Recent advances in self-consistent Green's function with Gorkov propagators

Carlo Barbieri

- Nambu covariant formalism for improving Gorkov SCGF

- The quest for consistent analysis of structure and scattering (from ab initio)

- Grouding DFT into ab initio.

- Newer tools for computing nuclear matter (SCGF and QMC).

frontiers Research Topics

Editors: L. Coraggio, S. Pastore, CB

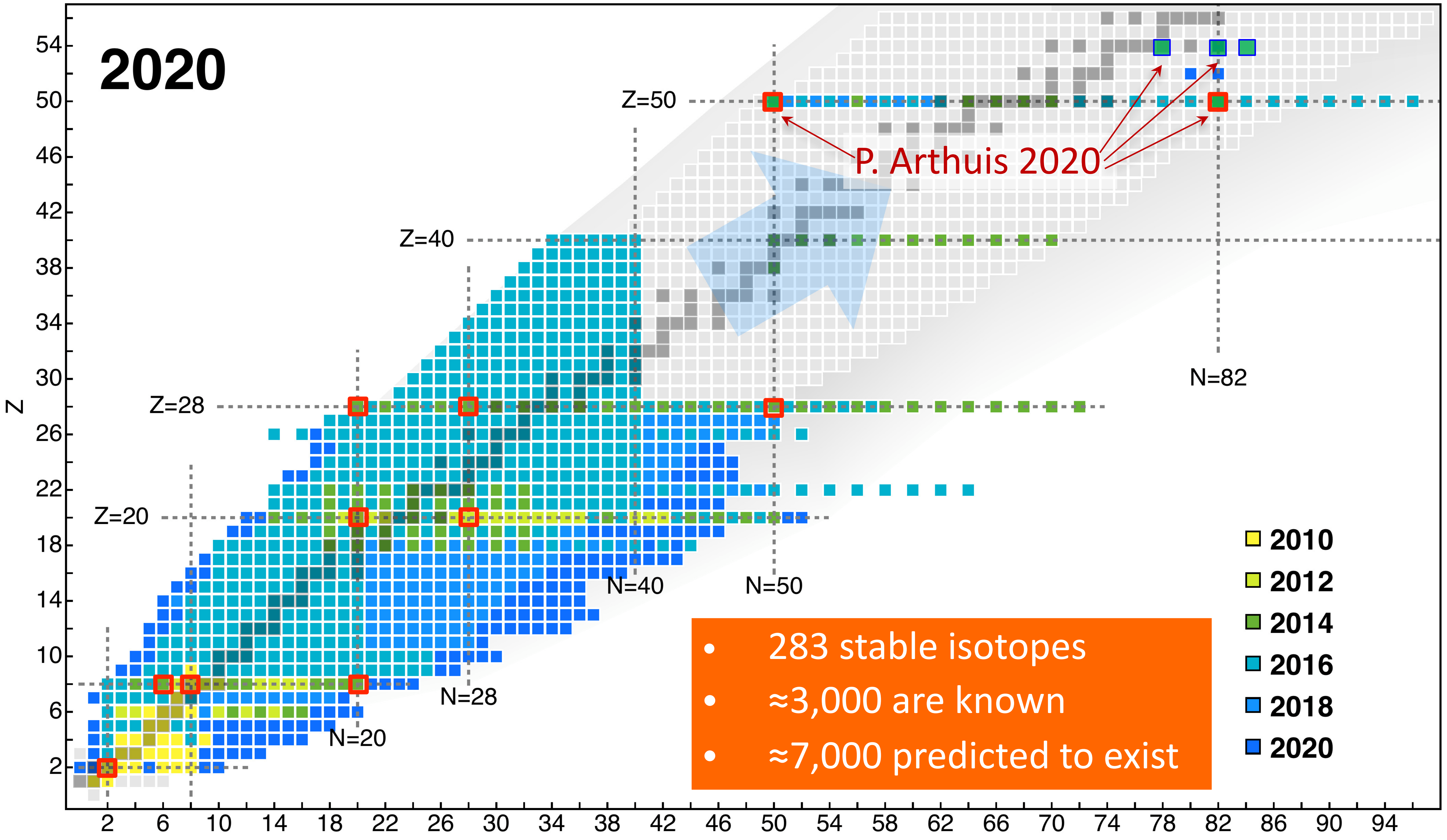
FRONTIERS topical review (doi: 10.3389/fphy.2020.626976) :

Frontiers in Physics **8**, 626976 (2021)

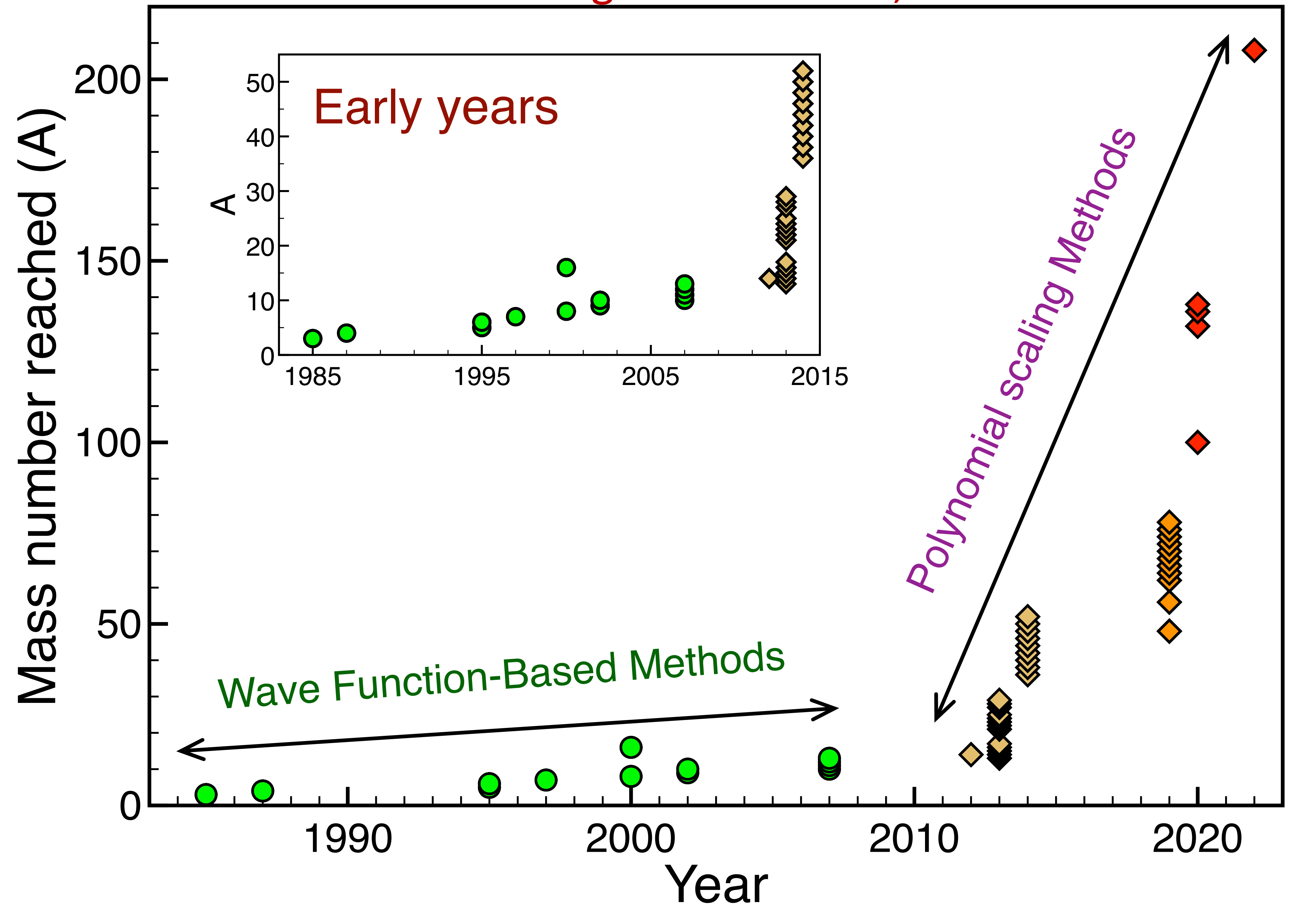
Reach of ab initio methods across the nuclear chart

Extension beyond few-nucleons thanks to:

- Soft (nearly perturbative) effective nuclear forces
- Diagrammatic many-body approaches



Legnaro Natl' Lab, Mid Term Plan 2022



Open challenges:

- Accuracy (better theory of nuclear forces)
- Mass number limit (optimised model spaces)
- Precision & scattering (high-order diag. resummations)

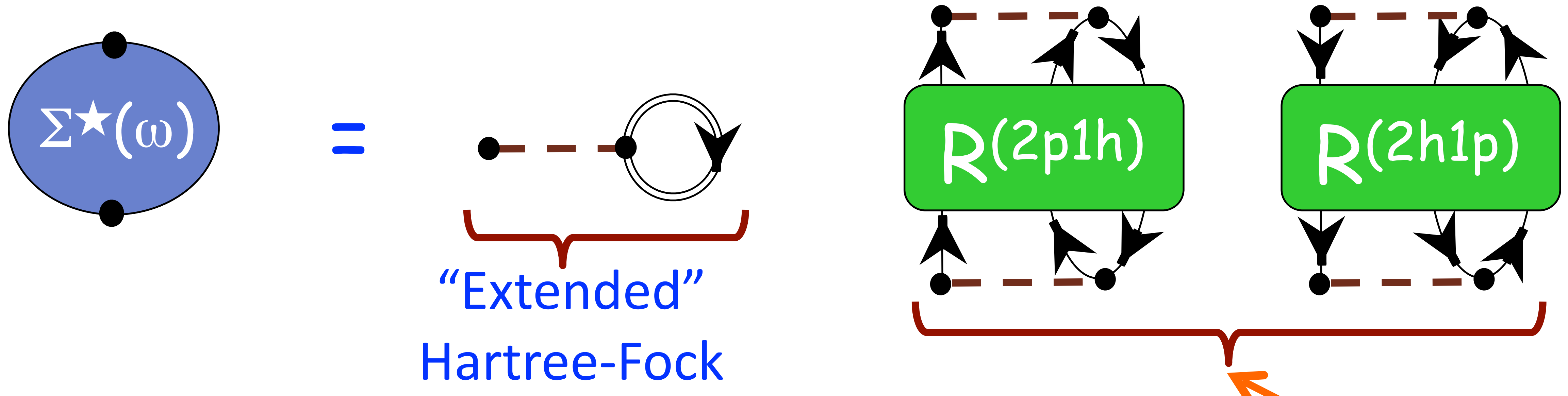
H. Hergert, Frontiers in Phys **8**, 379 (2020)
L. Coraggio, S. Pastore, **CB**, Frontiers in Phys **8**, 626976 (2021)

The Faddev-RPA and ADC(3) methods in a few words

Compute the nuclear self energy to extract both scattering (optical potential) and spectroscopy.
Both ladders and rings are needed for atomi nuclei:

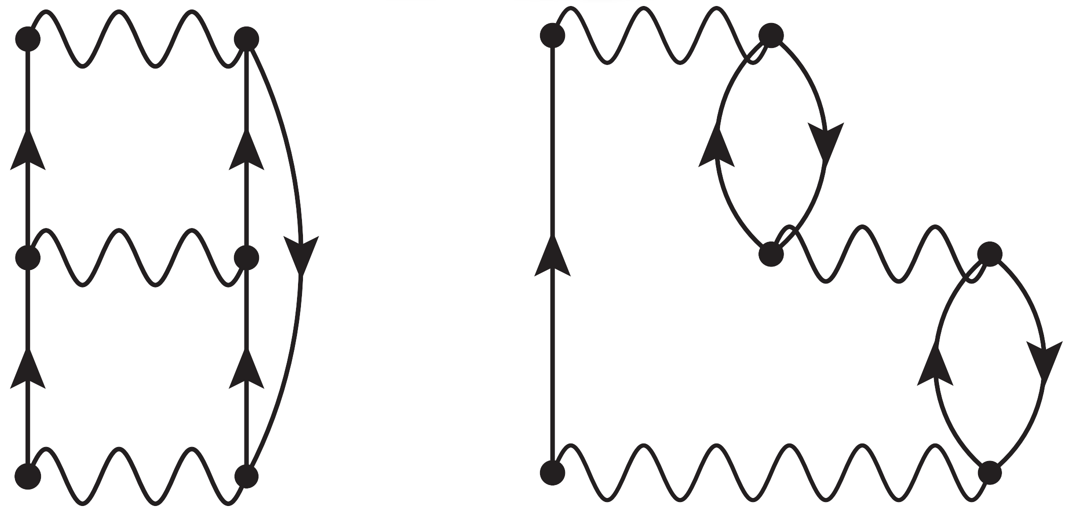
F-RPA:
*Phys. Rev. C**63**, 034313 (2001)*
*Phys. Rev. A**76**, 052503 (2007)*
*Phys. Rev. A**83**, 042517 (2011)*

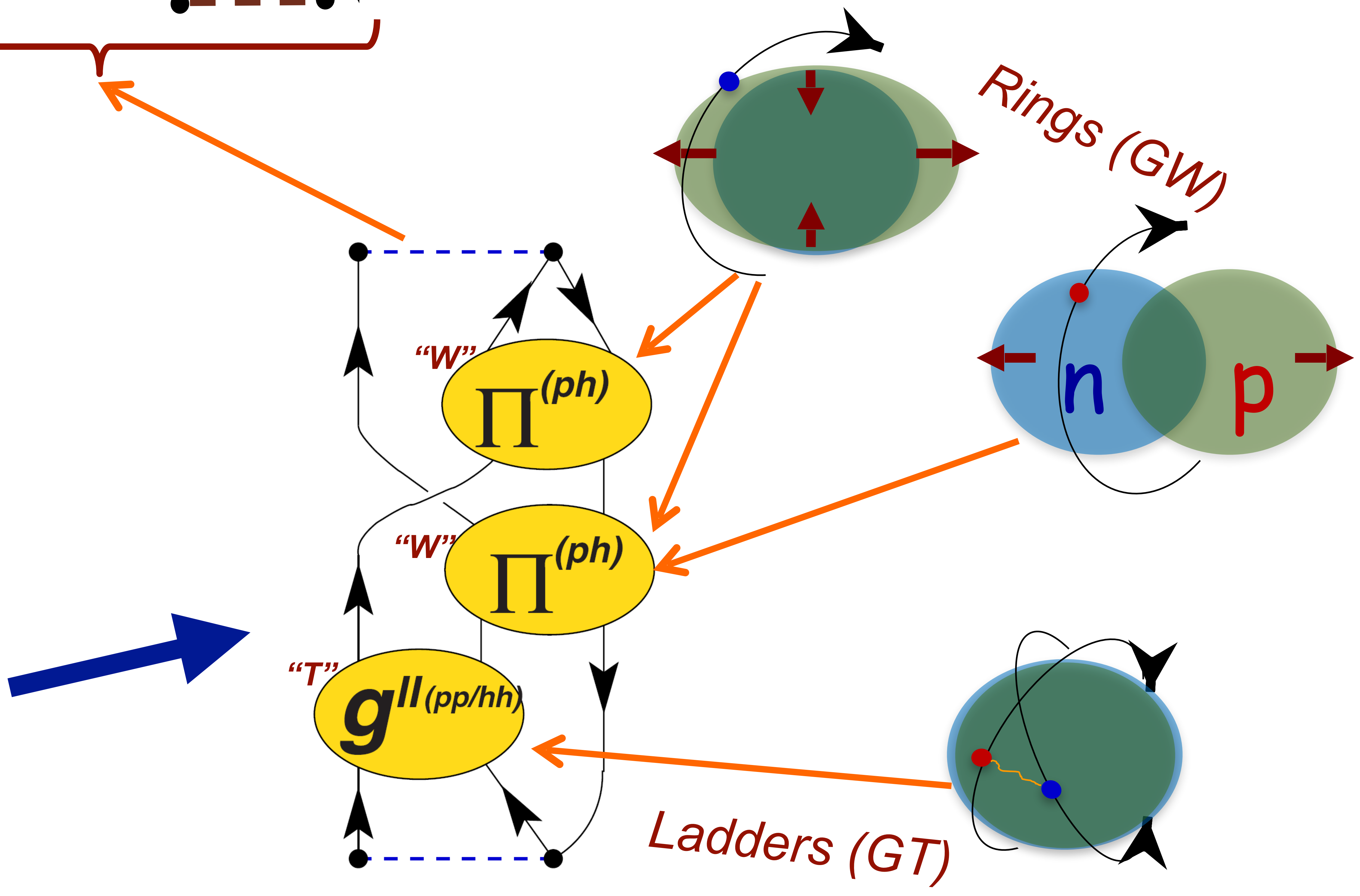
ADC(3):
*Lect. Notes in Phys **936** (2017)-*
Chapter 11.



All Ladders (GT) and ring modes (GW) are coupled to all orders. Two approaches:

- Faddev-RPA allows for RPA modes
- ADC(3) Tamn-Dancoff version using 3rd order diagrams as 'seeds':

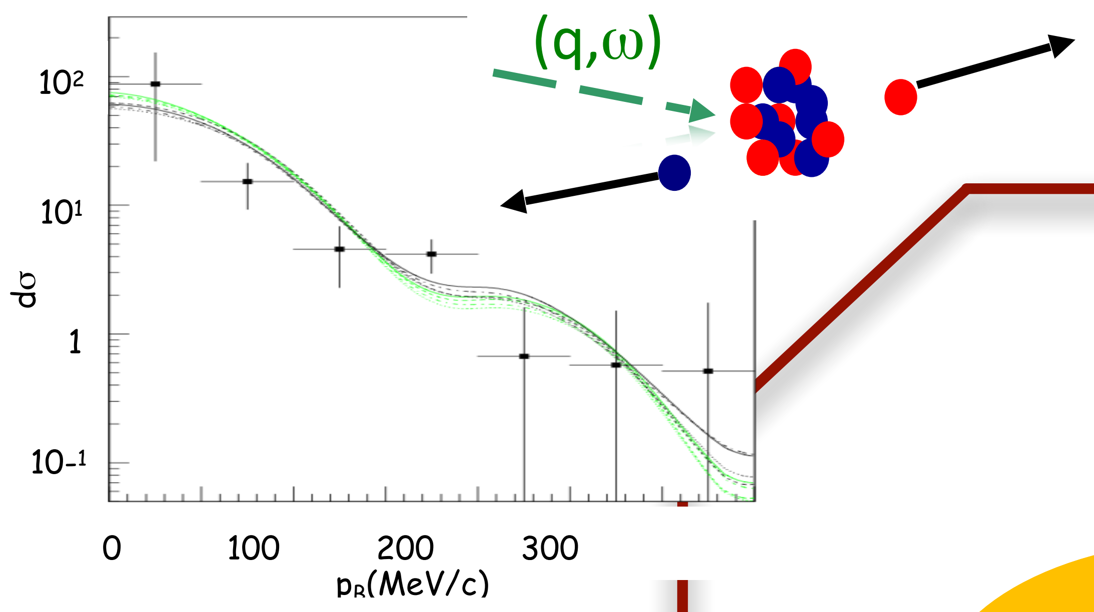




The Self-Consistent Green's Function with Faddev-RPA

Two-nucleon emission: $^{16}O(e,e'pn)^{14}N$

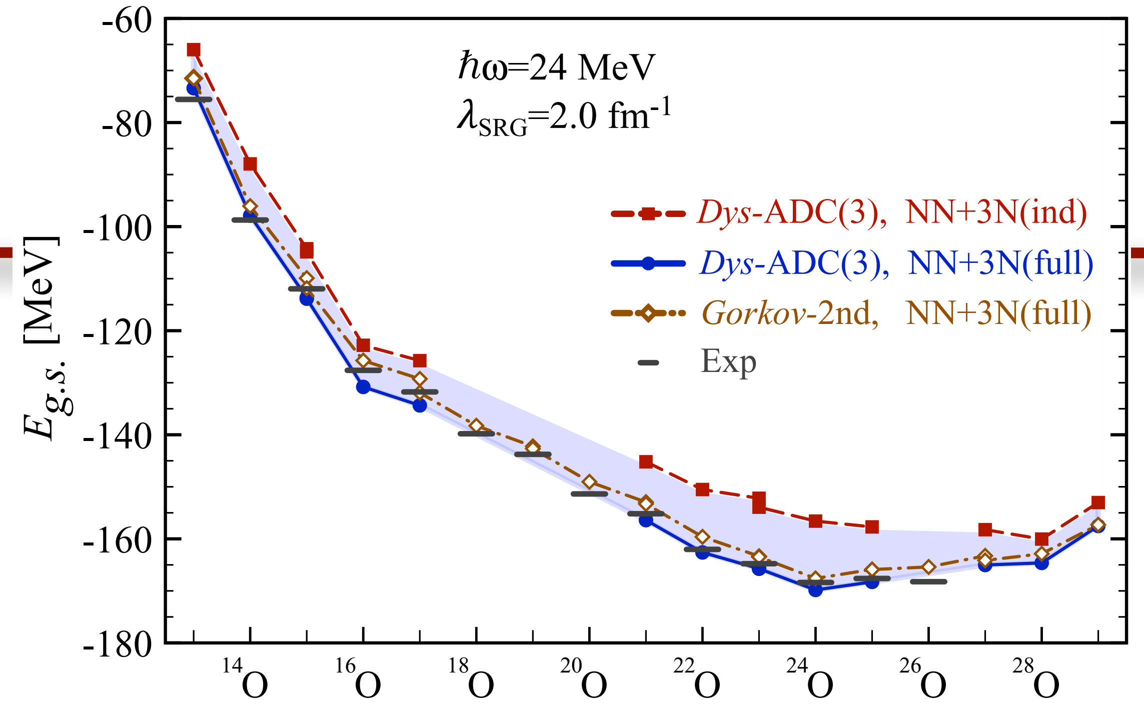
[Eur. Phys. J. A**43**, 137 (2010)]



Binding energies

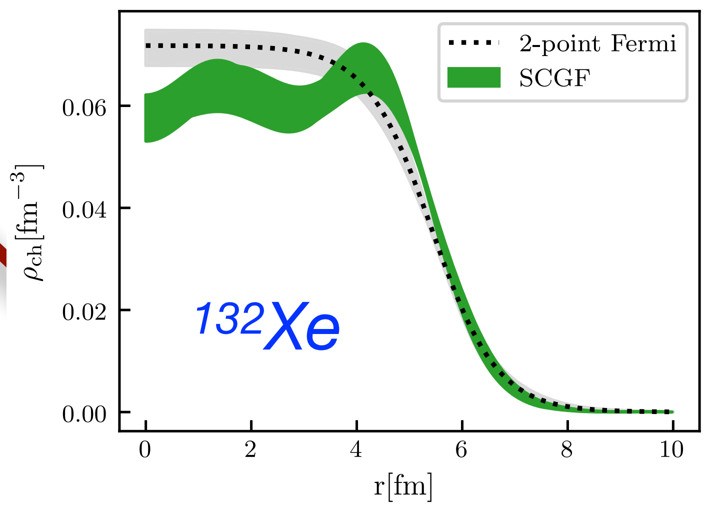
Oxygen drip line

[Phys Rev. Lett. **111**, 062501 (2013)]

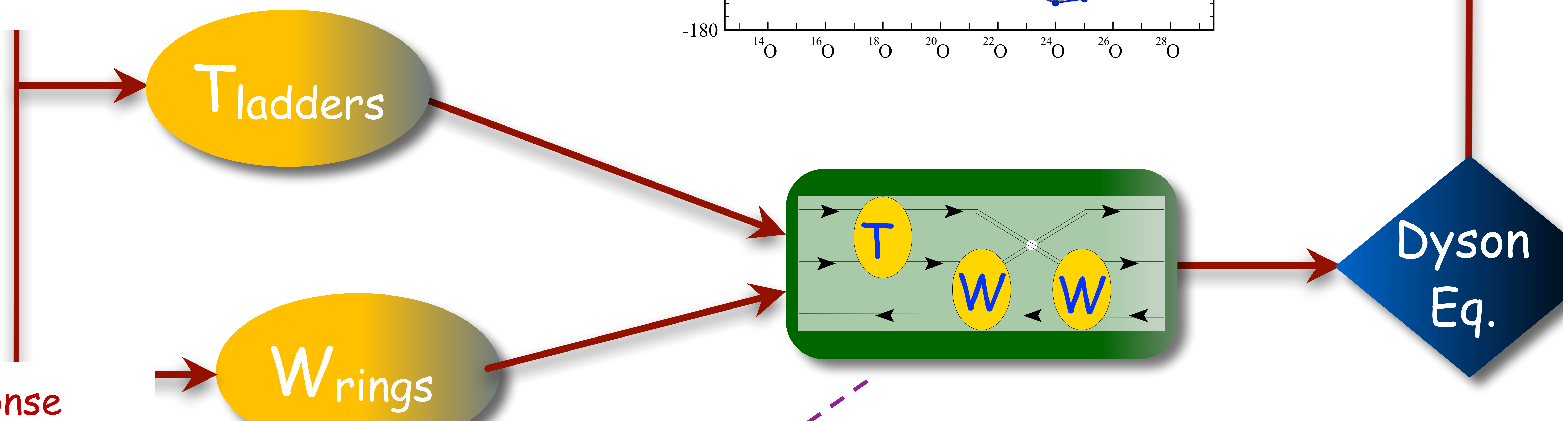


Charge & matter distribution

Neutron skins [Phys Rev. Lett. **125**, 182501 (2020)]



	SCGF	Exp.
^{100}Sn	4.525 – 4.707	
^{132}Sn	4.725 – 4.956	4.7093
^{132}Xe	4.700 – 4.948	4.7859
^{136}Xe	4.715 – 4.928	4.7964
^{138}Xe	4.724 – 4.941	4.8279



Spectroscopy

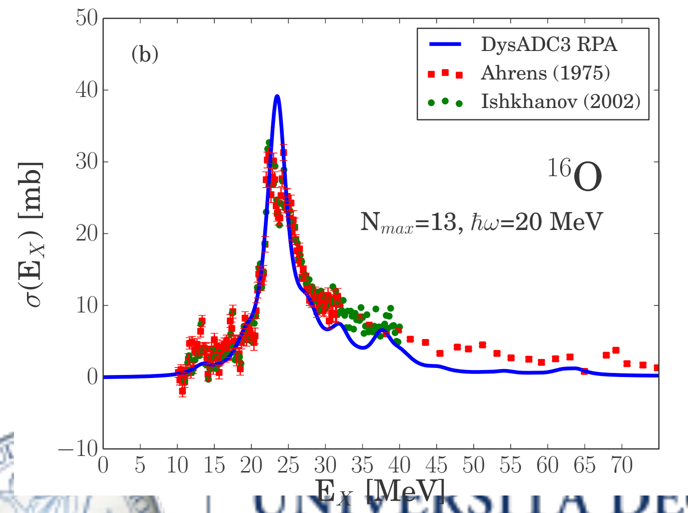
Ionisation energies and affinities for simple atoms and molecules

[Phys Rev. A. **83**, 042517 (2011); **85**, 012501 (2012)]

	Level	ADC(3)	FRPA	FRPA(c)	Expt.
HF					
	1π	16.48	16.05	16.35	16.05
	3σ	20.36	20.03	20.24	20.0
CO					
	5σ	13.94	14.37	13.69	14.01
	1π	16.98	16.95	16.84	16.91
	4σ	20.19	19.46	19.59	19.72
H_2O					
	$1b_1$	12.86	12.62	12.67	12.62
	$3a_1$	15.15	14.91	14.98	14.74
	$1b_2$	19.21	19.06	19.13	18.51
	$\bar{\Delta}$ (eV)	0.30(0.30)	0.25(0.23)	0.31(0.26)	
	Δ_{max} (eV)	0.70(0.70)	0.73(0.73)	0.88(0.62)	

Nuclear ELM response and dipole polarisability, α_D

[Phys Rev. C77, 024304 (2008)]

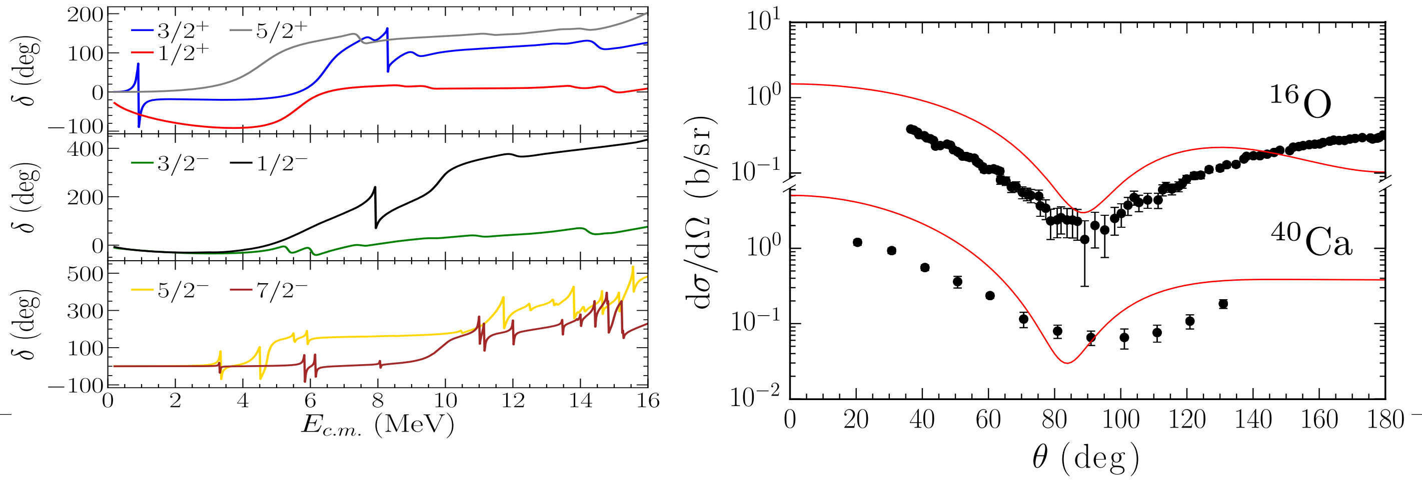


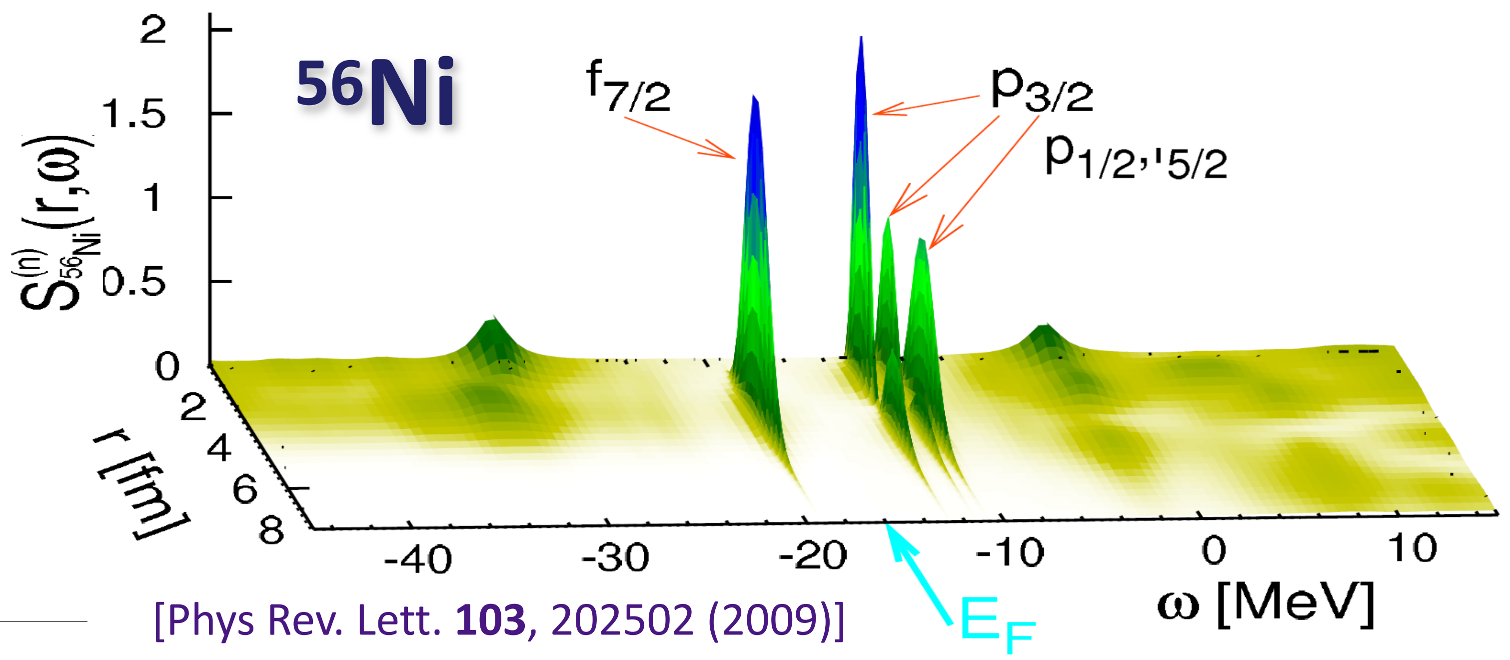
^{68}Ni:

	SCGF	Exp
E_{PDR} (MeV)	10.68 10.92	9.55(17)
E_{GDR} (MeV)	18.1	17.1(2)
α_D (fm^3)	3.60	3.40(23) 3.88(31)

Optical potential

Elastic neutron scattering [Phys Rev. Lett. **123**, 092501 (2013)]





[Phys Rev. Lett. **103**, 202502 (2009)]

Ab-initio Nuclear Computation & BcDor code

BoccaDorata code: https://gitlab.com/cbarbieri/BoccaDorata

- C++ class library for handling many-body propagators (MPI & OpenMP based).
- Computation of nuclear spectral functions, many-body propagators, RPA responses, coupled cluster equations and effective interaction/charges for the shell model.

Code history:

2006 — core functions and FRPA

shell model charges&interactions (lowest order)

2010 — new Gorkov formalism for open-shell nuclei (at 2nd order) (V. Soma, 2010–)

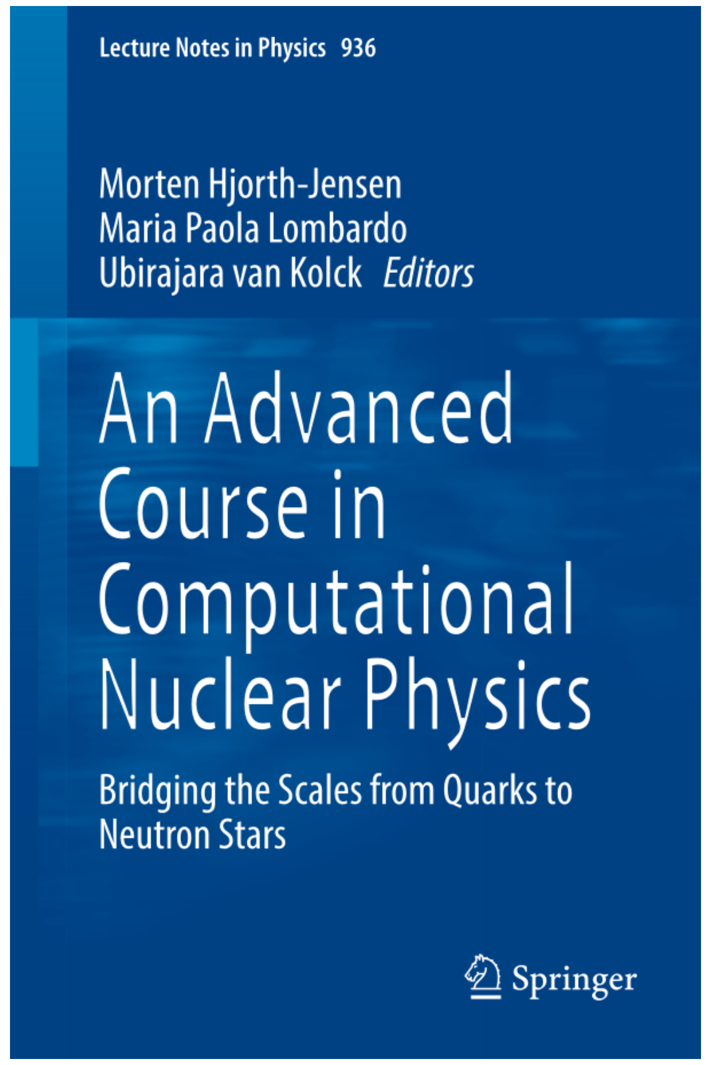
2012 — Coupled clusters equations

2013 — Three-nucleon forces (A. Cipollone, 2011–2015)

2014

2022 — Gorkov at 3rd order (will become massively parallel…)

applications -->



Self-consistent Green's function formalism and methods for Nuclear Physics

CB, A. Carbone, Lect. Notes in Phys. **936** (2017) – Chapter **11**

Reaching open-shell nuclei:

The Gorkov GF approach

V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)
V. Somà, CB, T. Duguet, Phys. Rev. C **87**, 011303R (2013)
V. Somà, CB, T. Duguet, Phys. Rev. C **89**, 024323 (2014)
CB, T. Duguet, V. Somà, Phys. Rev. C **105**, 044330 (2014)

Gorkov ansatz… for atomic nuclei

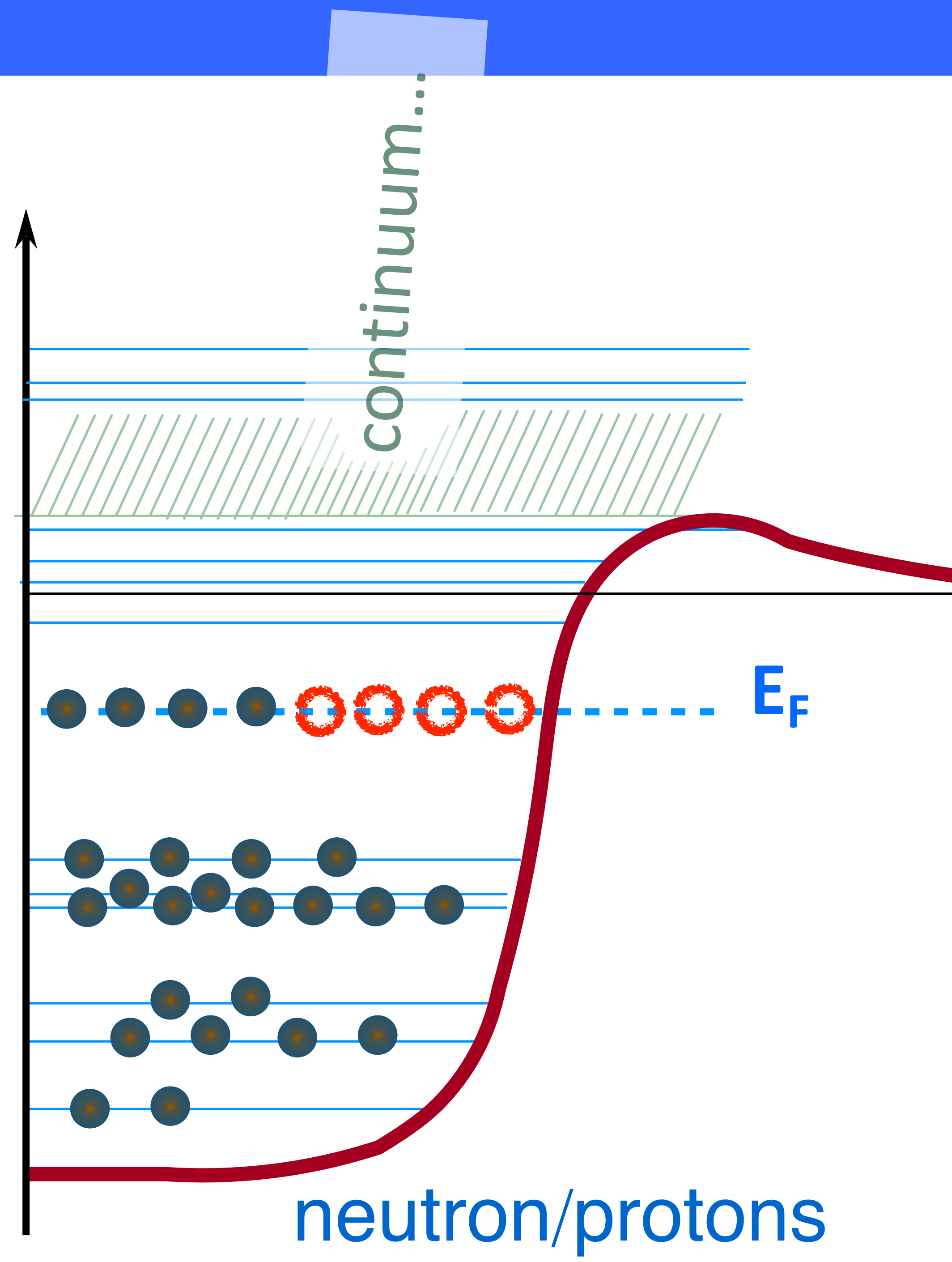
➢ ✺ Most atomic nuclei: partially filled orbits couple to collective vibrations

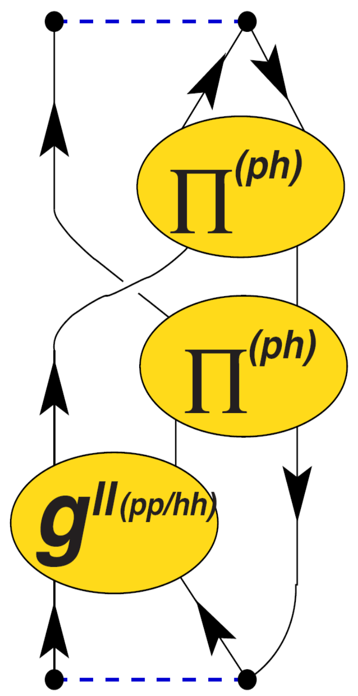
Expansion breaks down with vanishing *particle-hole* gaps

Pairing (two-nucleon) mitigates instabilities

Explicit configuration mixing

Single-reference: Bogoliubov (Gorkov)





➢ Ansatz $\boxed{E_0^{N\pm 2n} \approx E_0^N \pm 2n\mu \pm n\Delta\varepsilon_P \qquad \text{for } n = 1, 2, 3, \ldots,}$

➢ Auxiliary many-body state $|\Psi_0\rangle = \sum_{n=0}^{\infty} c_{2n} |\psi^{2n}\rangle$

V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)
CB, T. Duguet, V. Somà, Phys. Rev. C **105**, 044330 (2014)

Mixes various particle numbers

Introduce a "grand-canonical" potential $\Omega \equiv H - \mu N$

$\Rightarrow$ $|\Psi_0\rangle$ minimizes $\Omega_0 = \min_{|\Psi_0\rangle} \{\langle\Psi_0|\Omega|\Psi_0\rangle\}$ under the constraint $\mathrm{N} = \langle\Psi_0|N|\Psi_0\rangle$

Gorkov Green's functions and equations

Set of 4 Gorkov Green's functions:

$$\mathbf{G}_{\alpha\beta}(t,t') \equiv \begin{pmatrix} G^{11}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c_\alpha(t)c^\dagger_\beta(t')\right]|\Psi_0\rangle \equiv & G^{12}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c_\alpha(t)c_\beta(t')\right]|\Psi_0\rangle \equiv \\ G^{21}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c^\dagger_\alpha(t)c^\dagger_\beta(t')\right]|\Psi_0\rangle \equiv & G^{22}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c^\dagger_\alpha(t)c_\beta(t')\right]|\Psi_0\rangle \equiv \end{pmatrix}$$




[Gorkov 1958]

In terms of Nambu fields:

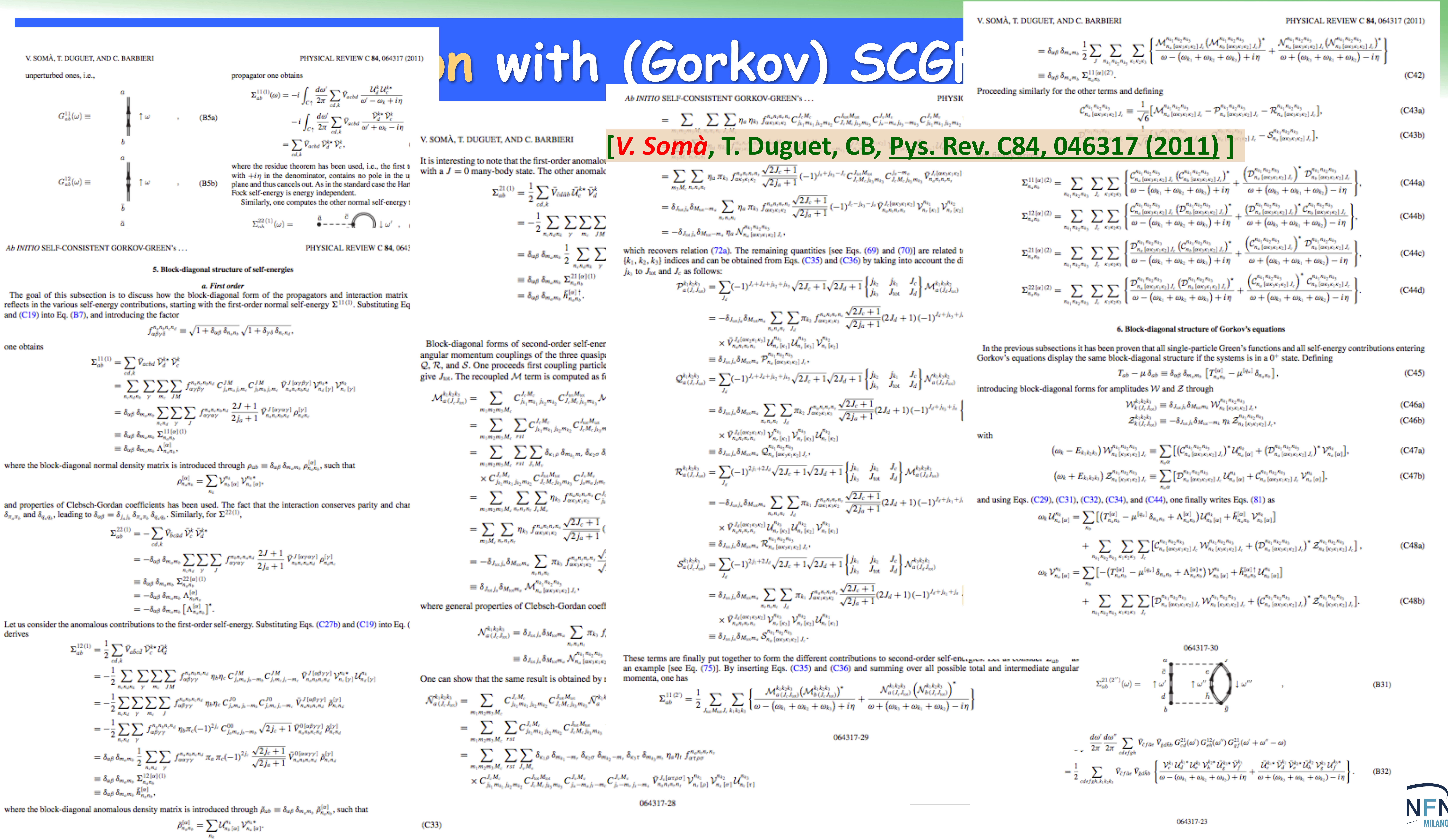
$$\mathbf{G}_{\alpha\beta}(t,t') = -i\langle\Psi_0|T\Big[\underbrace{\mathbf{A}_\alpha(t)\mathbf{A}^\dagger_\beta(t')}\Big]|\Psi_0\rangle \qquad \mathbf{A}_\alpha(t) \equiv \begin{bmatrix} c_\alpha(t) \\ c^\dagger_\alpha(t) \end{bmatrix}$$

[Anderson 1958
Nambu 1960]

Don't (anti)commute: in/out arrows and Nambu indices still matter!

...on with (Gorkov) SCGF

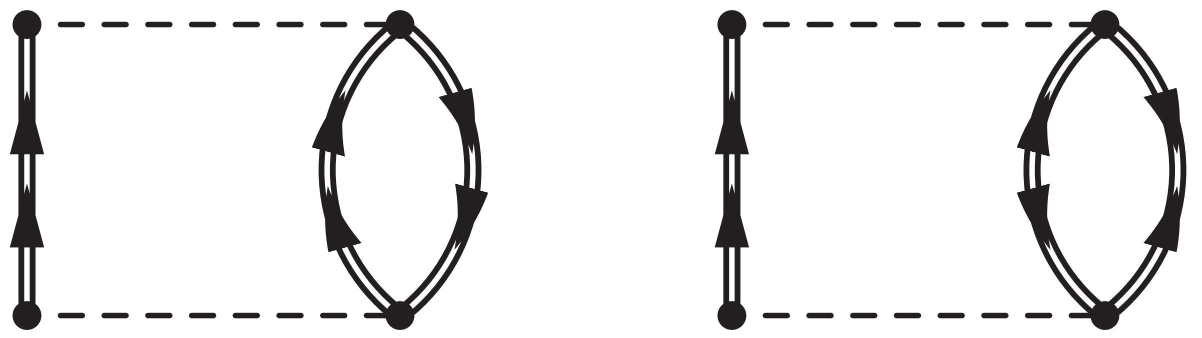
[*V. Somà*, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]



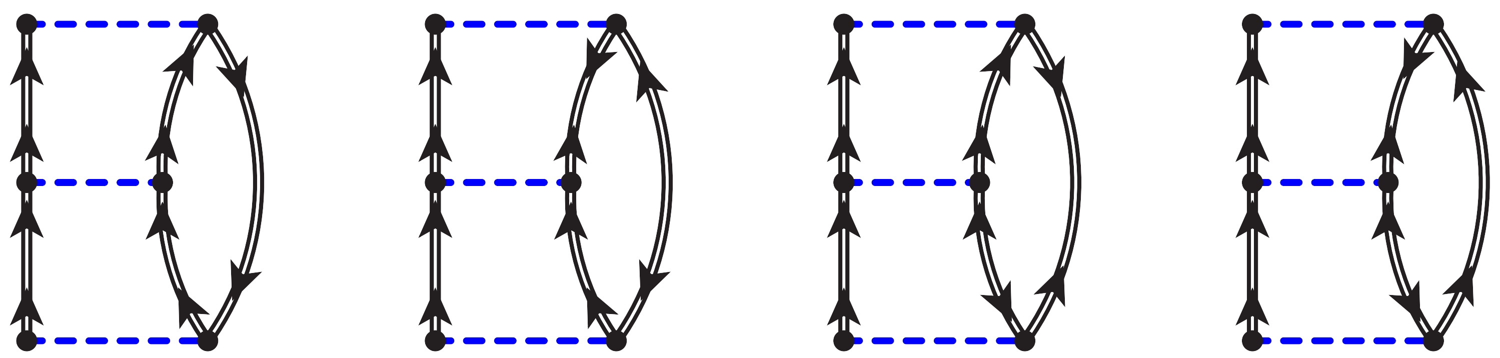
Nambu-Covariant approach to build (Gorkov) propagators

Gorkov at
2nd order:

$$\Sigma^{11}_{\alpha\beta}(\omega) \ =$$

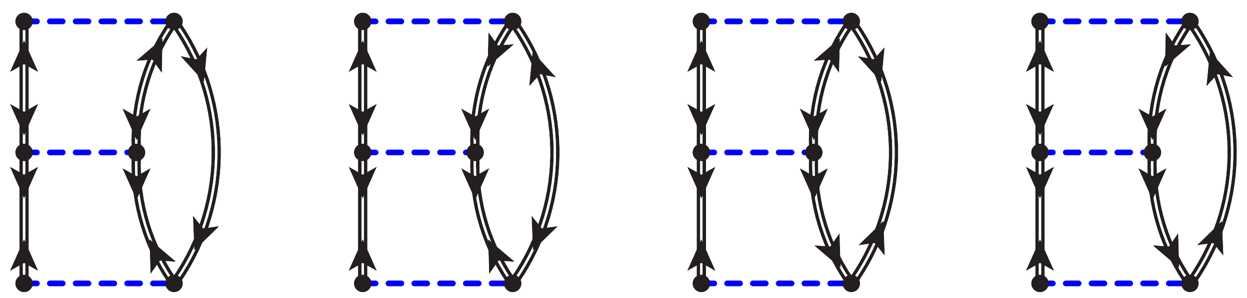


pp-ladders:

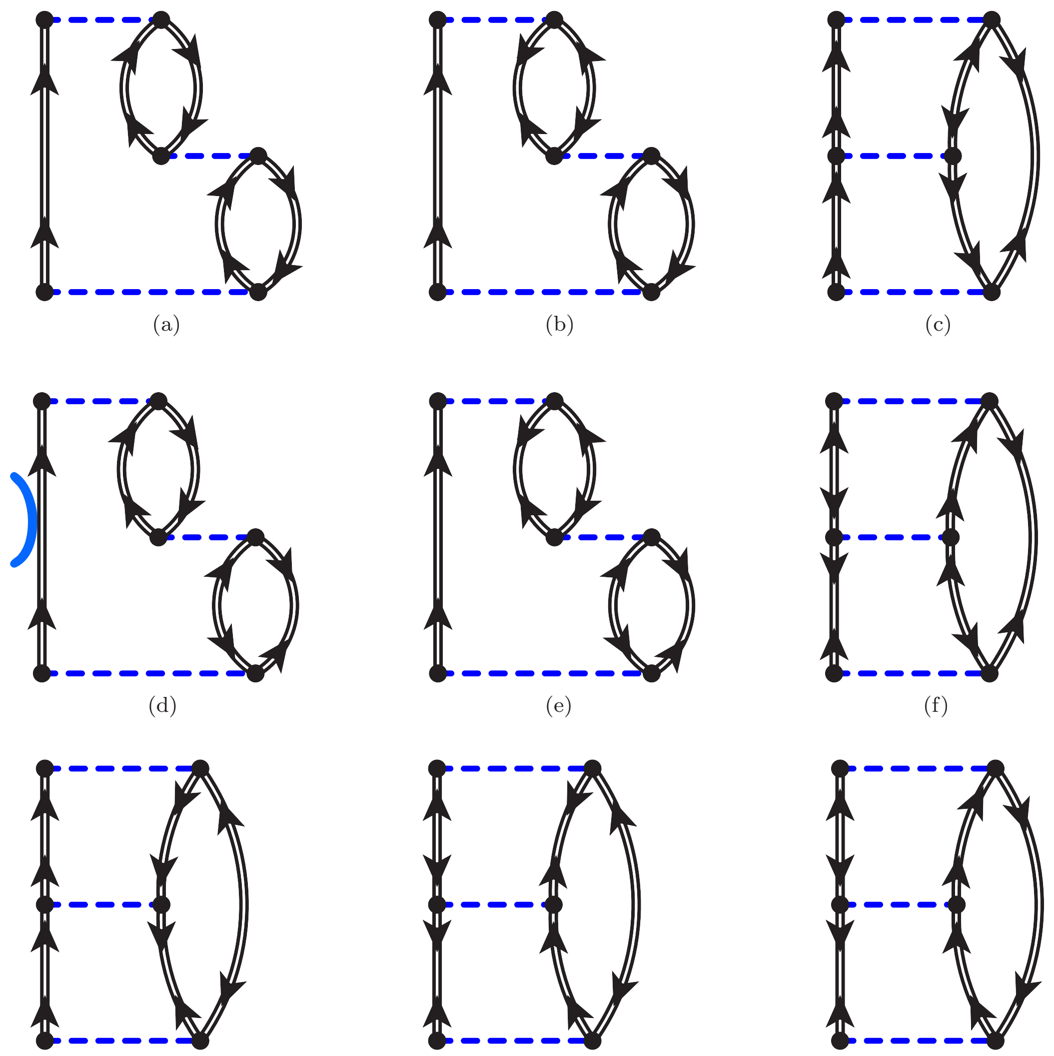


Gorkov at
3rd order:
(ONLY NN forces)

hh-interactions (hh int. among pp ladders!!!)



ph-rings:



(NN ONLY forces)

Nambu-Covariant approach to build (Gorkov) propagators

PHYSICAL REVIEW C **105**, 044330 (2022)

Gorkov algebraic diagrammatic construction formalism at third order

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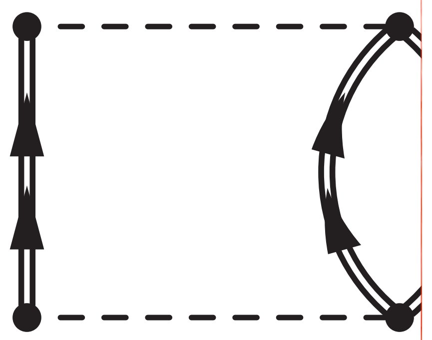
IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Gorkov at 2nd order:

$$\Sigma^{11}_{\alpha\beta}(\omega) \;=$$

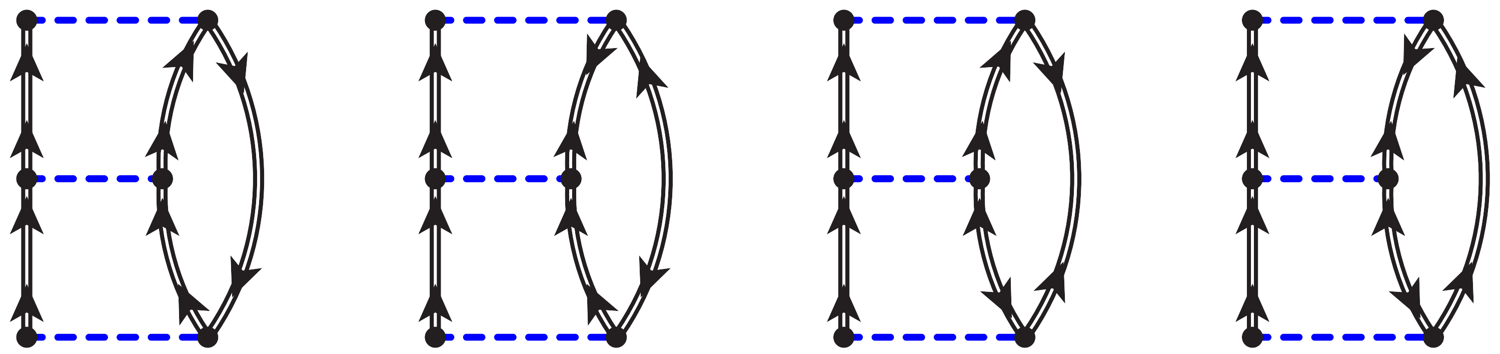


$$\widetilde{\Sigma}^{11}_{\alpha\beta}(\omega) = \sum_{rr'} \left\{ \mathcal{C}_{\alpha,r} \left[\frac{1}{\omega\mathbb{I} - \mathcal{E} + i\eta} \right]_{r,r'} \mathcal{C}^{\dagger}_{r',\beta} + \bar{\mathcal{D}}^{\dagger}_{\alpha,r} \left[\frac{1}{\omega\mathbb{I} + \mathcal{E}^{T} - i\eta} \right]_{r,r'} \bar{\mathcal{D}}_{r',\beta} \right\}, \tag{29a}$$

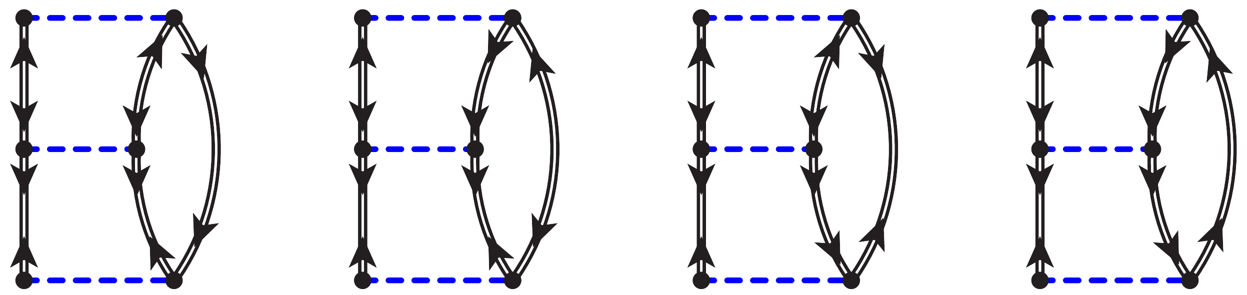
$$\widetilde{\Sigma}^{12}_{\alpha\beta}(\omega) = \sum_{rr'} \left\{ \mathcal{C}_{\alpha,r} \left[\frac{1}{\omega\mathbb{I} - \mathcal{E} + i\eta} \right]_{r,r'} \mathcal{D}^{*}_{r',\beta} + \bar{\mathcal{D}}^{\dagger}_{\alpha,r} \left[\frac{1}{\omega\mathbb{I} + \mathcal{E}^{T} - i\eta} \right]_{r,r'} \bar{\mathcal{C}}^{T}_{r',\beta} \right\}, \tag{29b}$$

Gorkov at 3rd order:
(ONLY NN forces)

pp-ladders:



hh-interactions (hh int. among pp ladders



(NN ONLY forces)

$$\mathcal{C}^{(\mathrm{IIa})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{P}_{123} \sum_{\substack{\mu\nu\lambda \\ k_4 k_5}} \frac{v_{\alpha\lambda,\mu\nu}}{2} \left(\bar{\mathcal{V}}^{k_4}_{\mu} \bar{\mathcal{V}}^{k_5}_{\nu}\right)^{*} t^{k_1 k_2}_{k_4 k_5} \bar{\mathcal{V}}^{k_3}_{\lambda}, \tag{43a}$$

$$\mathcal{C}^{(\mathrm{IIb})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{P}_{123} \sum_{\substack{\mu\nu\lambda \\ k_4 k_5}} v_{\alpha\lambda,\mu\nu} \left(\bar{\mathcal{V}}^{k_4}_{\nu} \mathcal{U}^{k_5}_{\lambda}\right)^{*} t^{k_1 k_2}_{k_4 k_5} \mathcal{U}^{k_3}_{\mu}, \tag{43b}$$

$$\mathcal{C}^{(\mathrm{IIc})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{P}_{123} \sum_{\substack{\mu\nu\lambda \\ k_4 k_5}} \frac{v_{\alpha\lambda,\mu\nu}}{2} \left(\bar{\mathcal{V}}^{k_4}_{\mu} \bar{\mathcal{V}}^{k_5}_{\nu}\right)^{*} t^{k_4 k_5}_{k_1 k_2} \bar{\mathcal{V}}^{k_3}_{\lambda}, \tag{47a}$$

$$\mathcal{C}^{(\mathrm{IId})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{P}_{123} \sum_{\substack{\mu\nu\lambda \\ k_4 k_5}} v_{\alpha\lambda,\mu\nu} \left(\bar{\mathcal{V}}^{k_4}_{\nu} \mathcal{U}^{k_5}_{\lambda}\right)^{*} t^{k_4 k_5}_{k_1 k_2} \mathcal{U}^{k_3}_{\mu}, \tag{47b}$$

$$\mathcal{E}^{(pp)}_{k_1 k_2, k_4 k_5} = \sum_{\alpha\beta\gamma\delta} \left(\mathcal{U}^{k_1}_{\alpha} \mathcal{U}^{k_2}_{\beta}\right)^{*} v_{\alpha\beta,\gamma\delta} \mathcal{U}^{k_4}_{\gamma} \mathcal{U}^{k_5}_{\delta}, \tag{45}$$

$$\mathcal{E}^{(hh)}_{k_1 k_2, k_4 k_5} = \sum_{\alpha\beta\gamma\delta} \bar{\mathcal{V}}^{k_1}_{\alpha} \bar{\mathcal{V}}^{k_2}_{\beta} v_{\alpha\beta,\gamma\delta} \left(\bar{\mathcal{V}}^{k_4}_{\gamma} \bar{\mathcal{V}}^{k_5}_{\delta}\right)^{*}. \tag{46}$$

$$\mathcal{C}^{(\mathrm{IIe})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\substack{\mu\nu\lambda \\ k_7 k_8}} v_{\alpha\lambda,\mu\nu} \left(\bar{\mathcal{V}}^{k_7}_{\nu} \mathcal{U}^{k_8}_{\lambda}\right)^{*} \mathcal{U}^{k_1}_{\mu} t^{k_8 k_2}_{k_7 k_3}, \tag{50a}$$

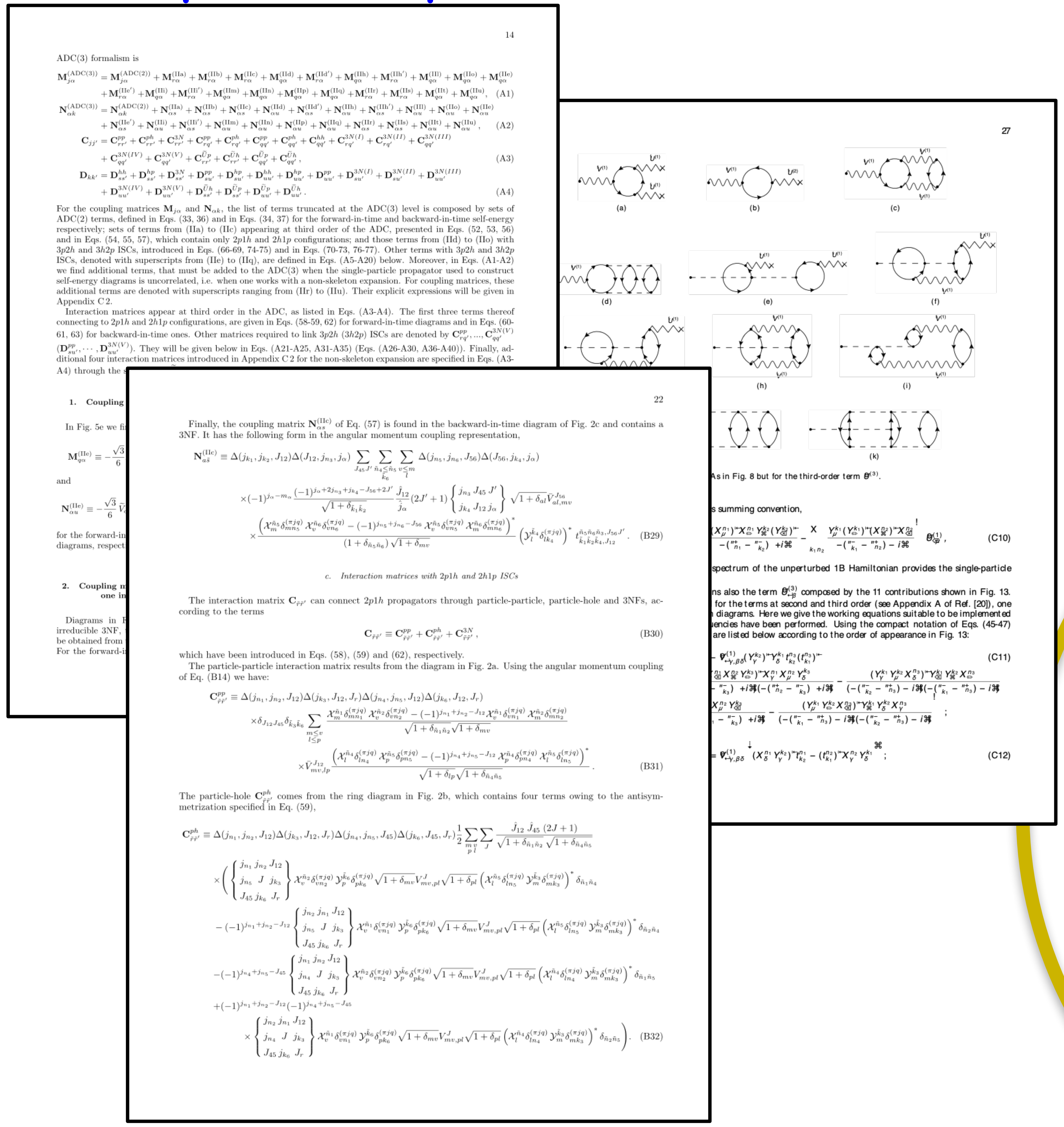
$$\mathcal{C}^{(\mathrm{IIf})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\substack{\mu\nu\lambda \\ k_7 k_8}} v_{\alpha\lambda,\mu\nu} \left(\mathcal{U}^{k_7}_{\lambda} \bar{\mathcal{V}}^{k_8}_{\mu}\right)^{*} \mathcal{U}^{k_1}_{\nu} t^{k_8 k_2}_{k_7 k_3}, \tag{50b}$$

$$\mathcal{C}^{(\mathrm{IIg})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\substack{\mu\nu\lambda \\ k_7 k_8}} v_{\alpha\lambda,\mu\nu} \left(\bar{\mathcal{V}}^{k_7}_{\mu} \bar{\mathcal{V}}^{k_8}_{\nu}\right)^{*} \bar{\mathcal{V}}^{k_1}_{\lambda} t^{k_8 k_2}_{k_7 k_3}, \tag{50c}$$

$$\mathcal{E}^{(\mathrm{Ic})}_{r,r'} = \tfrac{1}{6} \mathcal{A}_{123} \mathcal{A}_{456} \big(\delta_{k_1,k_4} \mathcal{E}^{(ph)}_{k_2 k_3, k_5 k_6}\big),$$

Inclusion of NNN forces

➔ 3p2h/3h2p terms relevant to next-generation high-precision methods.



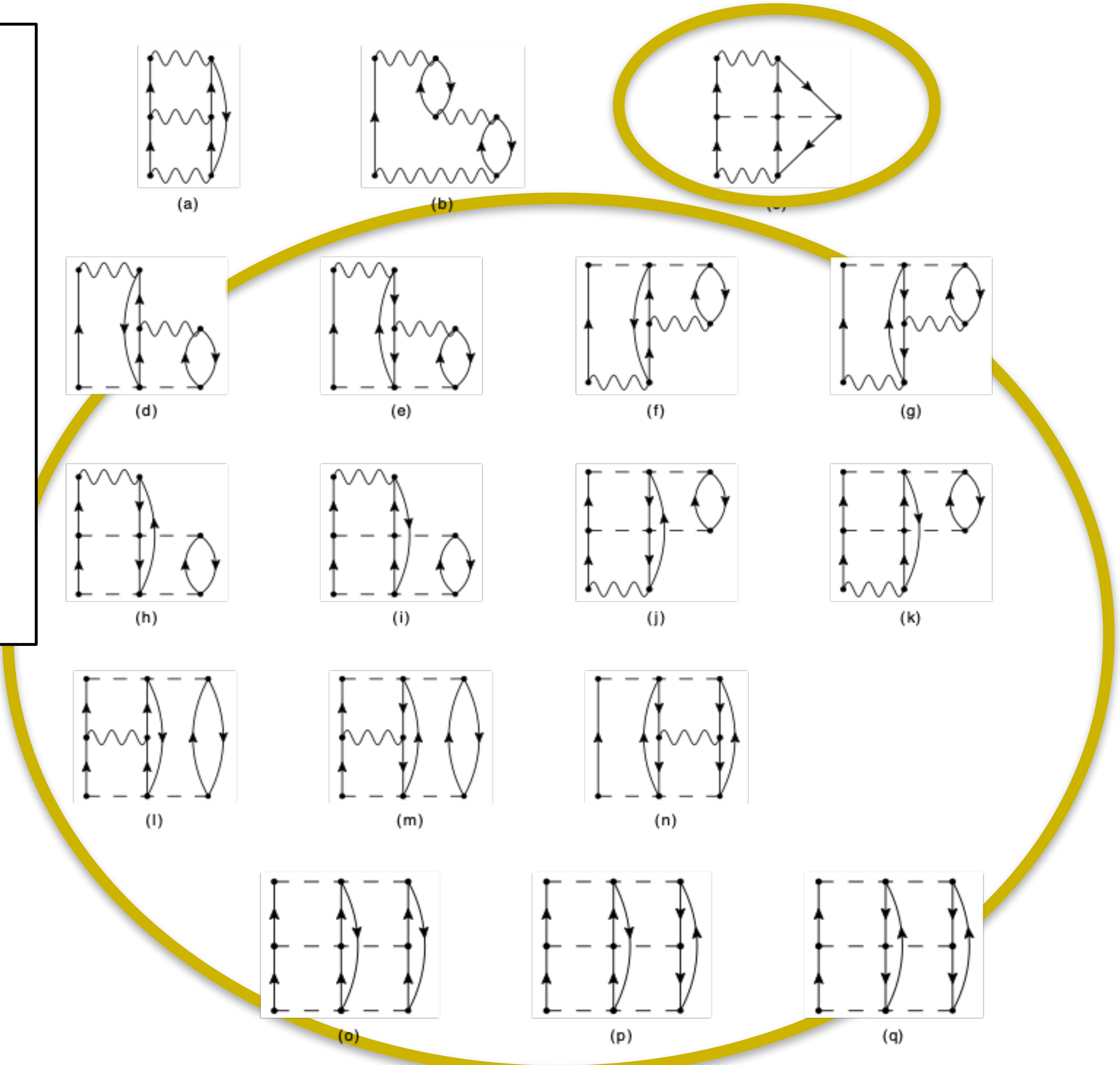


FIG. 5. 1PI, *skeleton* and *interaction irreducible* self-energy diagrams appearing at 3^{rd}-order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

Formalism already laid out:
F. Raimondi, CB, Phys. Rev. C**97**, 054308 (2018).

Gorkov Green's functions and equations

Set of 4 Gorkov Green's functions:

$$\mathbf{G}_{\alpha\beta}(t,t') \equiv \begin{pmatrix} G^{11}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c_\alpha(t)c^\dagger_\beta(t')\right]|\Psi_0\rangle \equiv & G^{12}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c_\alpha(t)c_\beta(t')\right]|\Psi_0\rangle \equiv \\ G^{21}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c^\dagger_\alpha(t)c^\dagger_\beta(t')\right]|\Psi_0\rangle \equiv & G^{22}_{\alpha\beta}(t,t') \equiv -i\langle\Psi_0|T\left[c^\dagger_\alpha(t)c_\beta(t')\right]|\Psi_0\rangle \equiv \end{pmatrix}$$

[Gorkov 1958]

In terms of Nambu fields:

$$\mathbf{G}_{\alpha\beta}(t,t') = -i\langle\Psi_0|T\left[\underbrace{\mathbf{A}_\alpha(t)\mathbf{A}^\dagger_\beta(t')}\right]|\Psi_0\rangle \qquad \mathbf{A}_\alpha(t) \equiv \begin{bmatrix} c_\alpha(t) \\ c^\dagger_\alpha(t) \end{bmatrix}$$

[Anderson 1958
Nambu 1960]

Don't (anti)commute: in/out arrows and Nambu indices still matter!

Nambu-Covariant approach to build (Gorkov) propagators

Combine w/ dual-basis:

$$\mathscr{H}_1^e \equiv \mathscr{H}_1 \times \mathscr{H}_1^\dagger$$

$$\mathcal{B}^e \equiv \mathcal{B} \cup \bar{\mathcal{B}}$$

(contravariant) (covariant)

$$\mathcal{B} \equiv \{\, |b\rangle \,\} \qquad \bar{\mathcal{B}} \equiv \{\, \langle \bar{b}| \,\}$$

$$\langle \bar{b} \,|\, c \rangle = \delta_{bc}$$

Generalised states:

$$\begin{pmatrix} |\Psi_1\rangle \\ \langle \Psi_1'| \end{pmatrix}$$

Inner product:

$$g\left(\begin{pmatrix} |\Psi_1\rangle \\ \langle \Psi_1'| \end{pmatrix}, \begin{pmatrix} |\Psi_2\rangle \\ \langle \Psi_2'| \end{pmatrix} \right) \equiv \langle \Psi_2' \,|\, \Psi_1 \rangle + \langle \Psi_1' \,|\, \Psi_2 \rangle$$

M. Drissi (Surrey, now @ TRIUMF, Canada)

Englobe Nambu indices in the basis:

$$|\beta\rangle \equiv |b,1\rangle \equiv \begin{pmatrix} |b\rangle \\ 0 \end{pmatrix}$$

$$|\bar{\beta}\rangle \equiv |b,2\rangle \equiv \begin{pmatrix} 0 \\ \langle \bar{b}| \end{pmatrix}$$

Generalised Nambu operators and commutation rules:

$$\mathrm{A}^{(b,1)} \equiv a_b \qquad \mathrm{A}^{(b,2)} \equiv \bar{a}_b \qquad \bar{\mathrm{A}}_{(b,1)} \equiv \bar{a}_b \qquad \bar{\mathrm{A}}_{(b,2)} \equiv a_b$$

$$\bar{\mathrm{A}}_\mu = \sum_\nu g_{\mu\nu}\, \mathrm{A}^\nu \qquad \bar{\mathrm{A}}_\mu = \sum_\nu g_\mu{}^\nu\, \bar{\mathrm{A}}_\nu \qquad \mathrm{A}^\mu = \sum_\nu g^{\mu\nu}\, \bar{\mathrm{A}}_\nu \qquad \mathrm{A}^\mu = \sum_\nu g^\mu{}_\nu\, \mathrm{A}^\nu$$

$$\{\, \mathrm{A}^\mu, \mathrm{A}^\nu \,\} = g^{\mu\nu} \qquad \{\, \mathrm{A}^\mu, \bar{\mathrm{A}}_\nu \,\} = g^\mu{}_\nu \qquad \{\, \bar{\mathrm{A}}_\mu, \mathrm{A}^\nu \,\} = g_\mu{}^\nu \qquad \{\, \bar{\mathrm{A}}_\mu, \bar{\mathrm{A}}_\nu \,\} = g_{\mu\nu}$$

M. Drissi, A. Rios, CB, arXiv:2107.09763 and arXiv:2107.09759

Nambu-Covariant approach to build (Gorkov) propagators

M. Drissi (Surrey, now @ TRIUMF, Canada)

Combine w/ dual-basis:

$$\mathscr{H}_1^e \equiv \mathscr{H}_1 \times \mathscr{H}_1^\dagger$$

$$\mathcal{B}^e \equiv \mathcal{B} \cup \bar{\mathcal{B}}$$

(contravariant) (covariant)

$$\mathcal{B} \equiv \{\, |b\rangle \,\} \qquad \bar{\mathcal{B}} \equiv \{\, \langle \bar{b}| \,\}$$

$$\langle \bar{b} \,|\, c \rangle = \delta_{bc}$$

Generalised states:

$$\begin{pmatrix} |\Psi_1\rangle \\ \langle \Psi_1'| \end{pmatrix}$$

Inner product:

$$g\left(\begin{pmatrix} |\Psi_1\rangle \\ \langle \Psi_1'| \end{pmatrix}, \begin{pmatrix} |\Psi_2\rangle \\ \langle \Psi_2'| \end{pmatrix} \right) \equiv \langle \Psi_2' \,|\, \Psi_1 \rangle + \langle \Psi_1' \,|\, \Psi_2 \rangle$$

Covariant (contravariant) of operators:

$$O \equiv \sum_{\substack{\mu_1 \dots \mu_k \\ \nu_1 \dots \nu_k}} o^{\mu_1 \dots \mu_k}{}_{\nu_1 \dots \nu_k} \, \bar{\mathrm{A}}_{\mu_1} \dots \bar{\mathrm{A}}_{\mu_k} \mathrm{A}^{\nu_1} \dots \mathrm{A}^{\nu_k} \qquad \text{(mixed)}$$

$$\equiv \sum_{\mu_1 \dots \mu_{2k}} o_{\mu_1 \dots \mu_{2k}} \, \mathrm{A}^{\mu_1} \dots \mathrm{A}^{\mu_{2k}} \qquad \text{(covariant)}$$

$$\equiv \sum_{\mu_1 \dots \mu_{2k}} o^{\mu_1 \dots \mu_{2k}} \, \bar{\mathrm{A}}_{\mu_1} \dots \bar{\mathrm{A}}_{\mu_{2k}} \qquad \text{(contravariant)}$$

$$o_{\mu_1 \dots \mu_{2k}} = \sum_{\alpha_1 \dots \alpha_k} g_{\mu_1 \alpha_1} \dots g_{\mu_k \alpha_k} \, o^{\alpha_1 \dots \alpha_k}{}_{\mu_{k+1} \dots \mu_{2k}}$$

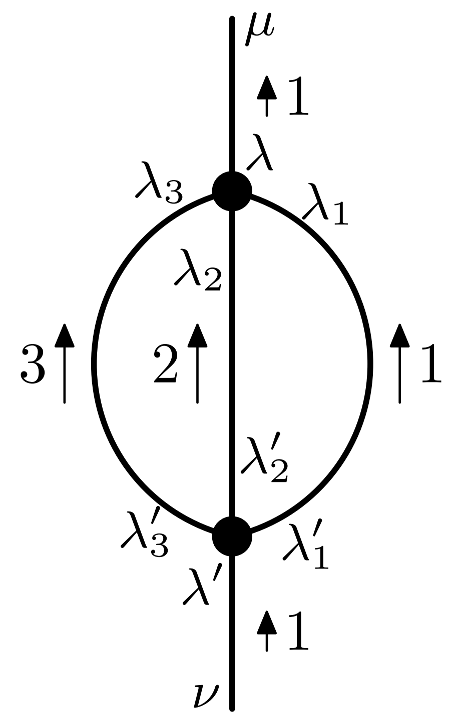
Observables are always scalars—they remain invariant under any change of basis.

M. Drissi, A. Rios, CB, arXiv:2107.09763 and arXiv:2107.09759

Nambu-Covariant approach to build (Gorkov) propagators

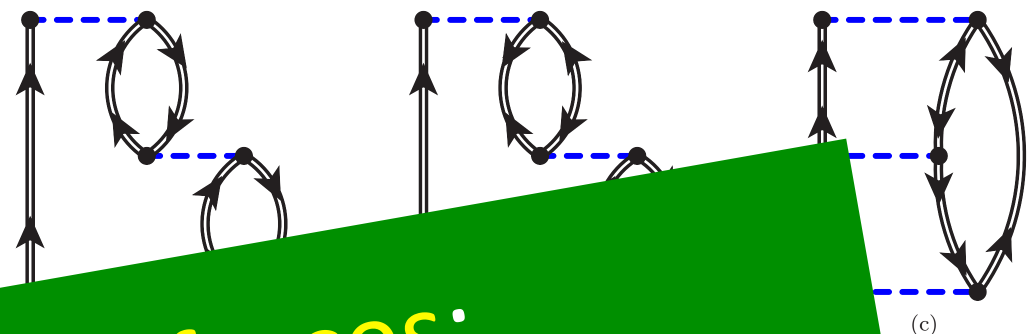
Gorkov at
2nd order:

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



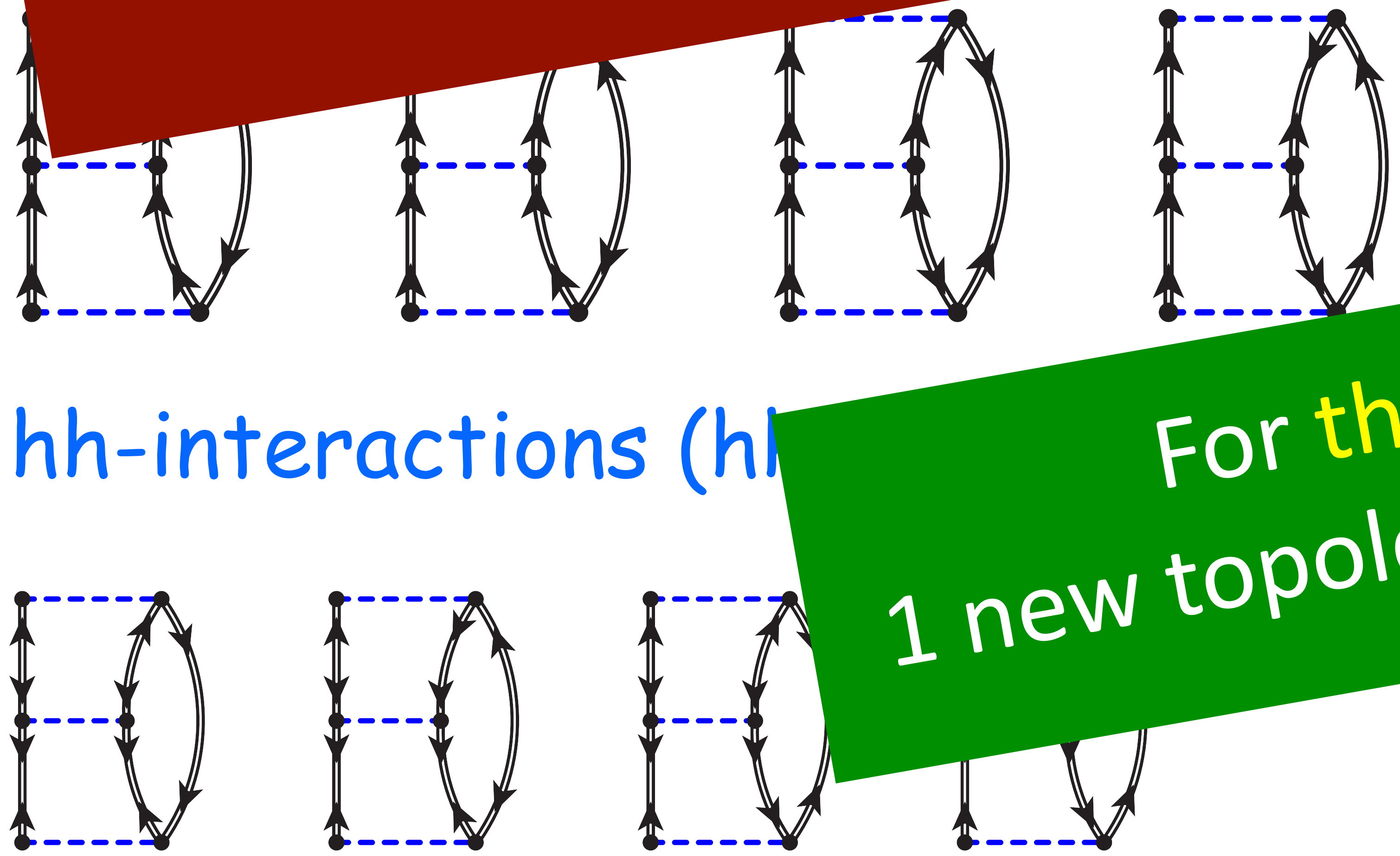
Just ONE topology at 2nd and 3rd order!
(2-body forces only)

ph-rings:

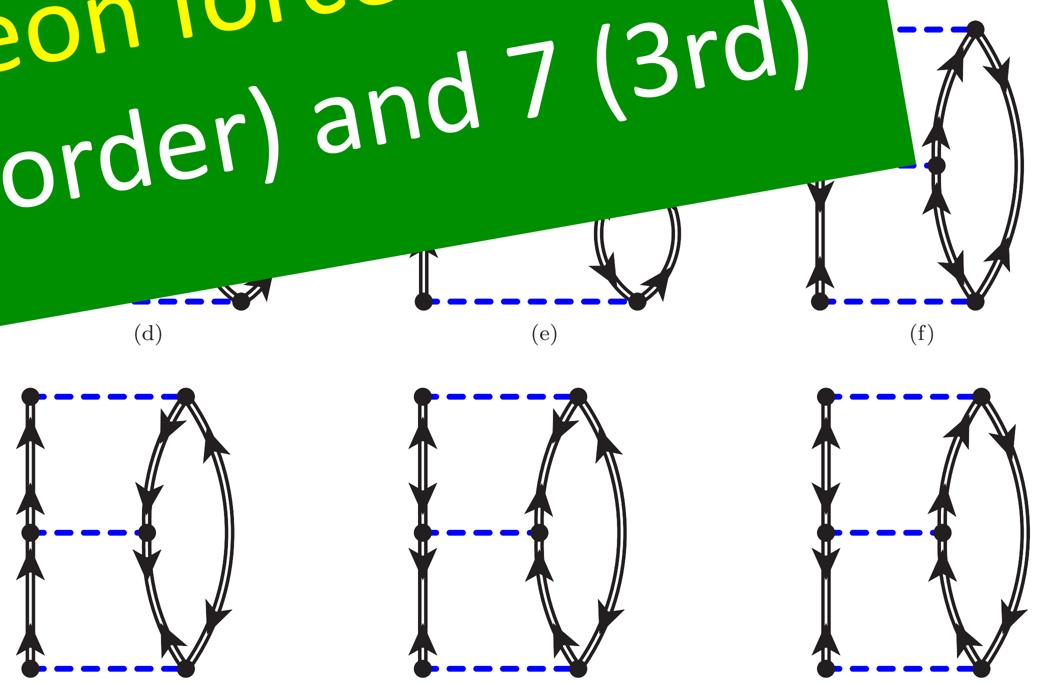


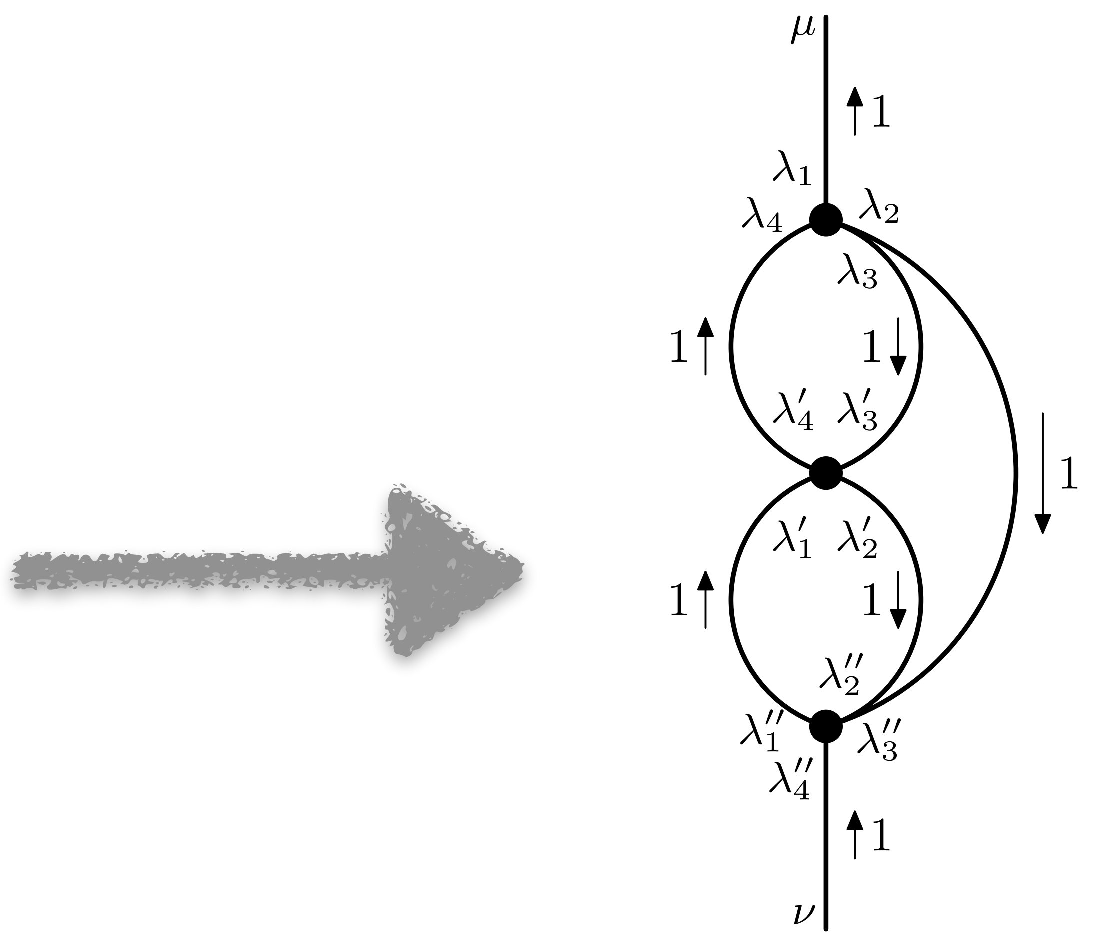
Gorkov at
3rd order:
(ONLY NN forces)

hh-interactions (hh



For three-nucleon forces:
1 new topology (2nd order) and 7 (3rd)

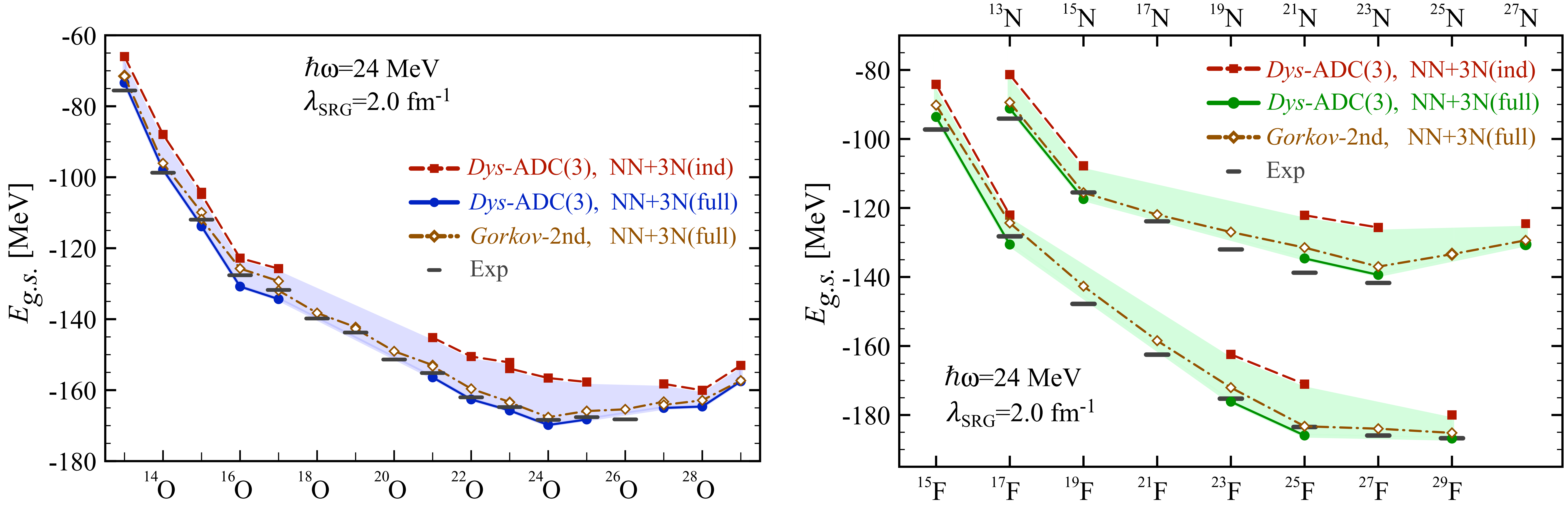




(NN ONLY forces)

Results for the N-O-F chains

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)
and Phys. Rev. C **92**, 014306 (2015)



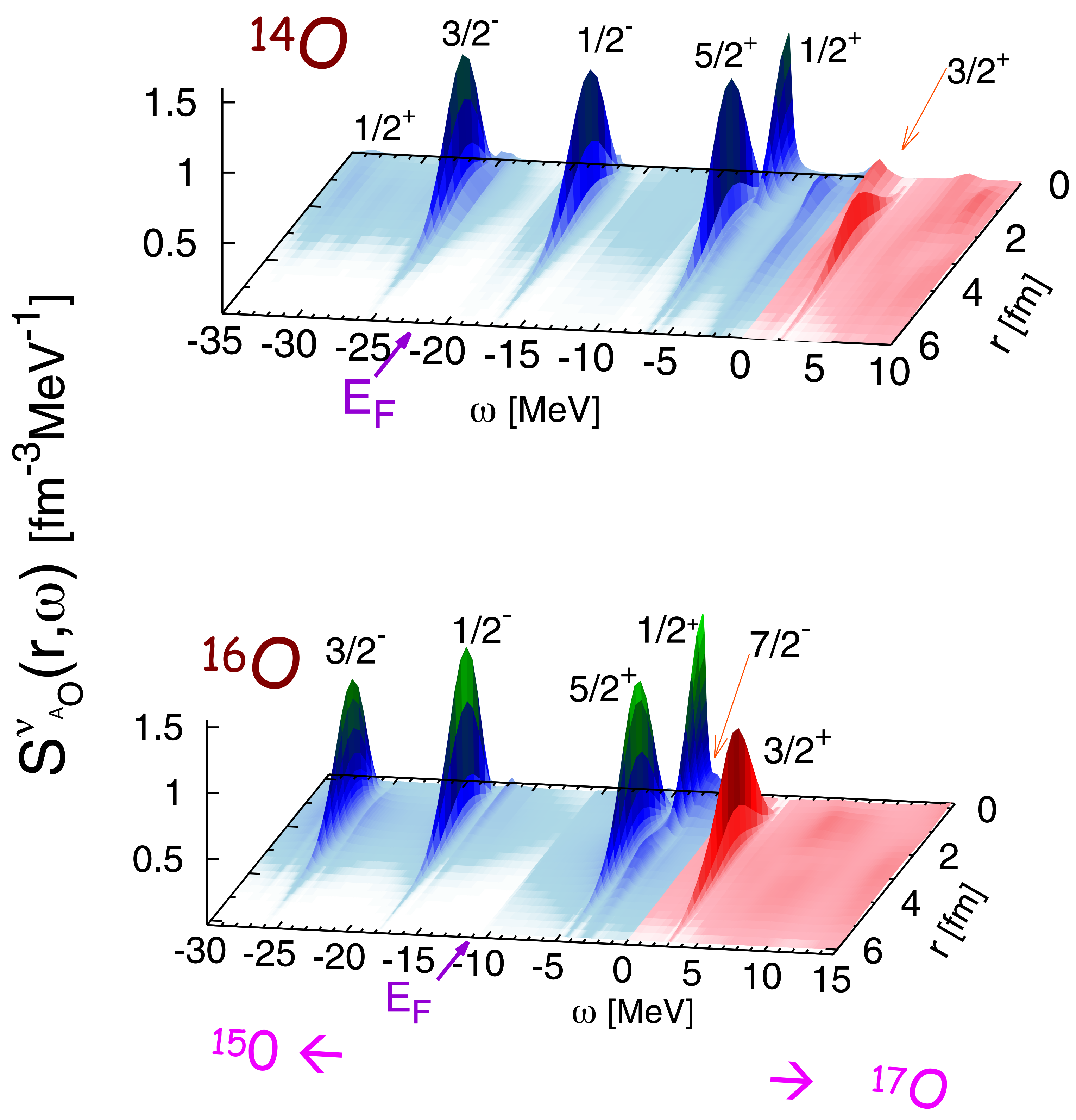
→ 3NF crucial for reproducing binding energies and driplines around oxygen

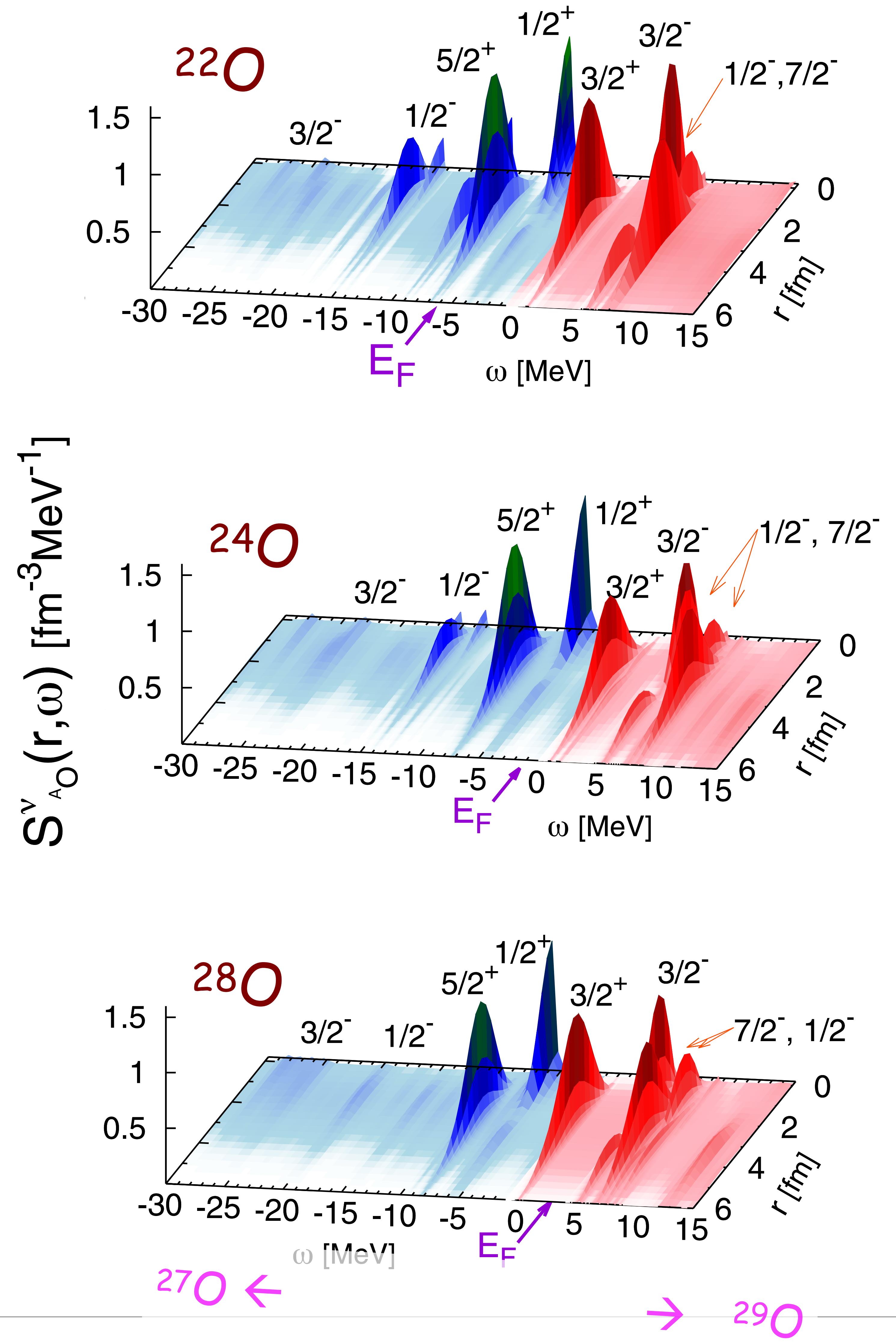
→ cf. microscopic shell model [Otsuka et al, PRL**105**, 032501 (2010).]

N3LO (Λ = 500Mev/c) chiral NN interaction evolved to 2N + 3N forces (2.0fm^{-1})
N2LO (Λ = 400Mev/c) chiral 3N interaction evolved (2.0fm^{-1})

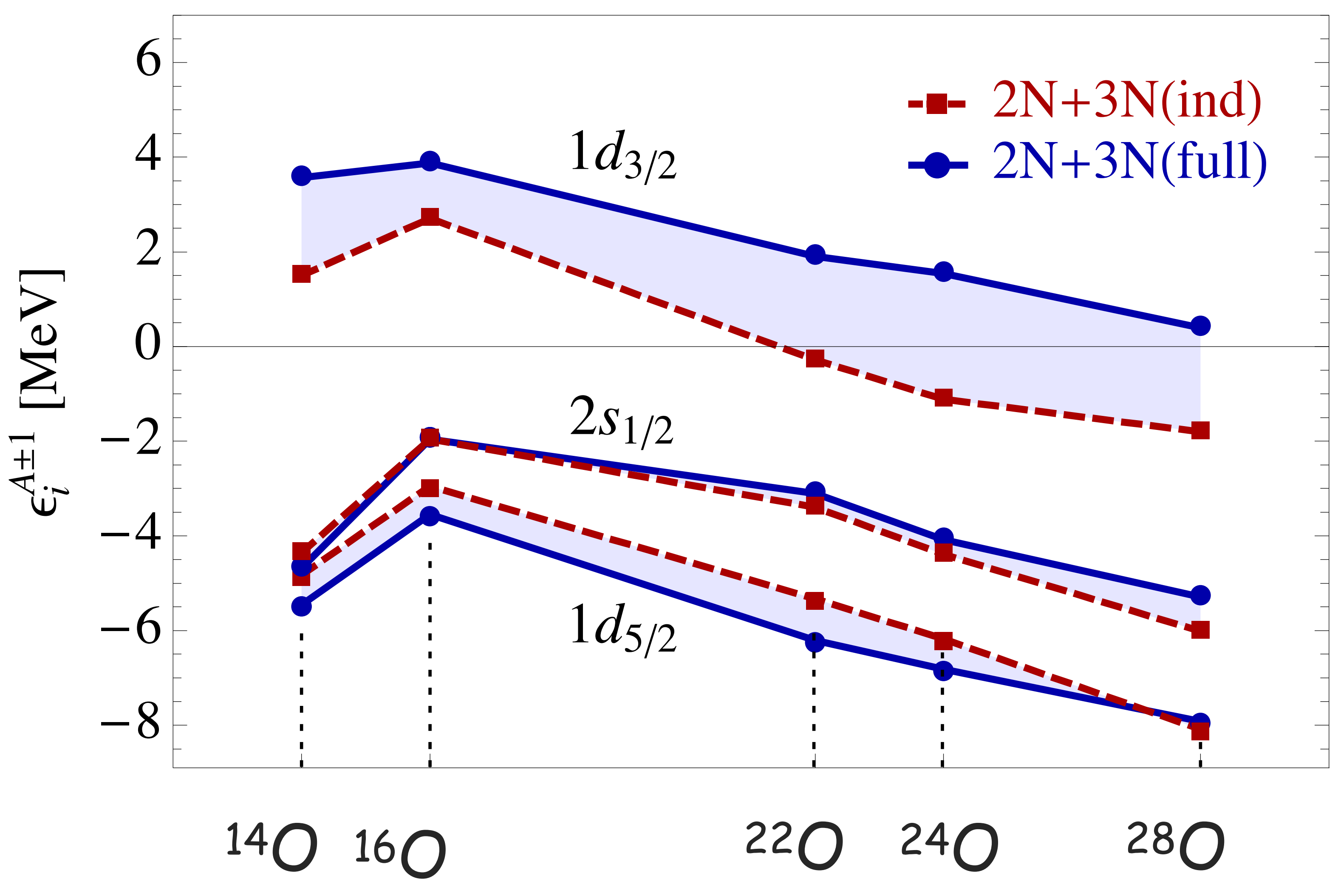
Neutron spectral function of Oxygens

A. Cipollone, CB, P. Navrátil, *Phys. Rev. C* **92**, *014306 (2015)*



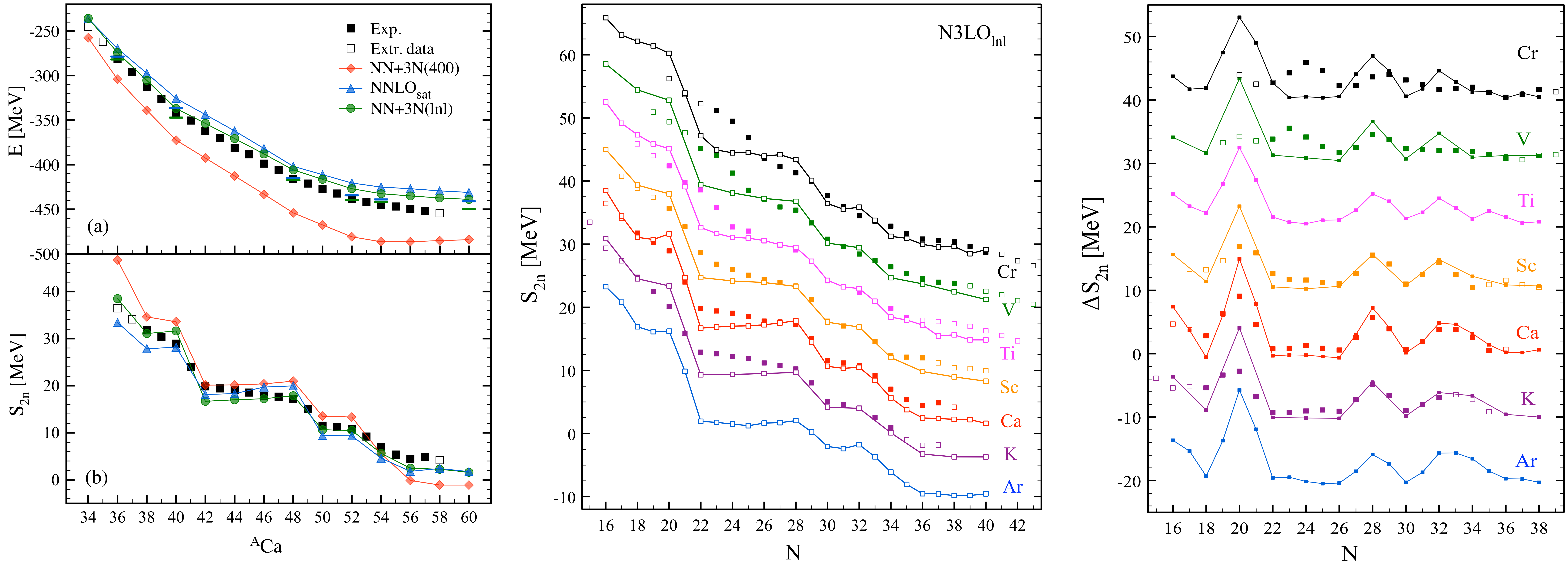


Neutron quasiparticle energies



N3LO(500) + nln 3NF

SCGF – Gorkov-ADC(2)

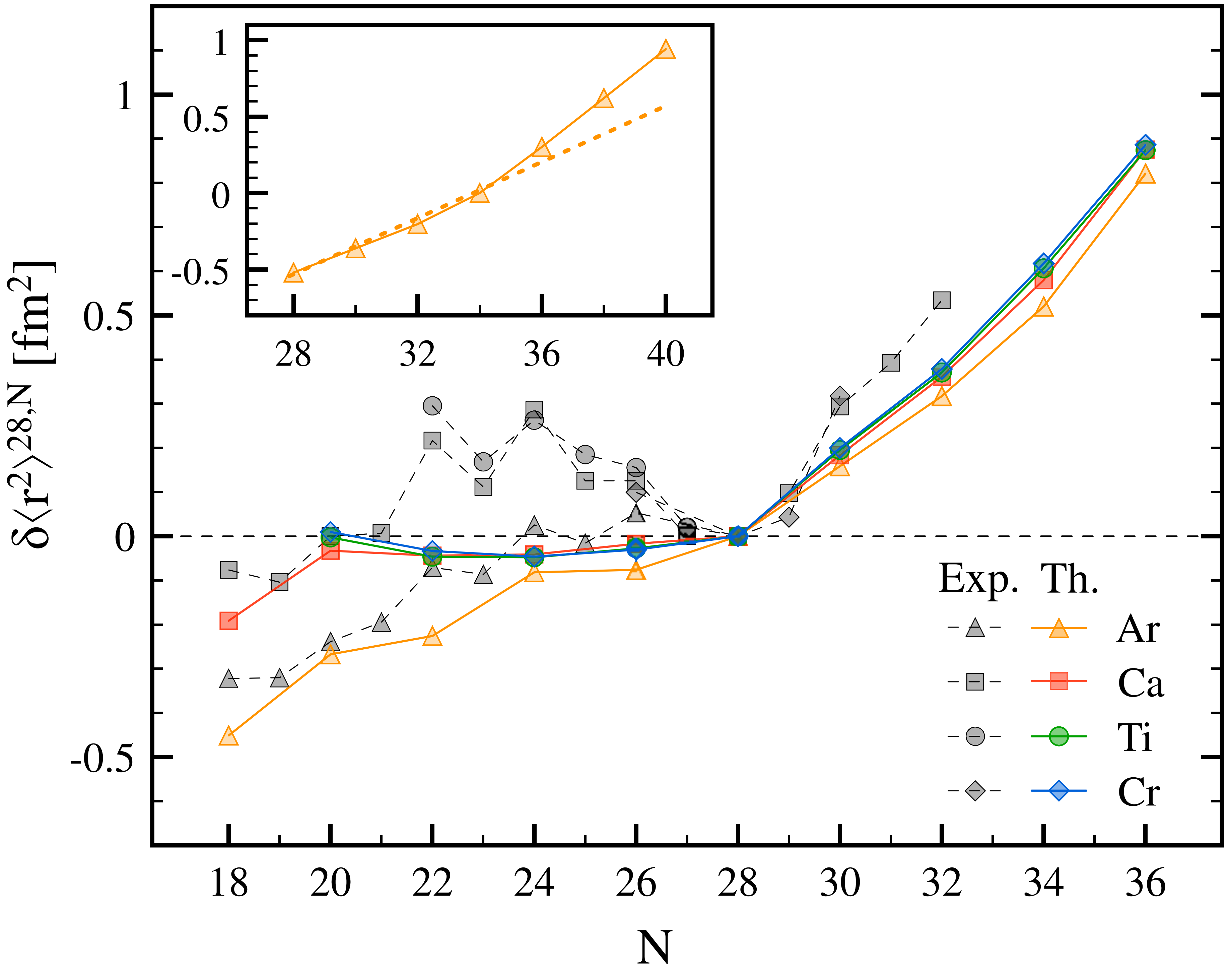


V. Somà, P. Navrátil, F. Raimondi, CB, T. Duguet – Phys. Rev. C**101**, 014318 (2020)

Eur. Phys. J. A**57** 135 (2021)

N3LO(500) + nln 3NF

SCGF – Gorkov-ADC(2)



- Bell-shaped behaviour in Ca40-48 requires particle-vibration coupling [ADC(3), FRPA]
- Universal behaviour of isotope shifts beyond N=28 neutrons
  (invariance on 20<Z<28)

V. Somà, P. Navrátil, CB, T. Duguet – Eur. Phys. J. A**57** 135 (2021)

N3LO(500) + nln 3NF

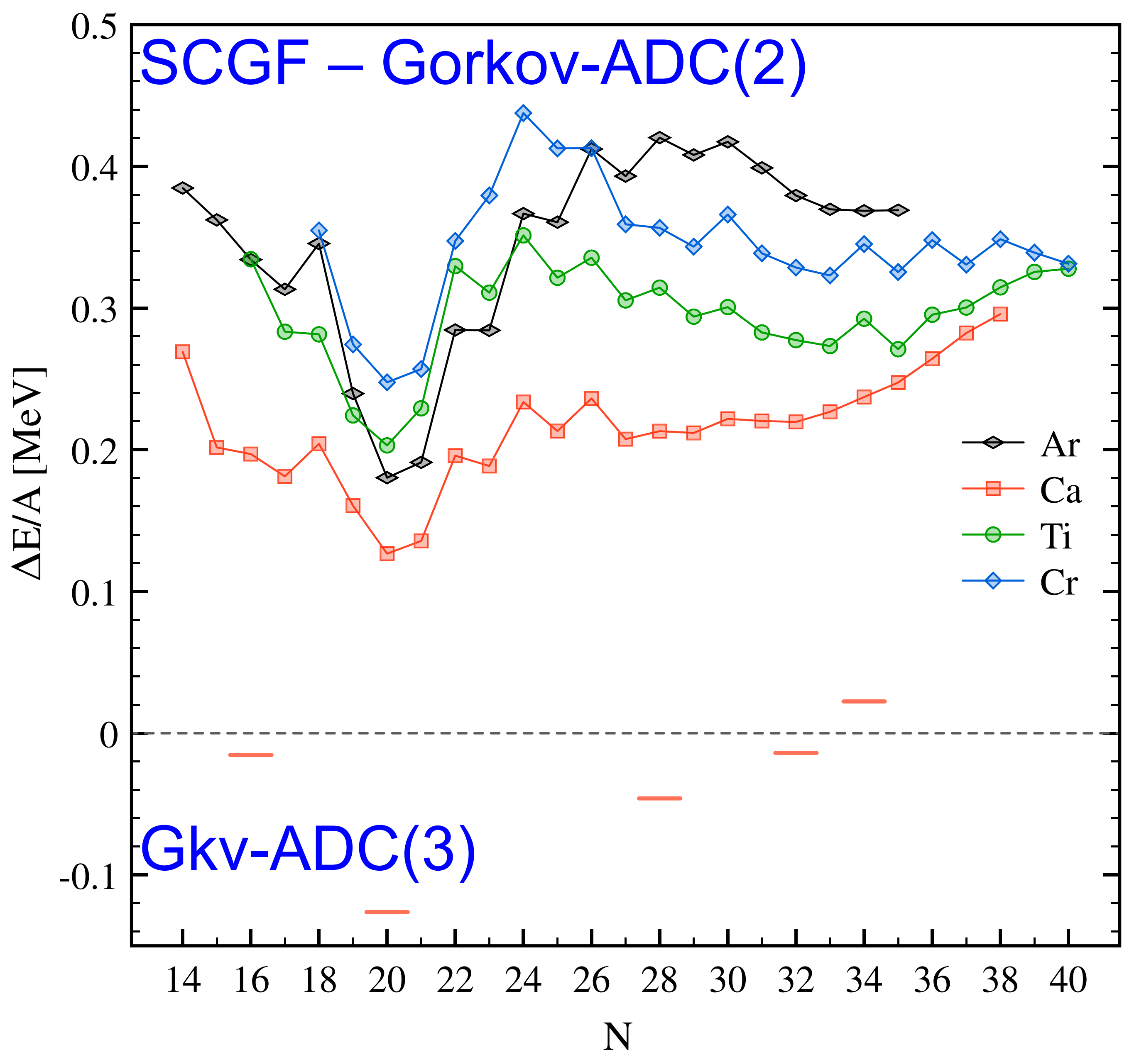
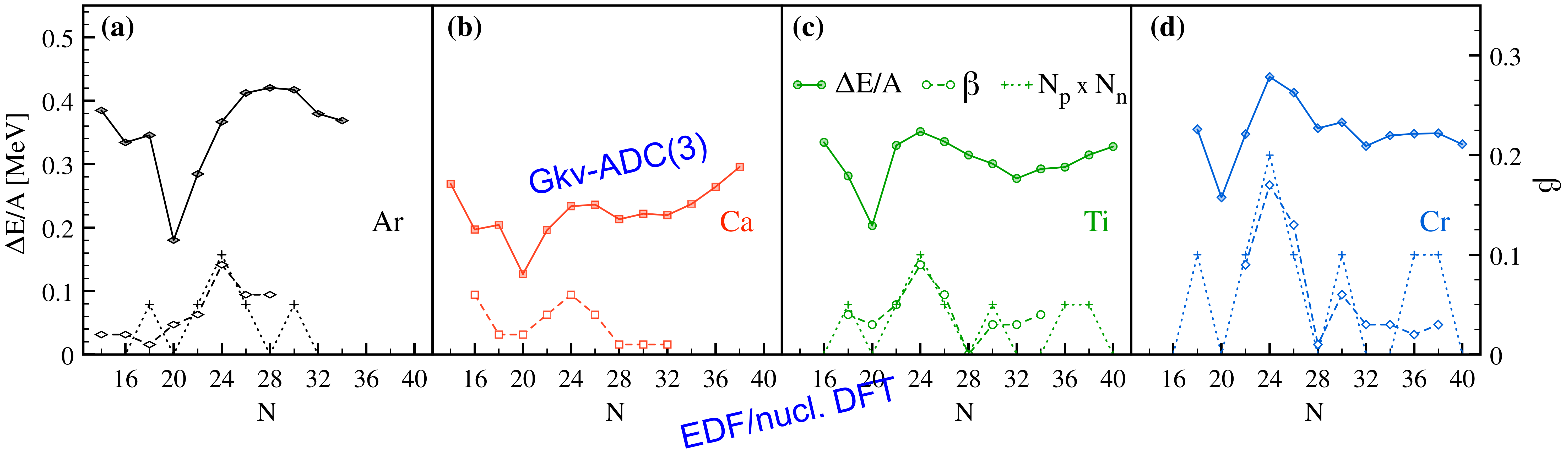


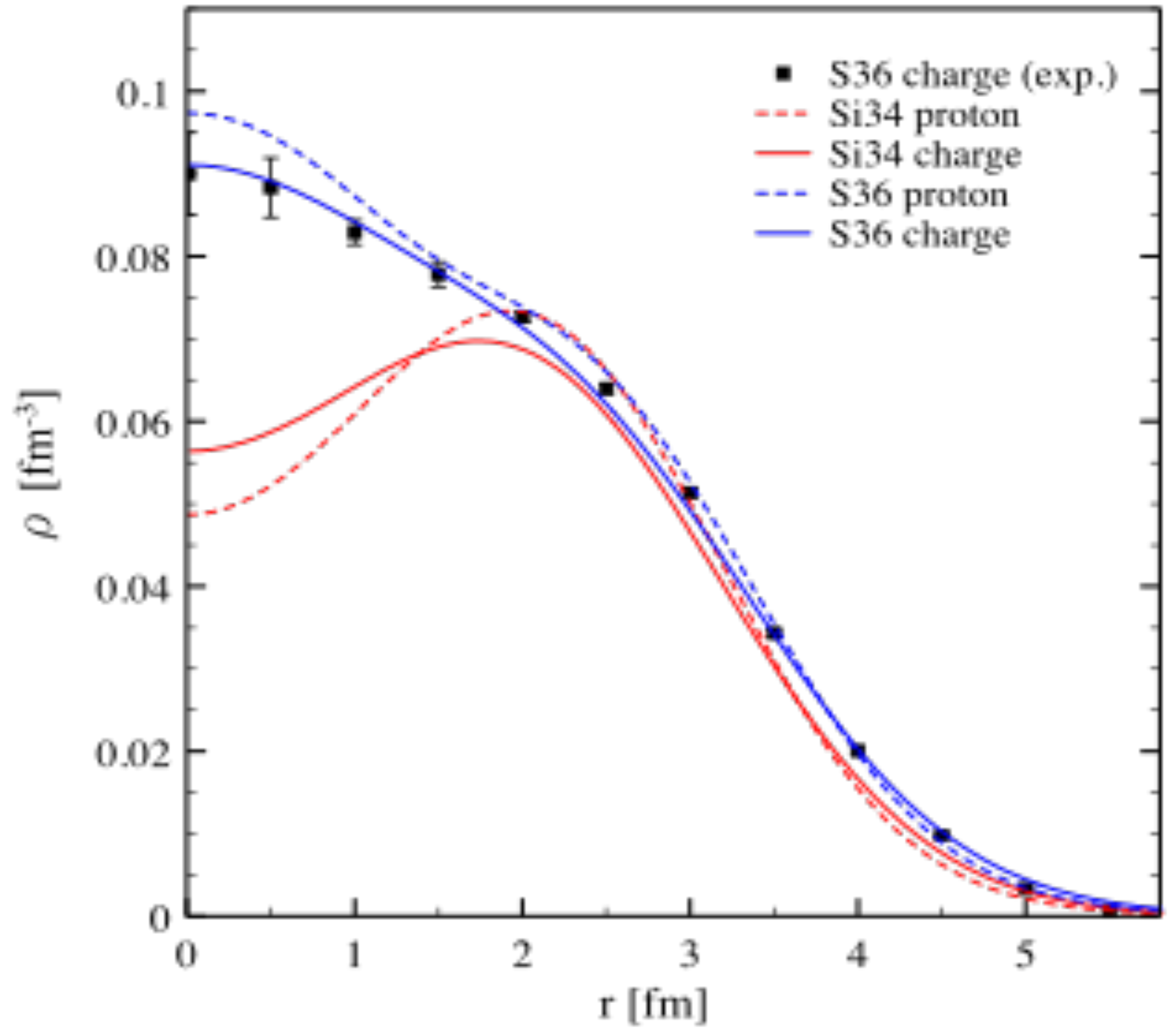
Fig. 8 Relative ADC(2) errors (theory-experiment) on total binding energies per nucleon along $Z = 18, 20, 22$ and 24 isotopic chains. ADC(3) errors are also reported for doubly closed-shell calcium isotopes and displayed as horizontal bars. Calculations and experimental data are taken from Fig. 1

- Accuracy for binding energies requires ADC(3)
- Larger discrepancies



V. Somà, P. Navrátil, CB, T. Duguet – Eur. Phys. J. A**57** 135 (2021)

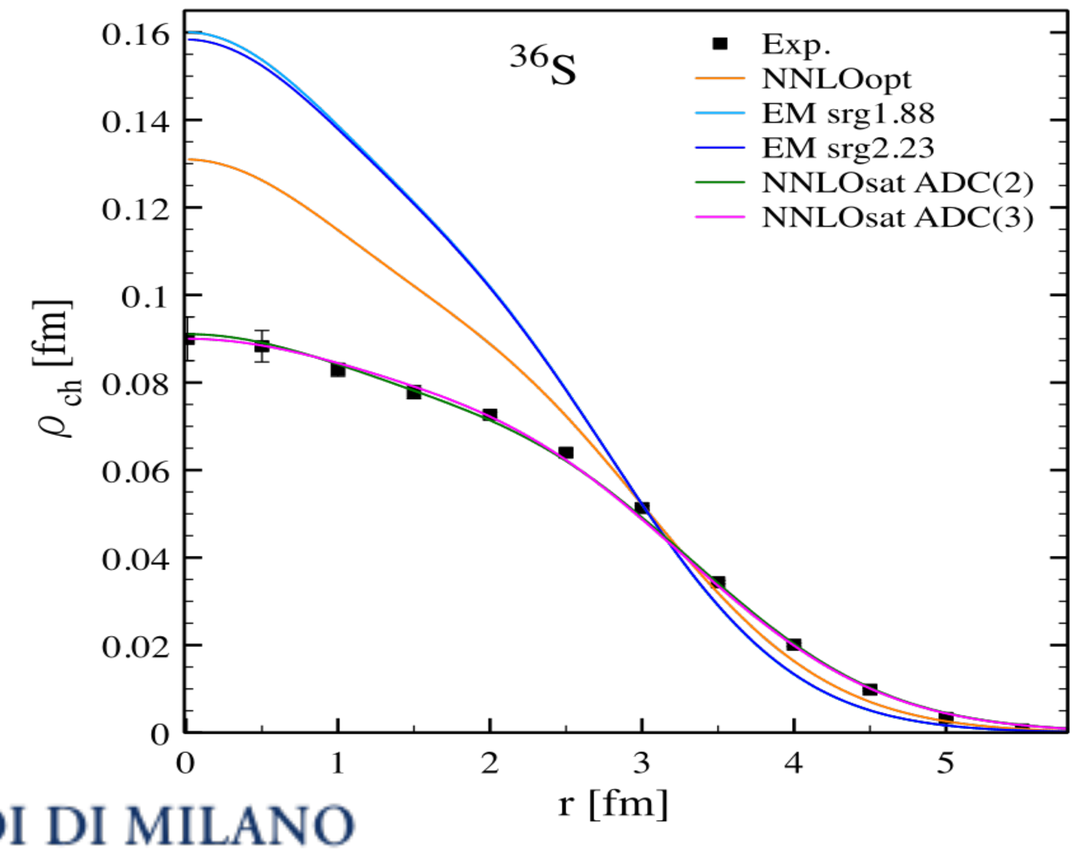
Bubble nuclei... ^{34}Si prediction

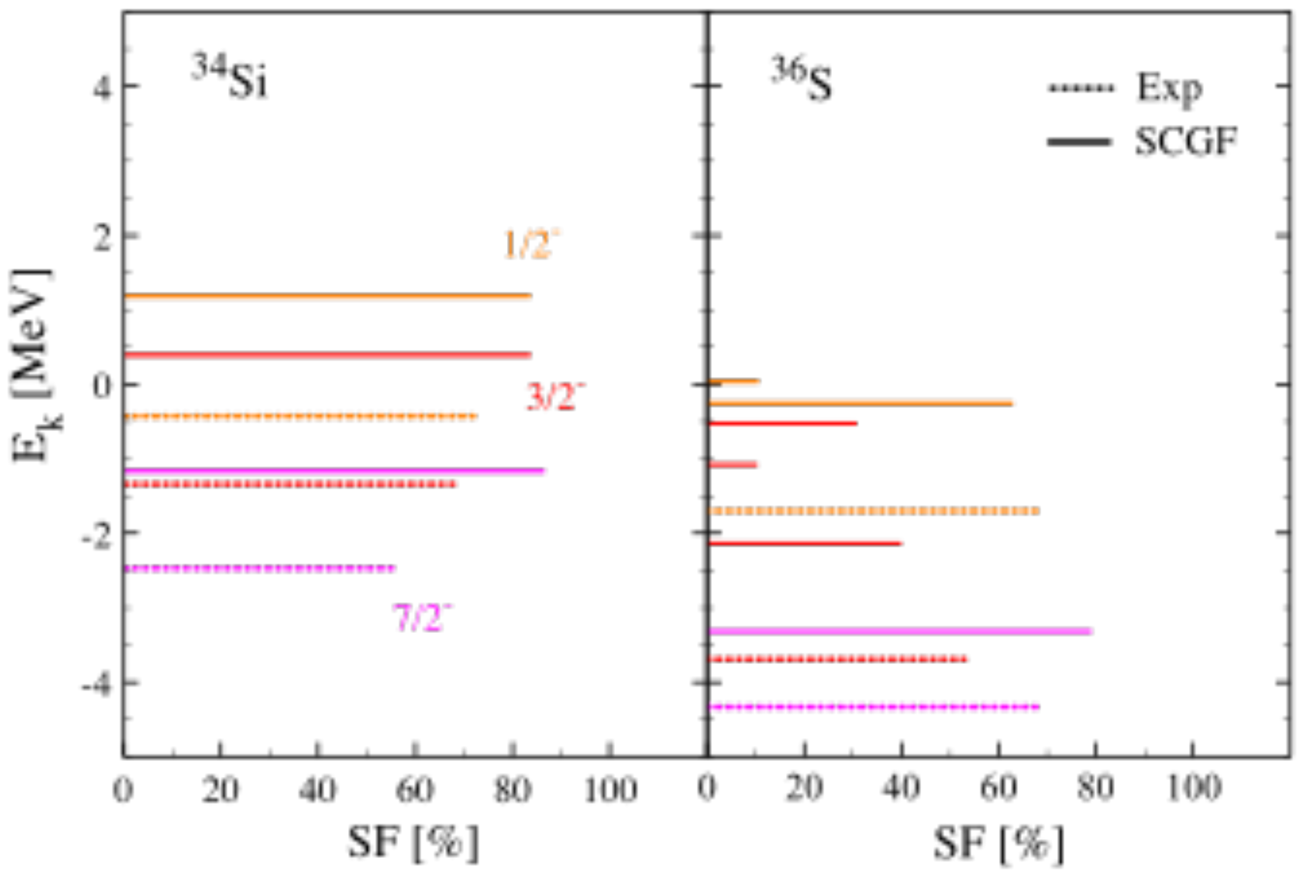


Duguet, Somà, Lecuse, CB, Navrátil,
Phys.Rev. C**95**, 034319 (2017)

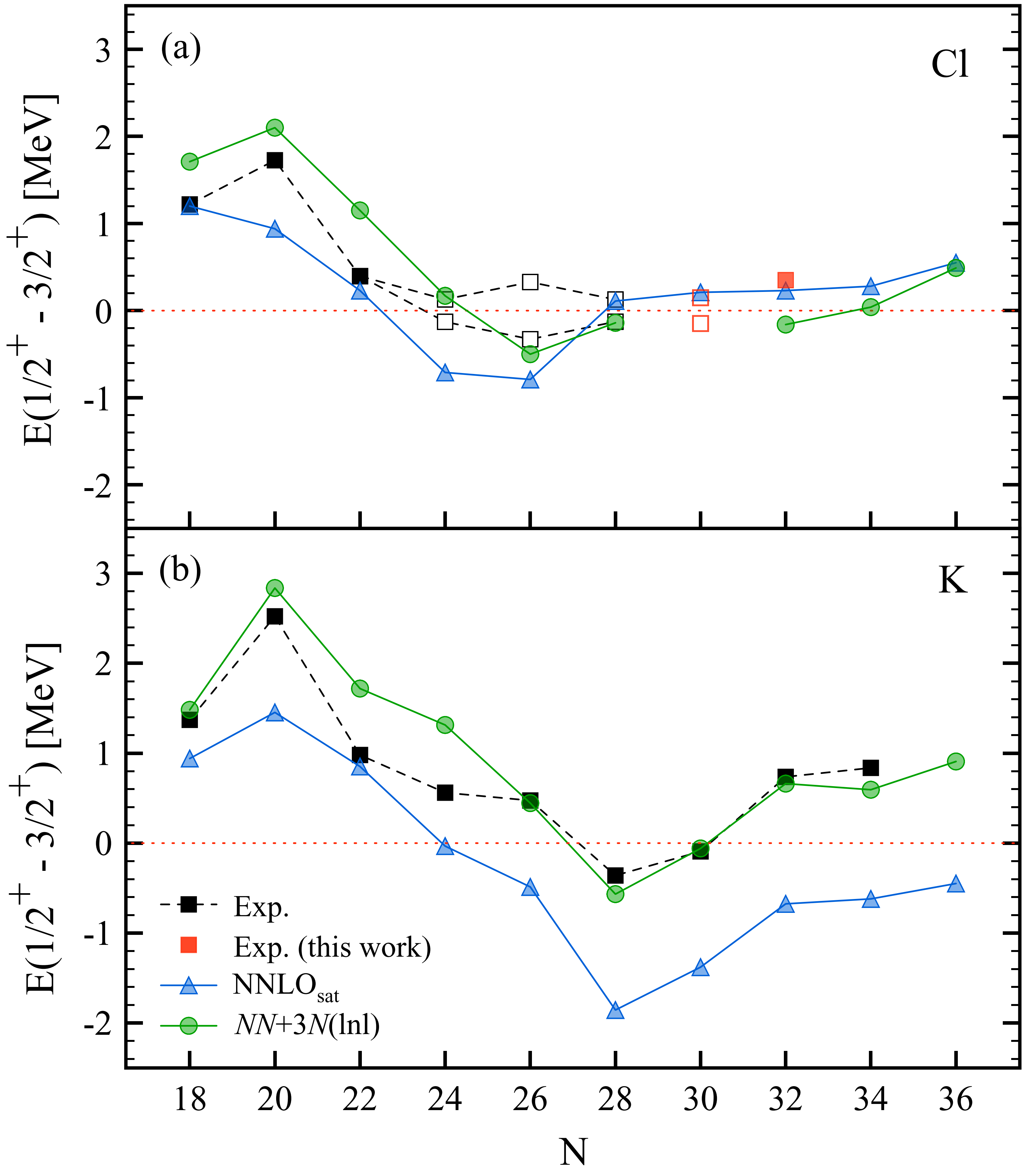
- ^{34}Si is unstable, charge distribution is still unknown
- Suggested central depletion from mean-field simulations
- Ab-initio theory confirms predictions
- Other theoretical and experimental evidence:
  Phys. Rev. ***C 79****, 034318 (2009),*
  Nature Physics ***13****, 152–156 (2017).*

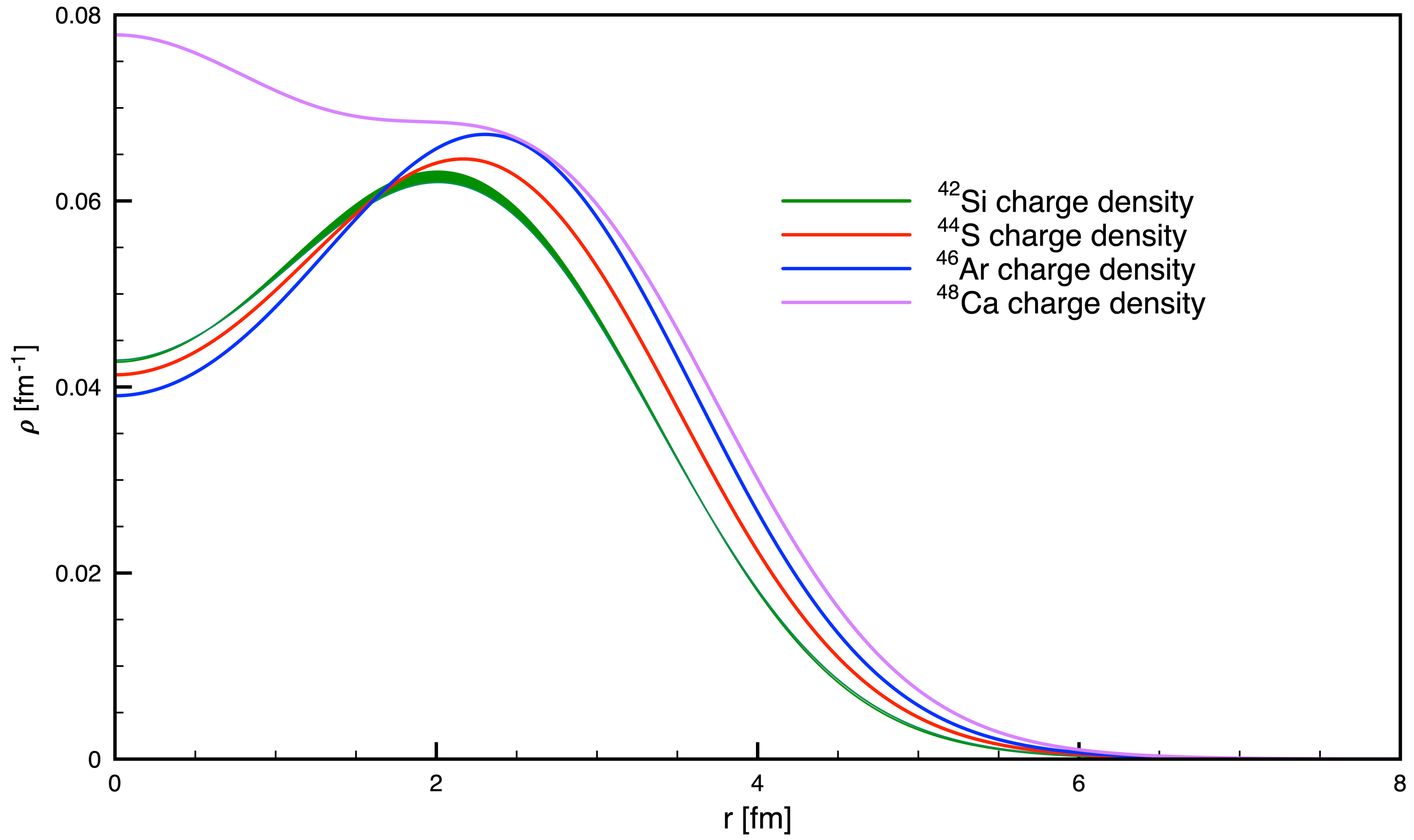
Validated by charge distributions and neutron quasiparticle spectra:





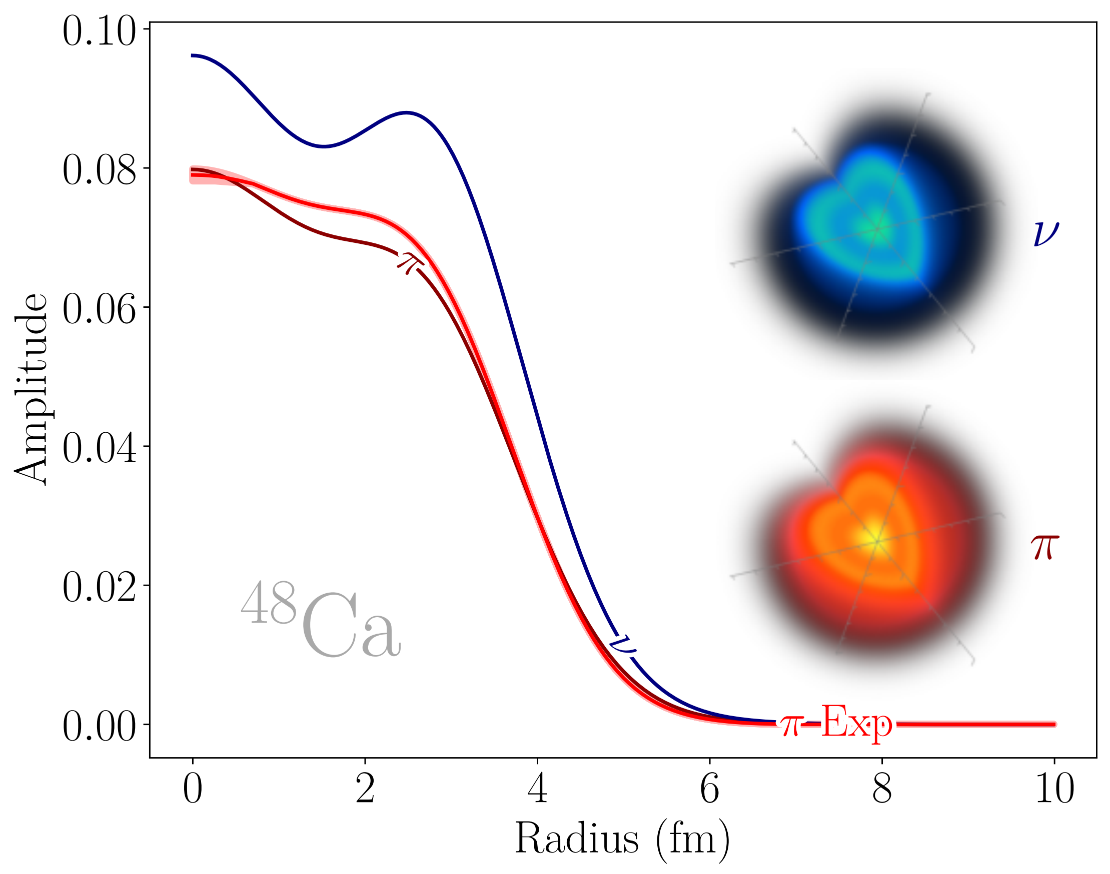
$d_{3/2}$ — $s_{1/2}$ inversion of protons and bubbles at N=28

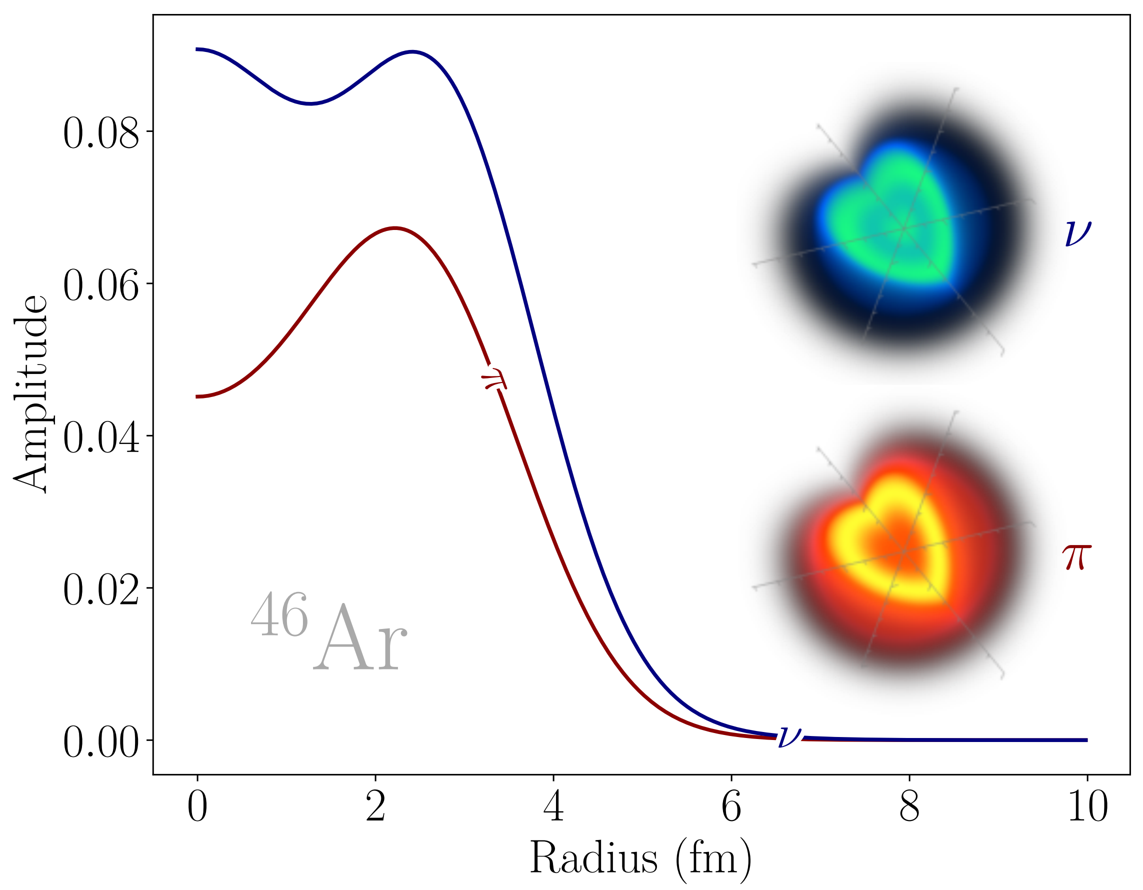




S. Brolli (BSc thesis)
CB

Charge bubble for ^{42}Si-^{46}Ar ??





D. Brugnara (PhD thesis) — GANIL

Papuga et al., PRL**110**, 172503 (2013); PRC**90**, 034321 (2014)
RIKEN, SEASTAR coll., Phys. Lett. **B802** 135215 (2020)
Linh, Gillibert, et al., PRC**104**, 044331 (2021)

Electron-Ion Trap colliders…

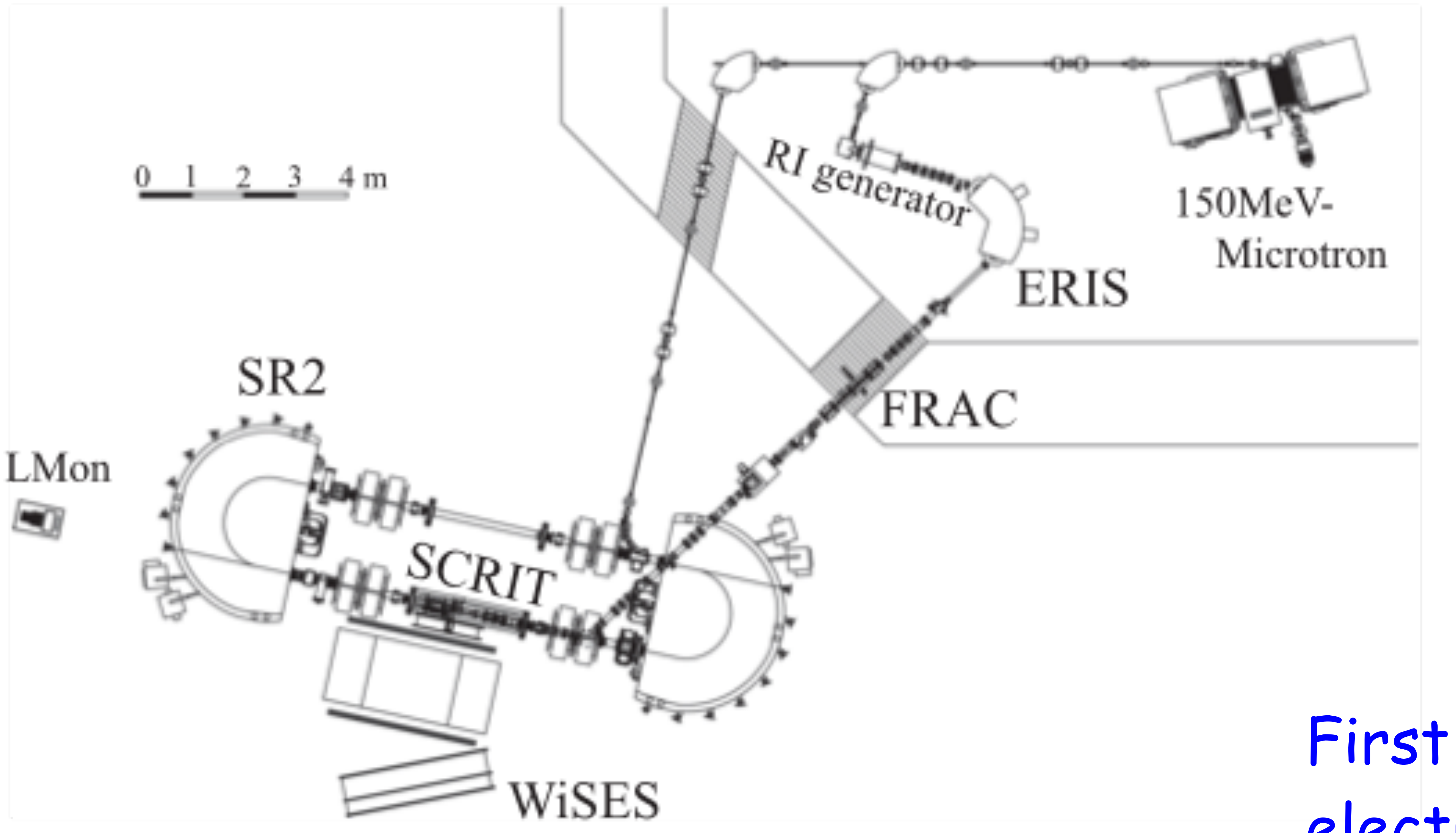


FIG. 1. Overview of the SCRIT electron scattering facility.

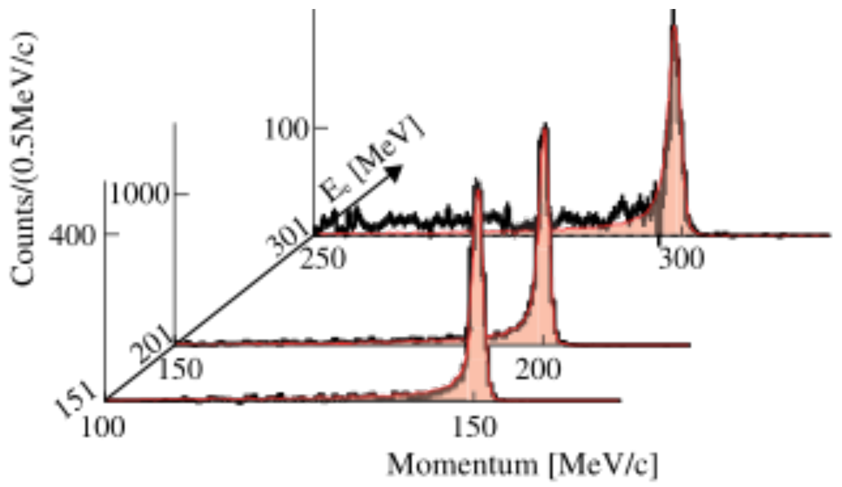
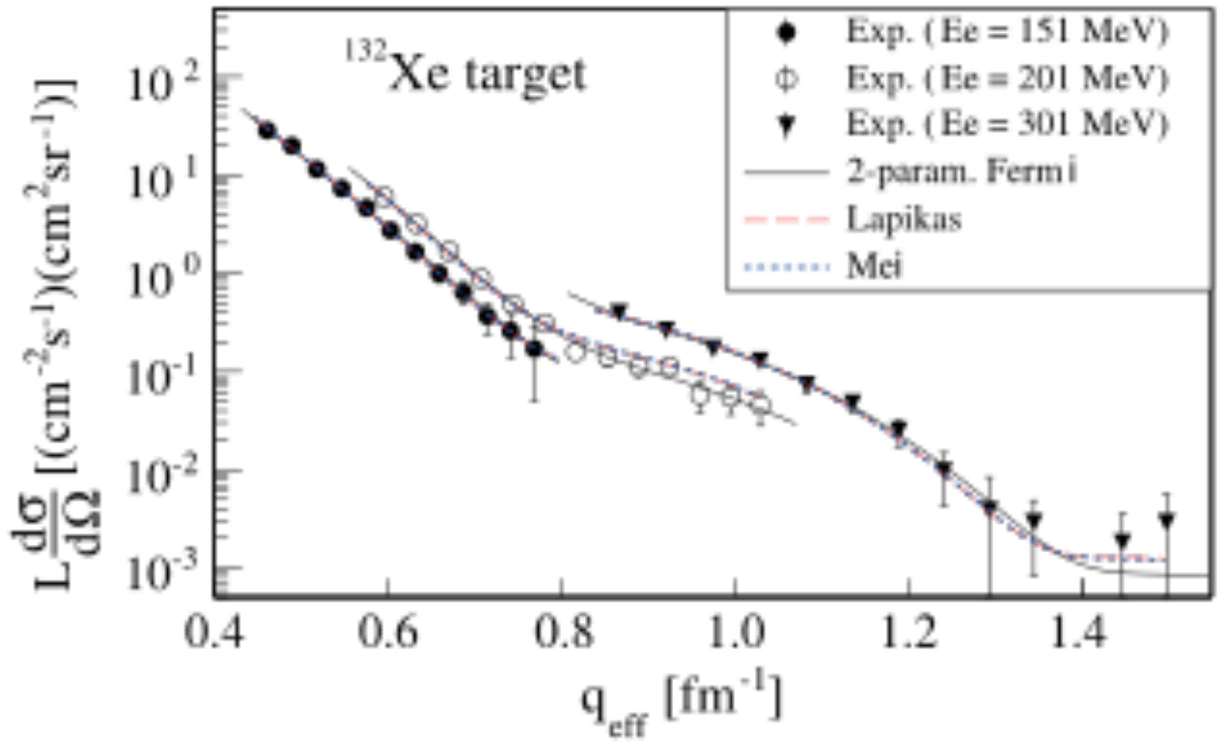


FIG. 3. Reconstructed momentum spectra of ^{132}Xe target after background subtraction. Red shaded lines are the simulated radiation tails following the elastic peaks.

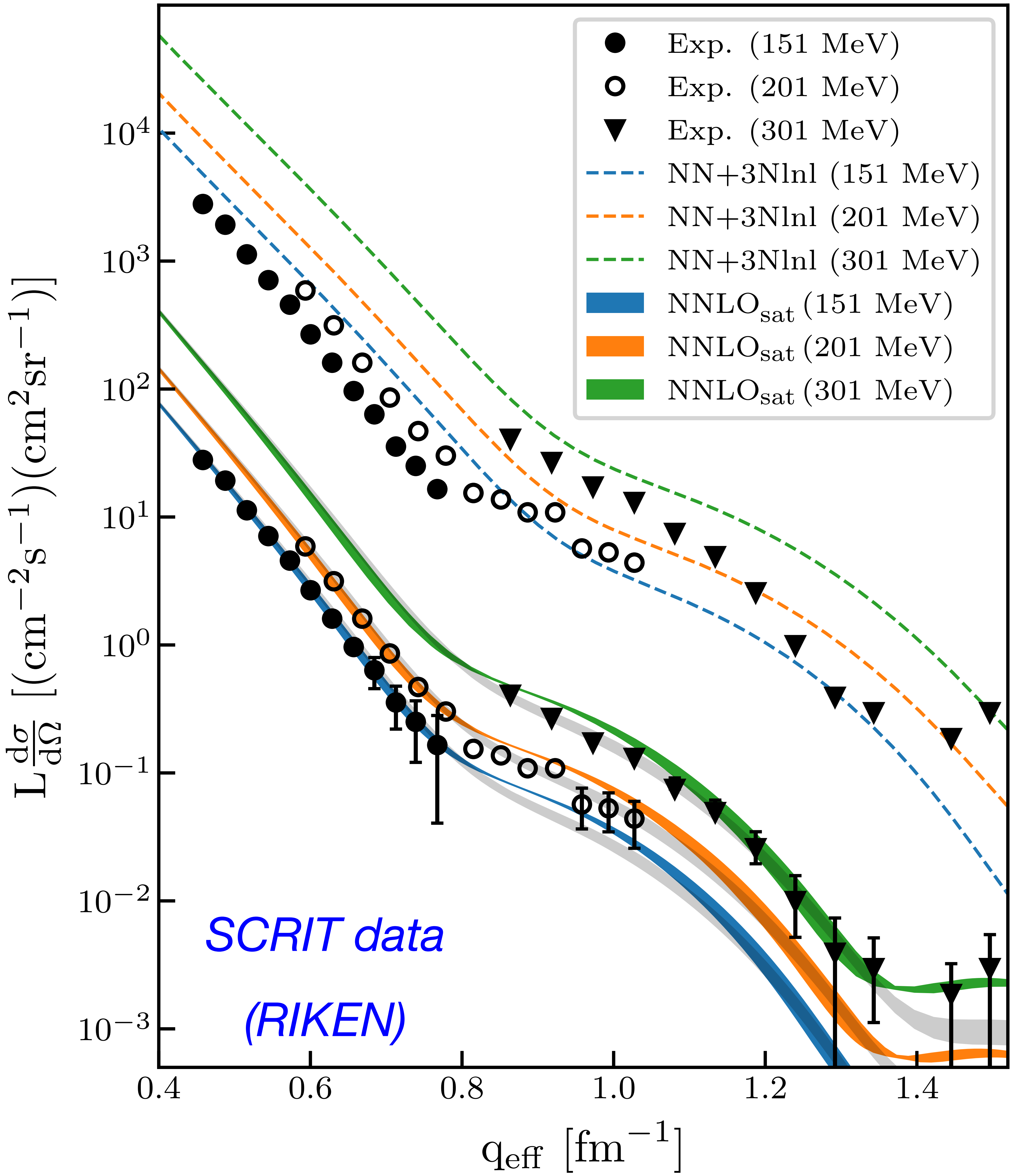


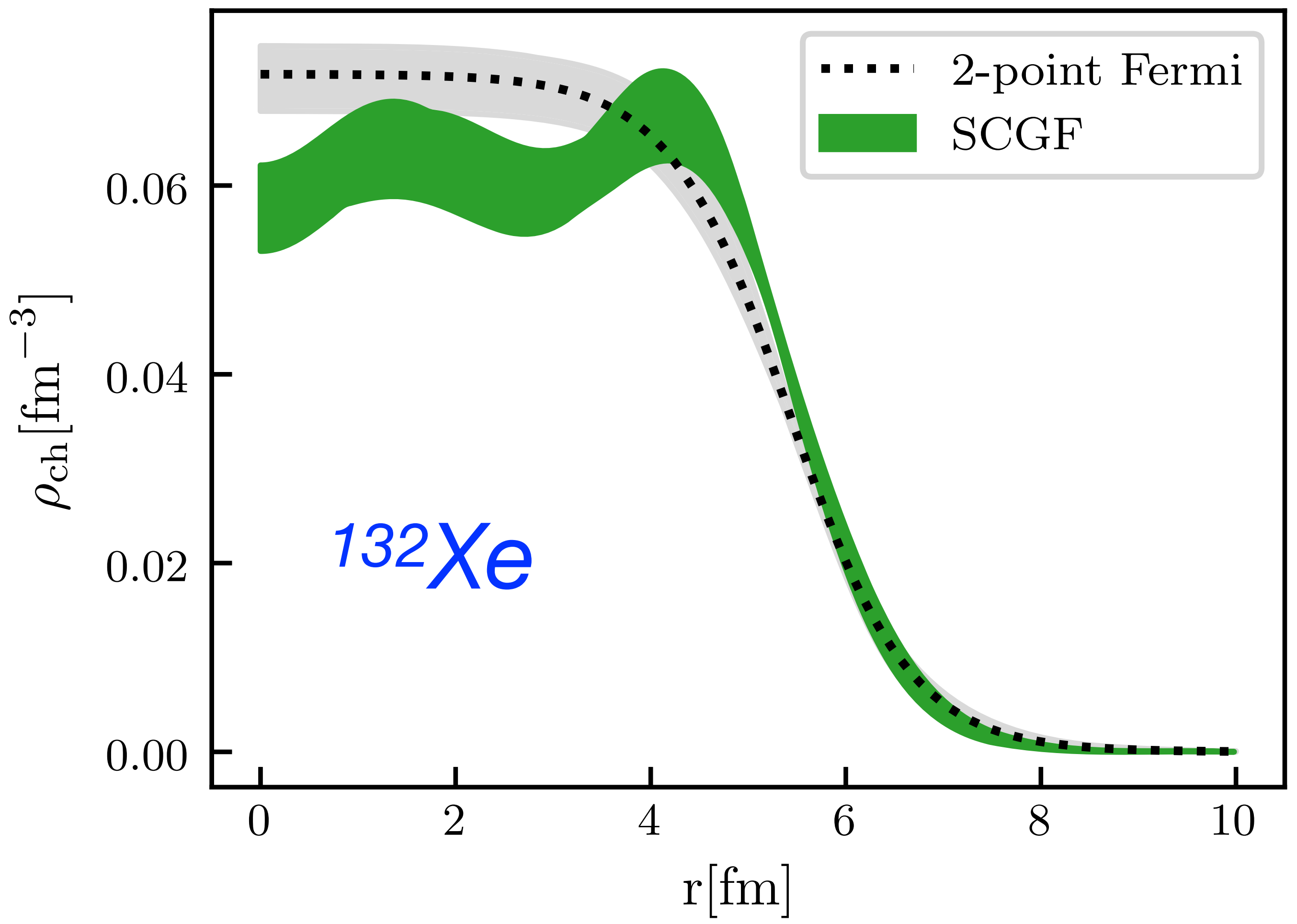
First ever measurement of charge radii through electron scattering with and ion trap setting that can be used on radioactive isotopes !!

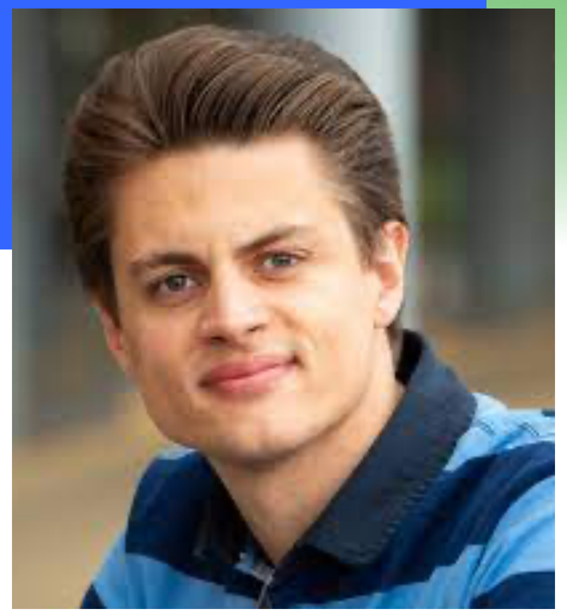
K. Tsukada *et al.*, Phy rev Lett **118**, 262501 (2017)

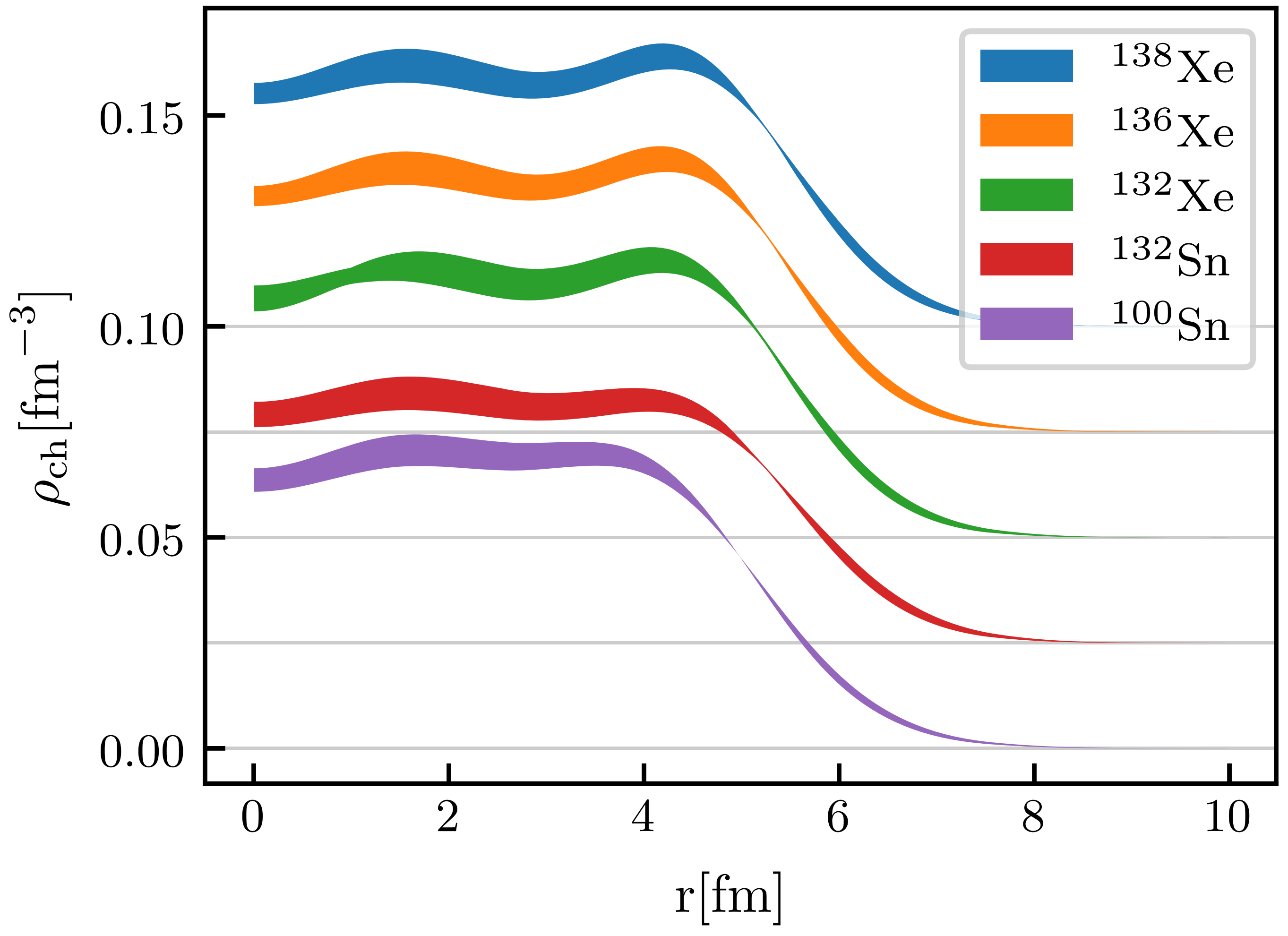
P. Arthuis, CB, M. Vorabbi, P. Finelli, Phys. Rev. Lett. ***125****, 182501 (2020)*

Charge density for Sn and Xe isotopes









	SCGF	Exp.
^{100}Sn	4.525 – 4.707	
^{132}Sn	4.725 – 4.956	4.7093
^{132}Xe	4.700 – 4.948	4.7859
^{136}Xe	4.715 – 4.928	4.7964
^{138}Xe	4.724 – 4.941	4.8279

*P. Arthuis, CB, M. Vorabbi, P. Finelli, Phys. Rev. Lett. **125**, 182501 (2020)*

Gorkov ADC(2) and Dyson ADC(3) with N3LO-lnl and NNLOsat Hamiltonians

Ab initio optical potentials from propagator theory

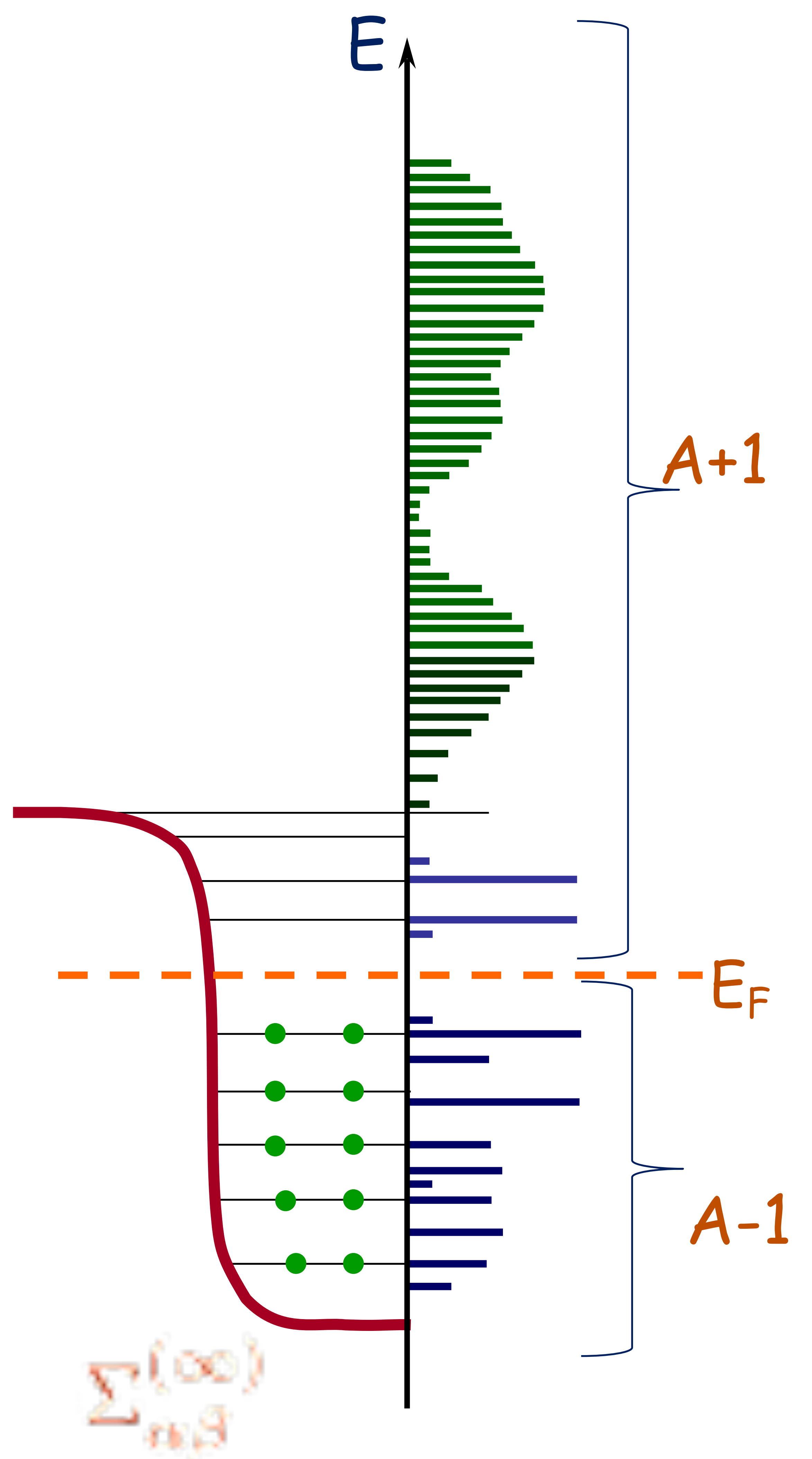
Relation to Fesbach theory:
Mahaux & Sartor, Adv. Nucl. Phys. 20 (1991)
Escher & Jennings Phys. Rev. C**66**, 034313 (2002)

Previous SCGF work:
CB, B. Jennings, Phys. Rev. C**72**, 014613 (2005)
S. Waldecker, CB, W. Dickhoff, Phys. Rev. C**84**, 034616 (2011)
A. Idini, CB, P. Navrátil, Phys. Rv. Lett. **123**, 092501 (2019)
M. Vorabbi, CB, et al., in preparation

State-of-the-art of the field:

C. Hebborn, et al., CB, "*Optical potentials for the rare-isotope beam era*", arXiv:2210.07293 (WP)
Jour. Phys. G (2023), in press.

Microscopic optical potential



Nuclear self-energy $\Sigma^\star(\mathbf{r},\mathbf{r}';\varepsilon)$:

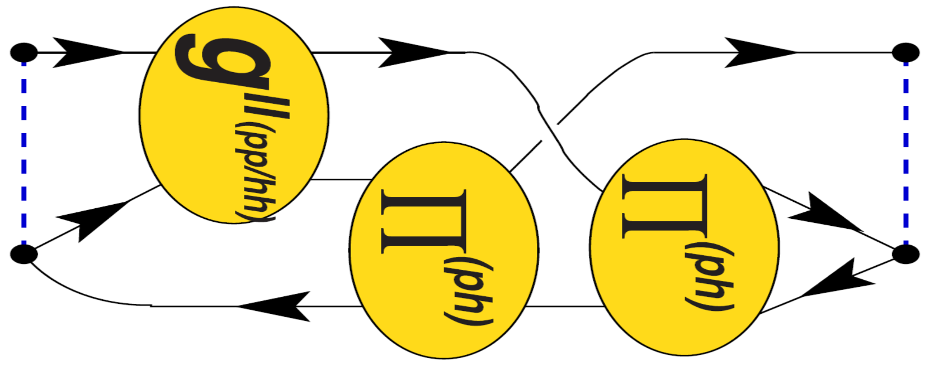
- contains *both particle* and *hole* props.
- it is proven to be a Feshbach opt. pot → in general it is *non-local !*

$$\Sigma^\star_{\alpha\beta}(\omega) = \Sigma^{(\infty)}_{\alpha\beta} + \sum_{i,j}\mathbf{M}^\dagger_{\alpha,i}\left(\frac{1}{E-(\mathbf{K}^>+\mathbf{C})+i\Gamma}\right)_{i,j}\mathbf{M}_{j,\beta}$$

$$+\sum_{r,s}\mathbf{N}_{\alpha,r}\left(\frac{1}{E-(\mathbf{K}^<+\mathbf{D})-i\Gamma}\right)_{r,s}\mathbf{N}^\dagger_{s,\beta}$$

mean-field

Particle-vibration couplings:



Solve scattering and overlap functions directly in momentum space:

$$\Sigma^{\star\, l,j}(k,k';E) = \sum_{n,\,n'} R_{n\,l}(k)\,\Sigma^{\star\, l,j}_{n,\,n'}\,R_{n\,l}(k')$$

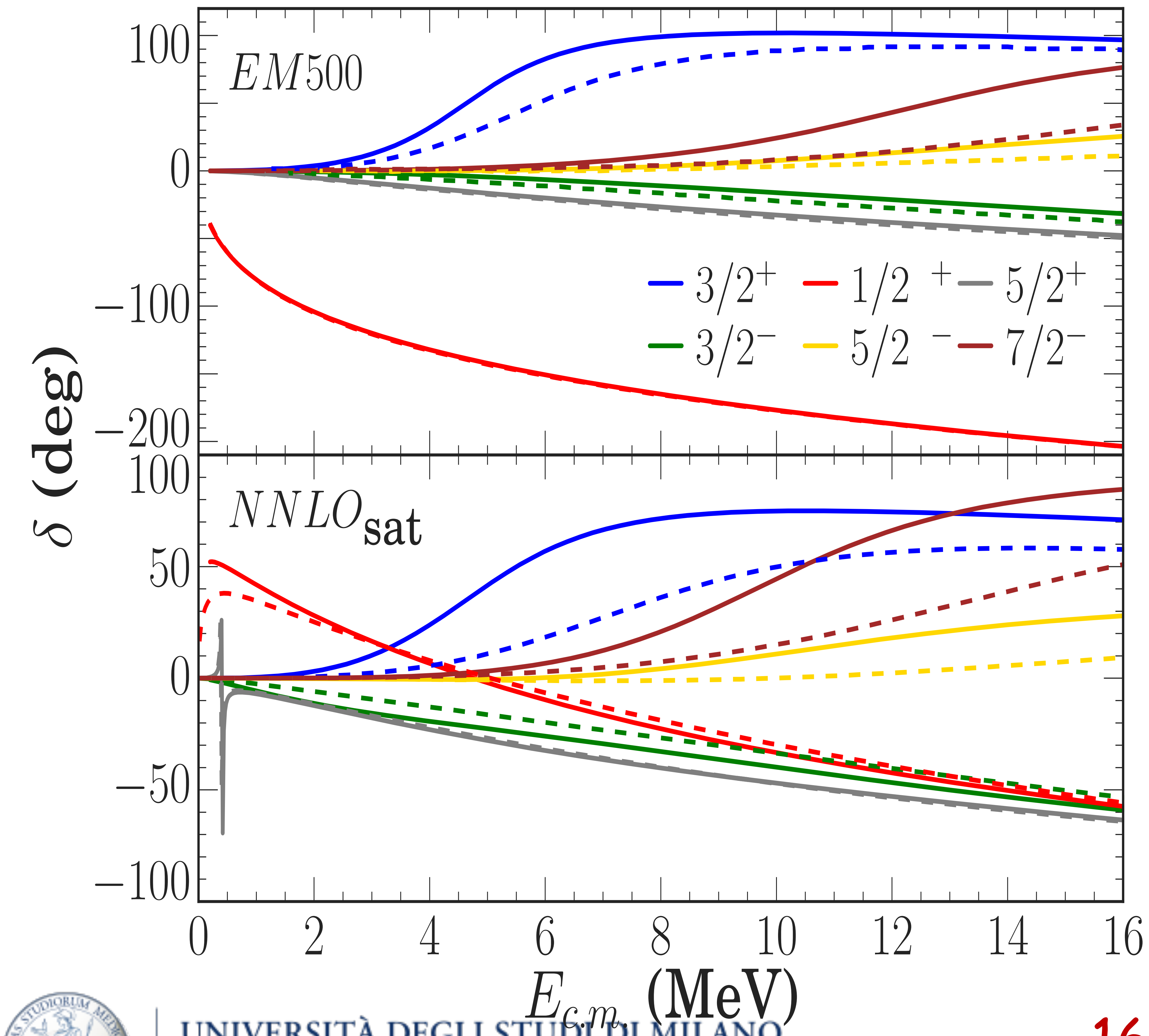
$$\frac{k^2}{2\mu}\psi_{l,j}(k) + \int \mathrm{d}k'\,k'^2\,\Sigma^{\star l,j}(k,k';E_{c.m.})\psi_{l,j}(k') = E_{c.m.}\psi_{l,j}(k)$$

Low energy scattering – from SCGF

[A. Idini, CB, Navratil,
Phys. Rev. Lett. **123**, 092501 (2019)]

Benchmark with NCSM-based scattering.

Scattering from mean-field only:



NCSM/RGM [**without** core excitations]

EM500: NN-SRG λ_{SRG}= 2.66 fm^{-1}, Nmax=18 (IT)
[PRC**82**, 034609 (2010)]

NNLOsat: Nmax=8 (IT-NCSM)

SCGF [$\Sigma^{(\infty)}$ only], always Nmax=13

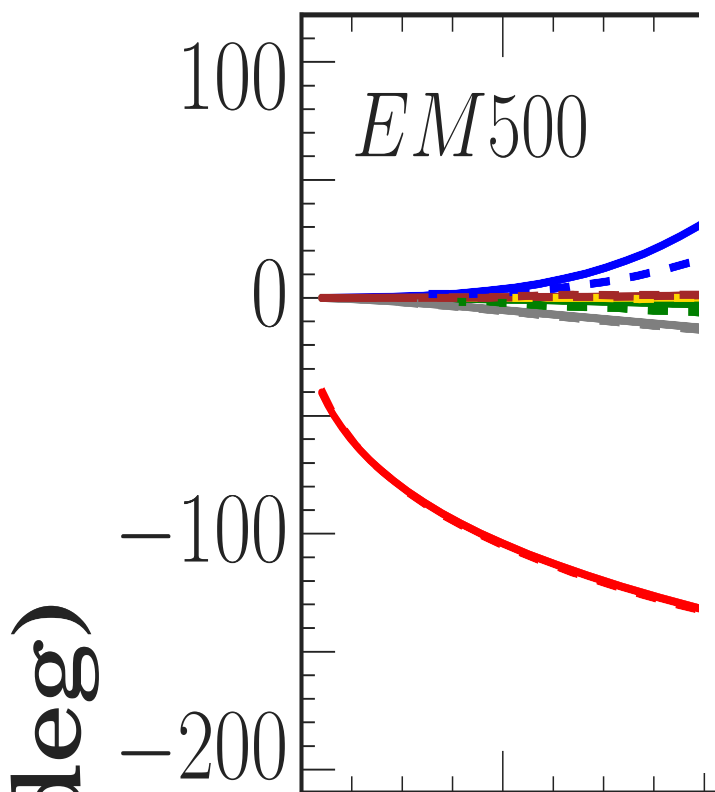
$^{16}O(n,n')^{16}O$

Low energy scattering – from SCGF

[A. Idini, CB, Navratil,
Phys. Rev. Lett. **123**, 092501 (2019)]

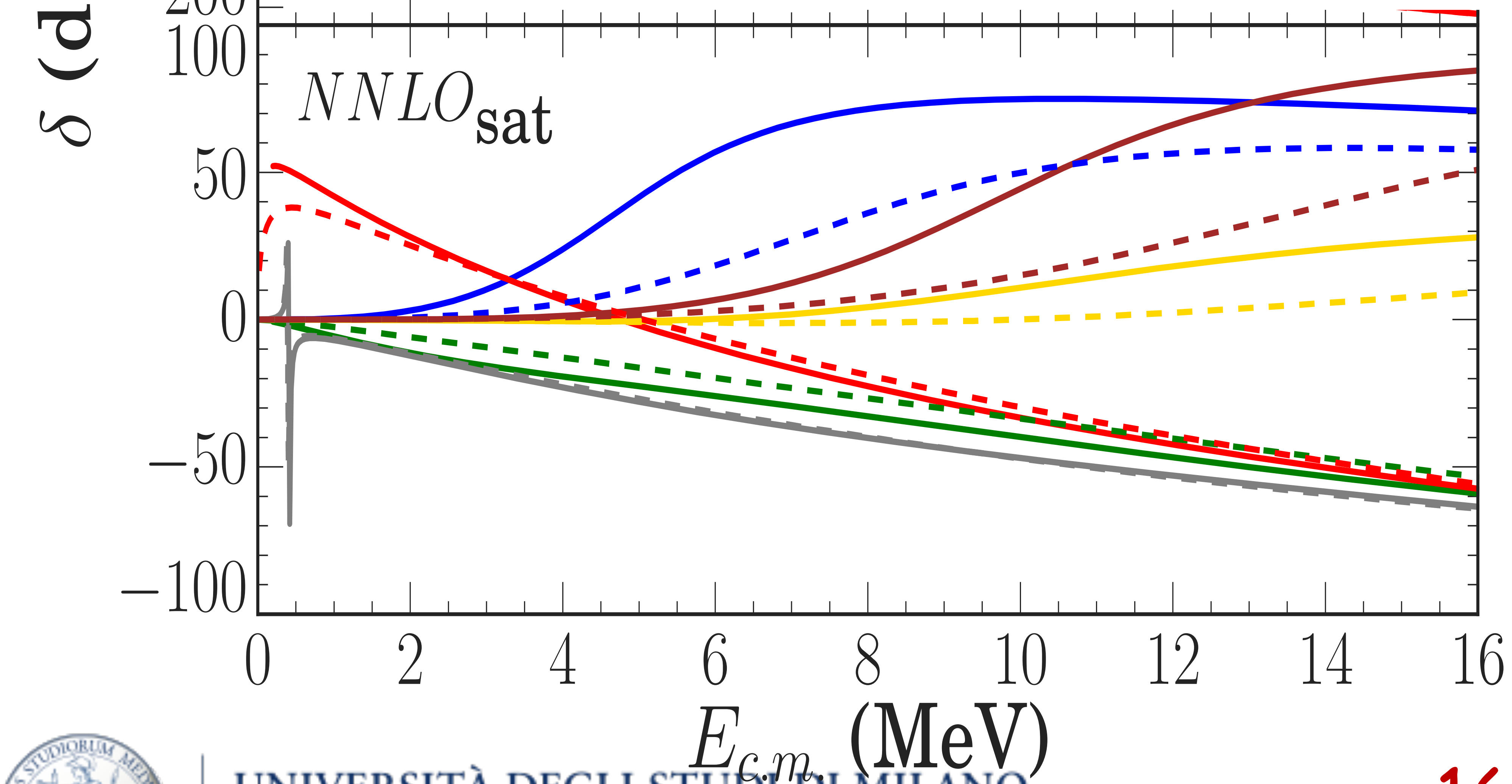
Benchmark with NCSM-based scattering.

Scattering from mean-field only:

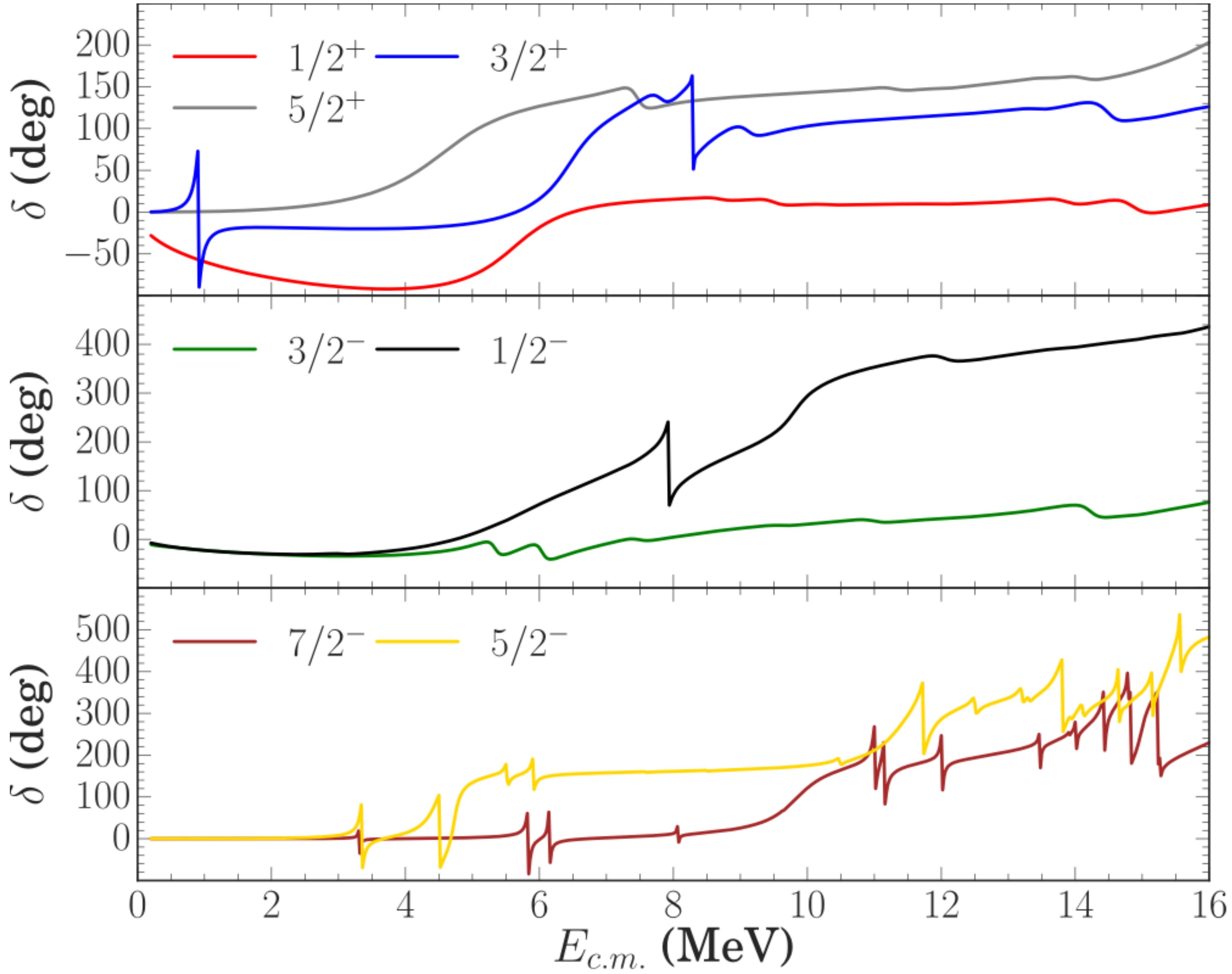


ε (MeV)	$5/2^+$	$1/2^+$	$1/2^-$	$5/2^-$	$3/2^-$	$3/2^+$	$5/2^+_*$	$5/2^-_*$	$7/2^-_*$
exp.	-4.14	-3.27	-1.09	-0.30	0.41	0.94	3.23	3.02	3.54
NNLO$_{sat}$	-5.06	-3.58	-0.15	-1.23	-2.24	0.91	4.57	3.36	3.37

TABLE I. Excitation spectrum of ^{17}O with respect to the $n+^{16}$O threshold, as obtained from Eq. (5) and the NNLO$_{sat}$ interaction and compared to the experiment [45]. Broad resonances in the continuum (most notably, the $5/2^+$) are computed at midpoint. The asterisks ($_*$) indicate higher excited states, above the lowest one, for each partial wave.



Full self-energy from SCGF:

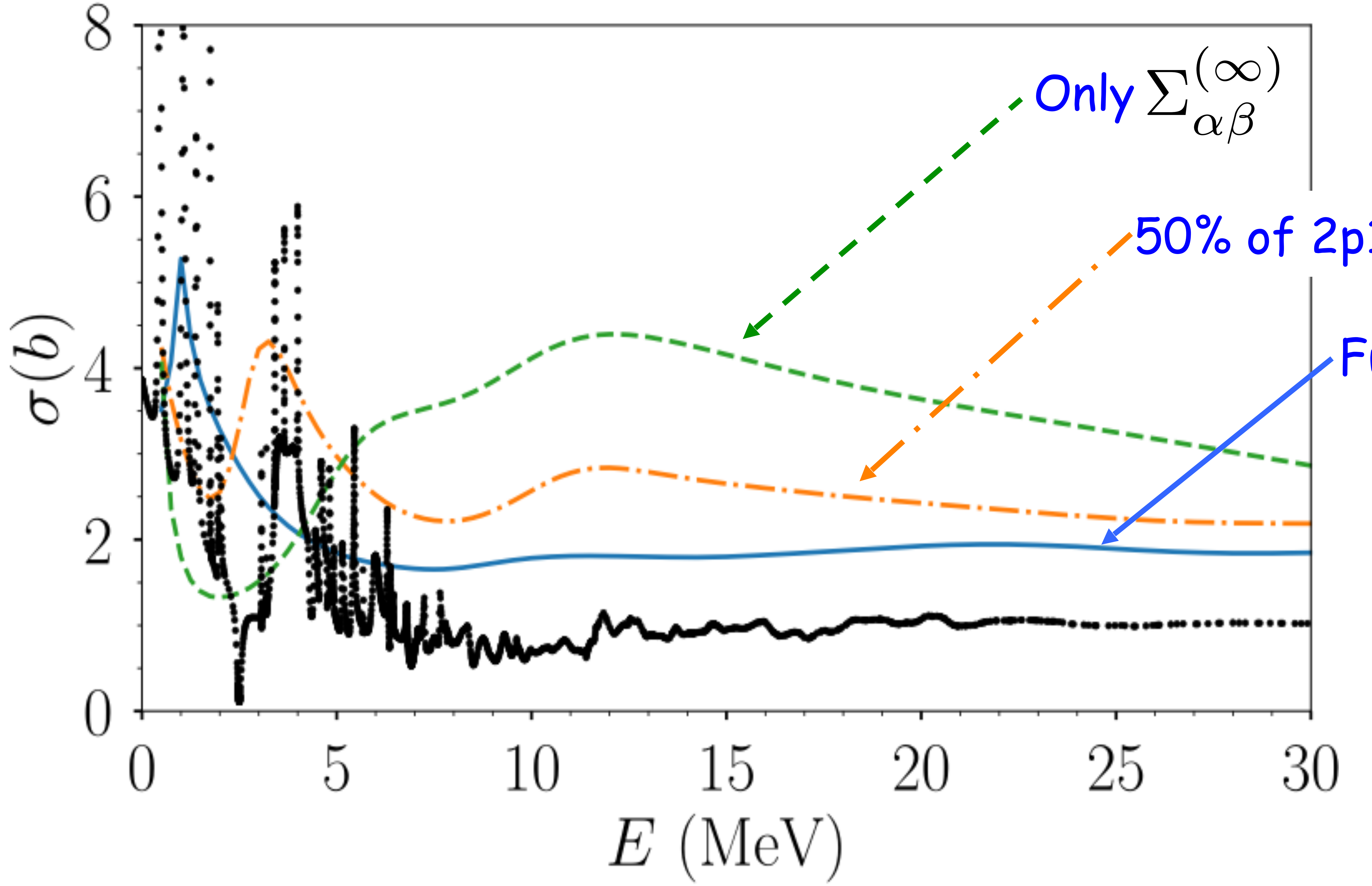


$^{16}O(n,n')^{16}O$

Role of intermediate state configurations (ISCs)

n-^{16}O, total elastic cross section

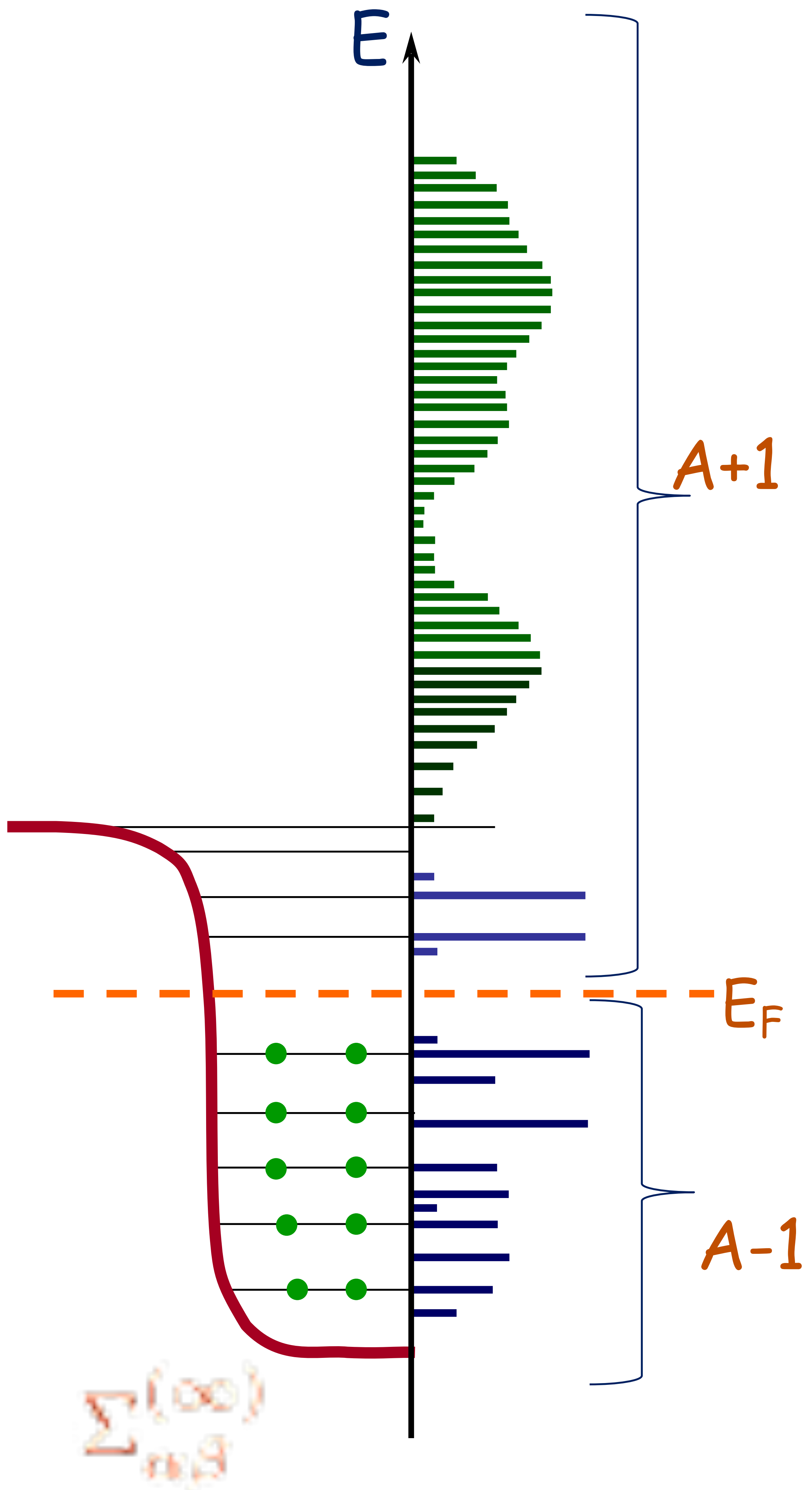
[A. Idini, CB, Navrátil,
Phys. Rev. Lett. **123**, 092501 (2019)]



High order configurations, or ADC(n>>3), to be critical for fully ab initio optical potentials

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \Sigma^{(\infty)}_{\alpha\beta} + \sum_{i,j} \mathbf{M}^{\dagger}_{\alpha,i} \underbrace{\left(\frac{1}{E - (\mathbf{K}^{>} + \mathbf{C}) + i\Gamma} \right)_{i,j}}_{\text{2p1h}} \mathbf{M}_{j,\beta} + \sum_{r,s} \mathbf{N}_{\alpha,r} \underbrace{\left(\frac{1}{E - (\mathbf{K}^{<} + \mathbf{D}) - i\Gamma} \right)_{r,s}}_{\text{2h1p}} \mathbf{N}^{\dagger}_{s,\beta}$$

Microscopic optical potential



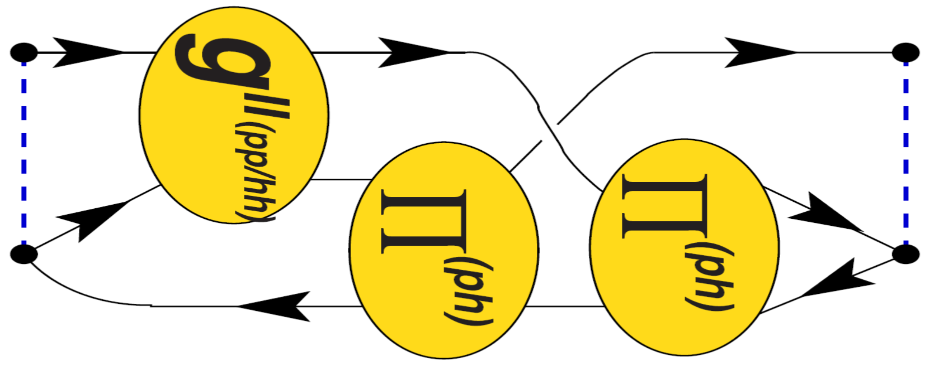
Nuclear self-energy $\Sigma^\star(\mathbf{r},\mathbf{r}';\varepsilon)$:

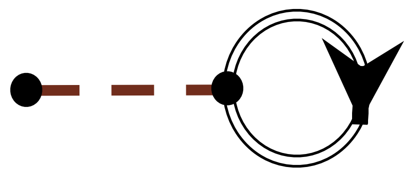
- contains *both particle* and *hole* props.
- it is proven to be a Feshbach opt. pot → in general it is *non-local !*

$$\Sigma^\star_{\alpha\beta}(\omega) = \Sigma^{(\infty)}_{\alpha\beta} + \sum_{i,j} \mathbf{M}^\dagger_{\alpha,i}\left(\frac{1}{E-(\mathbf{K}^> + \mathbf{C}) + i\Gamma}\right)_{i,j}\mathbf{M}_{j,\beta} + \sum_{r,s}\mathbf{N}_{\alpha,r}\left(\frac{1}{E-(\mathbf{K}^<+\mathbf{D}) - i\Gamma}\right)_{r,s}\mathbf{N}^\dagger_{s,\beta}$$

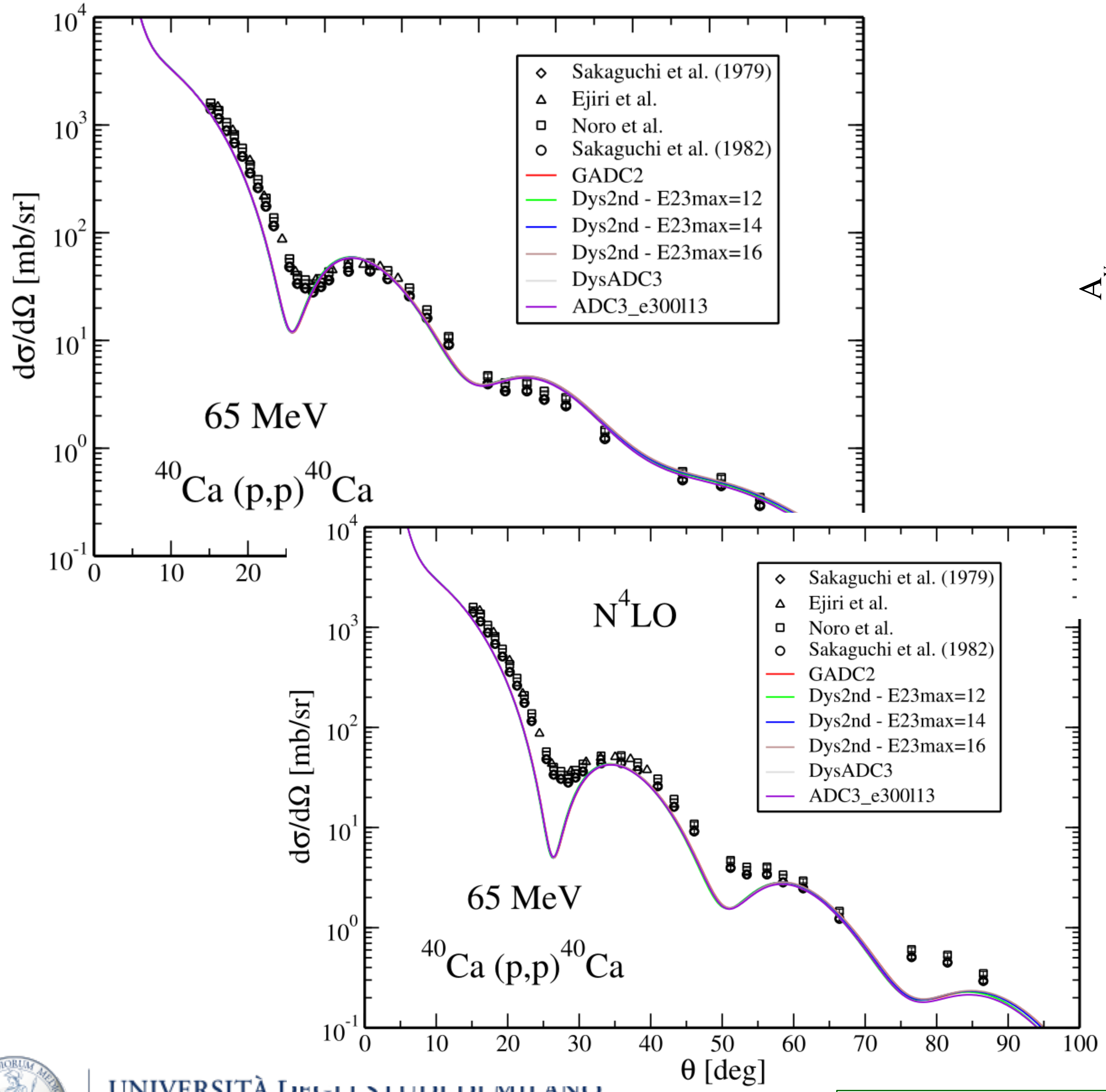
mean-field

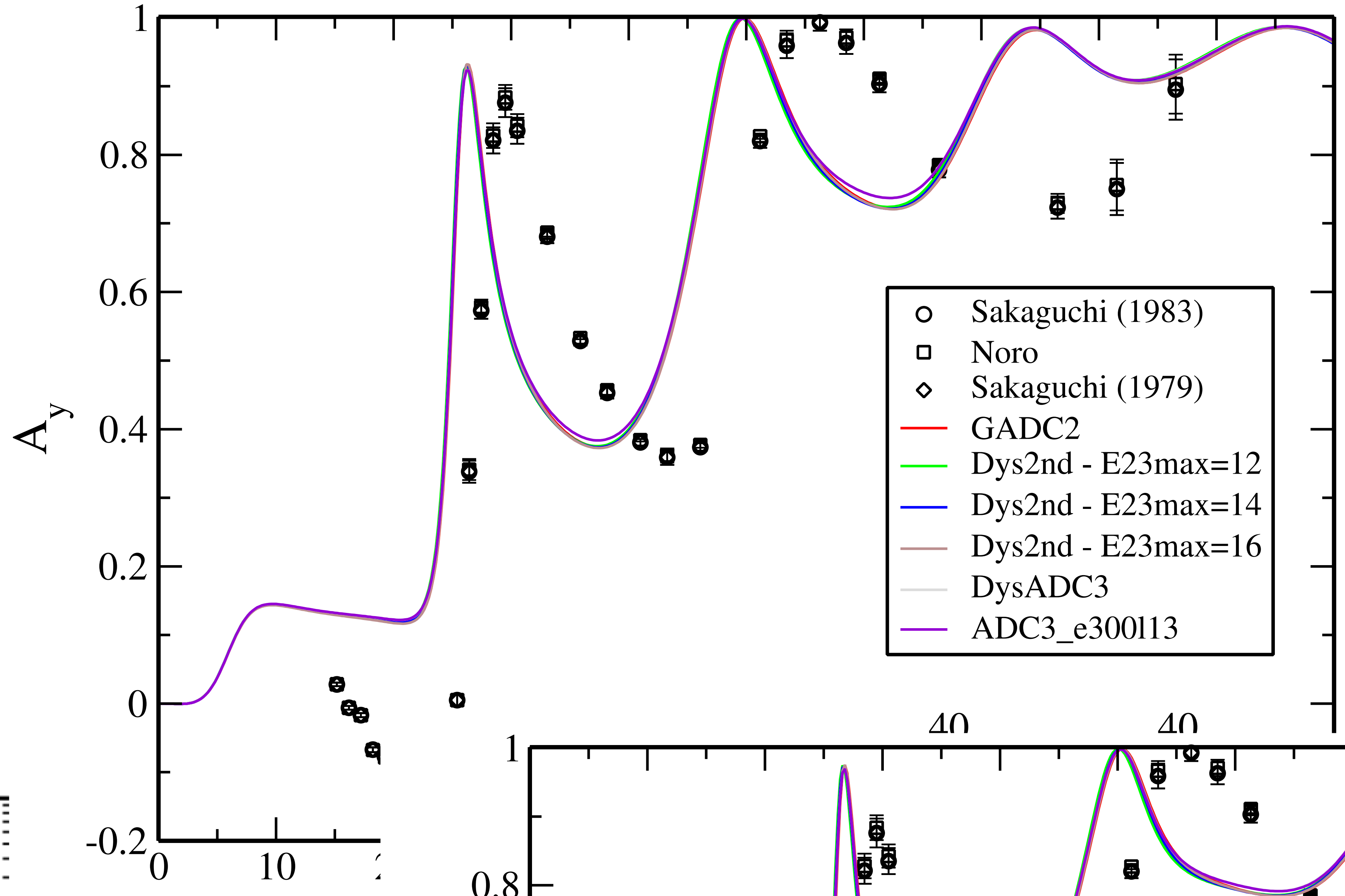
Particle-vibration couplings:

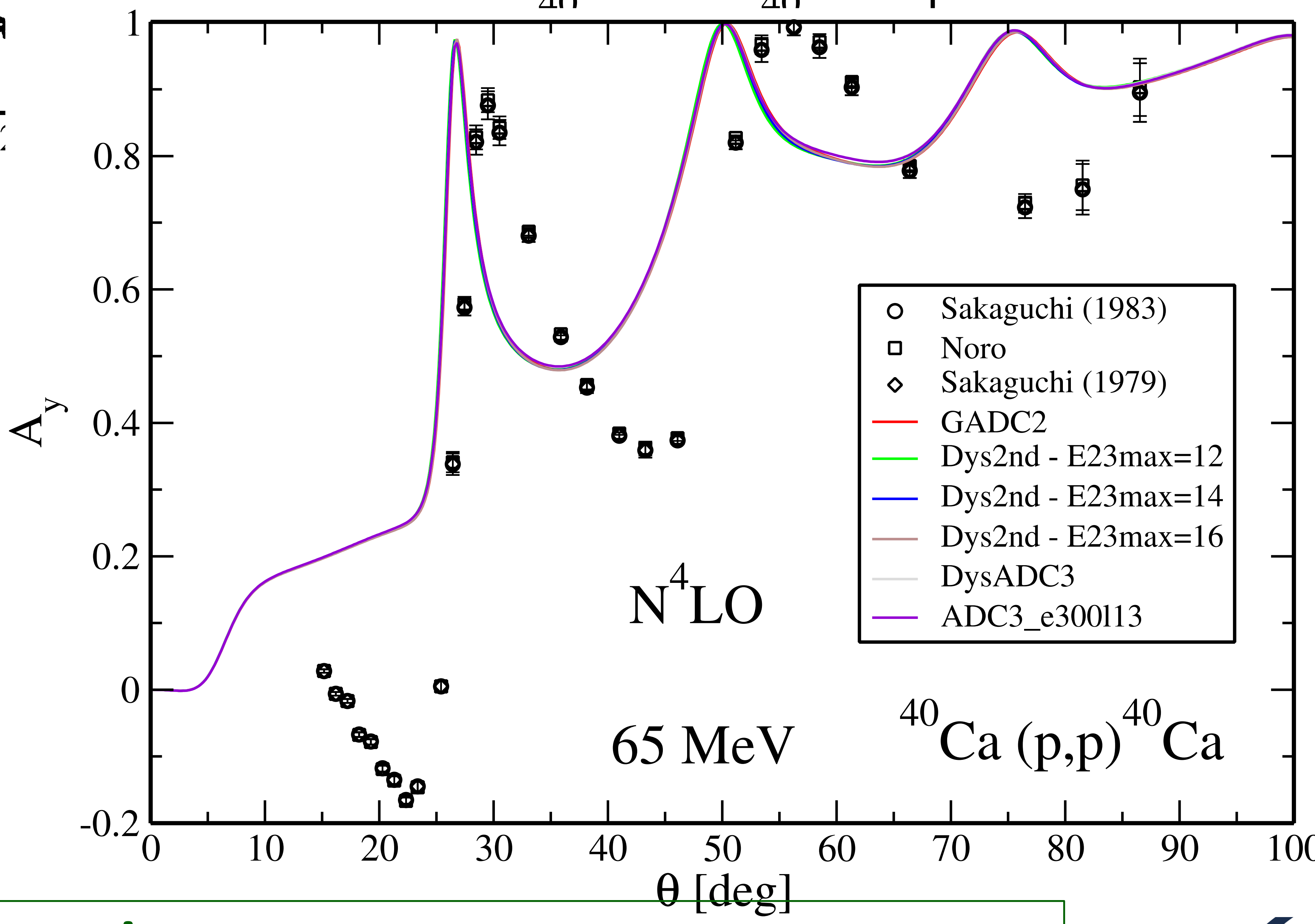


$$\Sigma^{(\infty)}_{\alpha\beta} =$$ 

Elastic nucleon nucleus scattering







M. Vorabbi
U. of surrey

M. Vorabbi et al. – **in preparation**

Nuclear Density Functional from Ab Initio Theory

PHYSICAL REVIEW C **104**, 024315 (2021)

Nuclear energy density functionals grounded in *ab initio* calculations

F. Marino,[1,2,*] C. Barbieri,[1,2] A. Carbone,[3] G. Colò,[1,2] A. Lovato,[4,5] F. Pederiva,[6,5] X. Roca-Maza,[1,2]
and E. Vigezzi[2]
[1]*Dipartimento di Fisica "Aldo Pontremoli," Università degli Studi di Milano, 20133 Milano, Italy*
[2]*Istituto Nazionale di Fisica Nucleare, Sezione di Milano, 20133 Milano, Italy*
[3]*Istituto Nazionale di Fisica Nucleare–CNAF, Viale Carlo Berti Pichat 6/2, 40127 Bologna, Italy*

DFT is in principle exact – but the energy density functional (EDF) is not known

For nuclear physics this is even more demanding: need to link the EDF to theories rooted in QCD!

Jacob's ladder

Machine-learn DFT functional
on the nuclear equation of state

→

Benchmark in finite systems

+ approximate GA

Nuclear Density Functional from Ab Initio Theory

Density functional theory (DFT)

$$E = \int d\mathbf{r}\,\mathcal{E}(\mathbf{r}) = E_{\mathrm{kin}} + E_{\mathrm{pot}} + E_{\mathrm{Coul}}$$

…exact if functional **was** known

Simplest approx is local density:

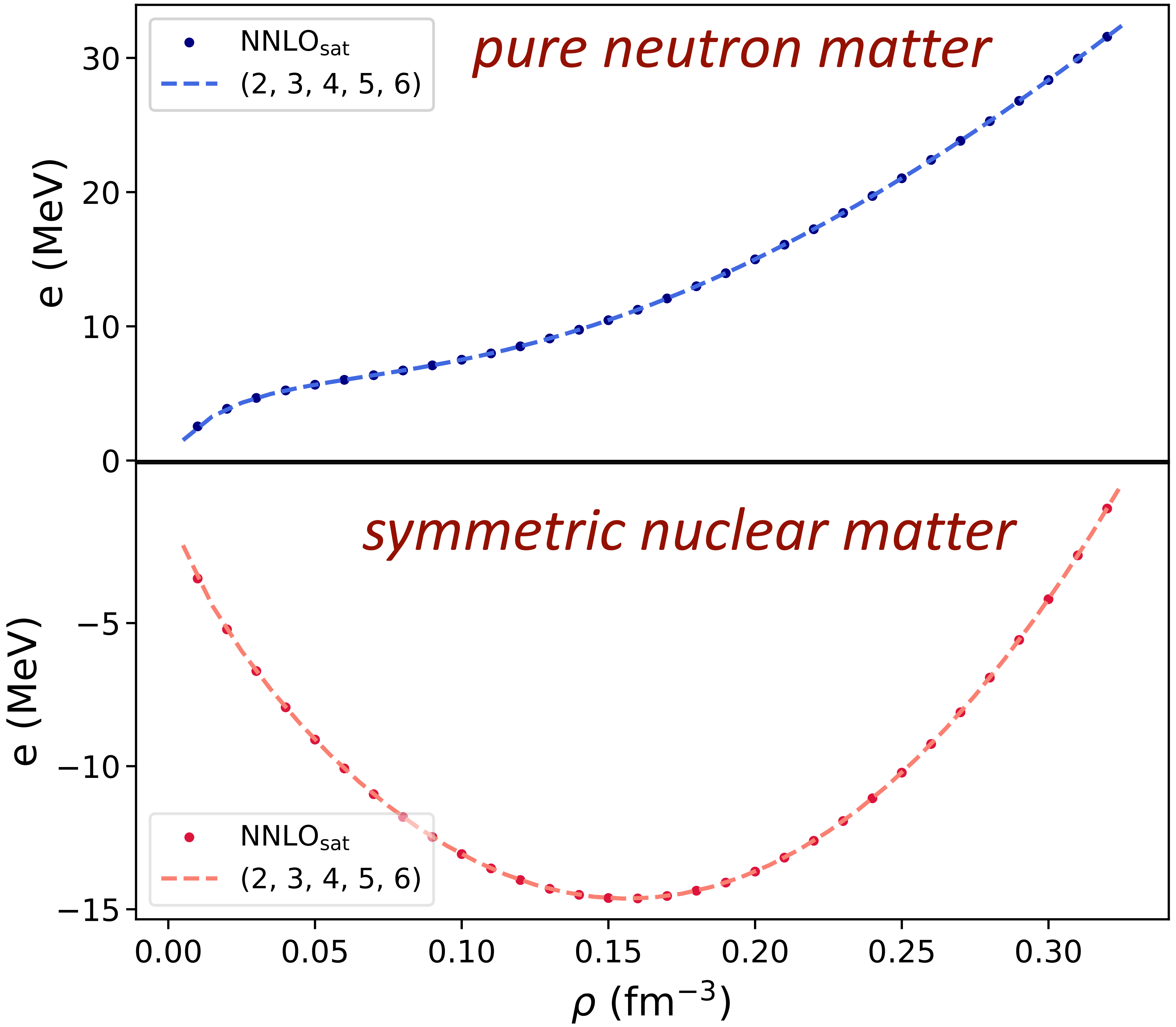
$$E_{\mathrm{LDA}} = E_{\mathrm{kin}} + E_{\mathrm{bulk}} + E_{\mathrm{Coul}}$$

$$\mathcal{E}_{\mathrm{bulk}}[\rho(\mathbf{r}), \beta(\mathbf{r})] = \rho(\mathbf{r}) v[\rho(\mathbf{r}), \beta(\mathbf{r})]$$

Then need to worry about gradients and surfaces:

$$E_{\mathrm{GA}} = E_{\mathrm{LDA}} + E_{\mathrm{surf}}$$

$$E_{\mathrm{surf}} = \int d\mathbf{r}\left[\sum_{t=0,1} C_t^{\Delta}\rho_t\Delta\rho_t \;-\frac{W_0}{2}\left(\rho\nabla\cdot\mathbf{J} + \sum_q \rho_q \nabla\cdot\mathbf{J}_q\right)\right]$$

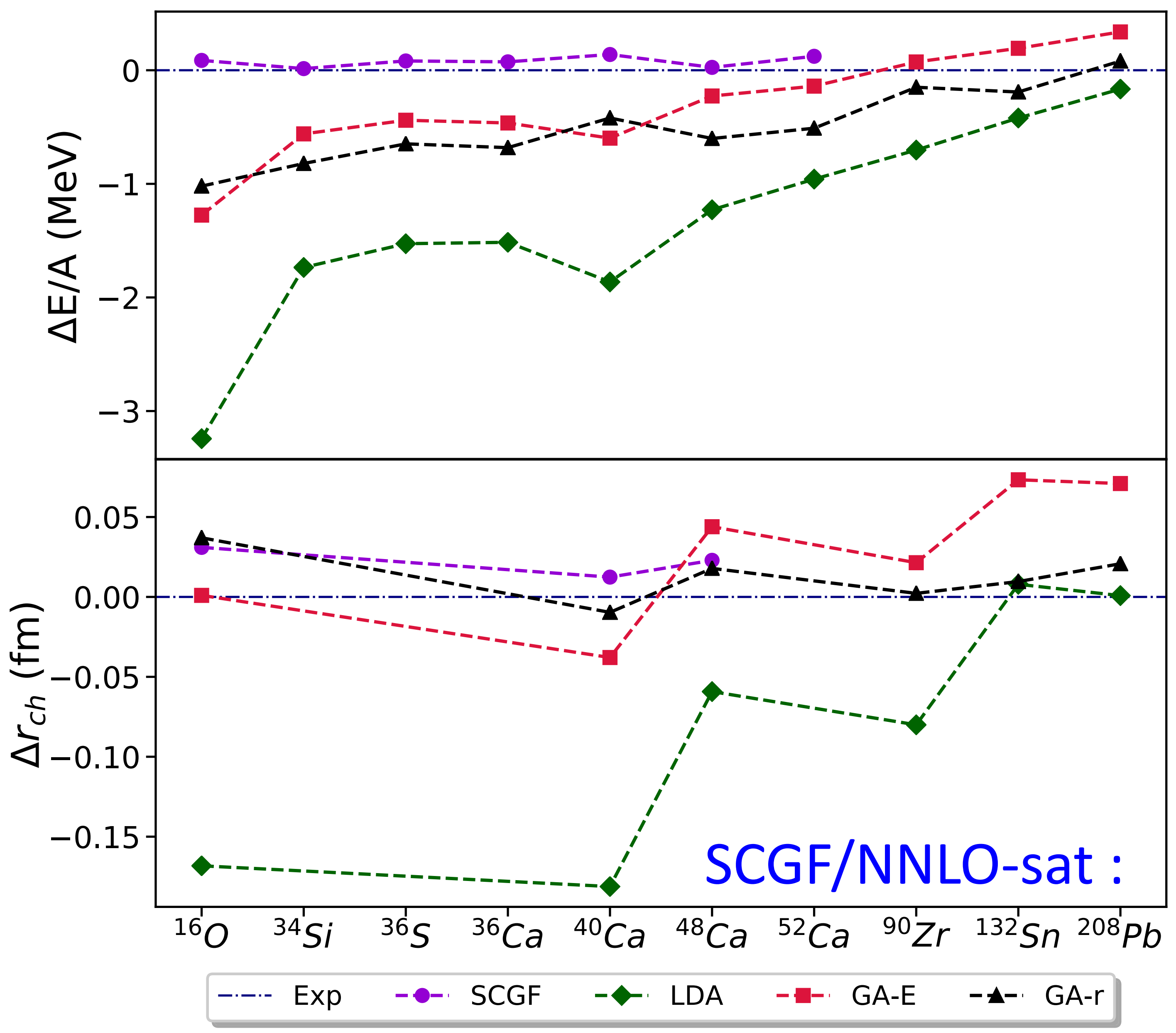


Machine-learn DFT functional on the nuclear equation of state

F. Marino, G. Colò, CB et al., Phys Rev. C**104**, 024315 (2021)

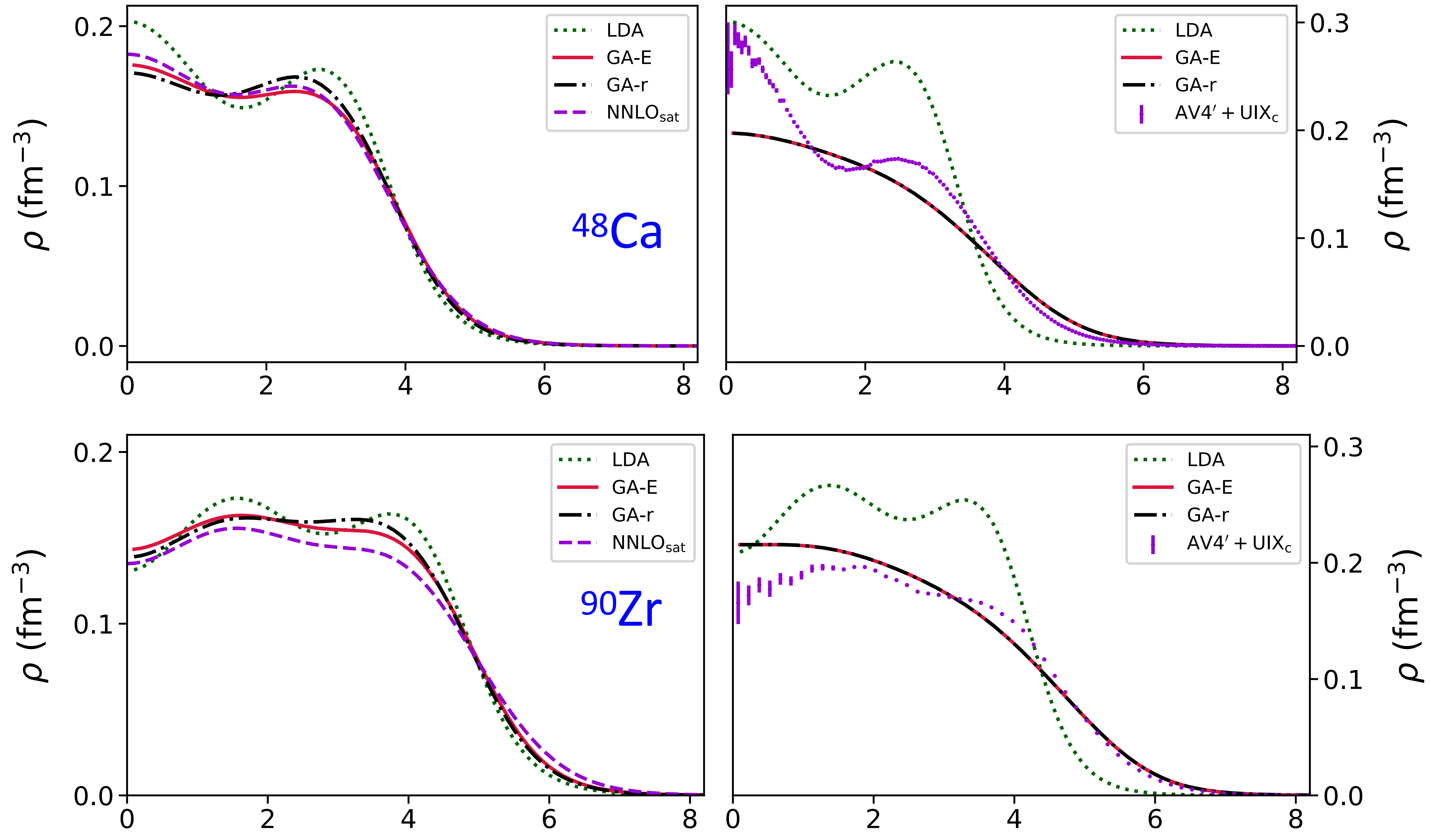
Benchmark on finite systems

Gradient terms are important (but they seem to work!):



SCGF/NNLO-sat :

AFDMC/AV4' :



Need to extract gradient information from non-uniform matter —> External (monocromatic) perturbation:

$$v(\mathbf{x}) = v_q e^{i\mathbf{q}\cdot\mathbf{x}} + c.c. = 2v_q \cos(\mathbf{q}\cdot\mathbf{x})$$

$$\delta\rho(\mathbf{x}) = 2\rho_q \cos(\mathbf{q}\cdot\mathbf{x})$$

F. Marino, G. Colò, CB et al., Phys Rev. C**104**, 024315 (2021)

ADC(3) computations for infinite matter

Finite size box (of length L) with periodic Boundary conditions:

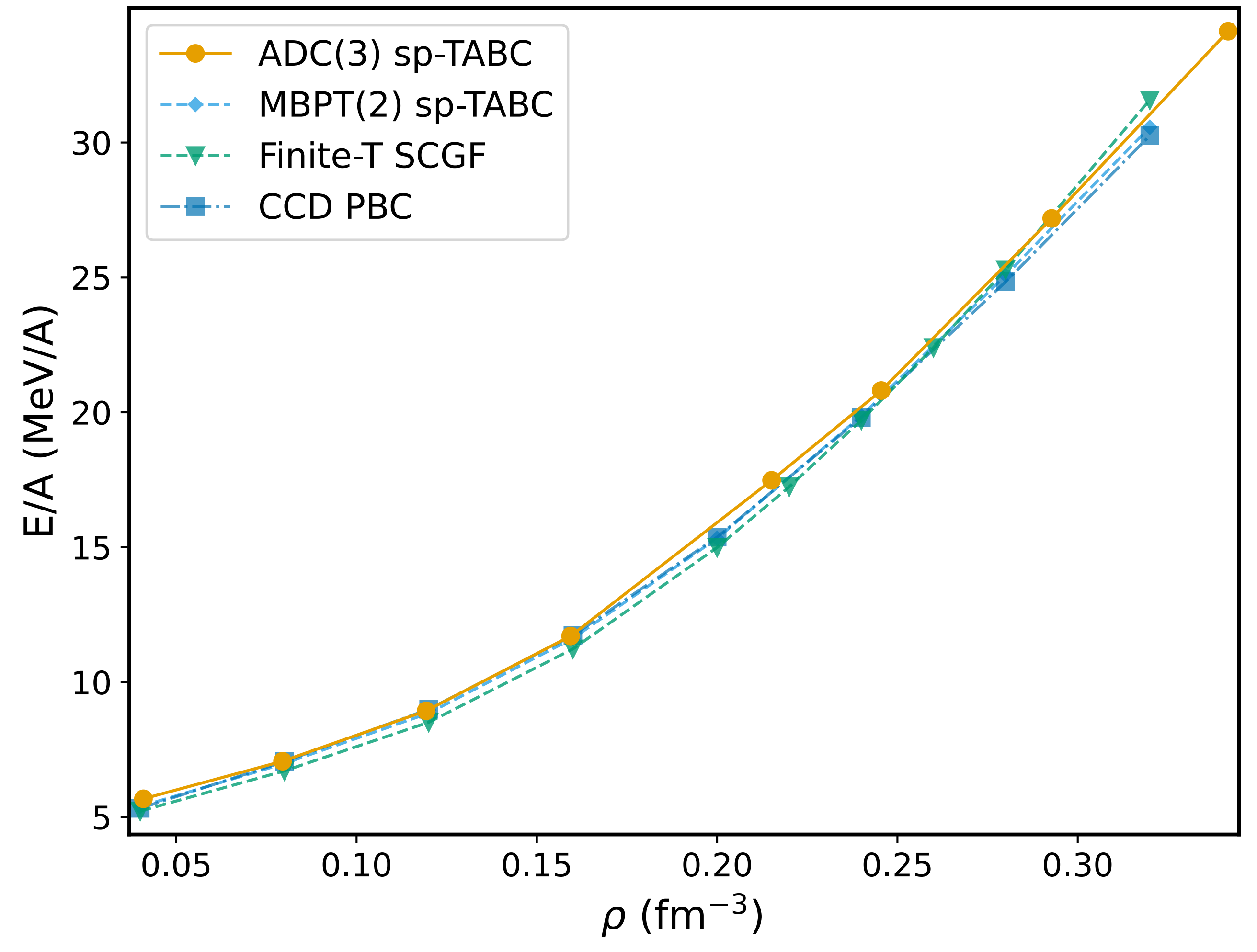
$$\rho = \frac{A}{L} \qquad p_F = \sqrt[3]{\frac{6\pi^2\rho}{\nu_d}}$$

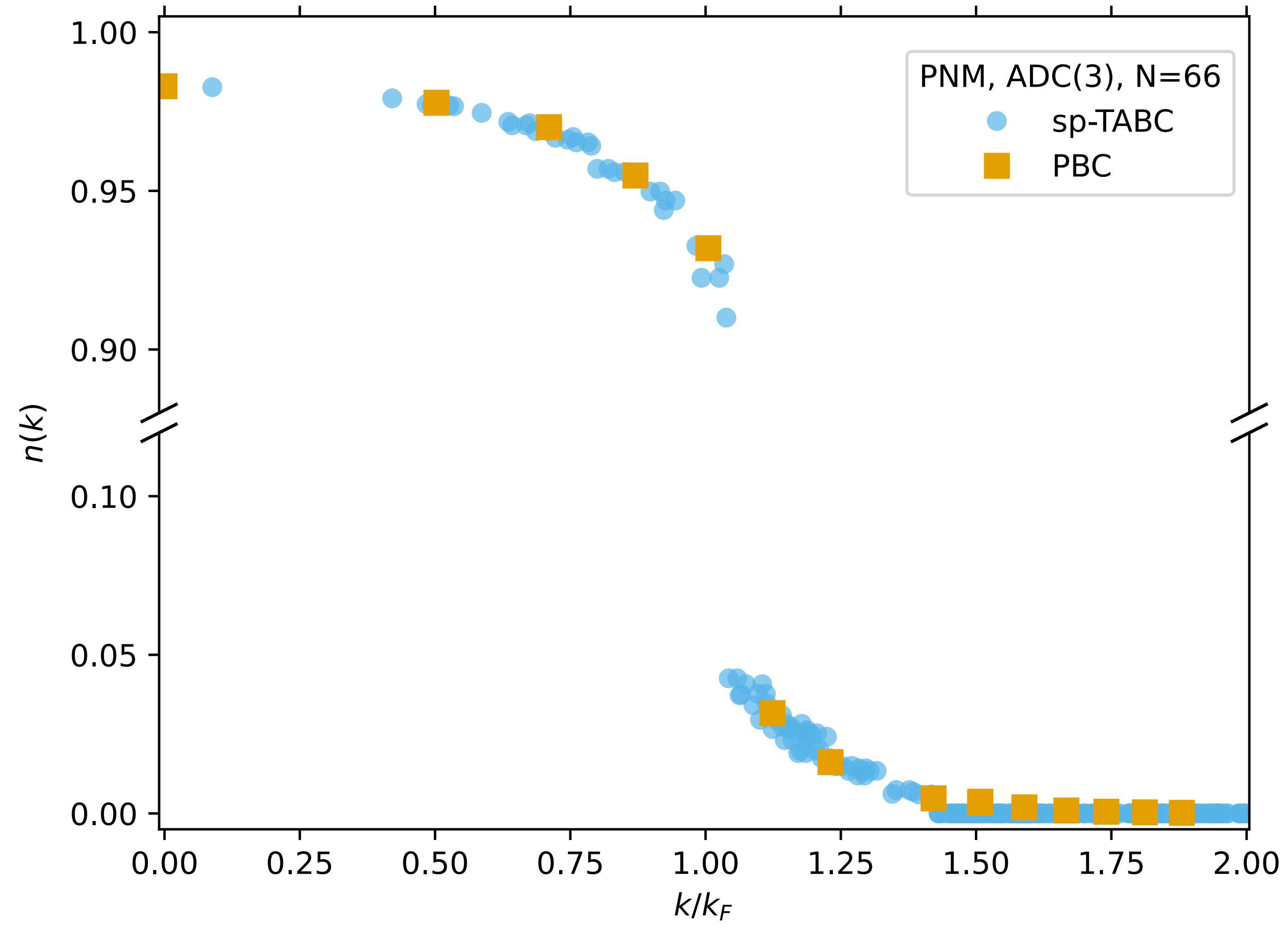
$$\widehat{H} = \sum_{\alpha} \varepsilon^0_\alpha\, a^\dagger_\alpha a_\alpha - \sum_{\alpha\beta} U_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{4}\sum_{\substack{\alpha\gamma\\ \beta\delta}} V_{\alpha\gamma,\beta\delta}\, a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta + \frac{1}{36}\sum_{\substack{\alpha\gamma\epsilon\\ \beta\delta\eta}} W_{\alpha\gamma\epsilon,\beta\delta\eta}\, a^\dagger_\alpha a^\dagger_\gamma a^\dagger_\epsilon a_\eta a_\delta a_\beta\,.$$

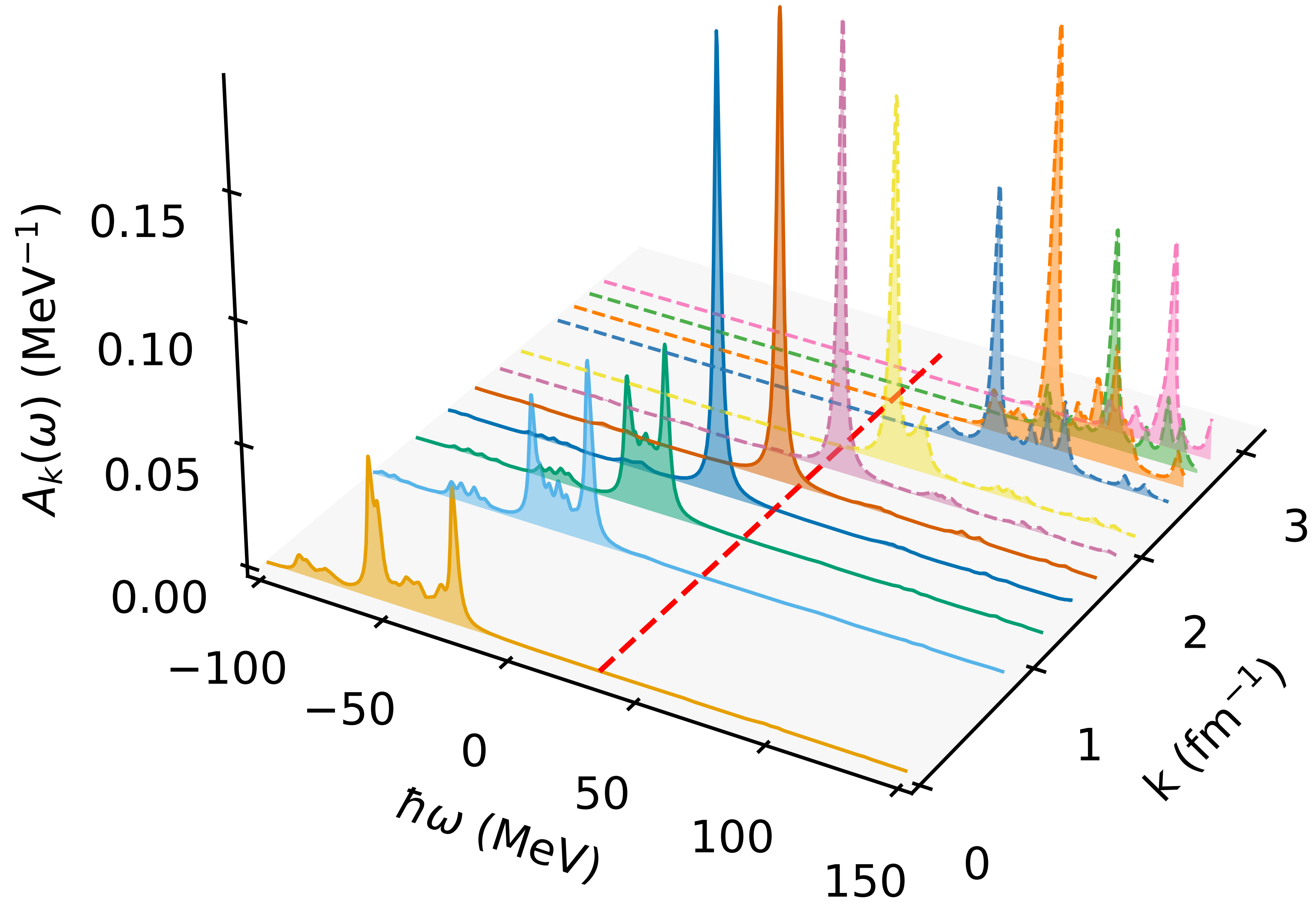
ADC(3) self energy:

$$\Sigma^{(\star)}_{\alpha\beta}(\omega) = -U_{\alpha\beta} + \Sigma^{(\infty)}_{\alpha\beta} + M^\dagger_{\alpha,r}\left[\frac{1}{\omega - [E^> + C]_{r,r'} + i\eta}\right]_{r,r'} M_{r',\beta}$$
$$+ N_{\alpha,s}\left[\frac{1}{\omega - (E^< + D) - i\eta}\right]_{s,s'} N^\dagger_{s',\beta}$$

A=66, 2+3 NF (NNLOsat)







F. Marino, C. McIlroy, CB et al., **in preparation**

Quantum Monte Carlo in configuration space

arXiv:2203.16167v2 [nucl-th]

Quantum Monte Carlo in Configuration Space with Three-Nucleon Forces

Pierre Arthuis[1,2,*] Carlo Barbieri[3,4,†] Francesco Pederiva,[5,6] and Alessandro Roggero[5,6,7]

[1] *Technische Universität Darmstadt, Department of Physics, 64289 Darmstadt, Germany*
[2] *ExtreMe Matter Institute EMMI and Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*

Configuration Interaction Monte Carlo (CIMC):

CI anstatz:

$$|\Psi\rangle = \sum_{\mathbf{n}} \langle \mathbf{n}|\Psi\rangle |\mathbf{n}\rangle \equiv \sum_{\mathbf{n}} \Psi(\mathbf{n})|\mathbf{n}\rangle$$

Immaginari time evolution to the ground state (DMF):

$$\Psi_{\tau+\Delta\tau}(\mathbf{m}) = \sum_{\mathbf{n}} \langle \mathbf{m}|P|\mathbf{n}\rangle \Psi_\tau(\mathbf{n}),$$

$$\langle \mathbf{m}|P|\mathbf{n}\rangle = \langle \mathbf{m}|e^{-\Delta\tau(H-E_T)}|\mathbf{n}\rangle$$

Monte Carlo smapling over configuration space:

$$|\mathbf{m}\rangle = a^\dagger_{p_1} \ldots, a^\dagger_{p_M} a_{h_1} \ldots, a_{h_M} |\Phi_{\rm HF}\rangle \equiv |\Phi^{p_1,\ldots,p_M}_{h_1,\ldots,h_M}\rangle$$

The specific CIMC algorithm is build in such a way that it preserves the variational principle.

A. Roggero, Ph.D. thesis and refs. therein.

Quantum Monte Carlo in configuration space

arXiv:2203.16167v2 [nucl-th]

Quantum Monte Carlo in Configuration Space with Three-Nucleon Forces

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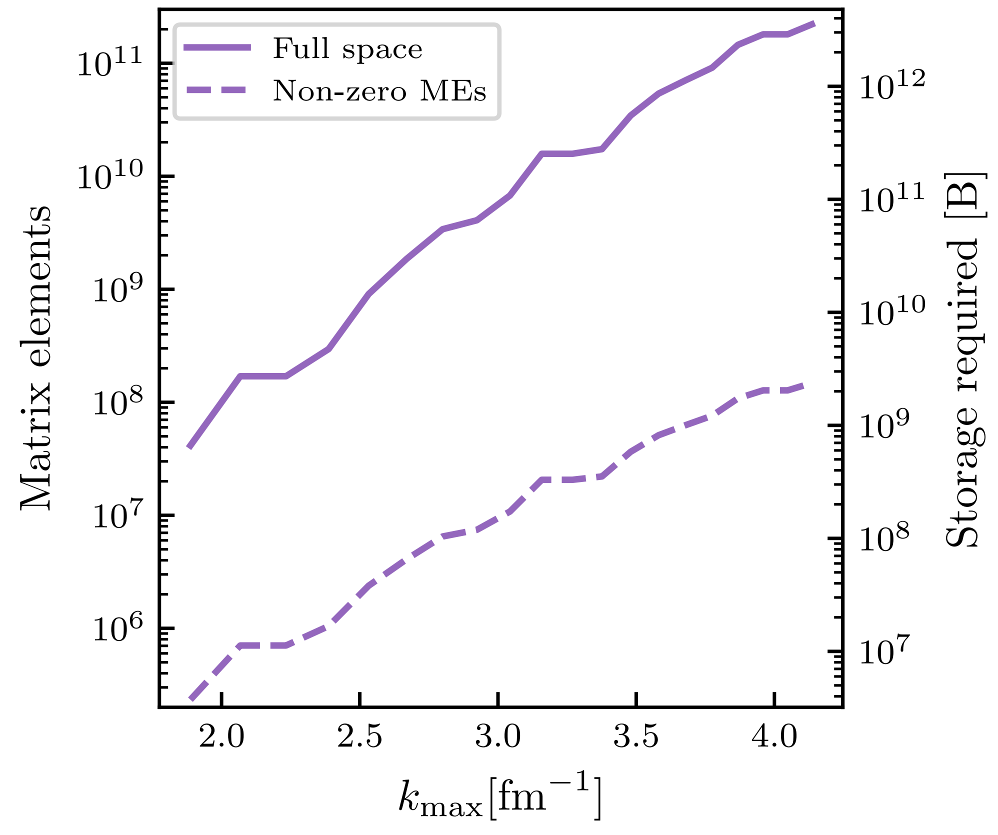
P. Arthuis (Surrey, now @ TU Darmstadt,

Configuration Interaction Monte Carlo (CIMC) for 3-nucleon forces:

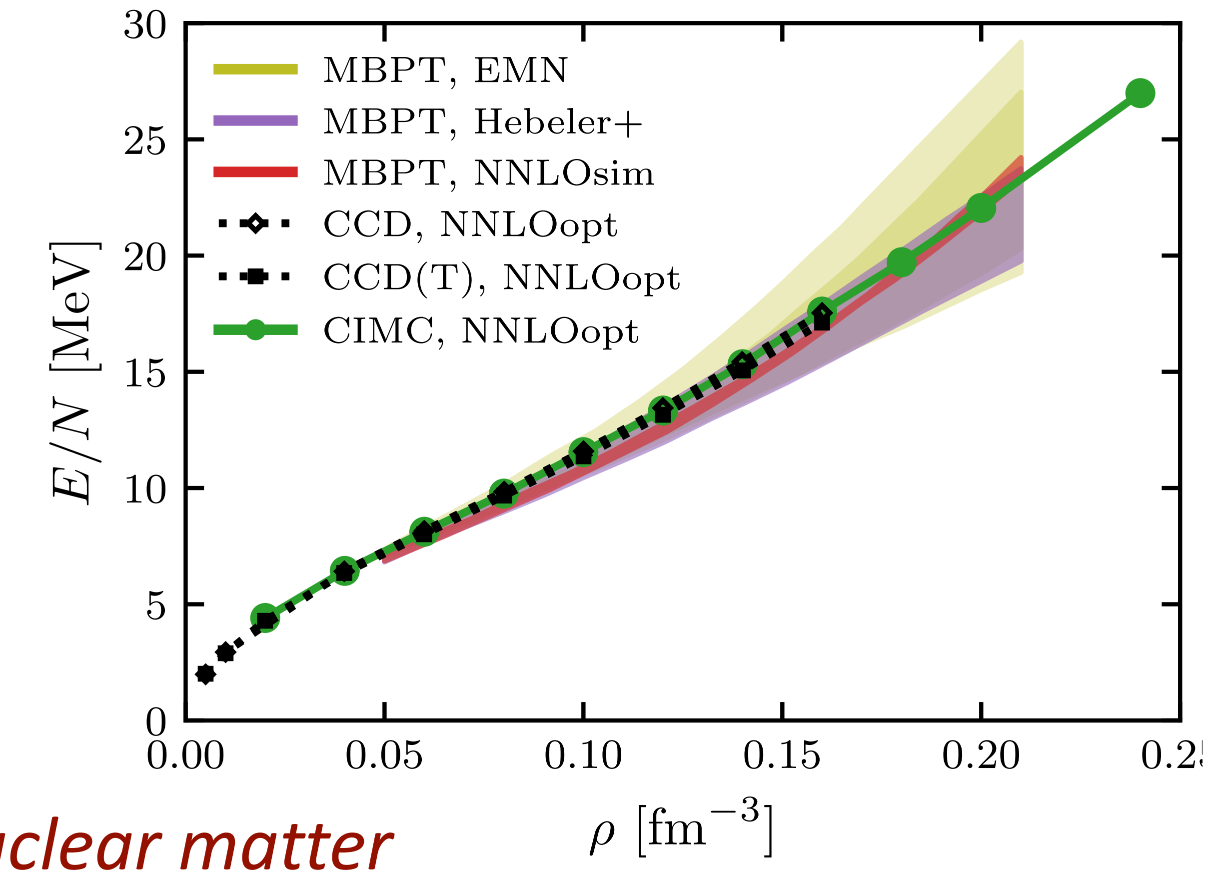
$$v^{(N.O.)}_{\alpha\beta,\gamma\delta} = \sum_{\mu\nu} v^{(3NF)}_{\alpha\beta\mu,\gamma\delta\nu}\, \rho_{\nu\mu}$$



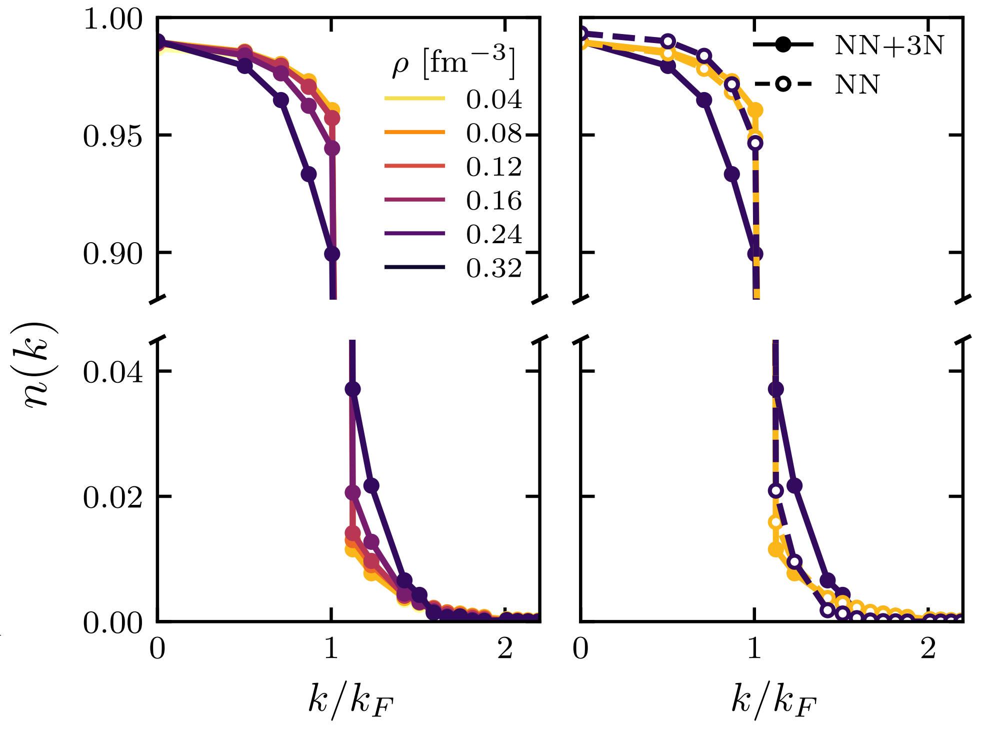
Efficient storage

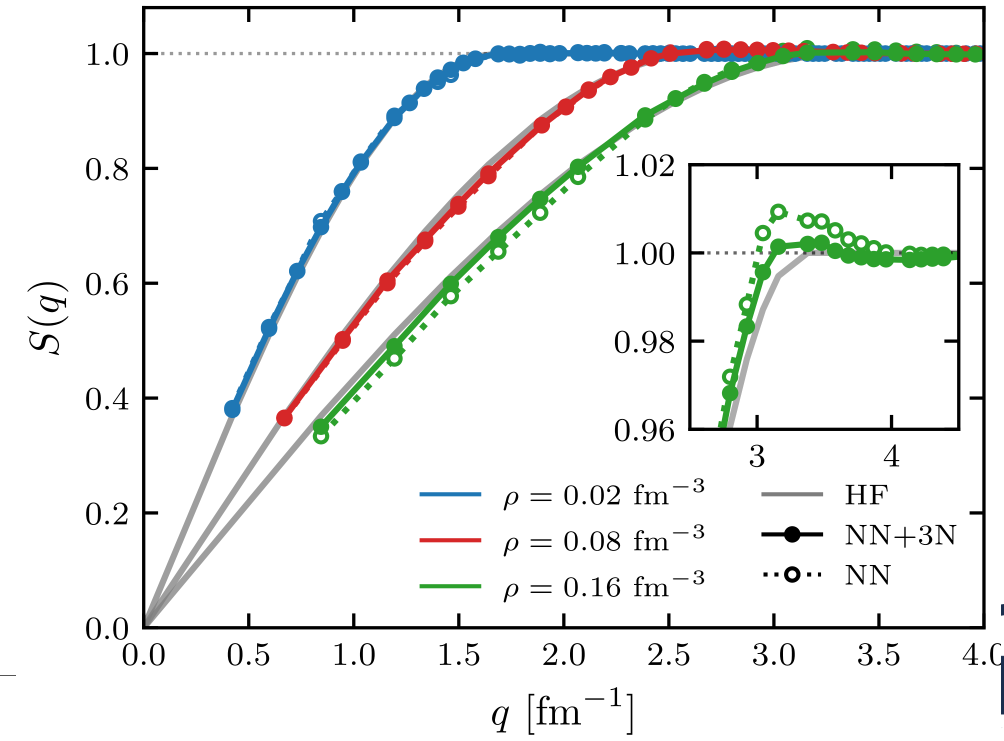
of 3NF mtx elements

66 neutrons, ρ = 0.16 fm^{-3}

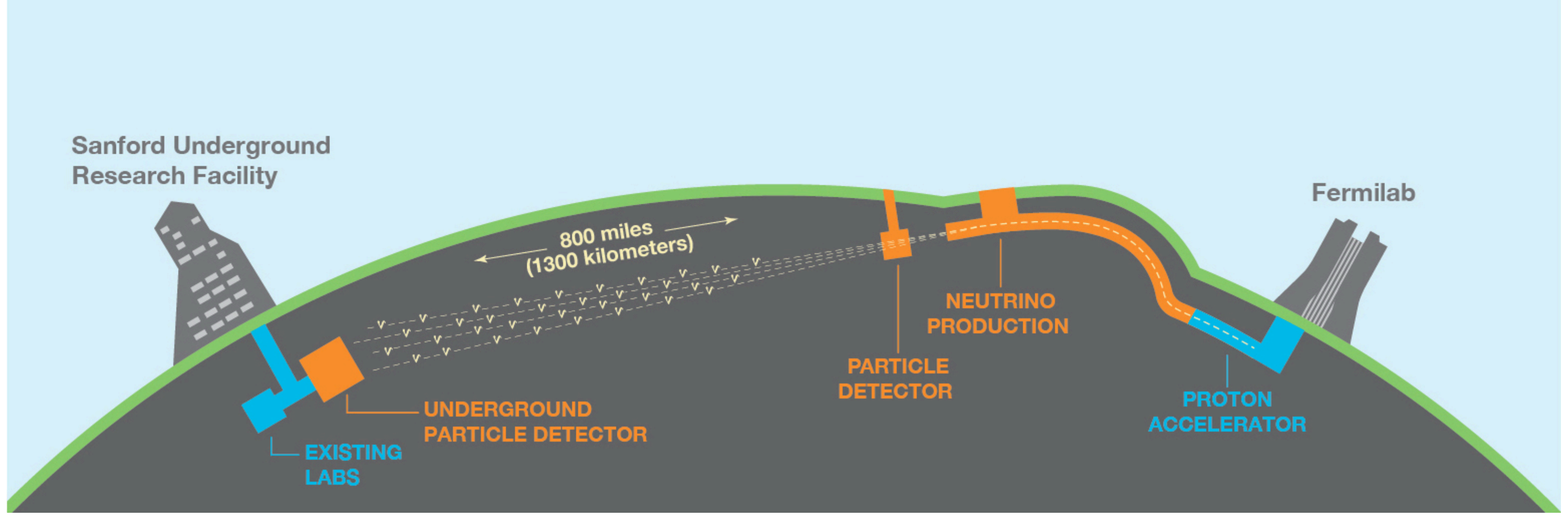


pure nuclear matter



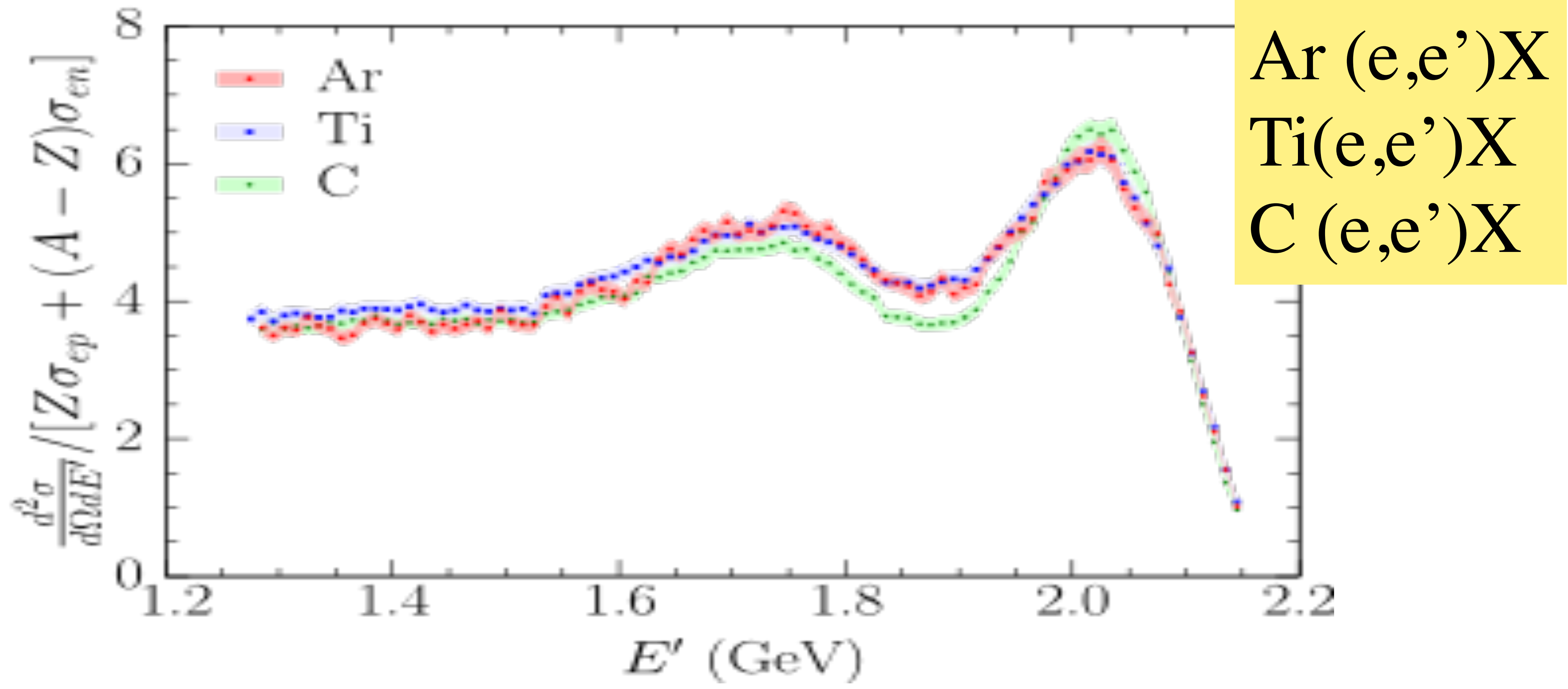


Neutrino Oscillations and Liquid Ar detectors



DUNE experiment will measure long base line neutrino oscillations to:

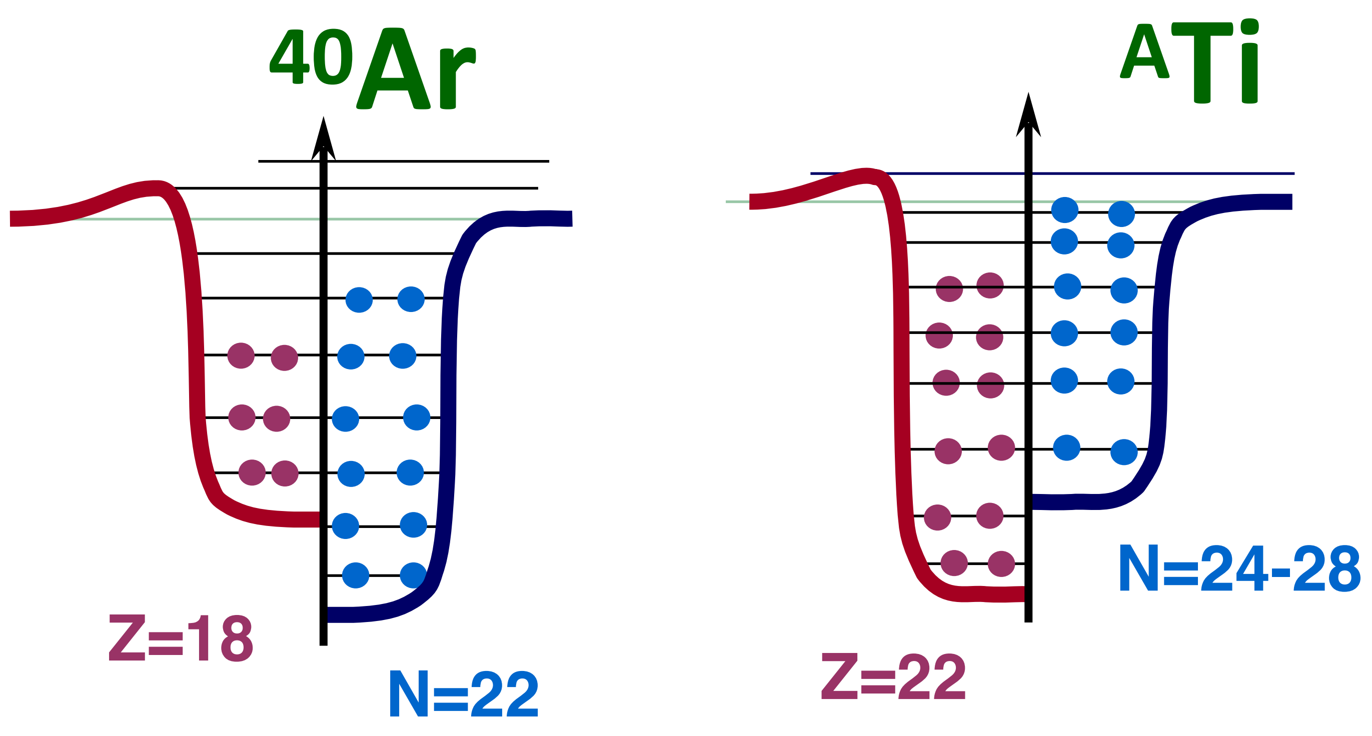
- Resolve neutrino mass hierarchy
- Search for CP violation in weak interaction
- Search for other physics beyond SM



^{40}Ar(e,e'p) and Ti(e,e'p) data

Jlab experiment E12-14-012 (Hall A)

Phys. Rev. C 98, 014617 (2018);

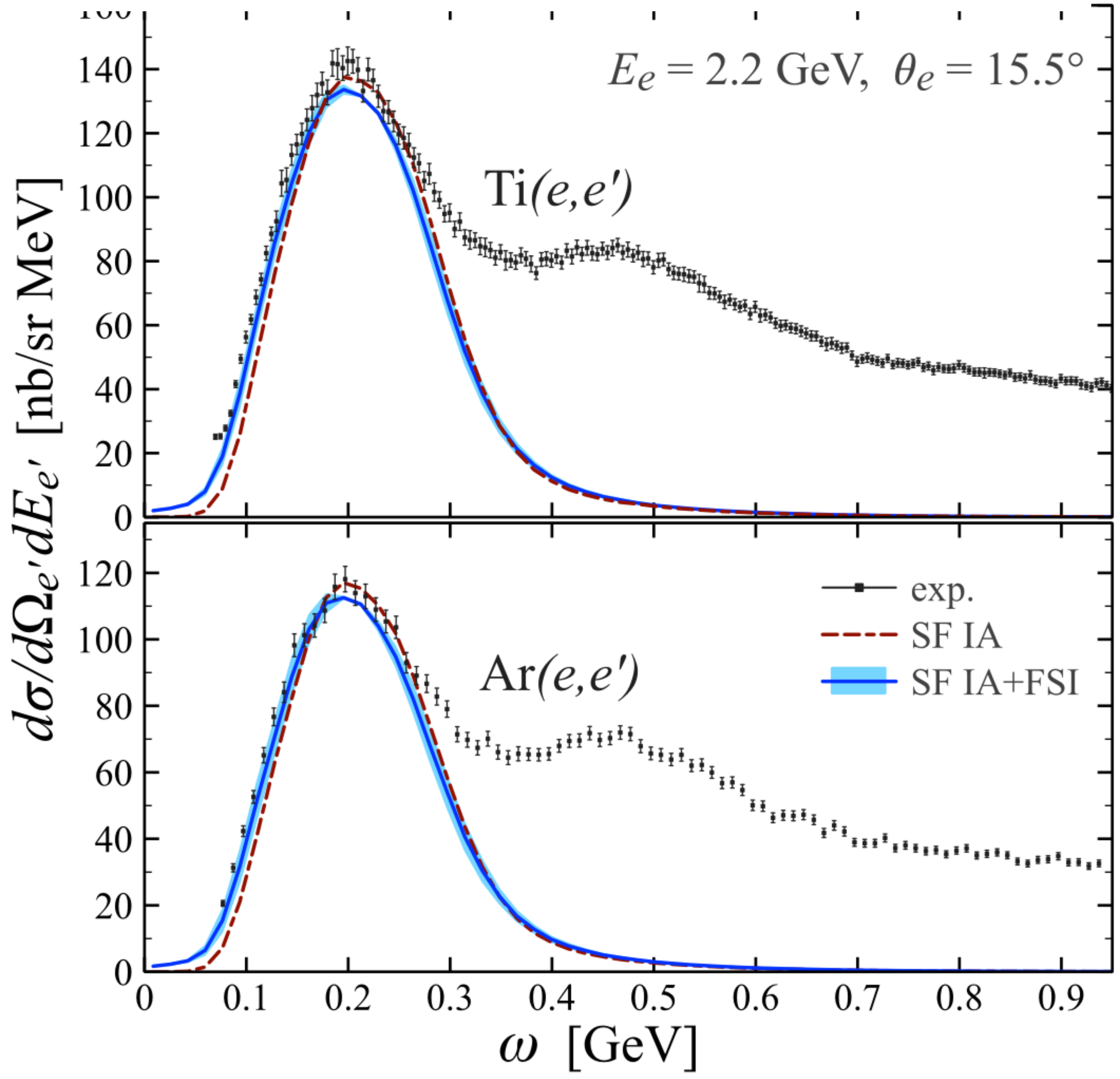


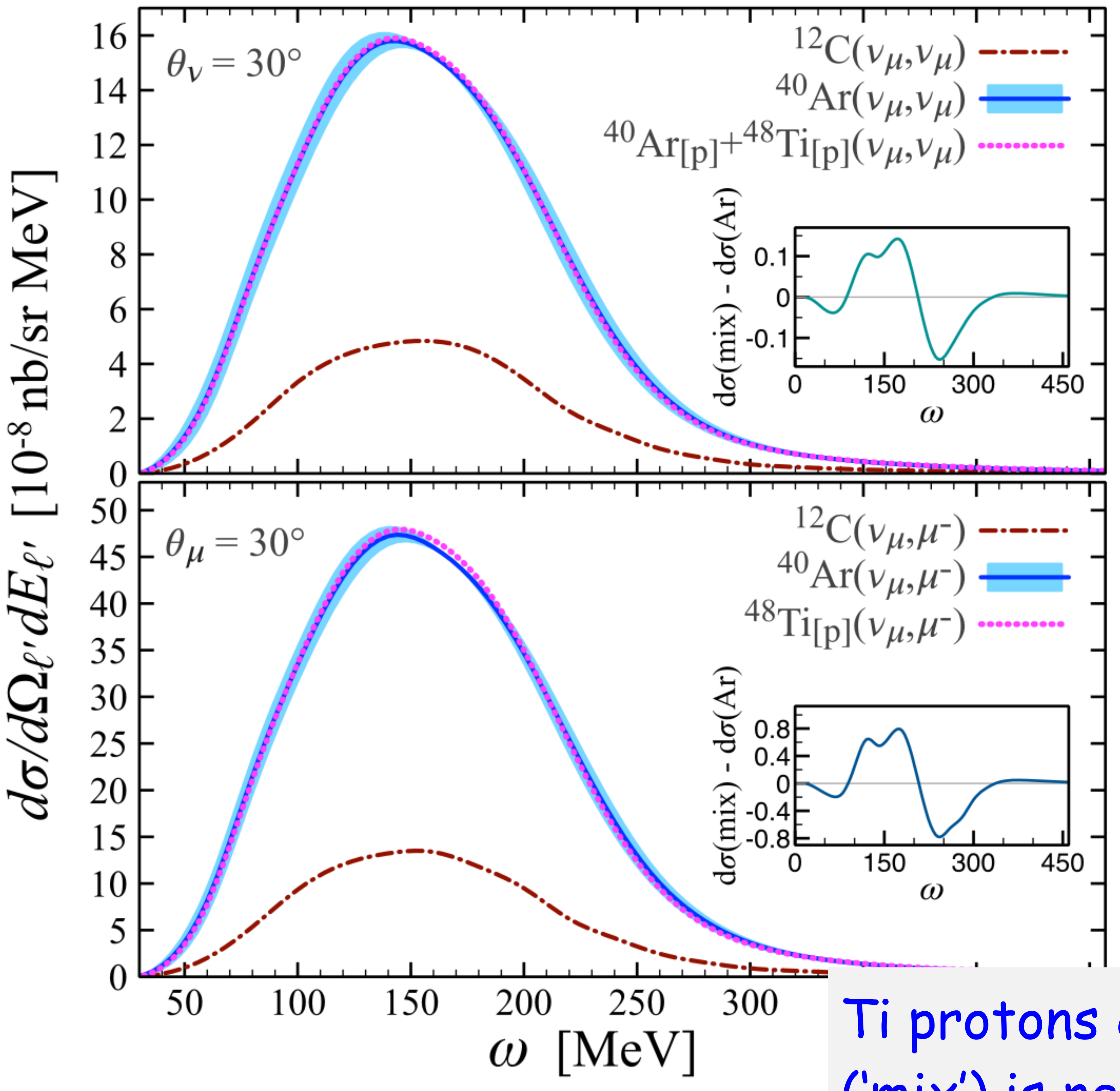
Proton distribution in Ti similar to neutron in ^{40}Ar

Electron and ν scattering on ^{40}Ar and Ti

Jlab experiment E12-14-012 (Hall A)

[Phys. Rev. C 98, 014617 (2018)]





Ti protons contribution ('mix') is nearly identical to neutrons in ^{40}Ar.

^{40}Ar(e,e'p) and Ti(e,e'p) data being analyzed

CB, N. Rocco, V. Somà, Phys. Rev. C**100**, 062501(R) (2019)

2023 Doctoral Training Program at ECT*

ECT*
EUROPEAN CENTRE FOR THEORETICAL STUDIES IN NUCLEAR PHYSICS AND RELATED AREAS
FONDAZIONE BRUNO KESSLER

Ab Initio Methods and Emerging Technologies for Nuclear Structure

Doctoral Training Programme 2023

Trento, 10 – 28 July 2023

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*Vittorio **Somà***, Université Paris-Saclay and CEA
Self-consistent Green's function methods

*Alexander **Tichai***, Technische Universität Darmstadt
Many-body perturbation theory

*Andreas **Ekström***, Chalmers University of Technology
Bayesian inference and modelling of nuclear forces

*Filippo **Vicentini***, Ecole Polytechnique and EPFL
Machine learning and neural network quantum states

*Alessandro **Lovato***, Argonne National Laboratory
Machine learning and Monte Carlo methods in Nuclear Physics

*Kyle **Wendt***, Lawrence Livermore National Laboratory
Optimal control for quantum simulations

Programme Coordinators

*Carlo **Barbieri***
University of Milan and INFN sezione di Milano

*Alessandro **Roggero***
University of Trento and INFN-TIFPA

Student Coordinator and Advisor

Alessandro **Roggero**
University of Trento and INFN-TIFPA

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Summary

Thank you for your attention!!!

→ Ab initio applications to structure and reactions are becoming increasingly powerful. Systematic applications beyond testing forces and structure becoming available

→ Particle-phonon coupling (ADC3/FRPA) being implemented for open shell

→ The covariant version of Nambu-Gorkov formalism in SCGF:

- Minimises the number of diagrams to handle
- Only basic topologies are retained.
- Facilitates automatic diagram generation at higher orders.

→ Applications… optical potentials, g.s. observables, one-nucleon spectroscopy

→ Systematic improvement of Nuclear DFT from ab initio in nuclear matter is promising

And thanks to my collaborators (over the years…)

Thank you for your attention!!!

E. Vigezzi, G. Colò, X. Roca-Maza,
F. Marino, A. Scalesi

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A. Cipollone,
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