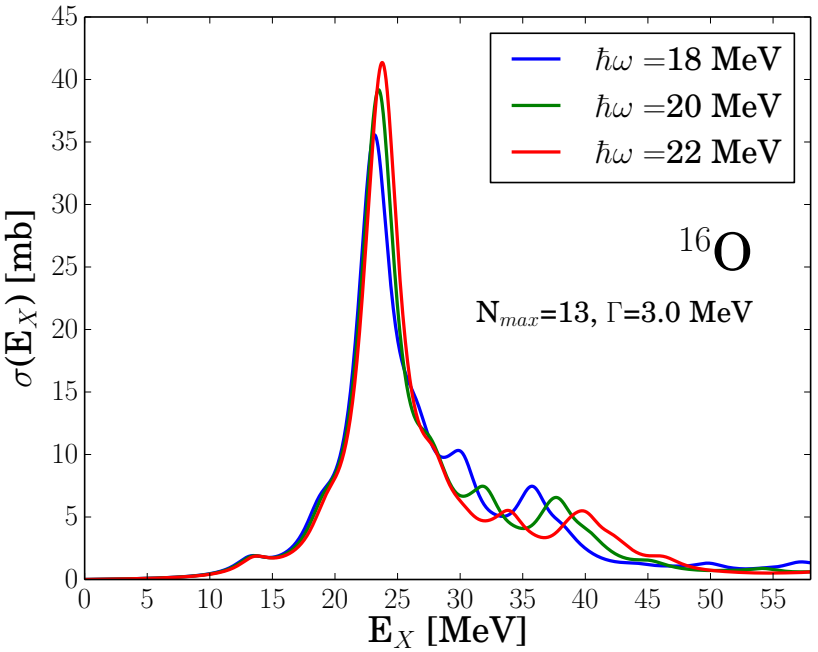
C. Barbieri, M. Hjorth-Jensen PRC 79, 064313 (2009)

Features of the calculation

- NN and 3N nuclear interaction $NNLO_{sat}$ (Phys. Rev. C 91, 051301(R))
- Electric dipole operator E1 $\hat{Q}_{1m}^{T=1} = \frac{N}{N+Z}\sum_{p=1}^{Z} r_p Y_{1m} - \frac{Z}{N+Z}\sum_{n=1}^{N} r_n Y_{1m}$
- Single-particle harmonic oscillator basis (N_{max}, $\hbar\omega$)



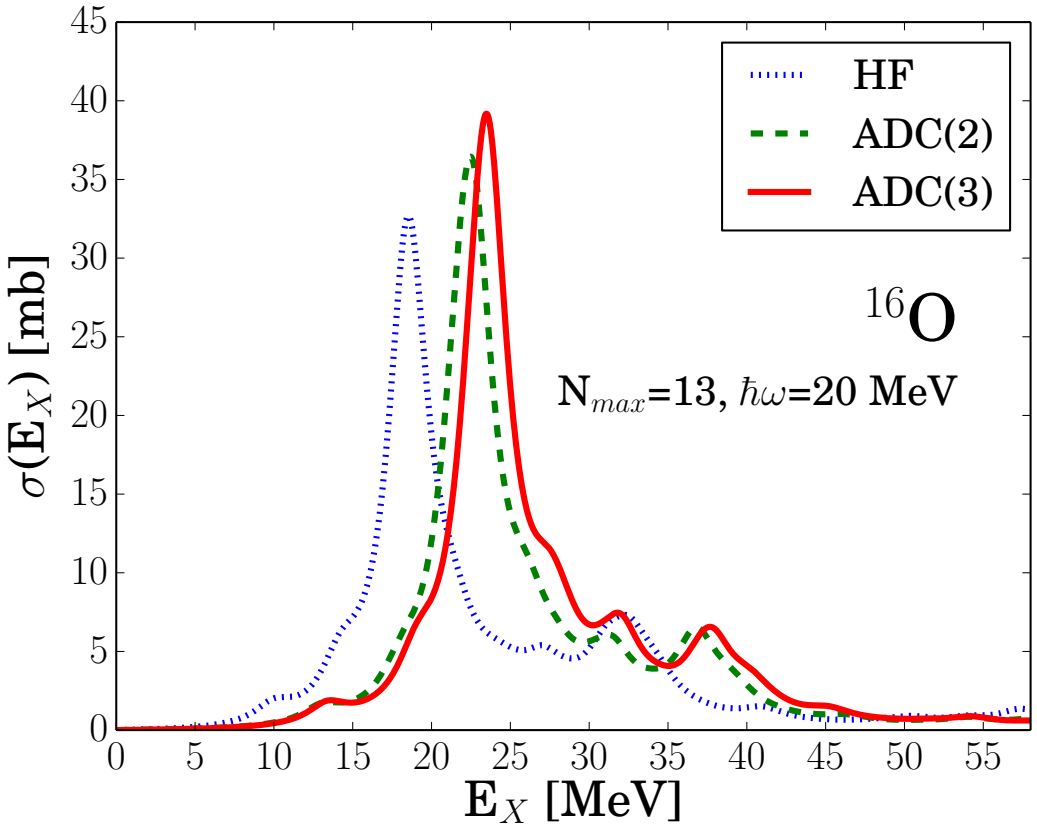
$\delta(\alpha_D, N_{max})$=2%



$\delta(\alpha_D, \hbar\omega)$=1.5%

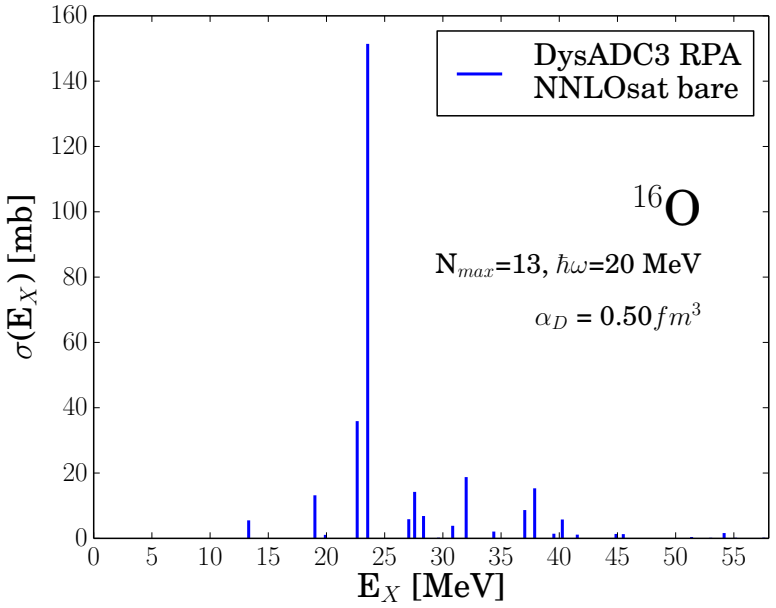
Many-body truncation convergence

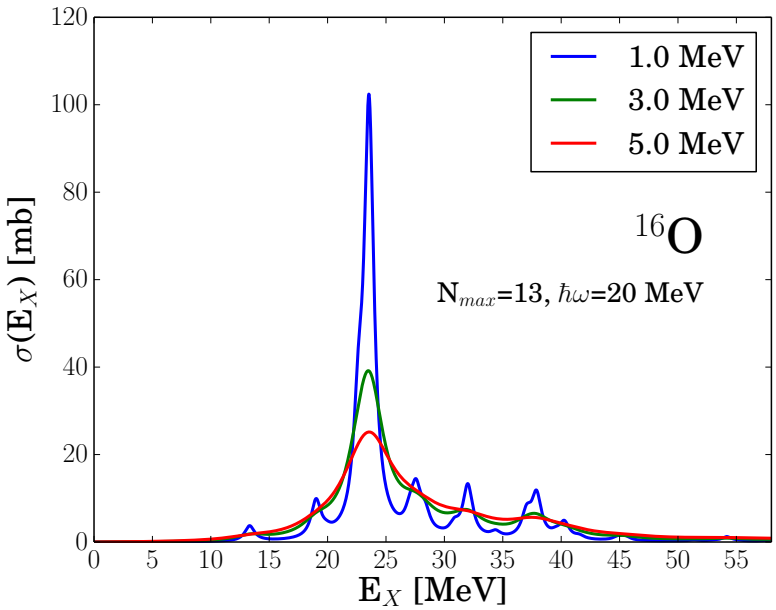
Convergence wrt inclusion of correlations in the reference propagator



- Impact of correlation beyond mean field
- Towards saturation of correlations from ADC(2) to ADC(3)

Discrete spectrum convolution



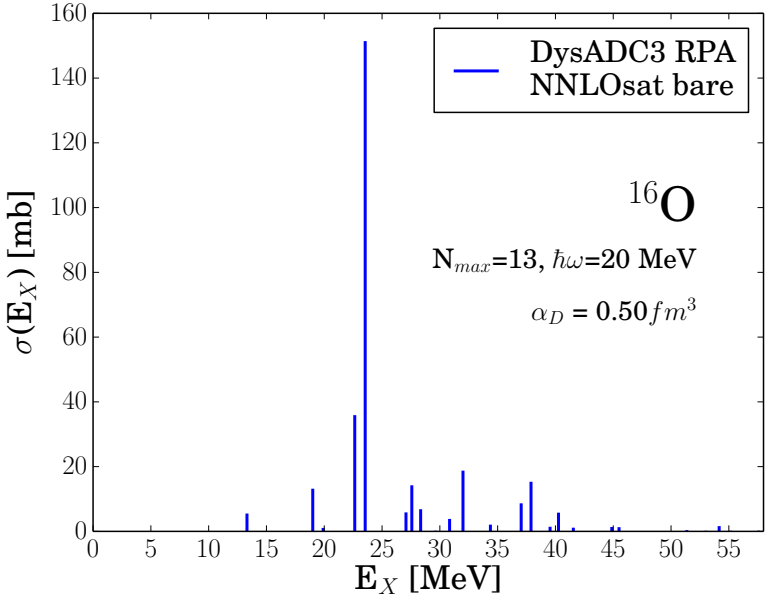


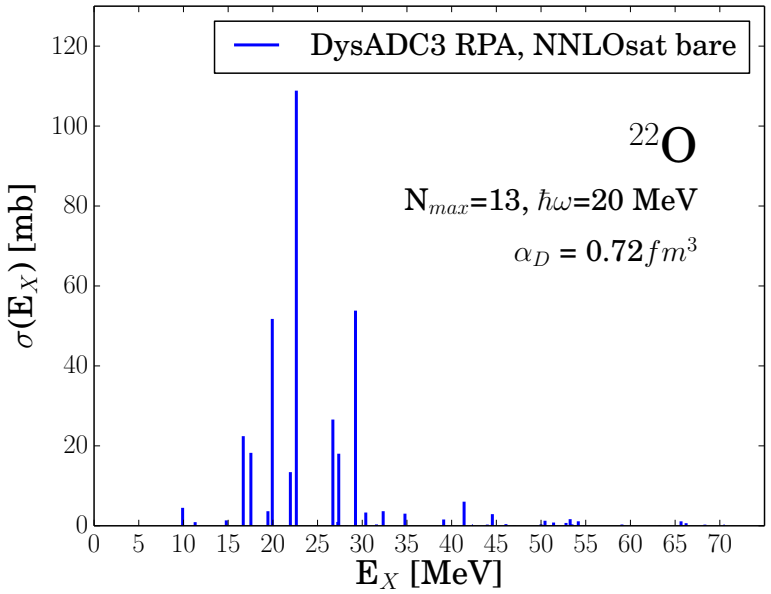
No treatment of the continuum

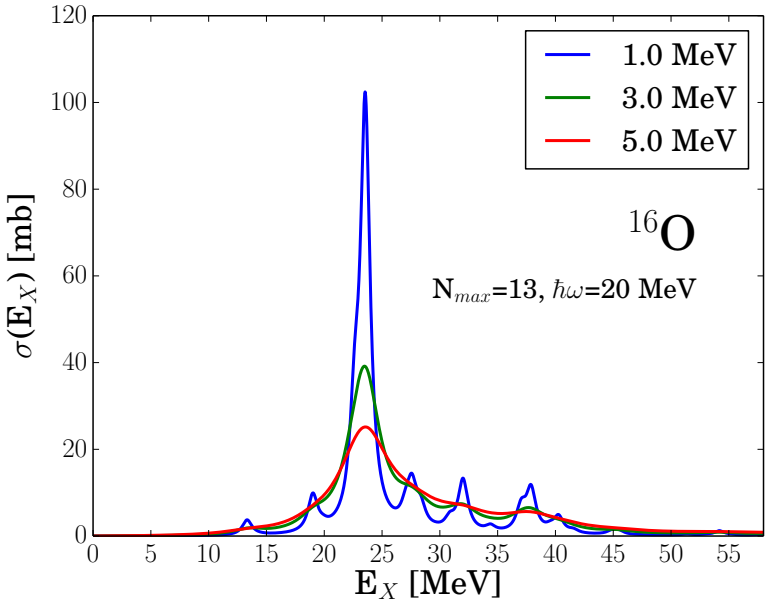
$$R_\Gamma(E) = \sum_n (\langle \Psi_n^A | \hat{\mathcal{Q}}_{1m}^{T=1} | \Psi_0^A \rangle)^2 \frac{\Gamma/2\pi}{(E_n^A - E)^2 + \Gamma^2/4}$$

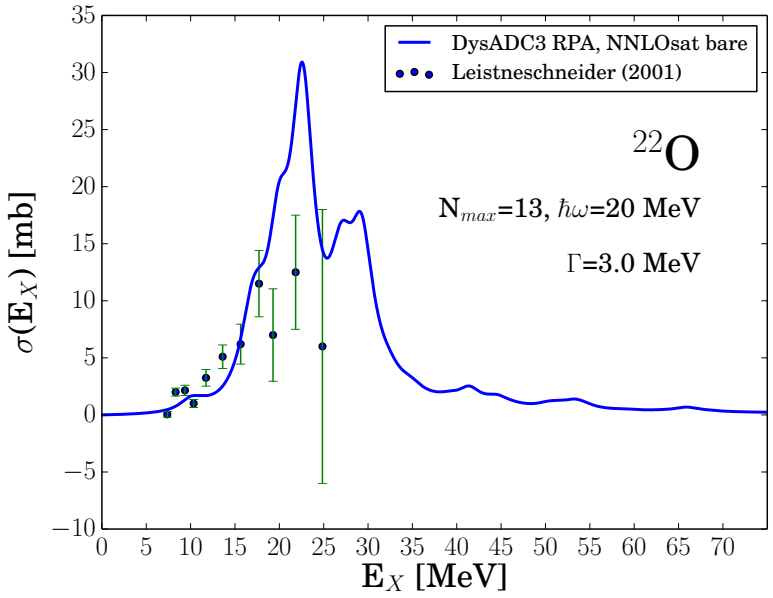
Γ width of the Lorentzian

Discrete vs convoluted photoabsorption σ

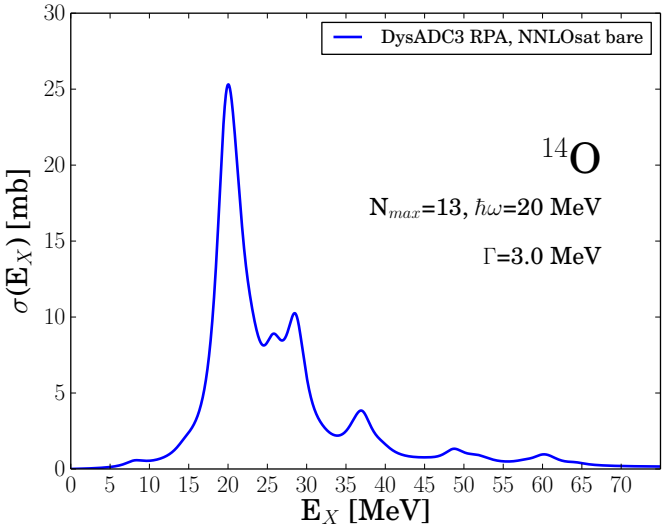


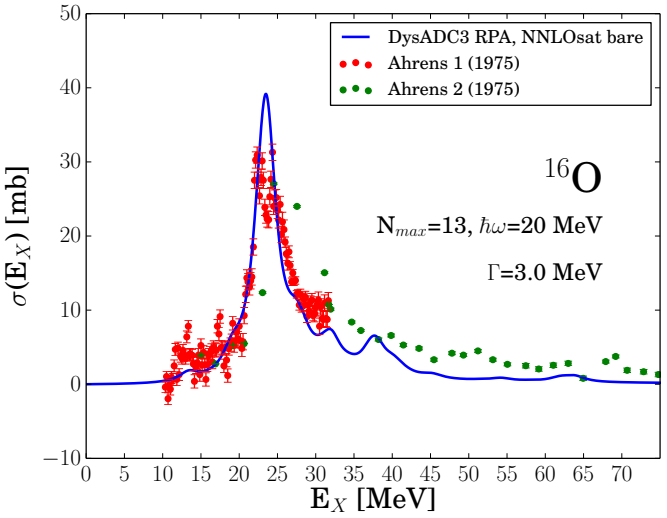


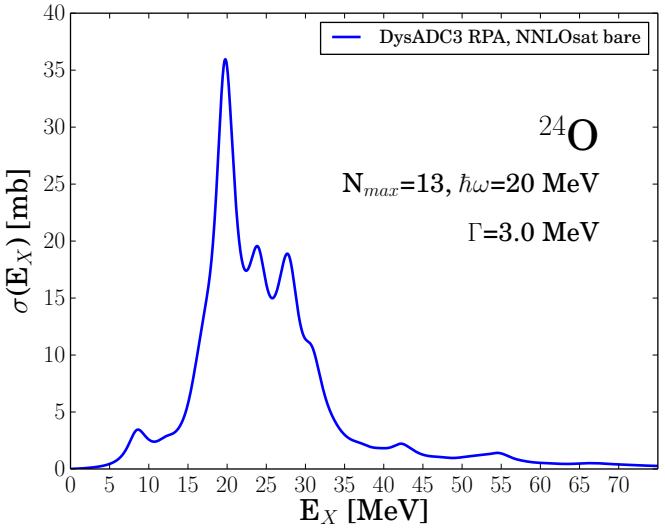


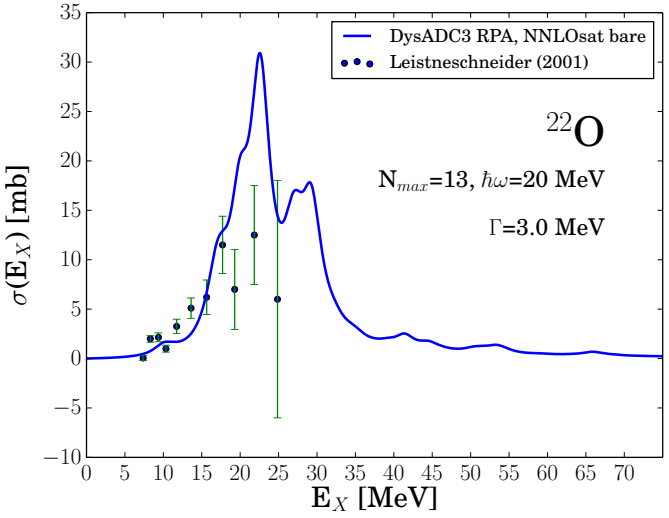


Results for Oxygen isotopes









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

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

Polarizability in ^{16}O and ^{22}O

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

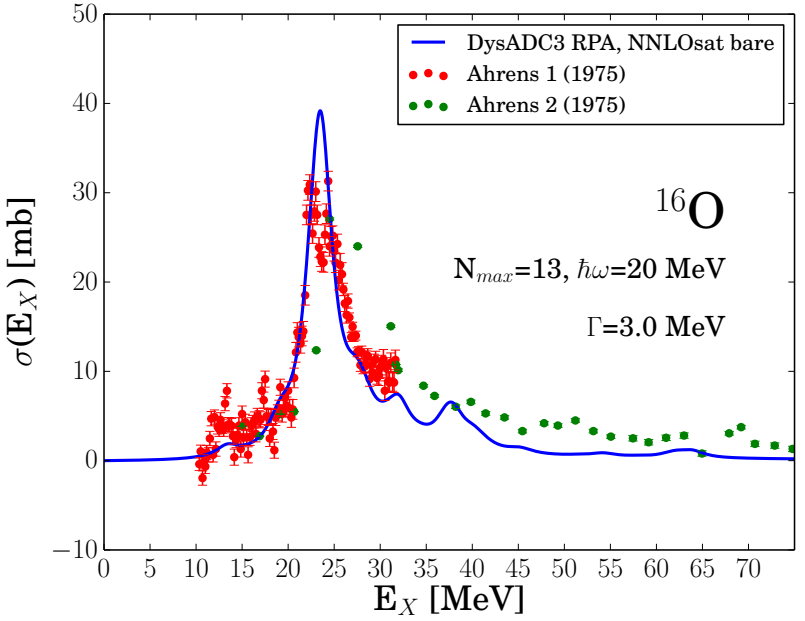
α_D (fm^3)	Exp	SCGF	CC-LIT
^{16}O	0.585(9)	0.50	0.57(1) * 0.528 **
^{22}O	0.43(4)	0.72	0.86(4) * na **

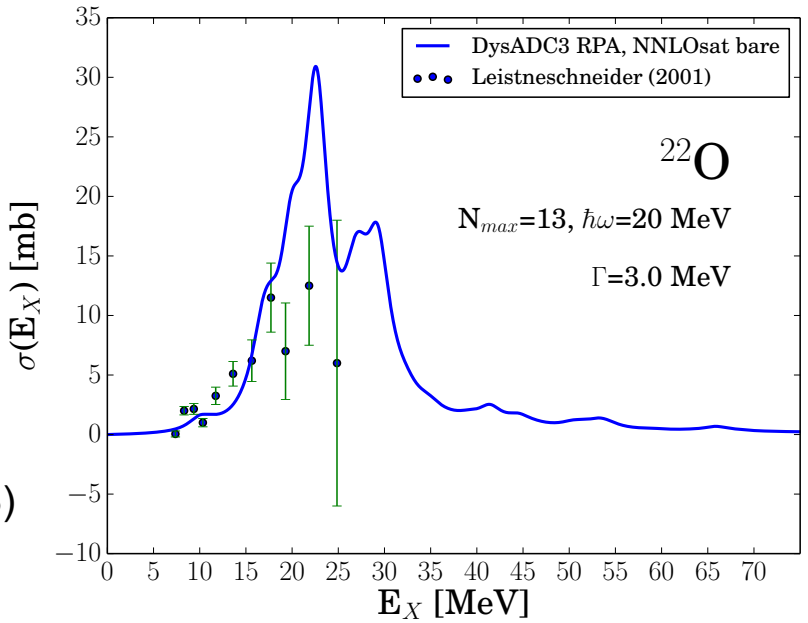
$\delta(\alpha_D,$ th-exp) ≃15% (^{16}O)

Coupled-Cluster + LIT

M. Miorelli, S. Bacca et al. Phys Rev C 98, 014324 (2018)

* Doubles/Doubles. ** Triples/Triples





Polarizability in ^{16}O and ^{22}O

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

α_D (fm^3)	Exp	SCGF	CC-LIT
^{16}O	0.585(9)	0.50	0.57(1) * 0.528 **
^{22}O	0.43(4)	0.72	0.86(4) * na **

$\delta(\alpha_D,$ th-exp) ≃15% (^{16}O)

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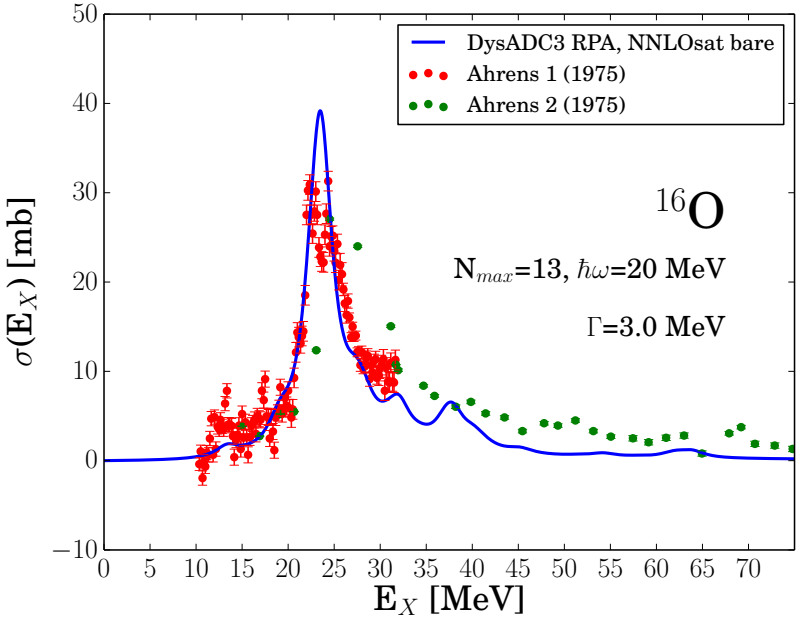
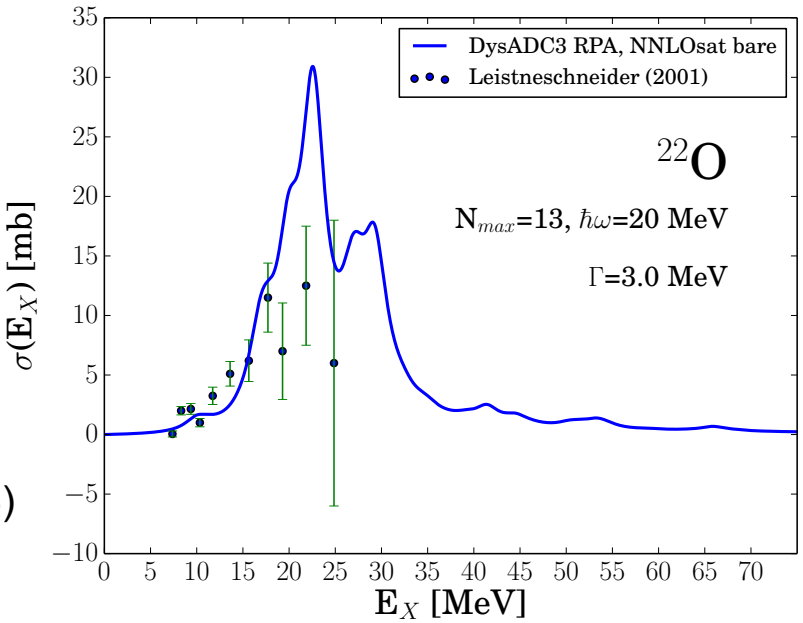
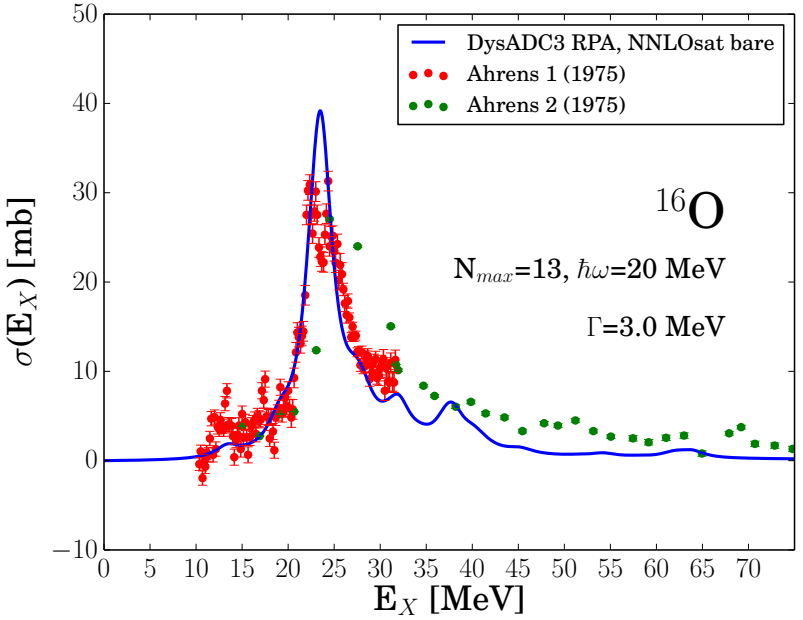


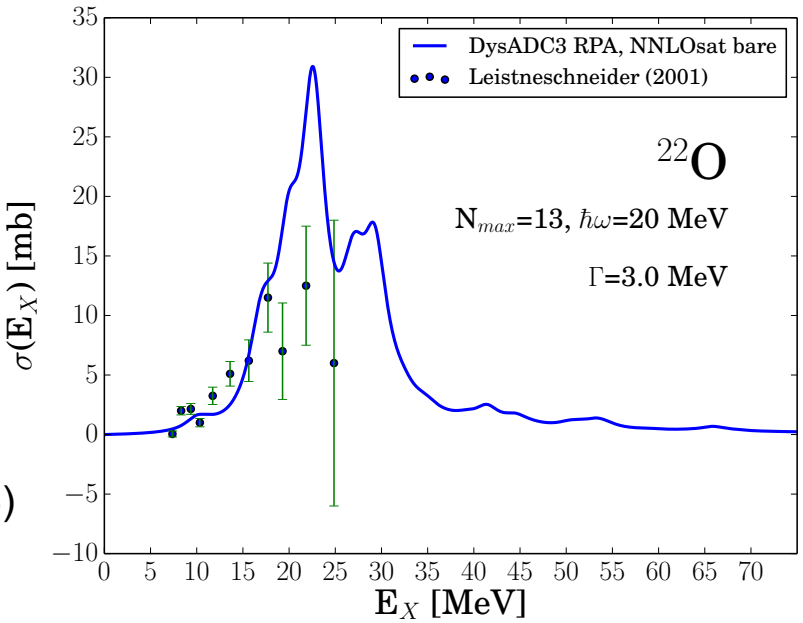


Polarizability in ^{16}O and ^{22}O

$$\alpha_D = 2\alpha \int dE \frac{R(E)}{E}$$

α_D (fm^3)	Exp	SCGF	CC-LIT
^{16}O	0.585(9)	0.50	0.57(1) * 0.528 **
^{22}O (< 3 MeV)	0.07(2)	0.05	0.05(1) * na **





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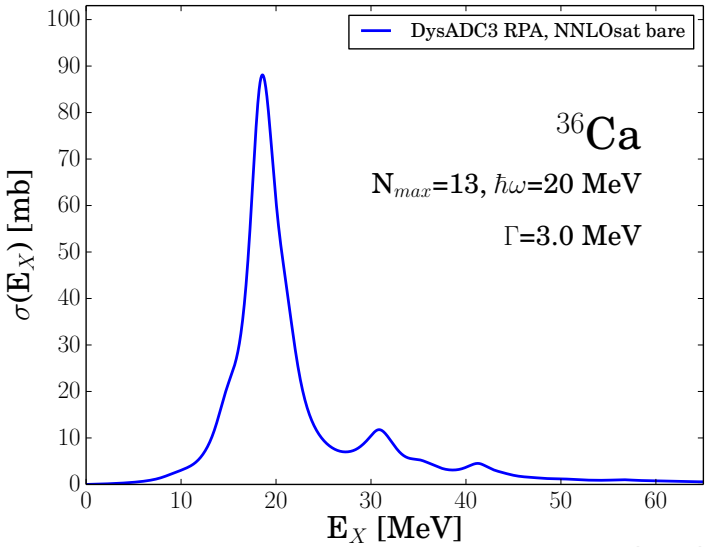
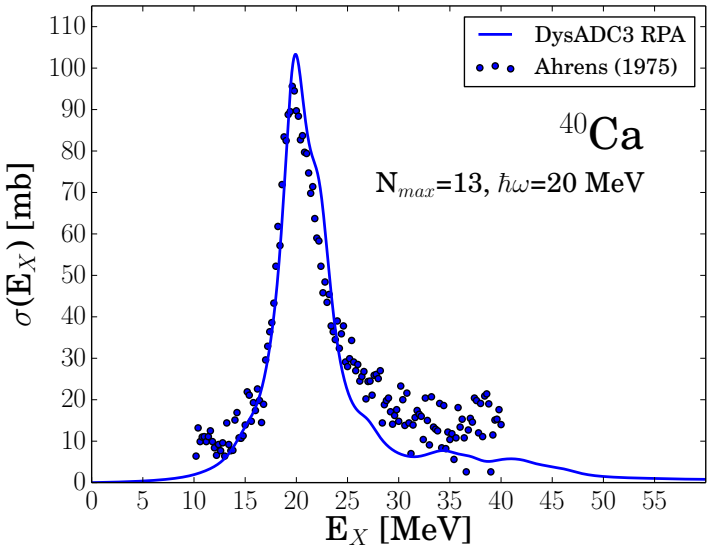
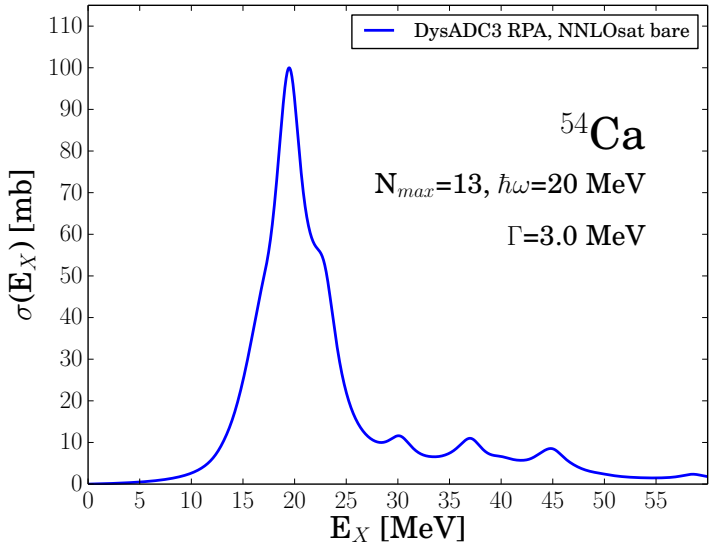
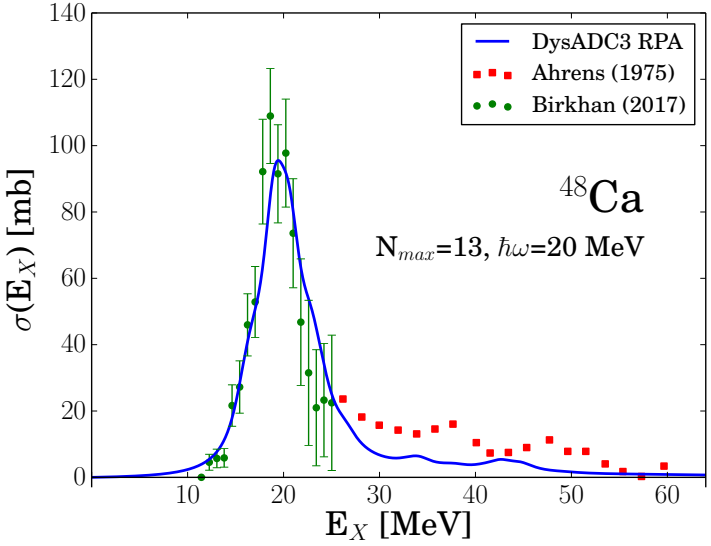
Results for Calcium isotopes





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





Polarizability in ^{40}Ca and ^{48}Ca

$$\alpha_D = 2\alpha \int dE \frac{R(E)}{E}$$

α_D (fm^3)	Exp	SCGF	CC-LIT
^{40}Ca	2.23(3)	1,79	1.87(3) * na **
^{48}Ca	2.07(22) (Birkhan et al)	2.06	2.45 * 2.25(8)**

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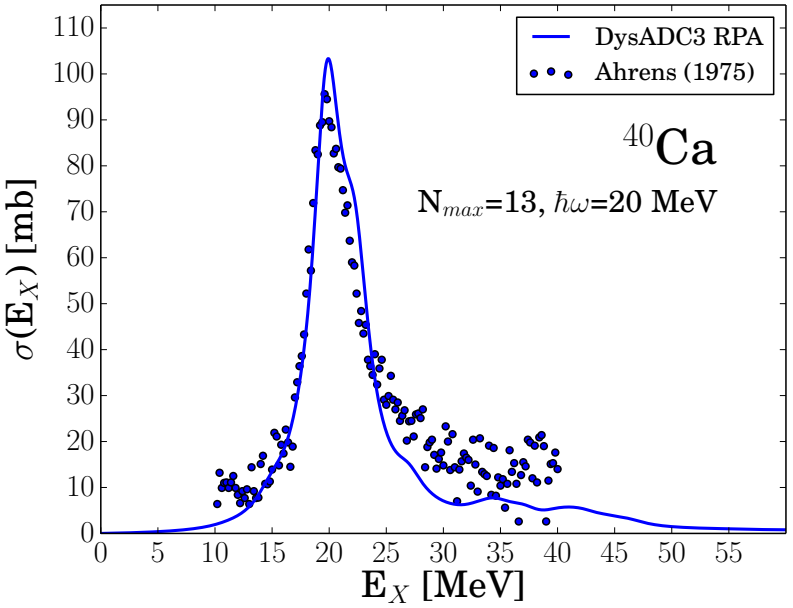
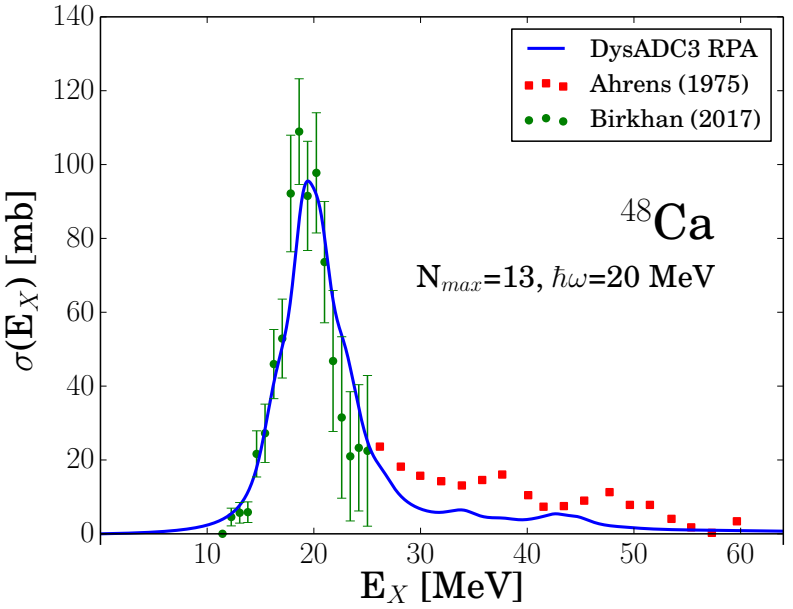
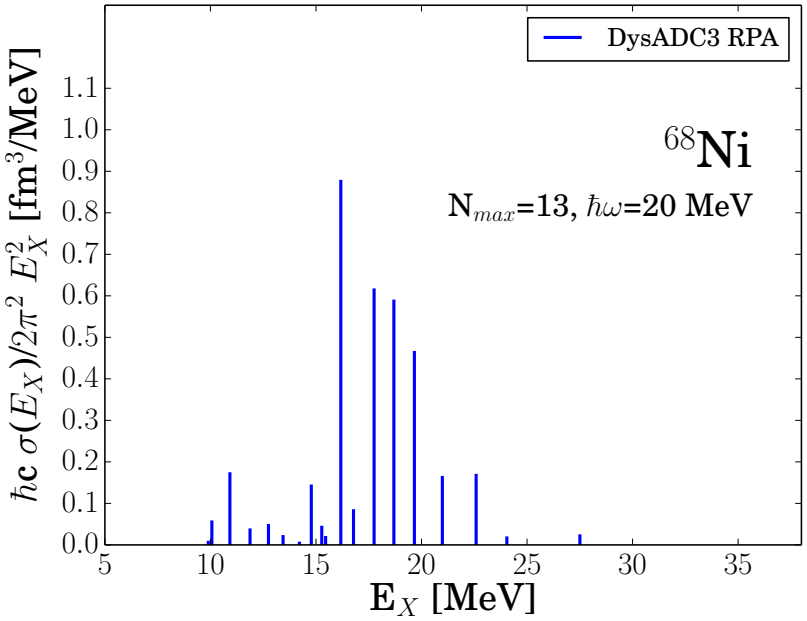
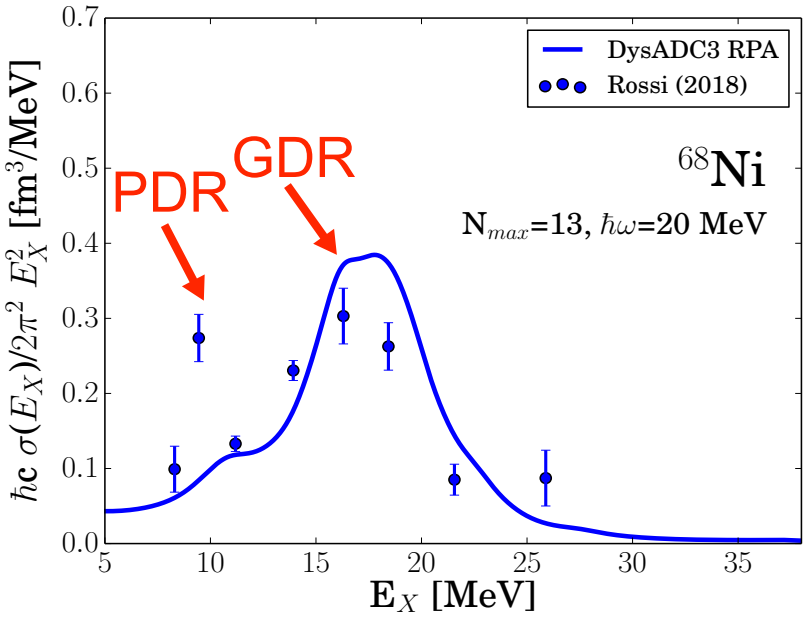




Results for ^{68}Ni





Comparison with experimental Coulomb excitation
(Rossi *et al* PRL, 111, 242503 (2013))

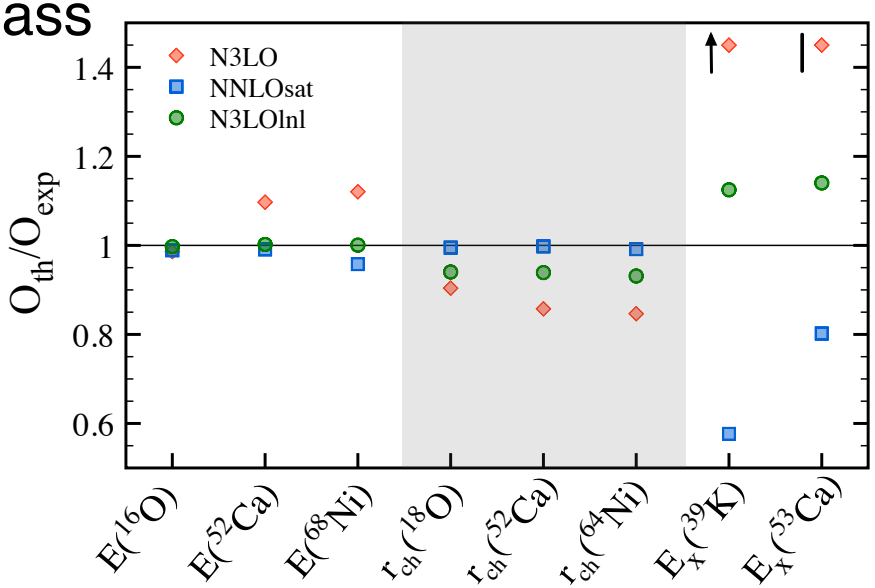
	Exp	SCGF
Pigmy (MeV)	9.55(17)	10.68 10.92
Giant (MeV)	17.1(2)	18.10
α_D (fm^3)	3.88(31)	3.60

$\delta(\alpha_D,\ \text{th-exp}) \simeq 7\%$

Conclusions

I)

- "Universal" Hamiltonian for medium-mass calculations not available yet
- Pragmatical approach



II)

- Dipole response and polarisability calculated from first principles
- Continuum to be included
- Correlations: going beyond DRPA approximation
- Polarization propagator based on Gorkov propagator (QDRPA)