Ab initio computations of the nuclear spectral function

Vittorio Somà
CEA Saclay, France

Neutrino detection and interactions: challenges and opportunities for ab initio nuclear theory

INT Seattle
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Collaborators:
Carlo Barbieri, Francesco Raimondi, Arnau Rios (University of Surrey), Thomas Duguet (CEA Saclay), Petr Navrátil (TRIUMF)

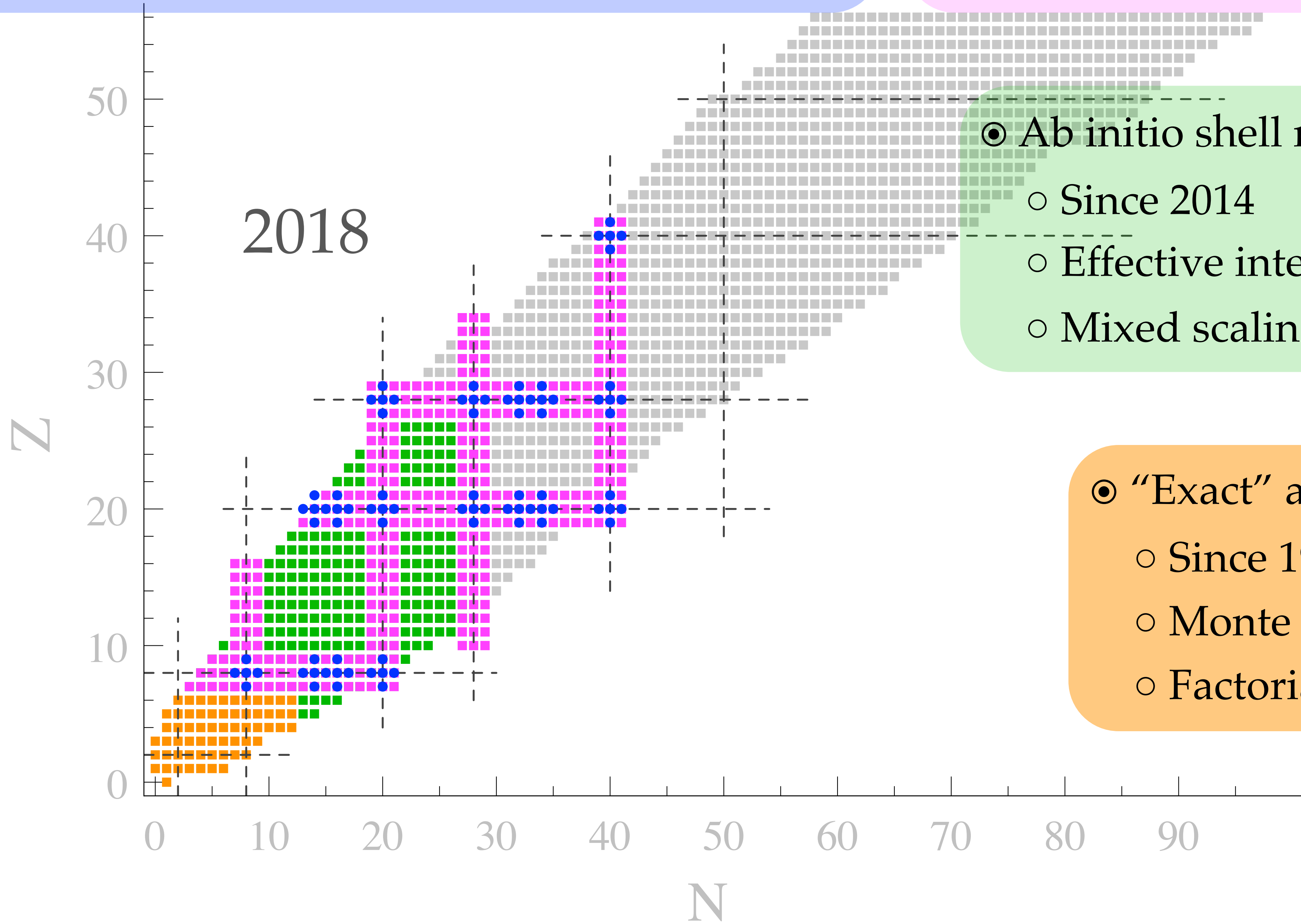
Outline

- **Introduction**
- **Self-consistent Green's function approach**
- **Applications**
  - Ground-state properties
  - Spectral function
  - Response function
- **Conclusions**

Evolution of ab initio nuclear chart

- Approximate approaches for closed-shell nuclei
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling

- Approximate approaches for open-shells
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling



- Ab initio shell model
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" approaches
  - Since 1980's
  - Monte Carlo, CI, ...
  - Factorial scaling

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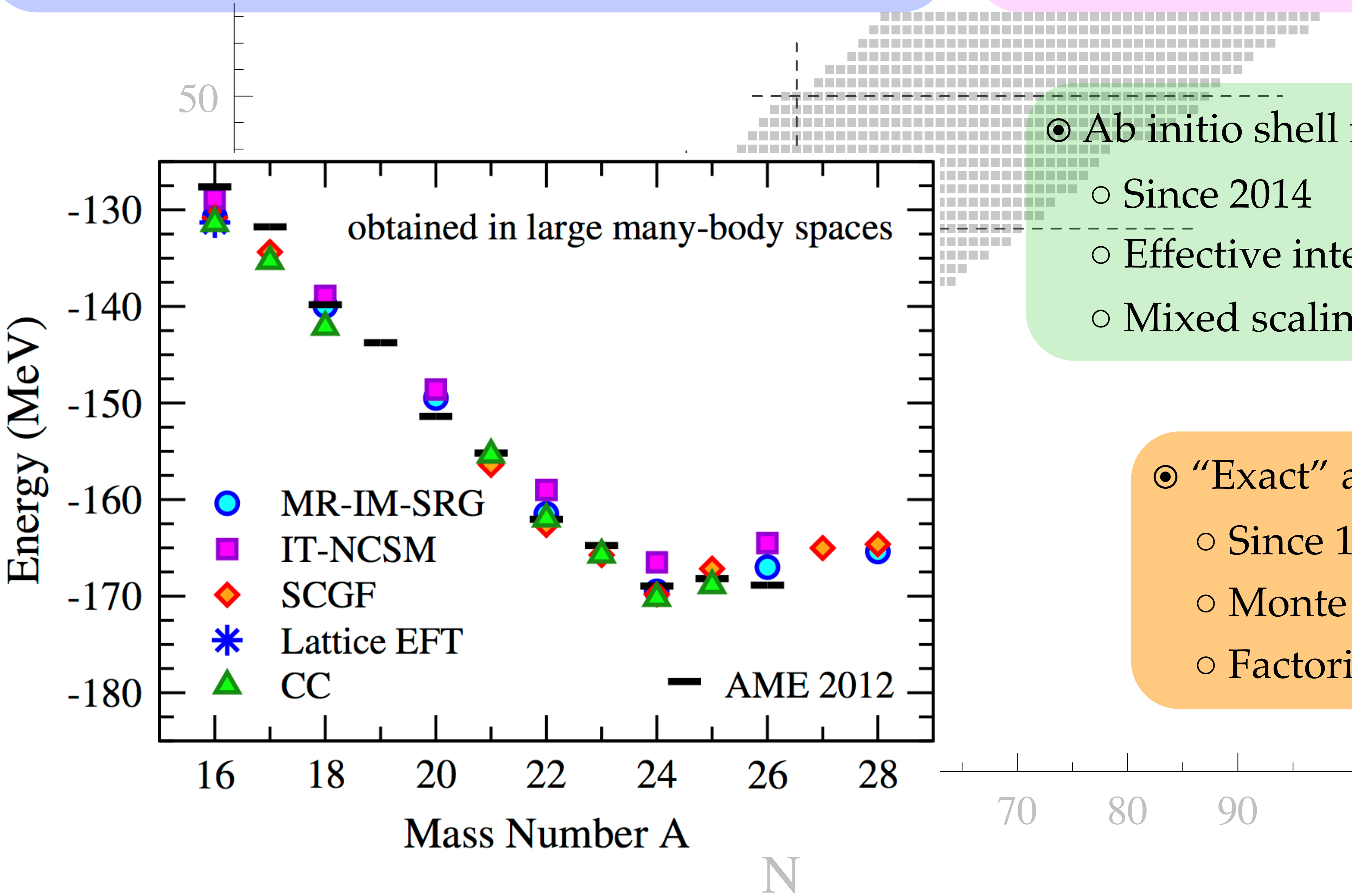

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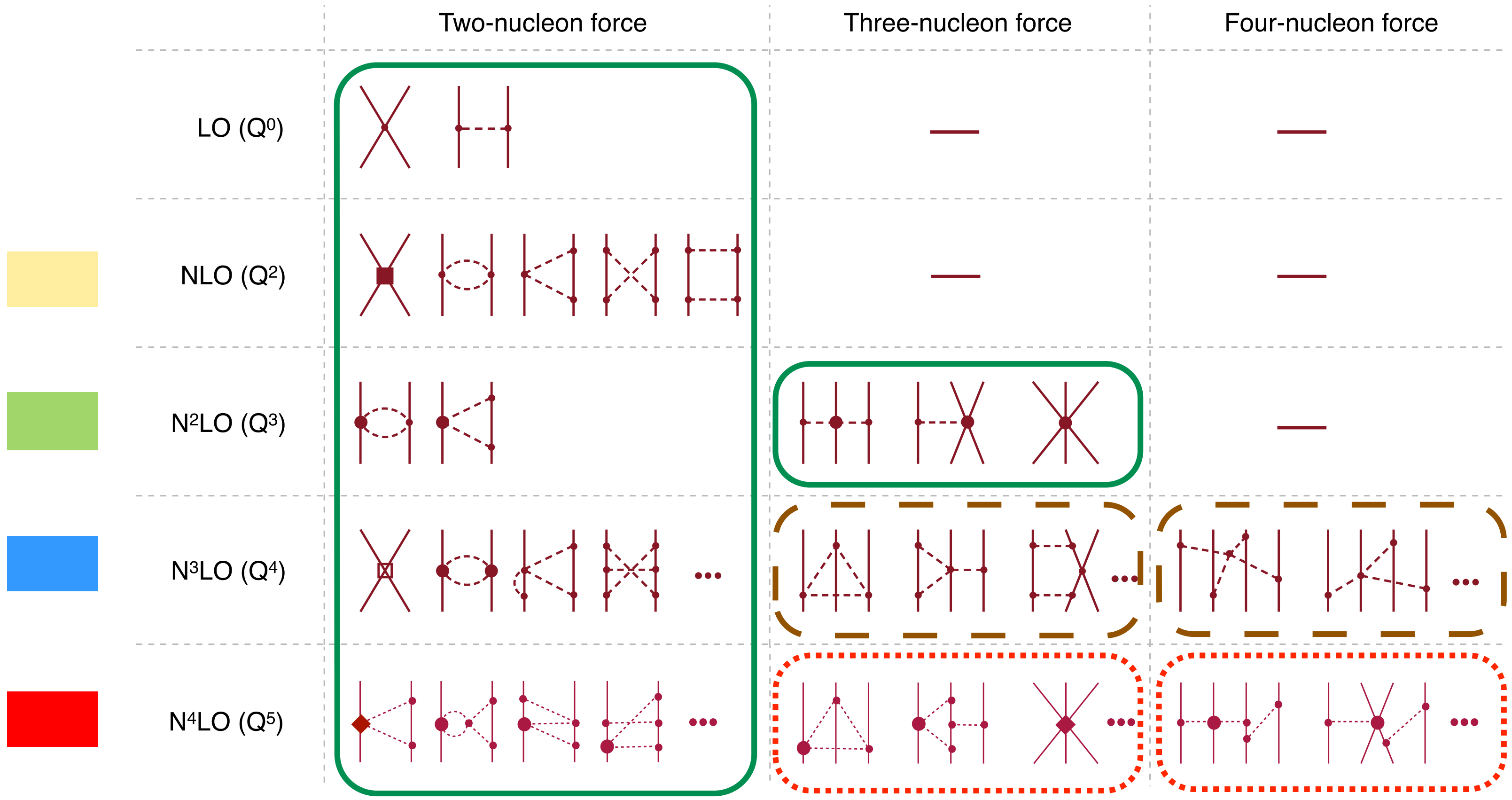
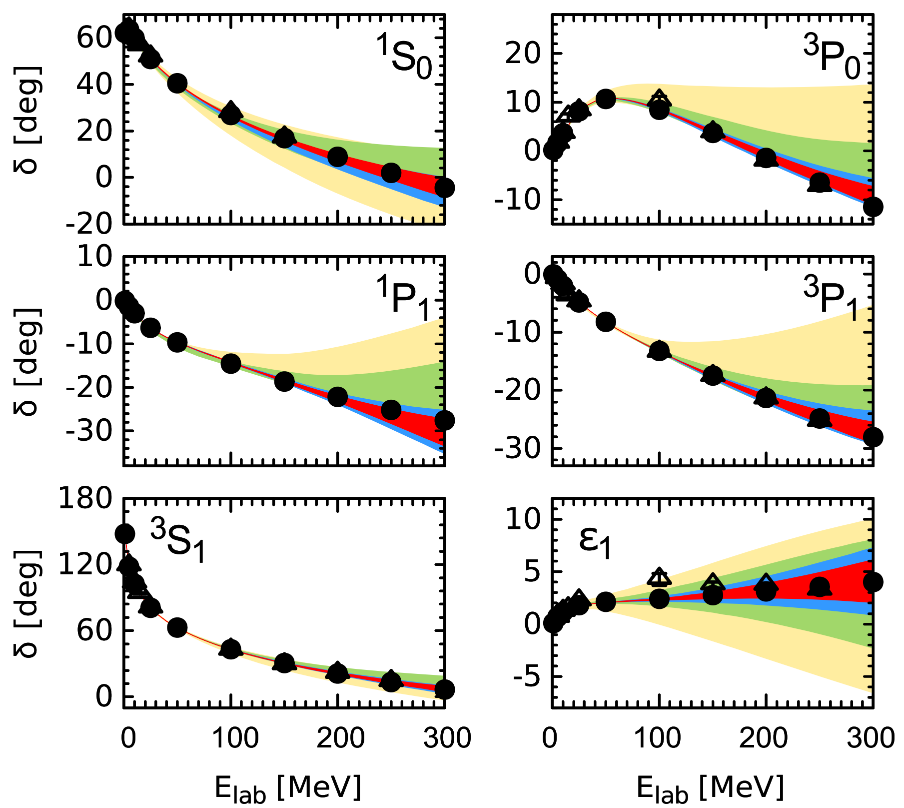
Chiral effective field theory & nuclear interactions

- Chiral EFT provides a **systematic** framework to construct *A*N interactions (*A*=2, 3, …)
- Main features:
  - High-energy physics unresolved → **soft potentials** → improved many-body convergence
  - Many-body forces and currents consistently derived
  - A **theoretical error** can be, in principle, assigned to each order in the expansion





[Meißner 2016]

➪ **Ideally: apply to the many-nucleon system (and propagate the theoretical error)**

Self-consistent Green's function approach

⊙ **Solution of the *A*-body Schrödinger equation** $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ **achieved by**

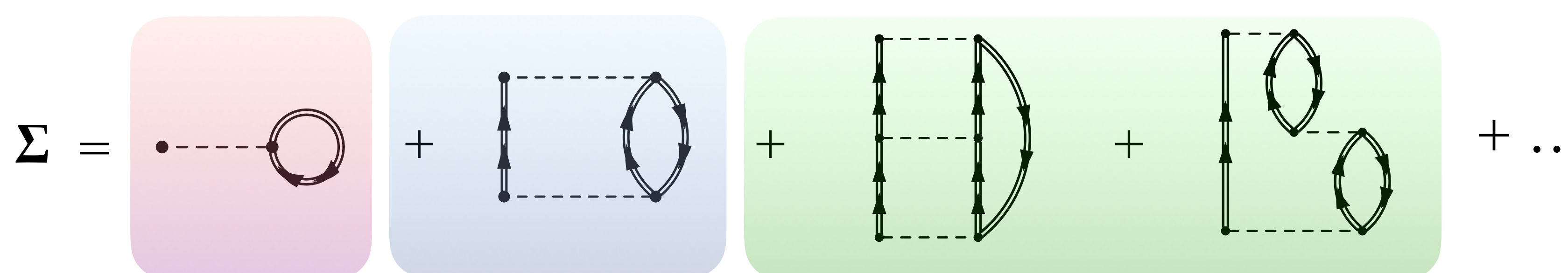
1) Rewriting it in terms of **1-, 2-, …. *A*-body objects** G_1=G, $G_{2, \dots}$ G_A (**Green's functions**)

2) Expanding these objects in perturbation (in practise **G** ➟ **one-body observables**, etc..)

○ **Self-consistent** schemes resum (infinite) subsets of perturbation-theory contributions

⊙ **Self-energy expansion**

Algebraic Diagrammatic Construction



ADC(1)=HF ADC(2) ADC(3) ADC(∞)=exact

⊙ **Access a variety of quantities**

○ One-body GF → Ground-state properties of even-even *A* + spectra of odd-even neighbours

○ Two-body GF → Excited spectrum of even-even *A*

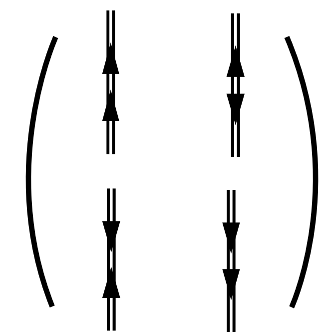
○ Self-energy → Optical potential for nucleon-nucleus scattering

Gorkov-Green's functions for open-shell systems

- Standard expansion schemes fail to account for superfluidity

- **Gorkov scheme generalises GF theory to superfluid systems** [Gorkov 1958]
  - Use **symmetry breaking** (particle number) to effectively include pairing correlations
  - Start expansion from symmetry-breaking reference $|\Psi_0\rangle \equiv \sum_{A}^{\text{even}} c_A \, |\psi_0^A\rangle$
  - 4 one-body Gorkov propagators

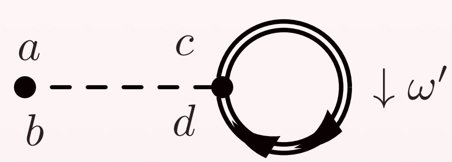
$$\mathbf{G}_{ab} = \begin{pmatrix} G_{ab}^{11} & G_{ab}^{12} \\ G_{ab}^{21} & G_{ab}^{22} \end{pmatrix} =$$



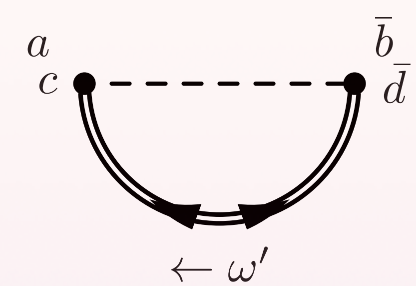
  - Symmetry must be eventually restored

- **Current implementation: ADC(2)** [Somà, Duguet & Barbieri 2011]

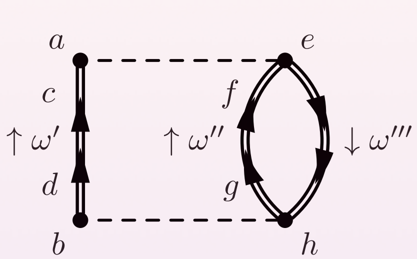
$\Sigma_{ab}^{11\,(1)} =$



$\Sigma_{ab}^{12\,(1)} =$



$\Sigma_{ab}^{11\,(2)}(\omega) =$



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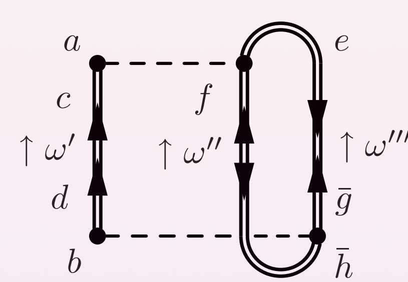
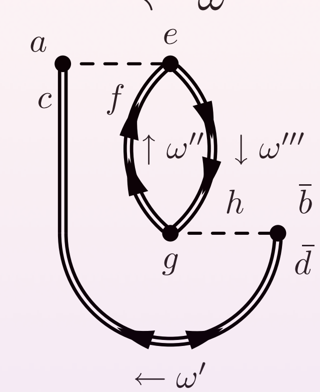


$\Sigma_{ab}^{12\,(2)}(\omega) =$



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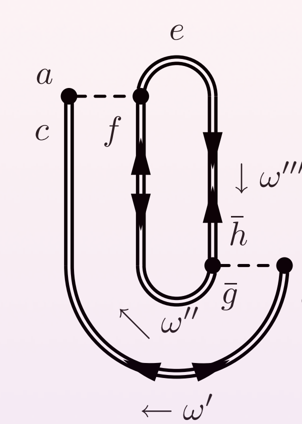
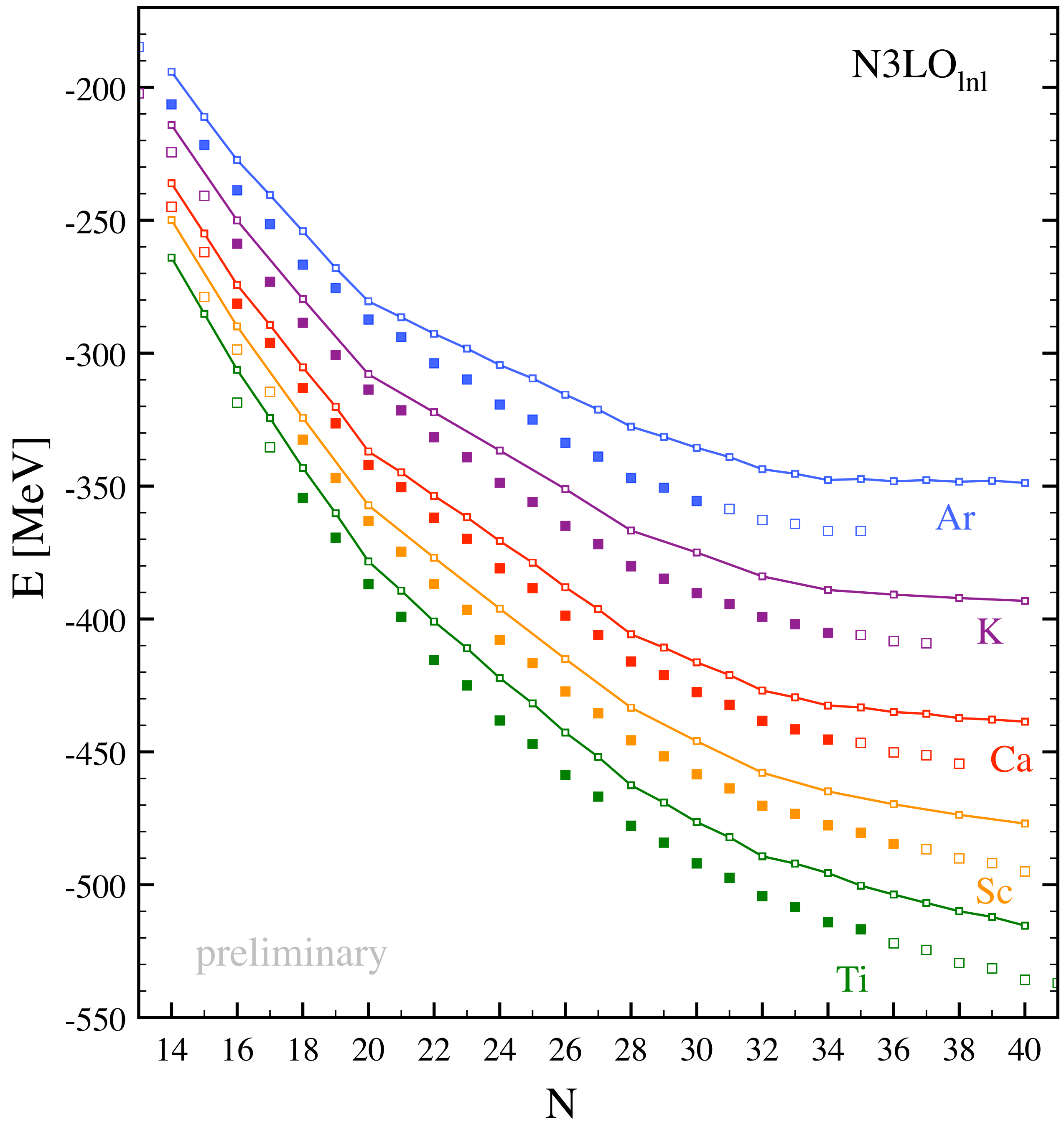


Systematics of medium-mass nuclei

- Calculation of complete mid-mass isotopic chains possible
  - Chiral N3LO 2N (500) + N2LO 3N (400 local / non-local) interaction, further SRG-ed to 2.0 fm^{-1}



- **Total energies**
  - Missing correlation energy from higher-order diagrams
  - Overall trends reasonable

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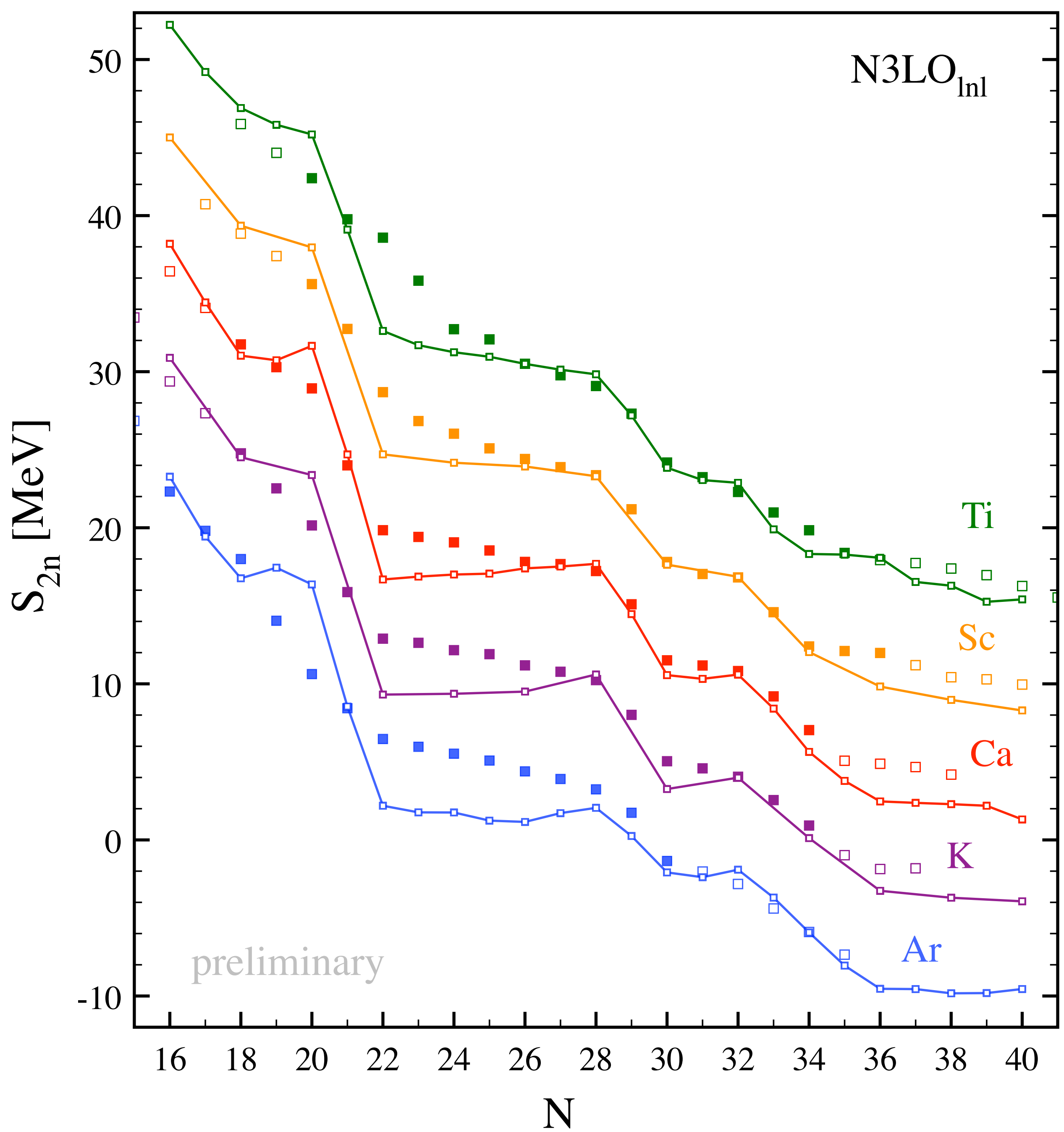
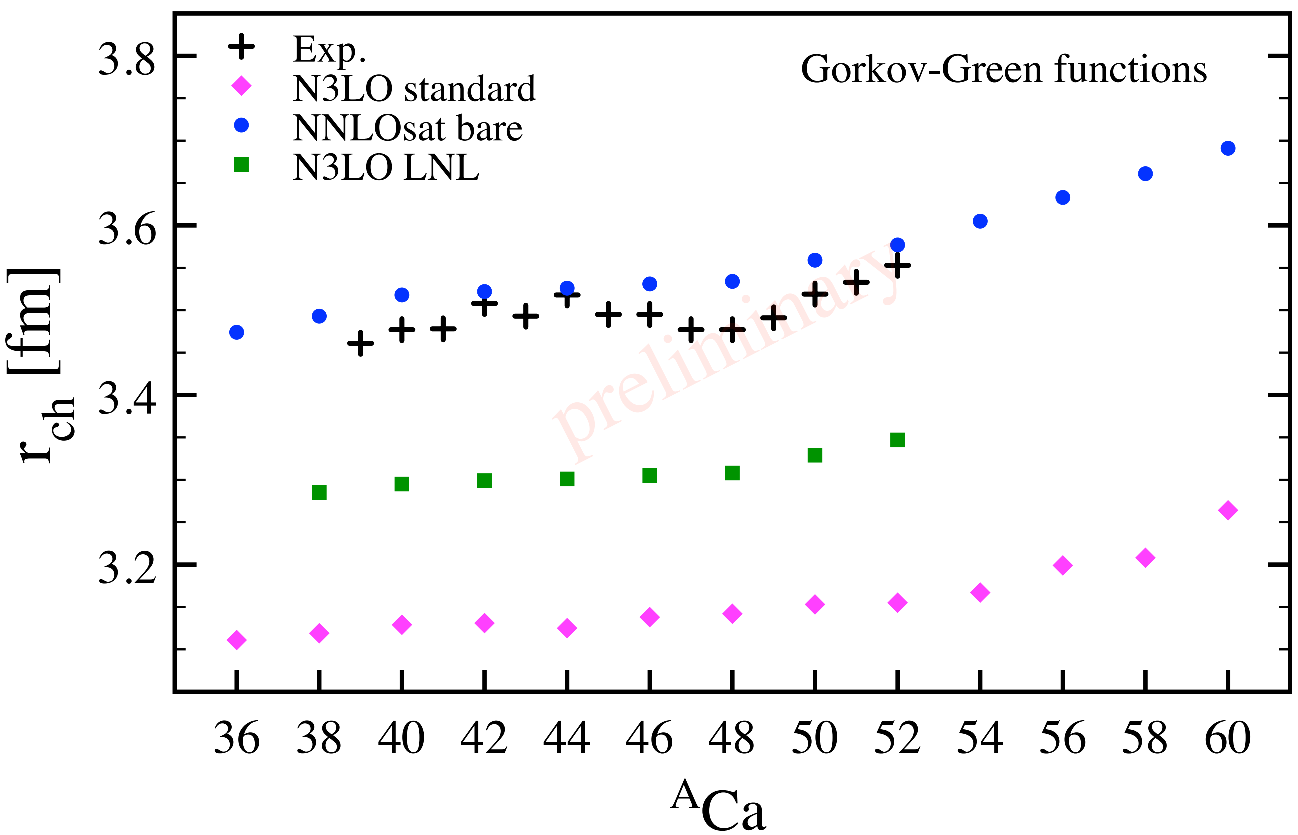
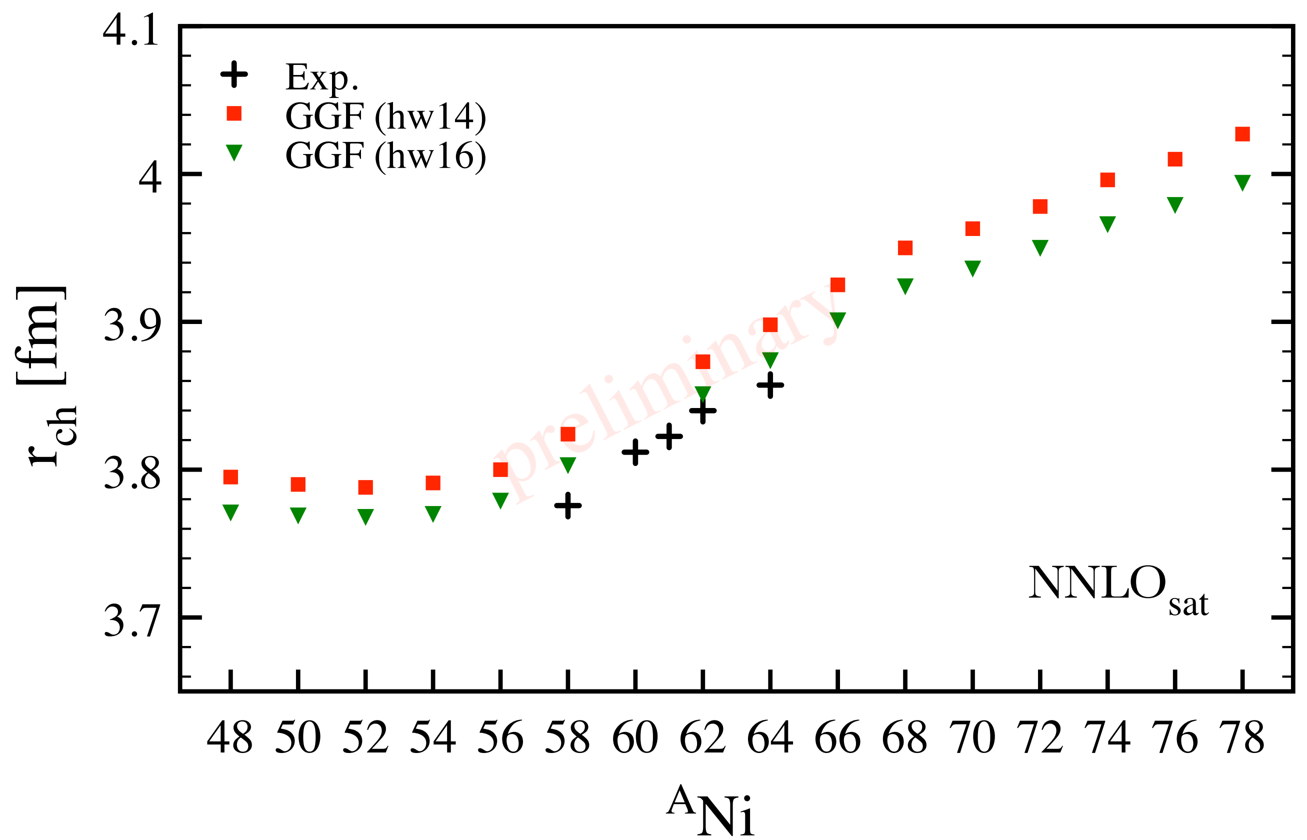


- **Total energies**
  - Missing correlation energy from higher-order diagrams
  - Overall trends reasonable
- **Energy differences (2N separation energies)**
  - *N*=20 gap overestimated
  - *N*=28 gap OK, pf shell well reproduced
  - Drip lines?

Systematics of medium-mass nuclei

⦿ Charge radii along calcium and nickel chains





○ Large sensitivity on the employed nuclear Hamiltonian

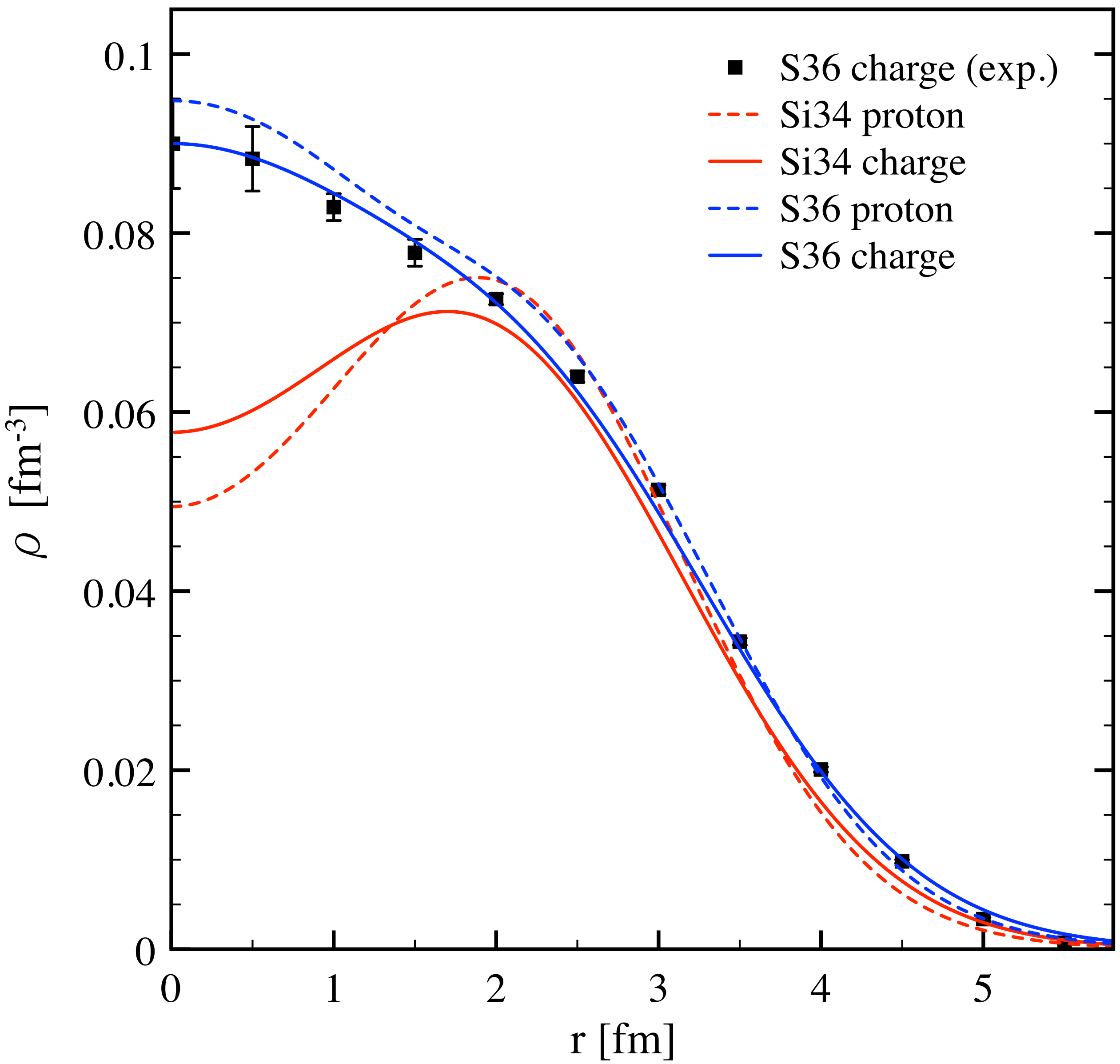
○ Discrepancies between different Hamiltonians depend on the observable

○ Good reproduction of nuclear radii with NNLOsat ↔ saturation properties

Charge density distribution of ^{34}Si

- **Unconventional depletion** ("bubble") in the centre of ρ_{ch} conjectured for ^{34}Si
  - Purely quantum mechanical effect (vacancy of $\ell = 0$ states embedded in larger-ℓ orbitals)
  - Conjectured associated effect on spin-orbit splitting (reduction for low-ℓ spin-orbit partners)

- **Charge density** computed through folding with the finite charge of the proton [Duguet *et al.* 2017]



$$\rho_{\mathrm{ch}}(r) = \sum_{i=1}^{3} \frac{\theta_i}{r_i\sqrt{\pi}} \int_0^{+\infty} dr' \frac{r'}{r} \rho_{\mathrm{p}}(r') \left[\mathrm{e}^{-\left(\frac{r-r'}{r_i}\right)^2} - \mathrm{e}^{-\left(\frac{r+r'}{r_i}\right)^2} \right]$$

➟ Folding smears out central depletion

➟ Good agreement with experiment for ^{36}S

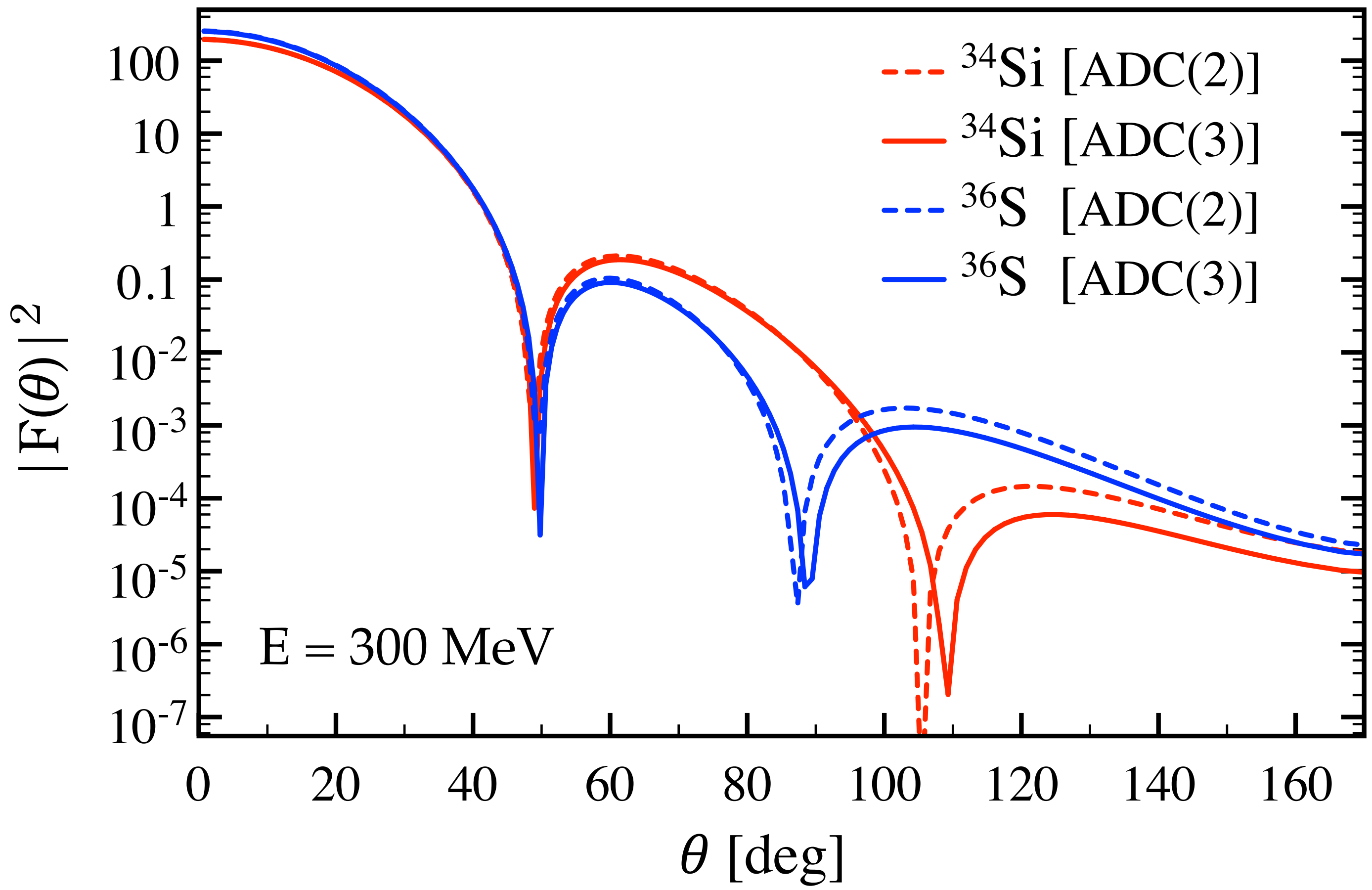
[Rychel *et al.* 1983]

➟ Central depletion predicted for ^{34}Si

Charge form factor of ^{34}Si

⦿ Charge form factor measured in (e,e) experiments sensitive to bubble structure?

$$F(q) = \int d\vec{r} \rho_{\rm ch}(r) e^{-i\vec{q}\cdot\vec{r}} \quad \text{and} \quad q = 2p \sin\theta/2$$



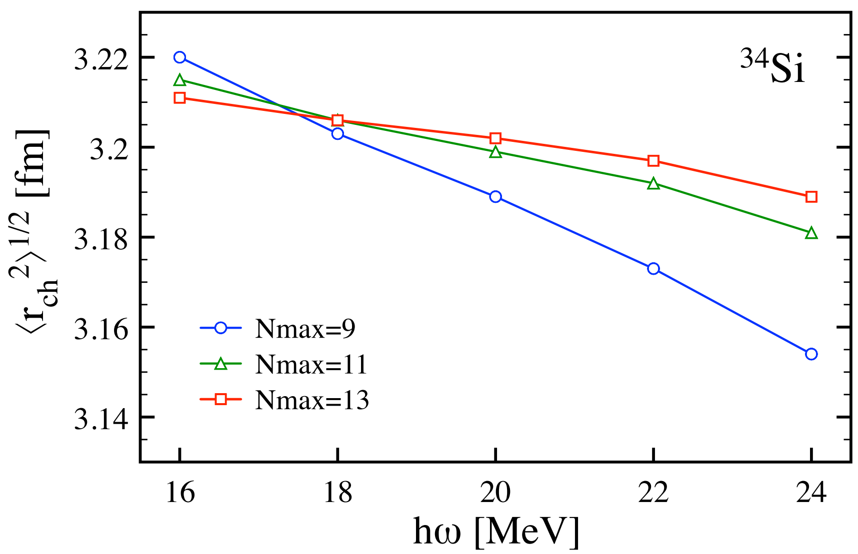
○ Central depletion reflects in larger F(θ) for angles θ>70° and shifted 2nd minimum

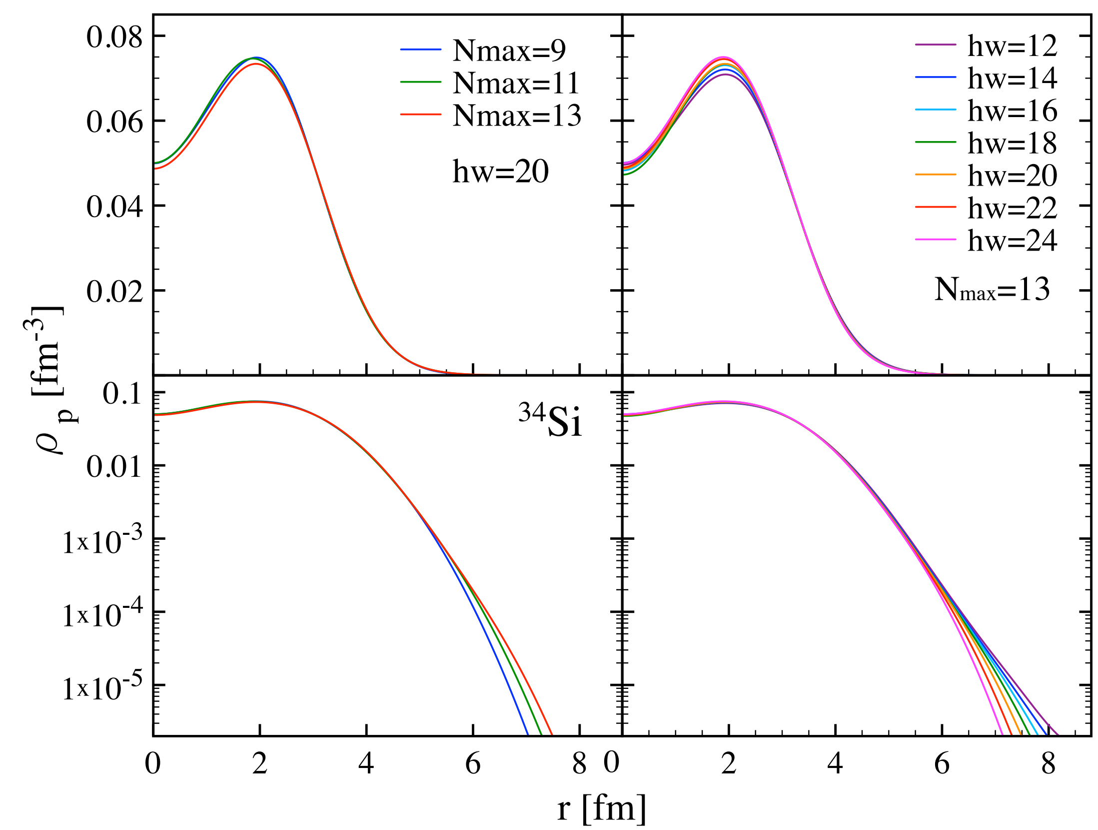
○ **Future electron scattering experiments might be able to see its fingerprints**

On convergence

- Calculations performed within different many-body truncations
  - ADC(1) = HF, ADC(2) & ADC(3)

- **Model space convergence**





- **Many-body convergence**

Binding energies

E [MeV]	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	-84.481	-274.626	-282.938	-283.427
^{36}S	-90.007	-296.060	-305.767	-308.714

ADC(3) brings only ~5% additional binding

Charge radii

$\langle r_{ch}^2 \rangle^{1/2}$	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	3.270	3.189	3.187	-
^{36}S	3.395	3.291	3.285	3.2985 ± 0.0024

Radii converged already at ADC(2) level

Spectral representation

Spectroscopic probabilities matrices

$$S_{\mu}^{+ab} \equiv \langle\Psi_0^{\text{A}}|a_a|\Psi_\mu^{\text{A+1}}\rangle\langle\Psi_\mu^{\text{A+1}}|a_b^\dagger|\Psi_0^{\text{A}}\rangle$$

$$S_{\nu}^{-ab} \equiv \langle\Psi_0^{\text{A}}|a_a^\dagger|\Psi_\nu^{\text{A-1}}\rangle\langle\Psi_\nu^{\text{A-1}}|a_b|\Psi_0^{\text{A}}\rangle$$

Spectroscopic factors

$$SF_\mu^+ \equiv \text{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\mu^+\right] = \sum_{a\in\mathcal{H}_1} |U_\mu^a|^2$$

$$SF_\nu^- \equiv \text{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\nu^-\right] = \sum_{a\in\mathcal{H}_1} |V_\nu^a|^2$$

$$G_{ab}(z) = \sum_\mu \frac{\langle\Psi_0^A|a_a\,|\,\Psi_\mu^{A+1}\rangle\langle\Psi_\mu^{A+1}\,|\,a_b^\dagger|\Psi_0^A\rangle}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{\langle\Psi_0^A|a_b^\dagger\,|\,\Psi_\nu^{A-1}\rangle\langle\Psi_\nu^{A-1}\,|\,a_a|\Psi_0^A\rangle}{z - E_\nu^- - i\eta}$$

Eigenstates of A+1

Eigenstates of A-1

One-nucleon addition separation energies

$$E_\mu^+ \equiv E_\mu^{A+1} - E_0^A$$

One-nucleon removal separation energies

$$E_\nu^- \equiv E_0^A - E_\nu^{A-1}$$

Combining numerator and denominator result in the spectral function

Spectral function

$$\mathbf{S}(z) \equiv \sum_{\mu\in\mathcal{H}_{A+1}} \mathbf{S}_\mu^+\ \delta(z - E_\mu^+) + \sum_{\nu\in\mathcal{H}_{A-1}} \mathbf{S}_\nu^-\ \delta(z - E_\nu^-)$$

Spectral strength distribution

$$\mathcal{S}(z) \equiv \text{Tr}_{\mathcal{H}_1}[\mathbf{S}(z)]$$

$$= \sum_{\mu\in\mathcal{H}_{A+1}} SF_\mu^+\,\delta(z - E_\mu^+) + \sum_{\nu\in\mathcal{H}_{A-1}} SF_\nu^-\,\delta(z - E_\nu^-)$$

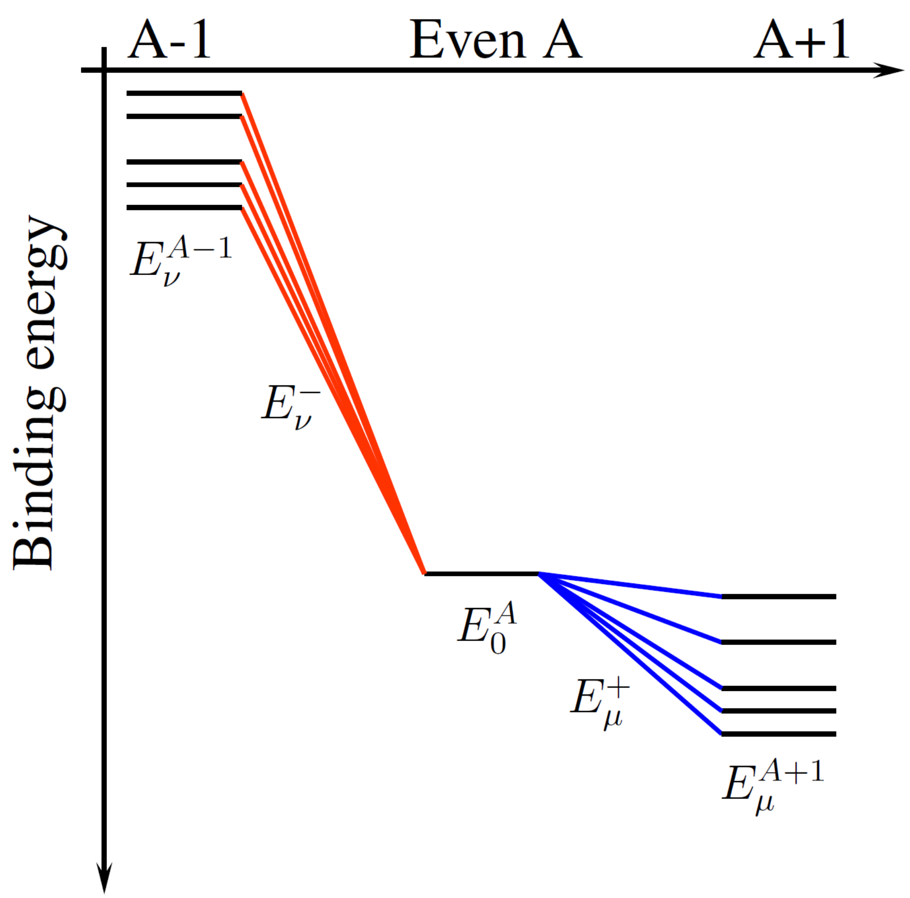
Spectral representation

$$G_{ab}(z) = \sum_\mu \frac{U_a^\mu (U_b^\mu)^*}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{(V_a^\nu)^* V_b^\nu}{z - E_\nu^- - i\eta}$$

Separation energies

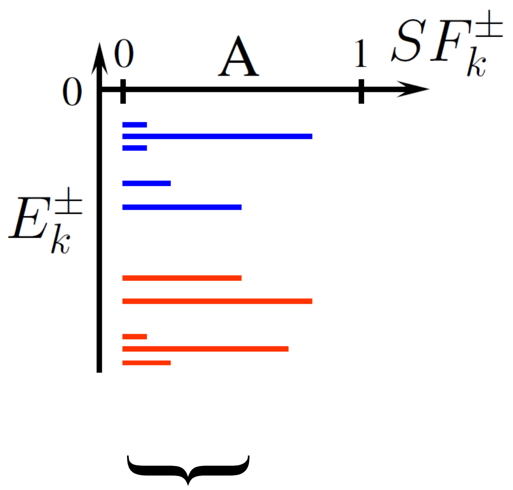
$$E_\mu^+ \equiv E_\mu^{A+1} - E_0^A$$

$$E_\nu^- \equiv E_0^A - E_\nu^{A-1}$$



Spectral strength distribution

$$\mathcal{S}(z) = \sum_{\mu \in \mathcal{H}_{A+1}} SF_\mu^+ \, \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_\nu^- \, \delta(z - E_\nu^-)$$



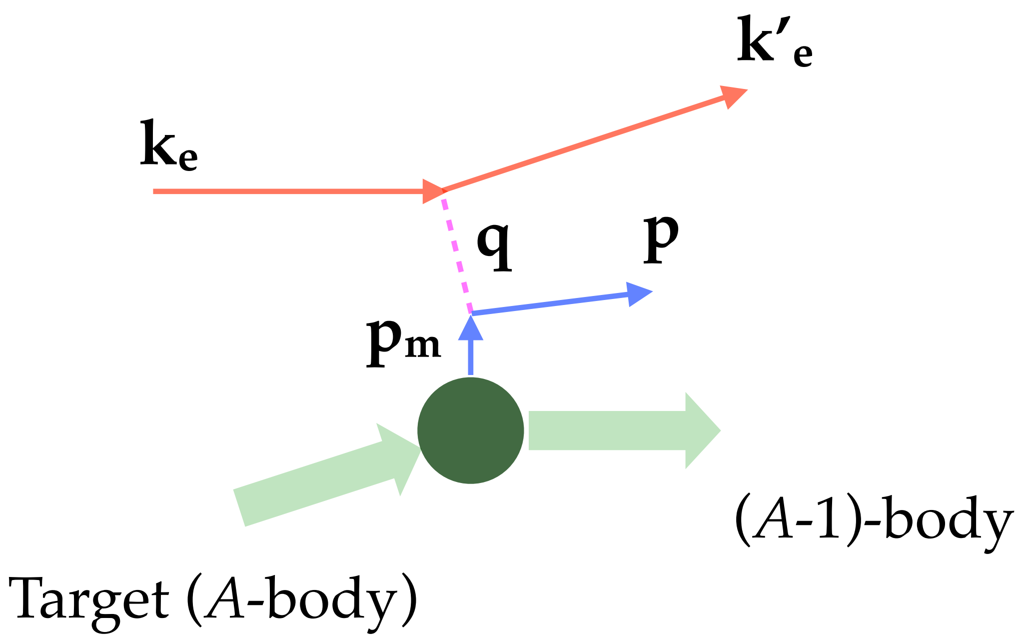
Spectroscopic factors

$$SF_\mu^+ \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\mu^+\right] = \sum_{a \in \mathcal{H}_1} \left|U_\mu^a\right|^2$$

$$SF_\nu^- \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\nu^-\right] = \sum_{a \in \mathcal{H}_1} \left|V_\nu^a\right|^2$$

Spectral strength in experiments

⊙ Clean connection to (*e*,*e′p*) experiments



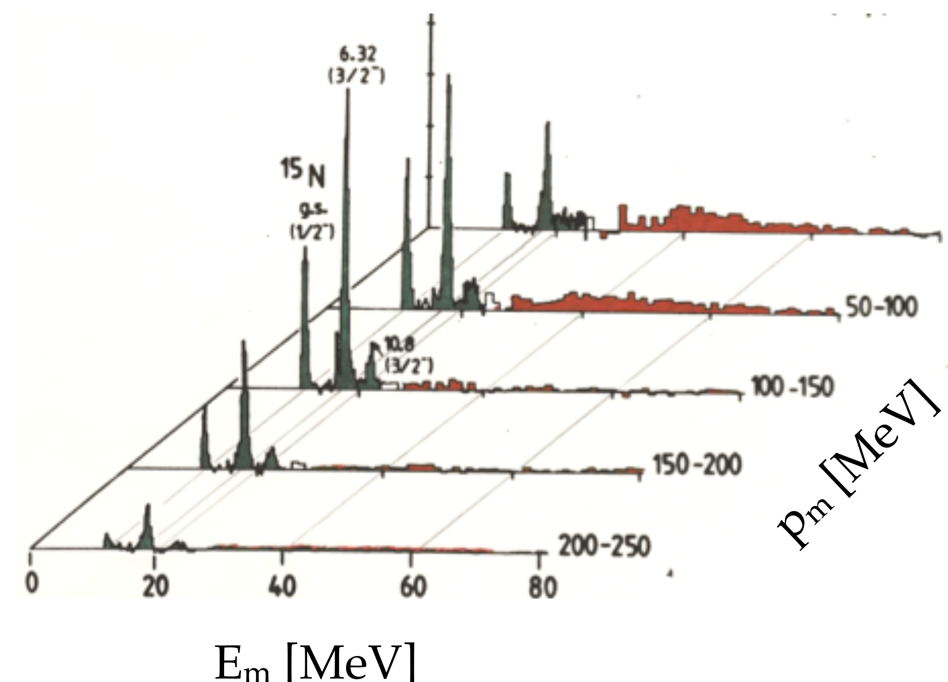
○ Measuring **q** and **p** gives information on $\mathbf{p_m}$

○ Similarly for missing energy E_m

○ Spectral strength distribution ↔ $P(p_m, E_m)$

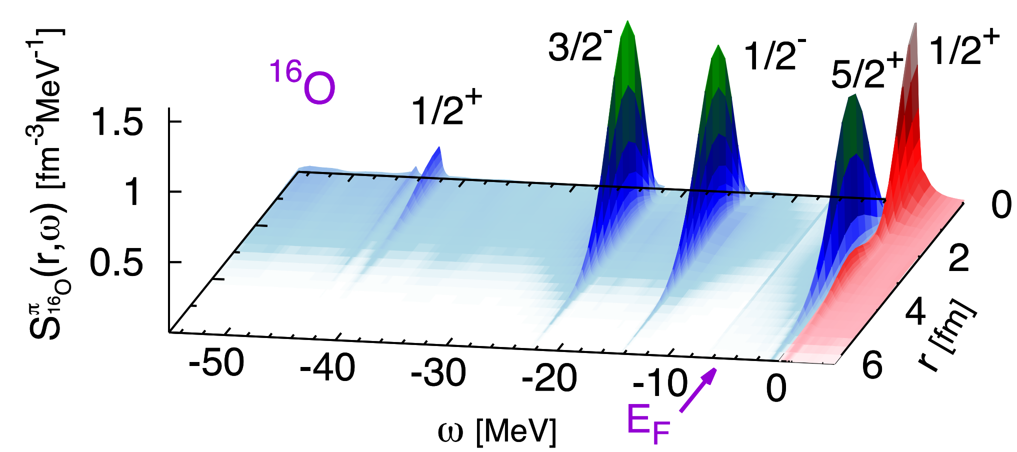
⊙ Spectroscopy via knockout / transfer exp.

Results from (e,e′p) on ^{16}***O (ALS in Saclay)***



[Mougey *et al.* 1980]

SCGF calculations

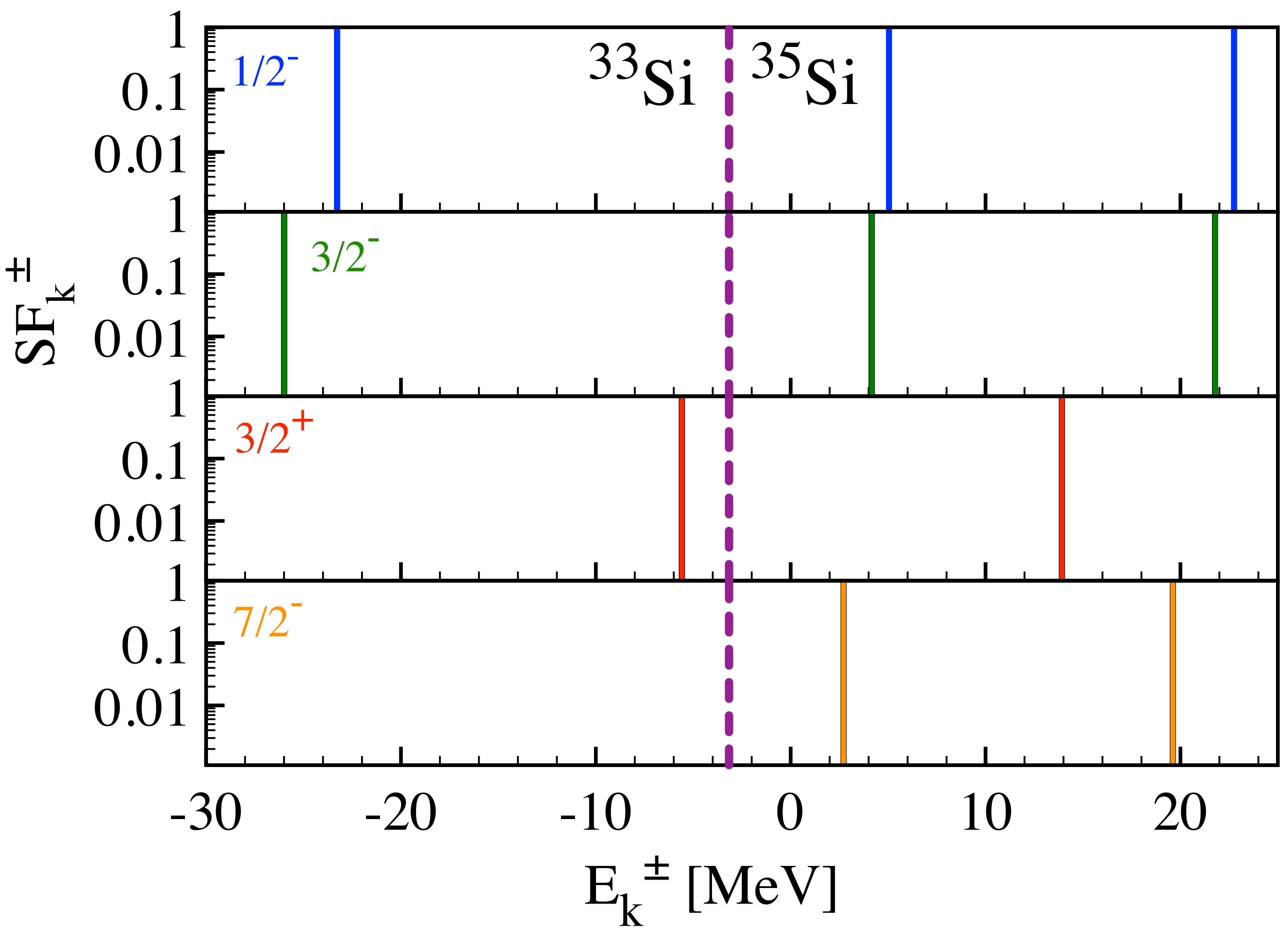


[Cipollone *et al.* 2015]

Spectral strength distribution

- ^{34}Si neutron addition & removal strength

ADC(1)

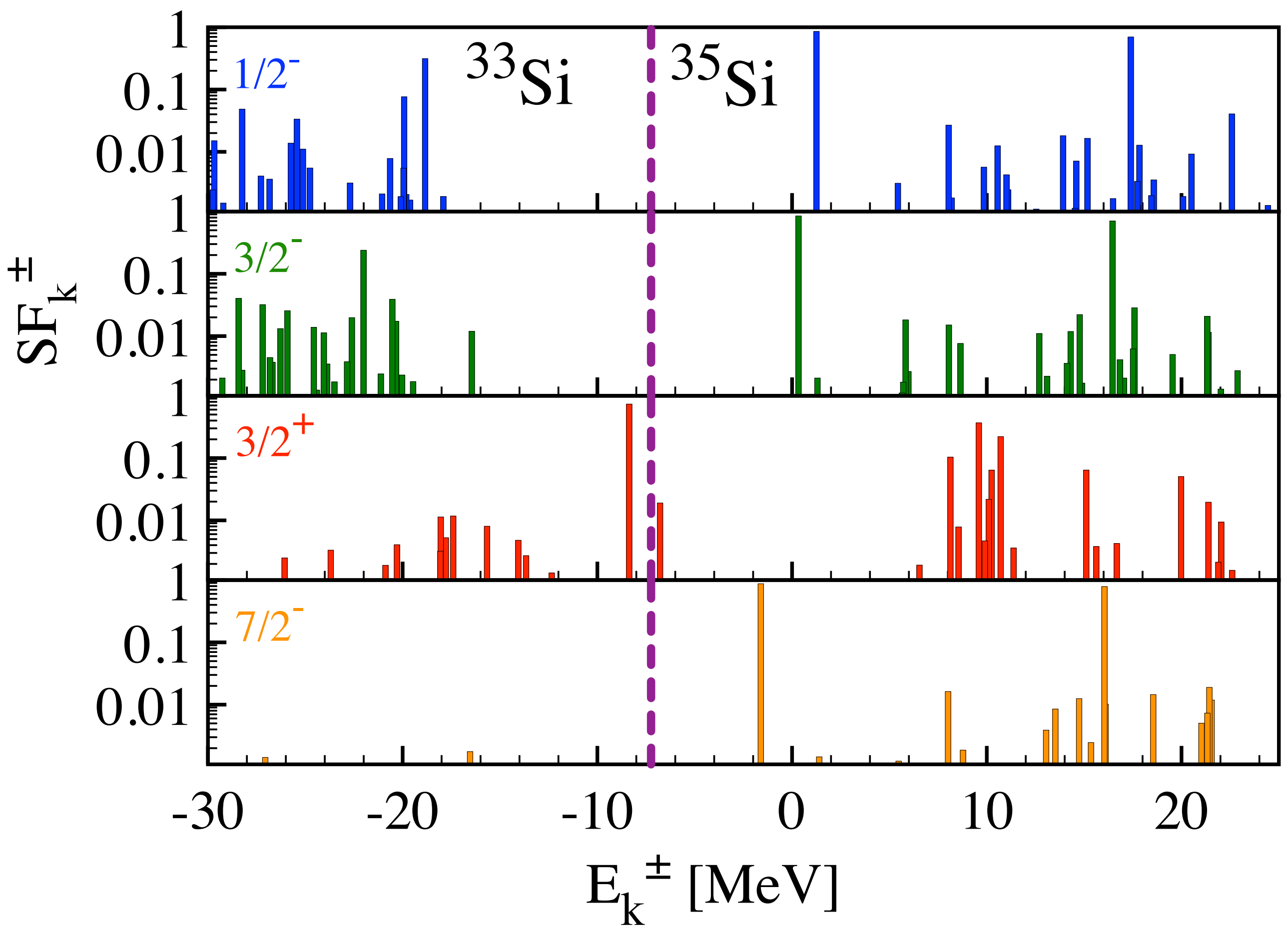


- Independent-particle picture

Spectral strength distribution

- ^{34}Si neutron addition & removal strength

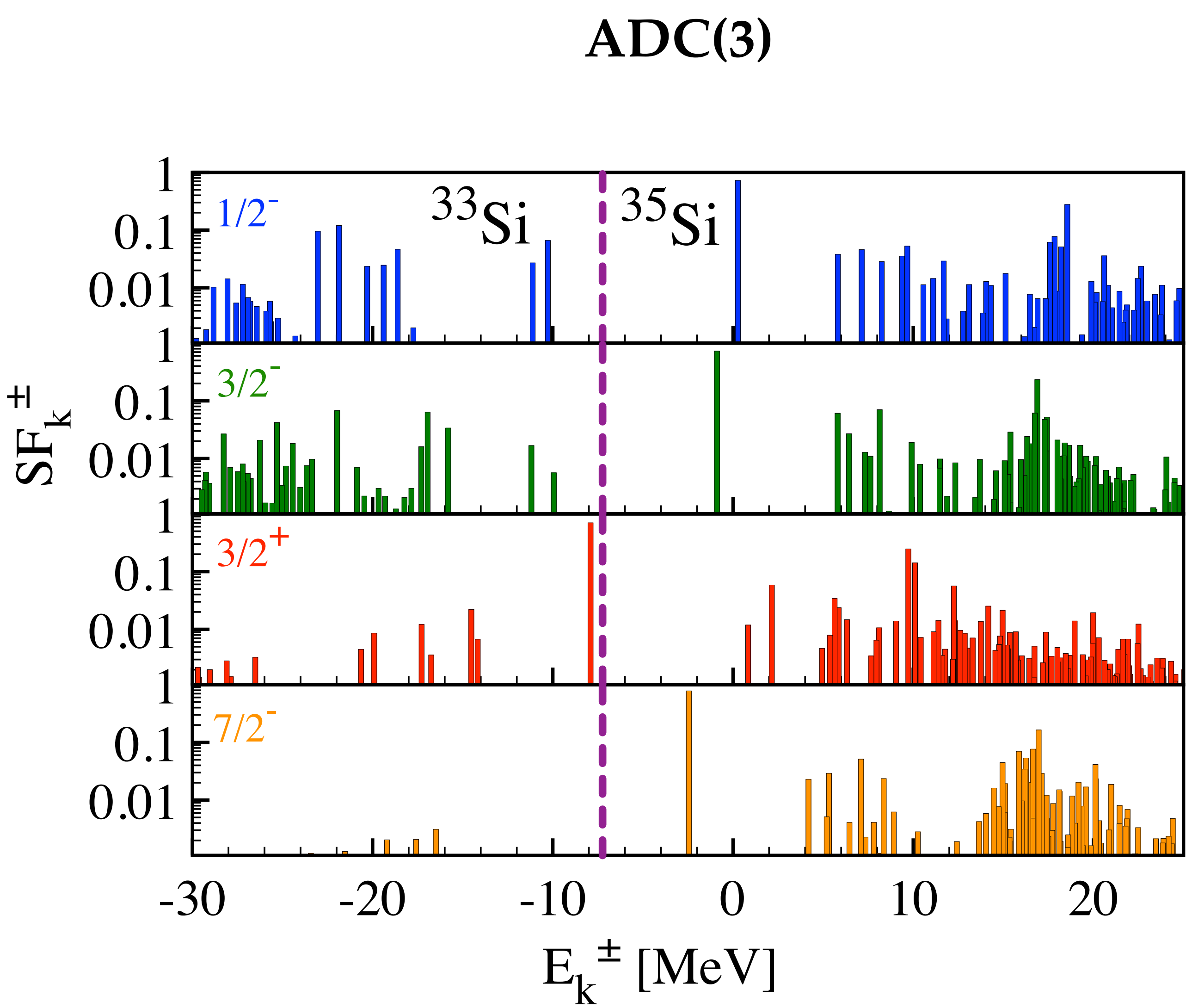
ADC(2)



- Second-order dynamical correlations fragment IP peaks

Spectral strength distribution

- ^{34}Si neutron addition & removal strength

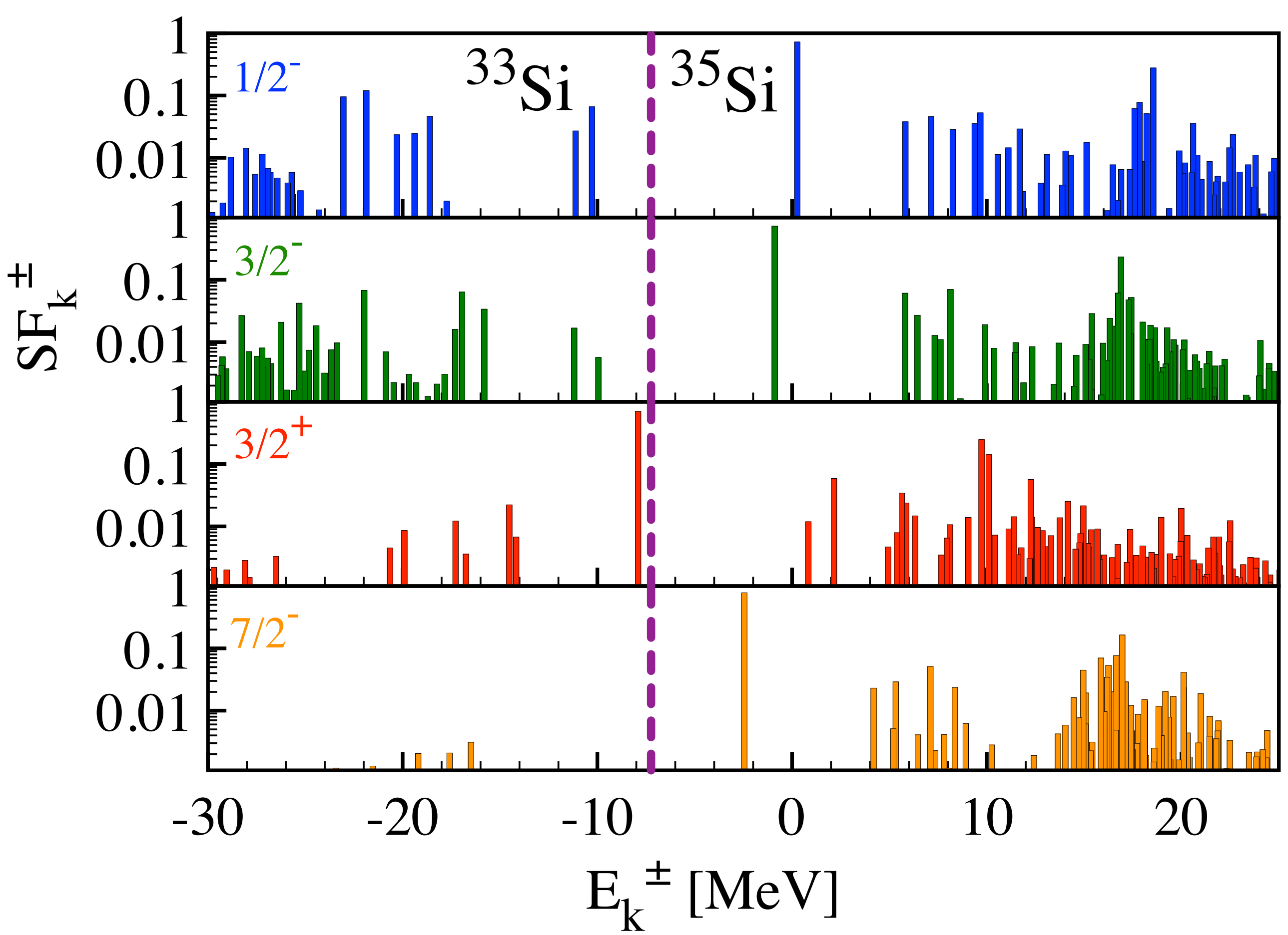


- Third-order compresses the spectrum (main peaks)
- Further fragmentation is generated

Spectral strength distribution

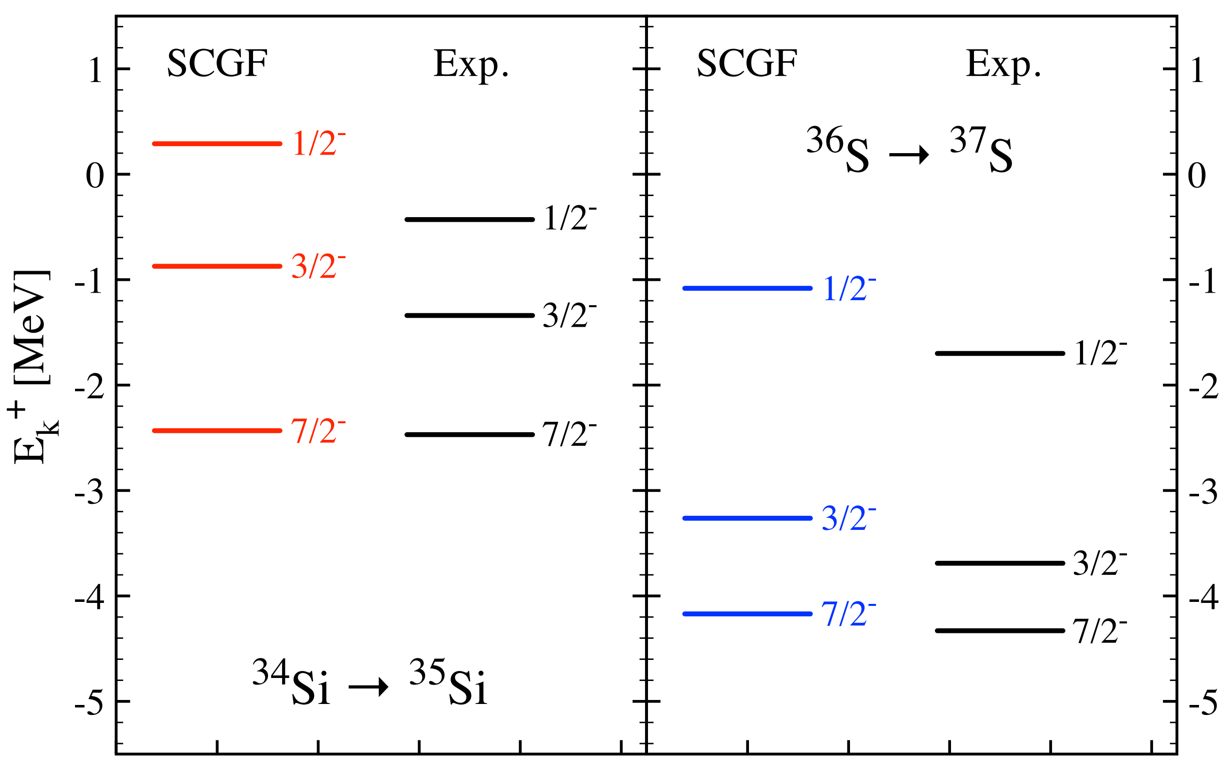
⦿ ^{34}Si neutron addition & removal strength

ADC(3)



One-neutron addition

Exp. data: [Thorn *et al.* 1984] [Eckle *et al.* 1989] [Burgunder *et al.* 2014]



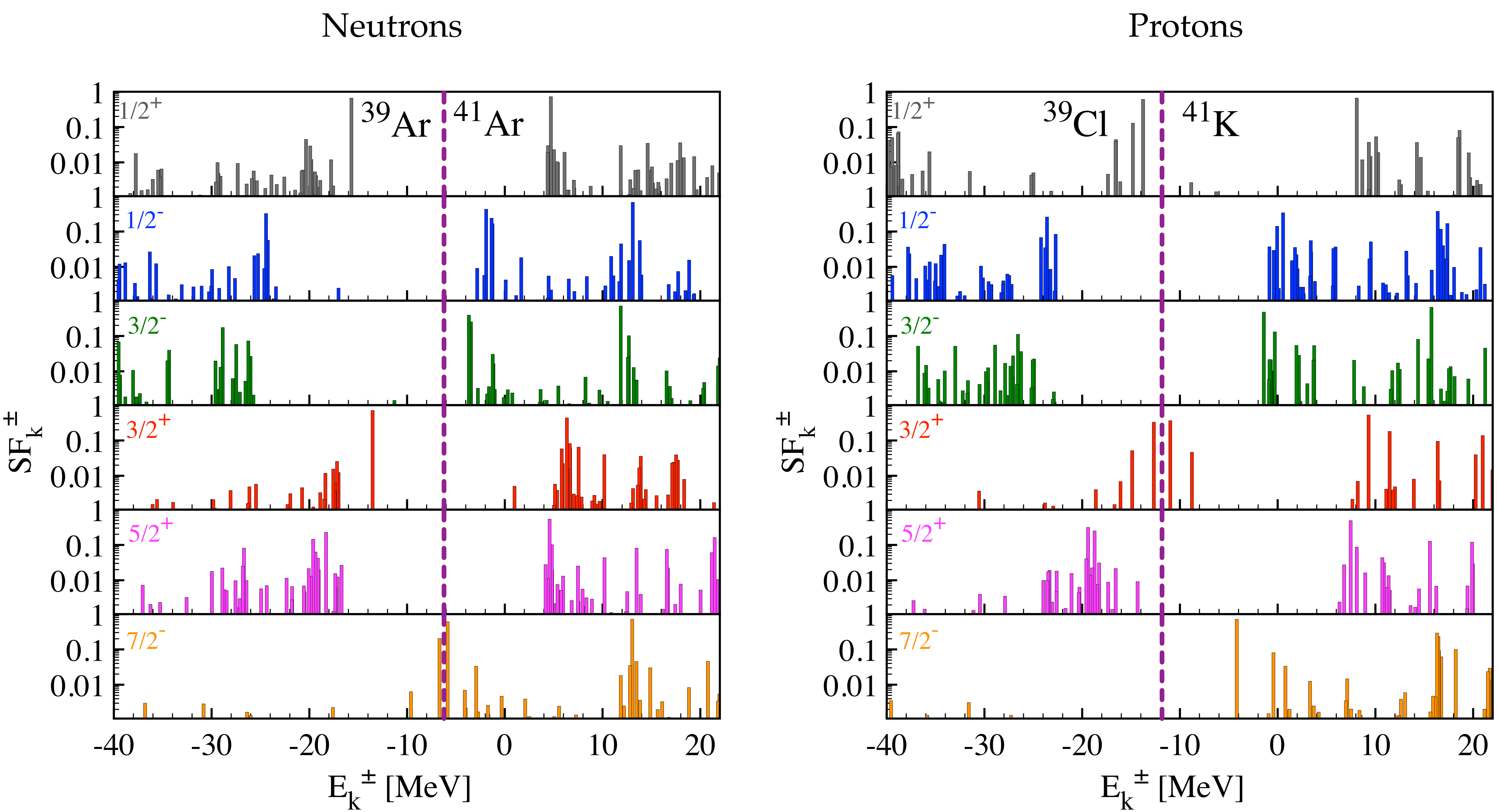
○ Third-order correlations compress the spectrum

○ Further fragmentation is generated

Reduction of $E_{1/2^-}$ - $E_{3/2^-}$ spin-orbit splitting (unique in the nuclear chart) well reproduced

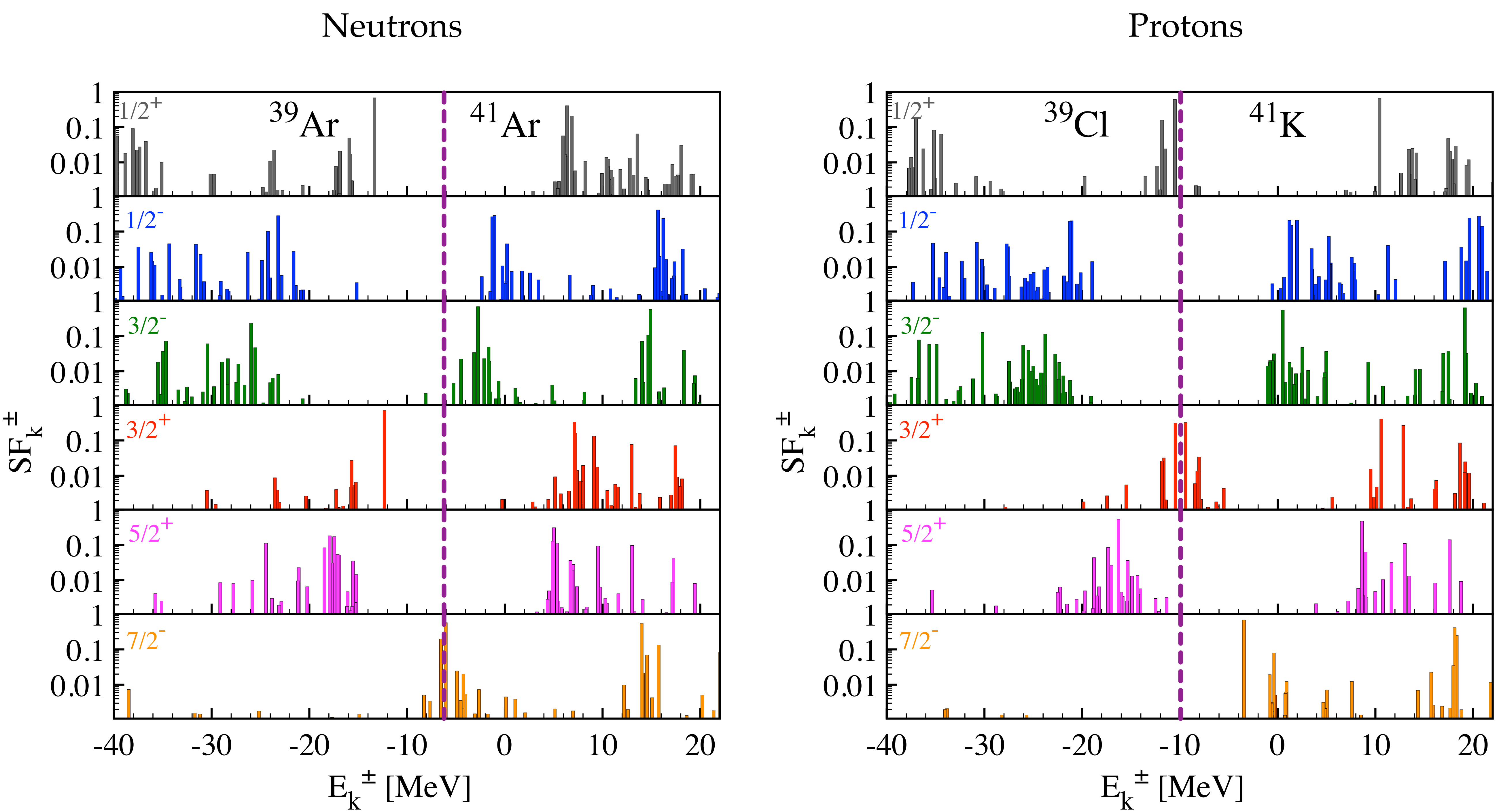
Spectral function of ^{40}Ar

⊙ ADC(2) truncation, N3LO local-nonlocal interaction



Spectral function of ^{40}Ar

- ADC(2) truncation, $NNLO_{sat}$ interaction



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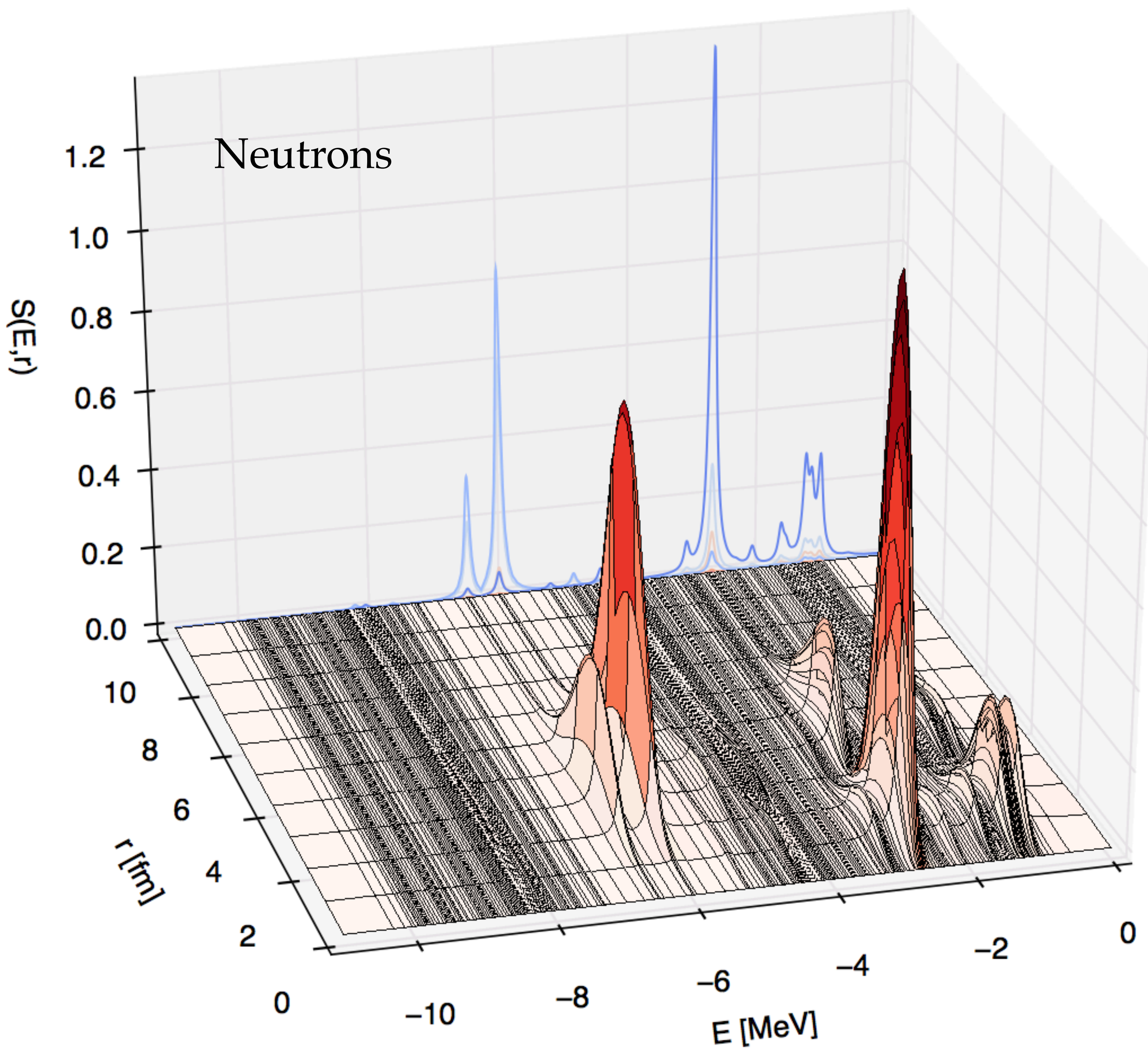
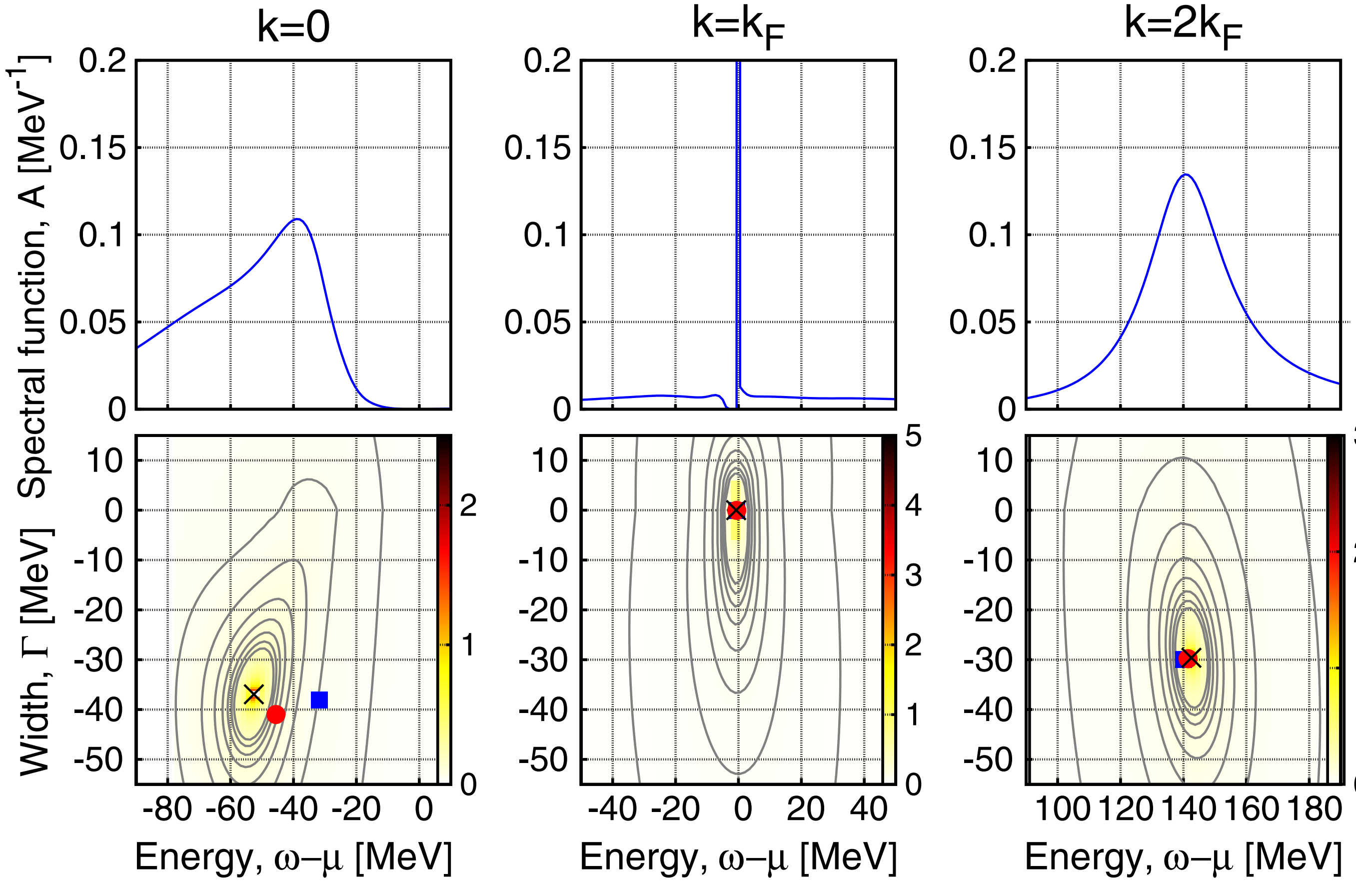
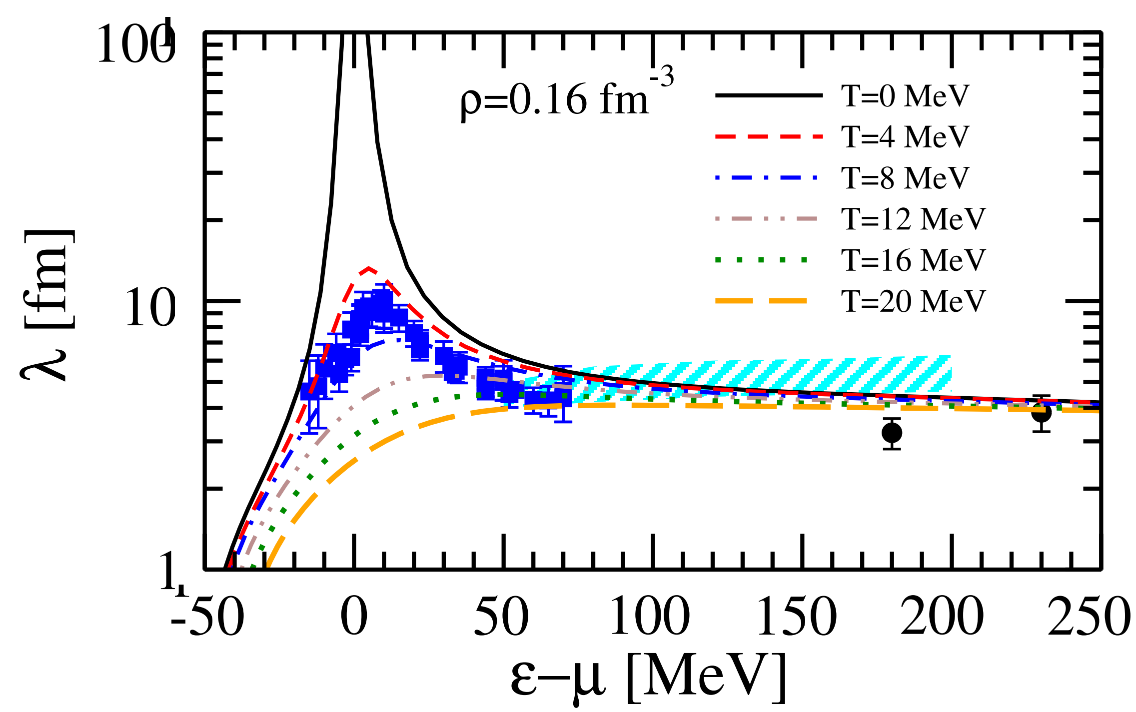


Fragmentation of single-particle strength in infinite matter

- **Spectral function depicts correlations**
  - Broad peak signals depart from mean-field/independent particle picture
  - Well-defined (long-lived) quasiparticles at the Fermi surface
  - Long mean free path for E < E_F





[Rios, Somà 2012]

Electromagnetic response

- Nuclear response produced by an isovector dipole operator

$$R(E) = \sum_{\nu} |\langle \Psi_\nu^A | \hat{D} \,|\, \Psi_0^A \rangle|^2 \, \delta(E_\nu - E)$$

$$\sum_{ab} \langle a | \hat{D} \,|\, b \rangle \, \langle \Psi_\nu^A | c_a^\dagger c_b \,|\, \Psi_0^A \rangle$$

Electric dipole excitation operator

Polarisation propagator computed in RPA

- Total photoabsorption cross section

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

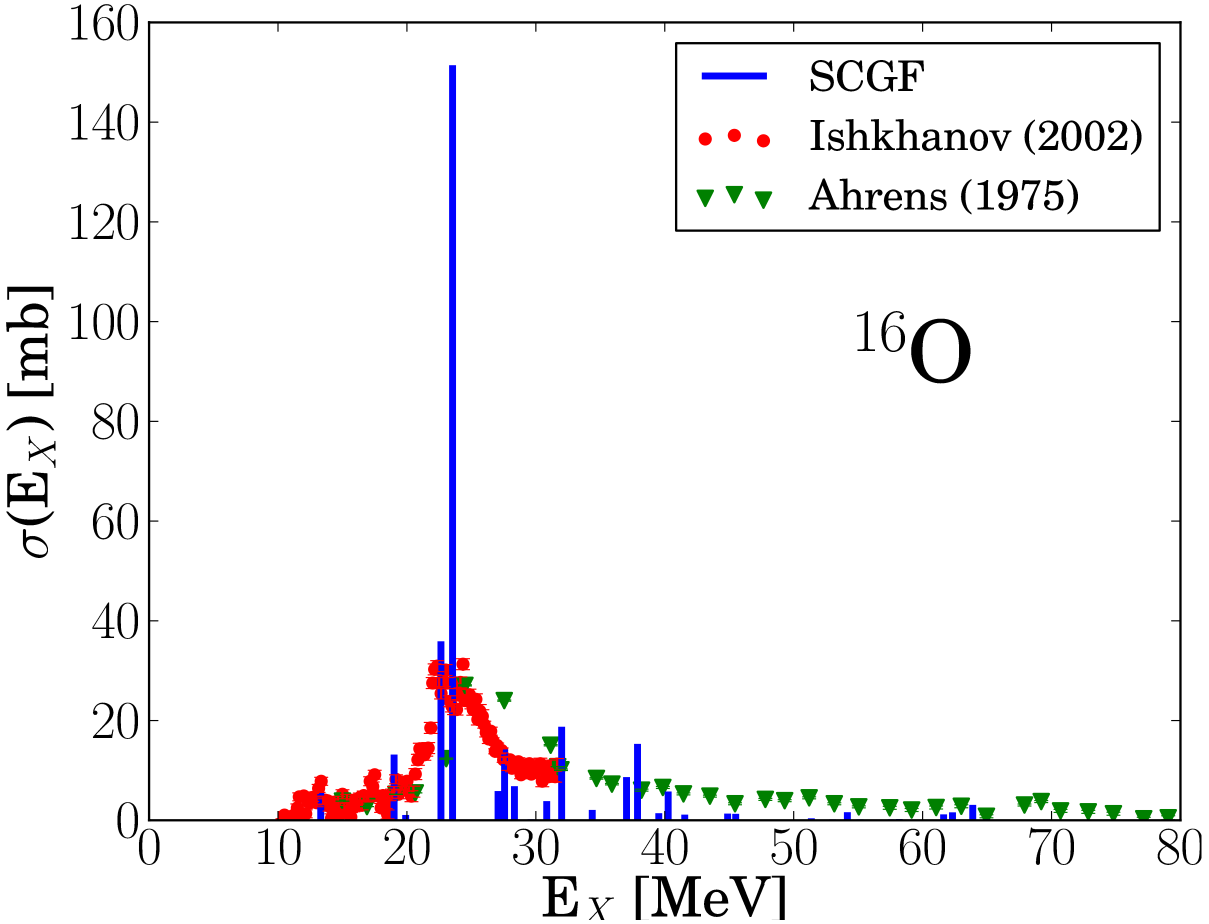
- Dipole polarisability

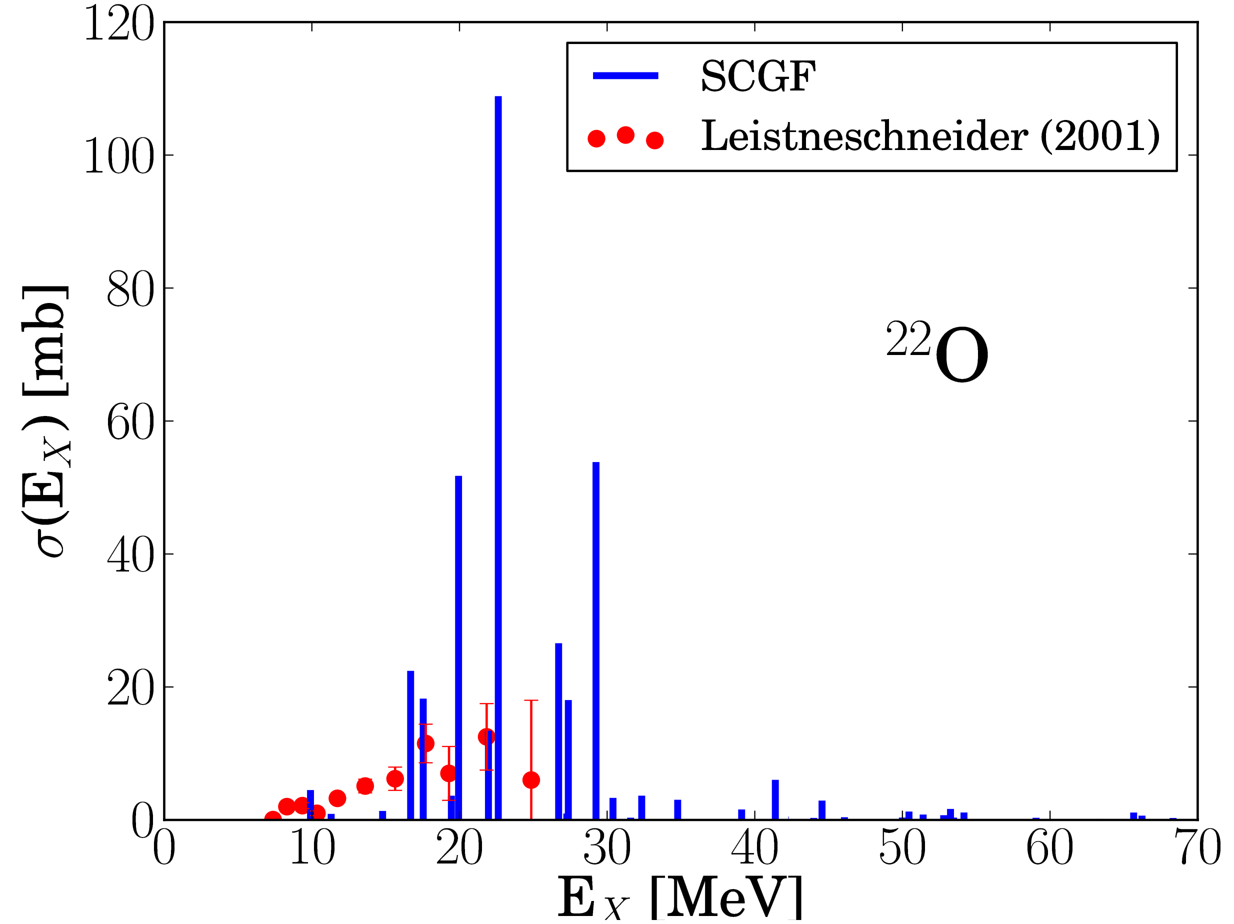
$$\alpha_D = 2\alpha \int dE \, \frac{R(E)}{E}$$

Electromagnetic response

⦿ Computed σ from RPA response vs. σ from photoabsorption and Coulomb excitation

[Raimondi *et al.* in preparation]





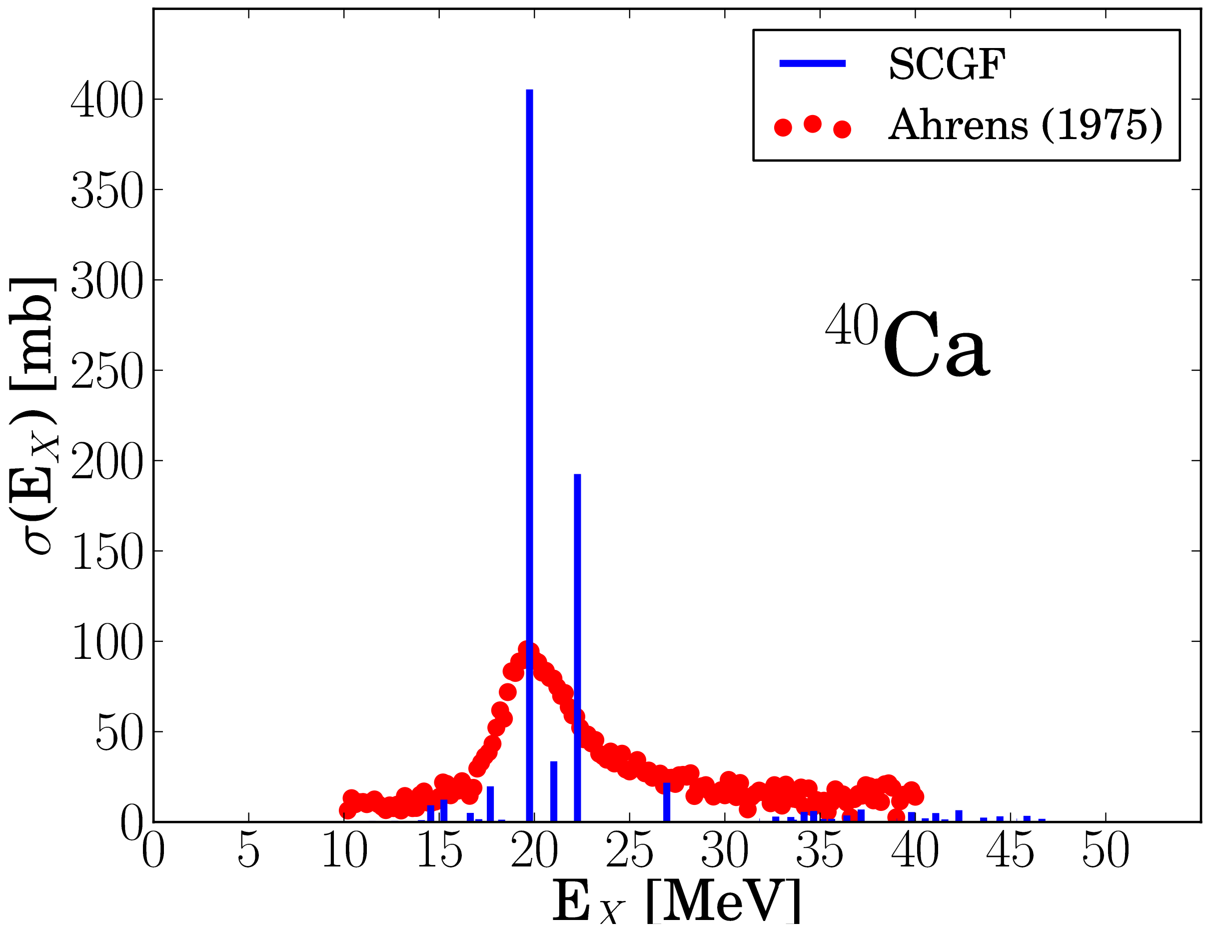
- ○ GDR position of ^{16}O well reproduced
- ○ Hint of a soft dipole mode in ^{22}O
- ○ Comparison with CC LIT results for α_D

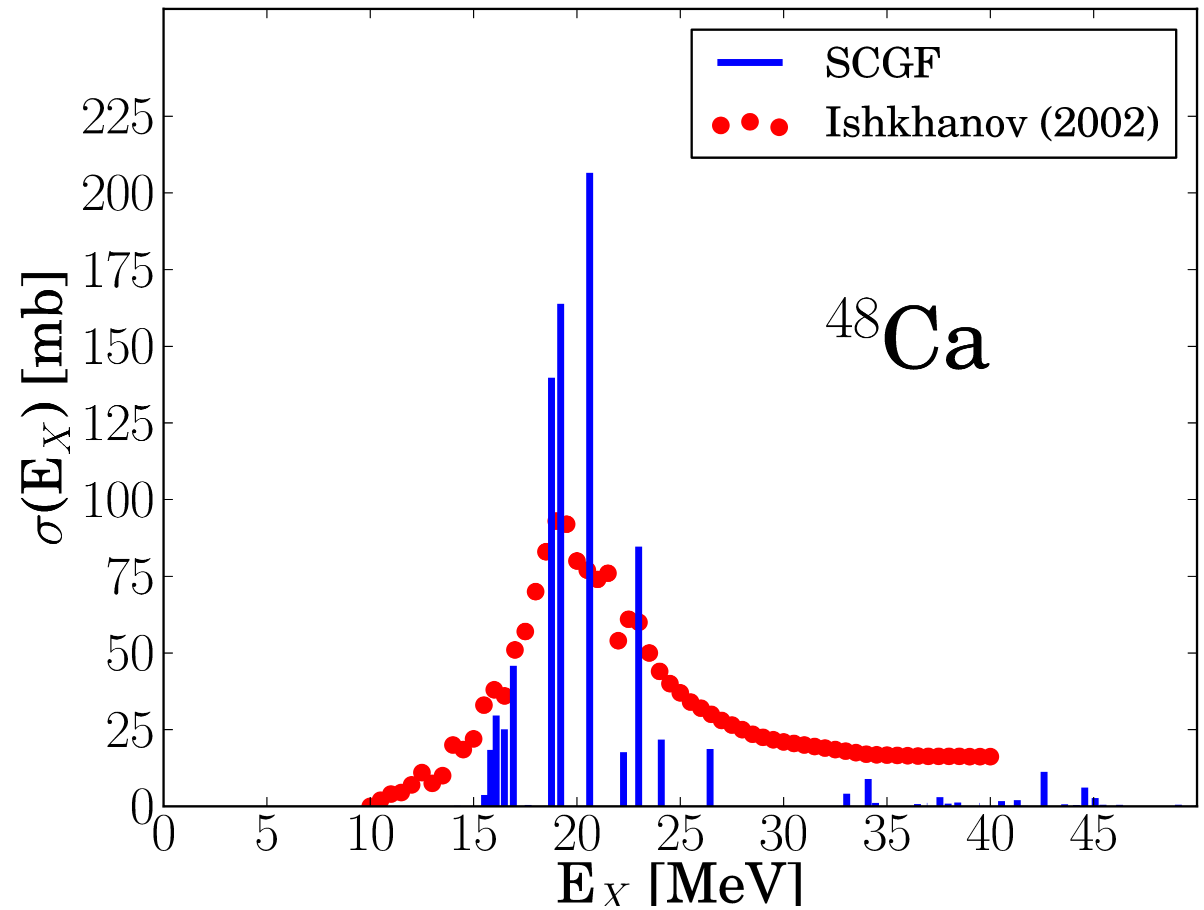
Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{16}O	0.50	0.57(1)	0.585(9)
^{22}O	0.72	0.86(4)	0.43(4)

Electromagnetic response

- Computed σ from RPA response vs. σ from photoabsorption and Coulomb excitation

[Raimondi *et al.* in preparation]





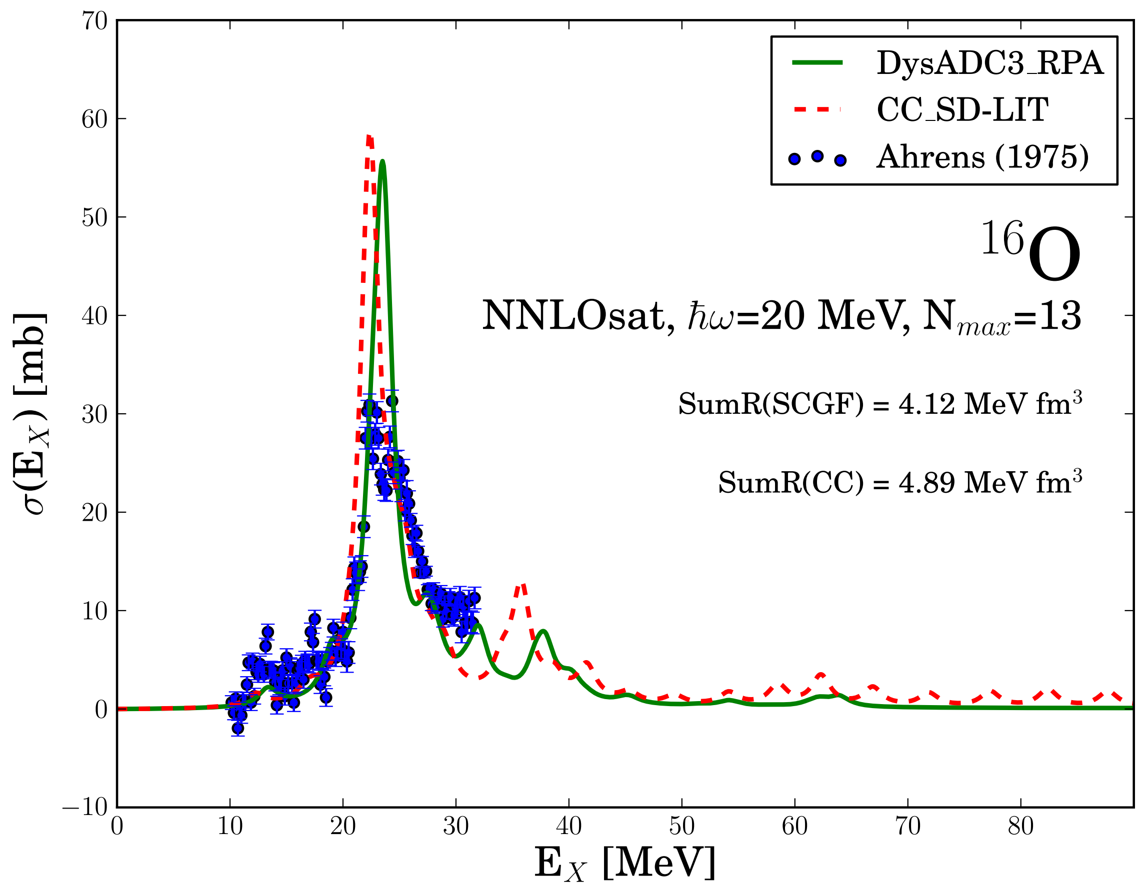
- ○ GDR positions reproduced
- ○ Total sum rule OK but poor strength distribution
- ○ Comparison with CC LIT results for α_D

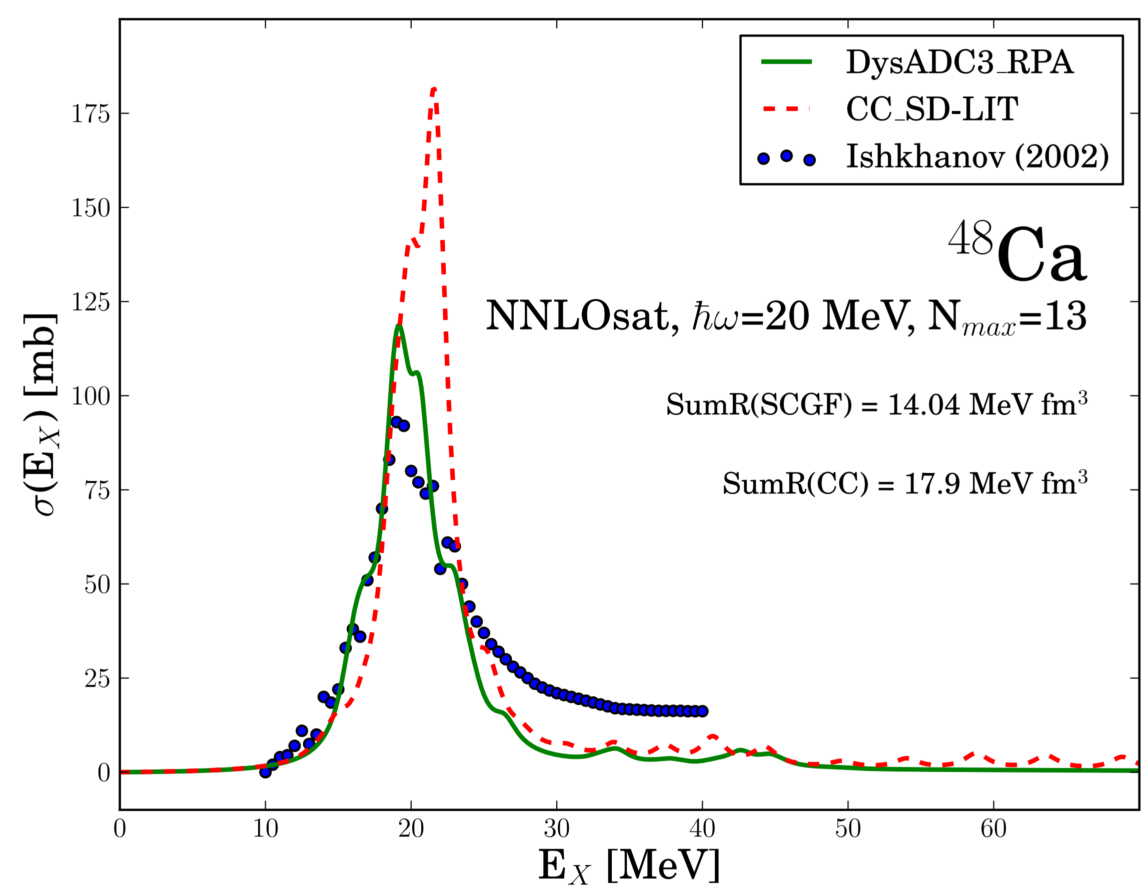
Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{40}Ca	1.79	1.47 $(1.87)_{thresh}$	1.87(3)
^{48}Ca	2.08	2.45	2.07(22)

Electromagnetic response

⦿ Comparison with coupled-cluster Lorentz integral transform (CC-LIT)

[Raimondi *et al.* in preparation]





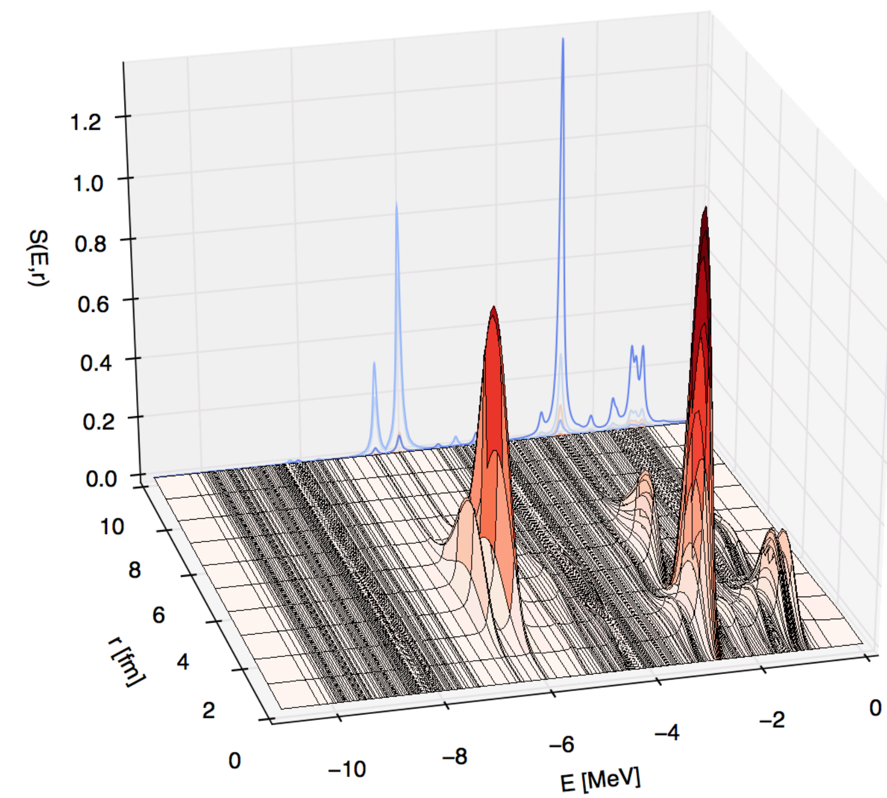
○ Different ways of including correlations

GF → RPA (first-order 2-body correlator) on top of fully correlated reference state

CC → SD (analogous to second RPA) on top of HF reference state

Conclusions

- **Ab initio calculations routinely access mid-mass nuclei**
  - Many-body formalism well grounded
  - Interactions currently represent largest source of uncertainty
  - Pragmatic choices lead to successful applications
  - Thorough assessment of theoretical error?



- **Self-consistent Green's function approach gives access to a variety of observables**
  - Ground-state properties along isotopic chains, spectral functions, response functions
  - Case of ^{40}Ar to be investigated in ADC(3) scheme (work in progress…)