TRIUMF Workshop on Progress in Ab Initio Nuclear Theory Feb. 27-March 1, 2024

UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA
INFN MILANO

Reach and opportunities for Green's function methods in nuclear physics

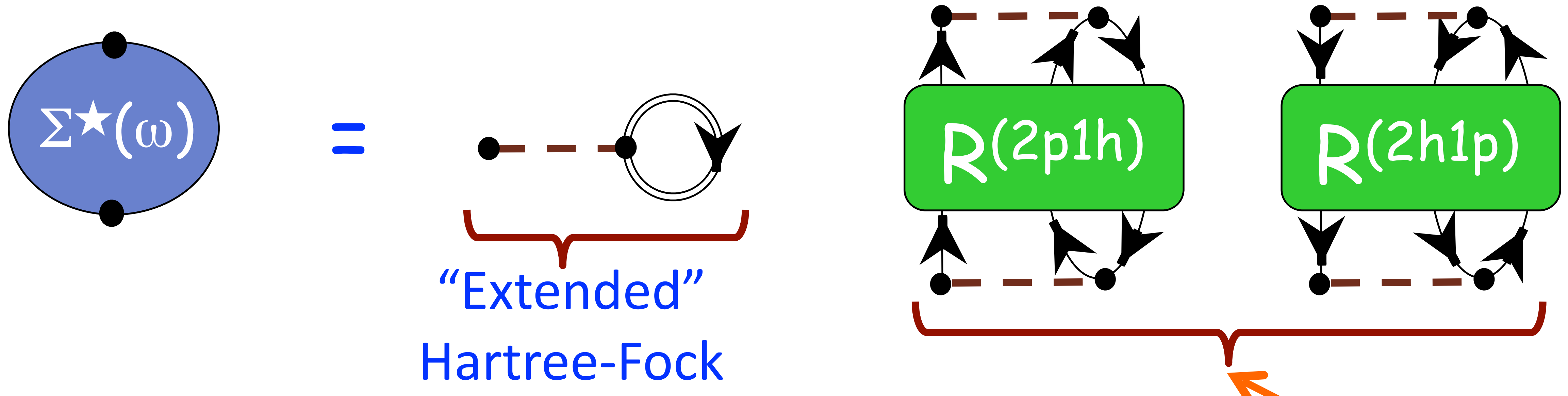
Carlo Barbieri

Outline:

- Optical potentials
- Infinite matter
- Diagrammatic Monte Carlo

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:

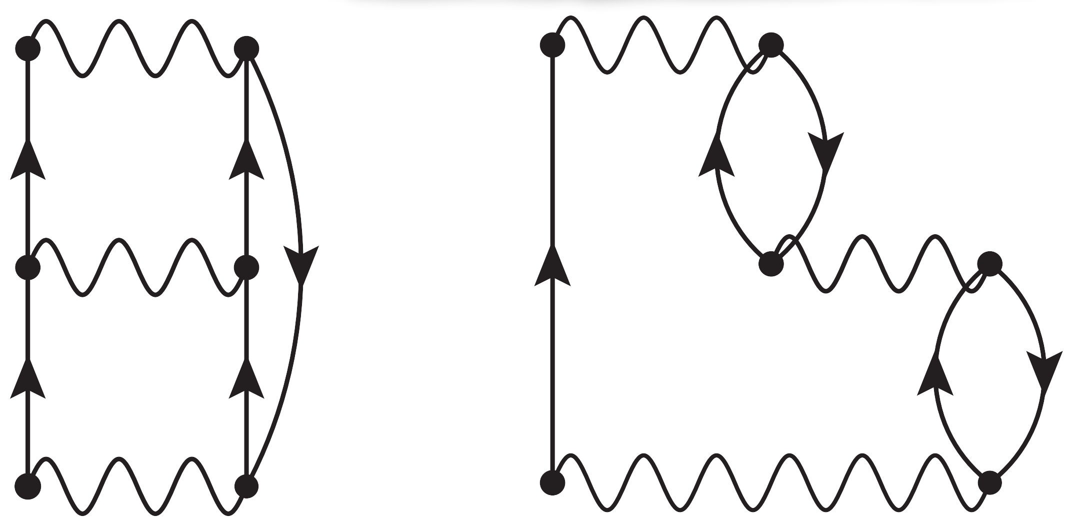


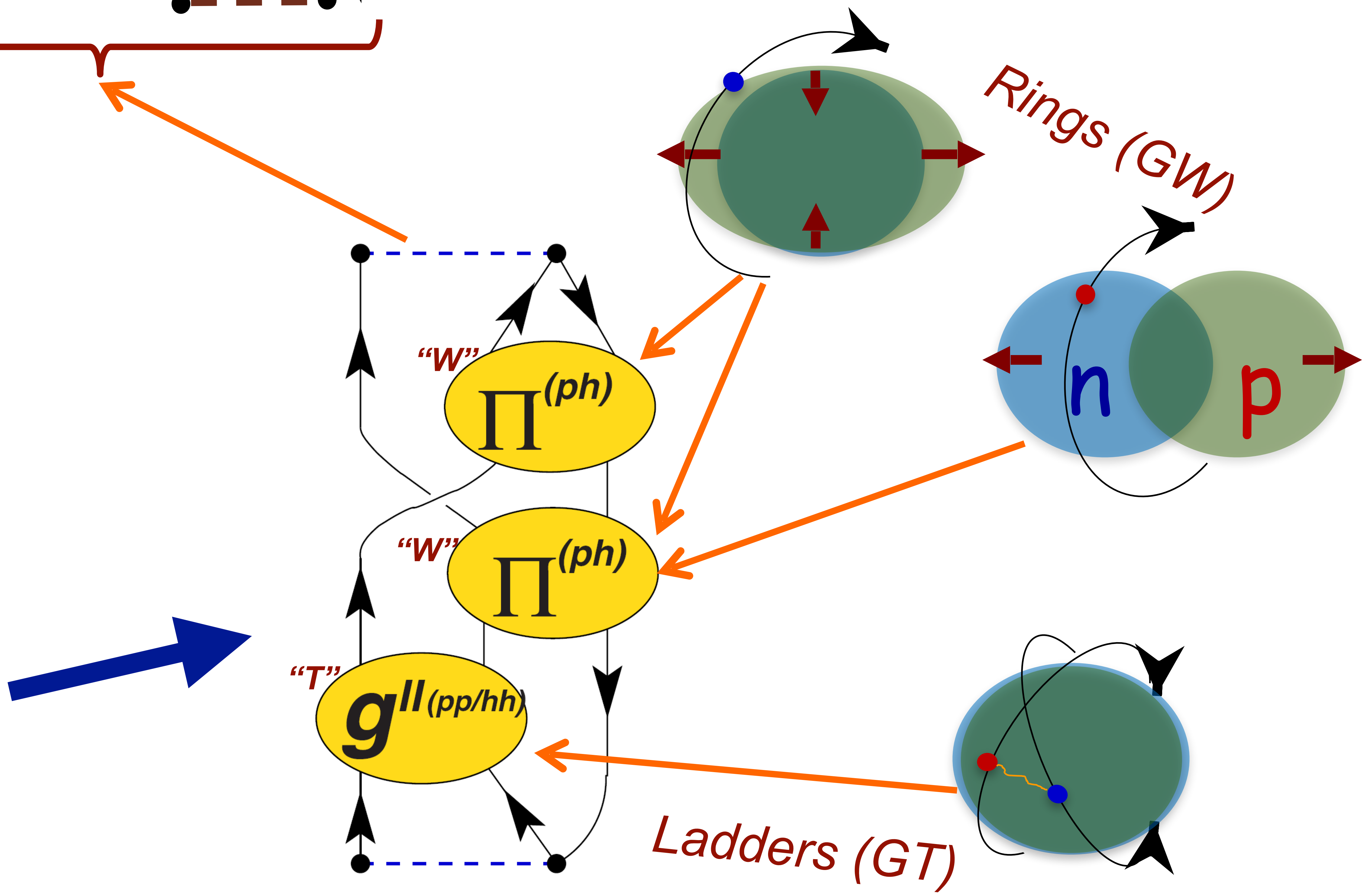
F-RPA:
*Phys. Rev. C**63**, 034313 (2001)*
*Phys. Rev. A**76**, 052503 (2007)*
*Phys. Rev. A**83**, 042517 (2011)*

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':

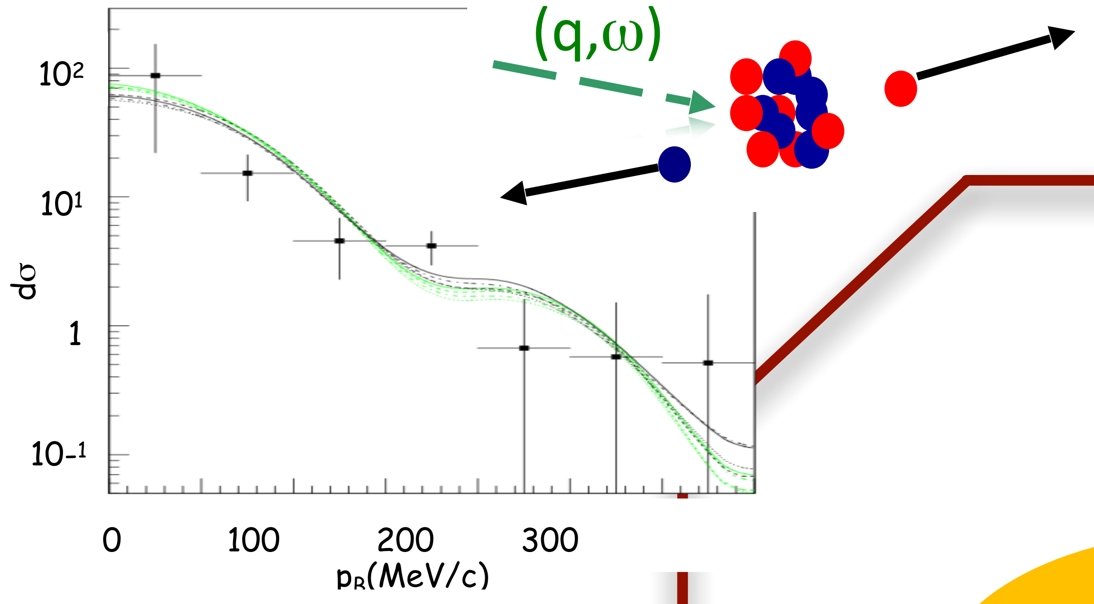




The Self-Consistent Green's Function with Faddev-RPA

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

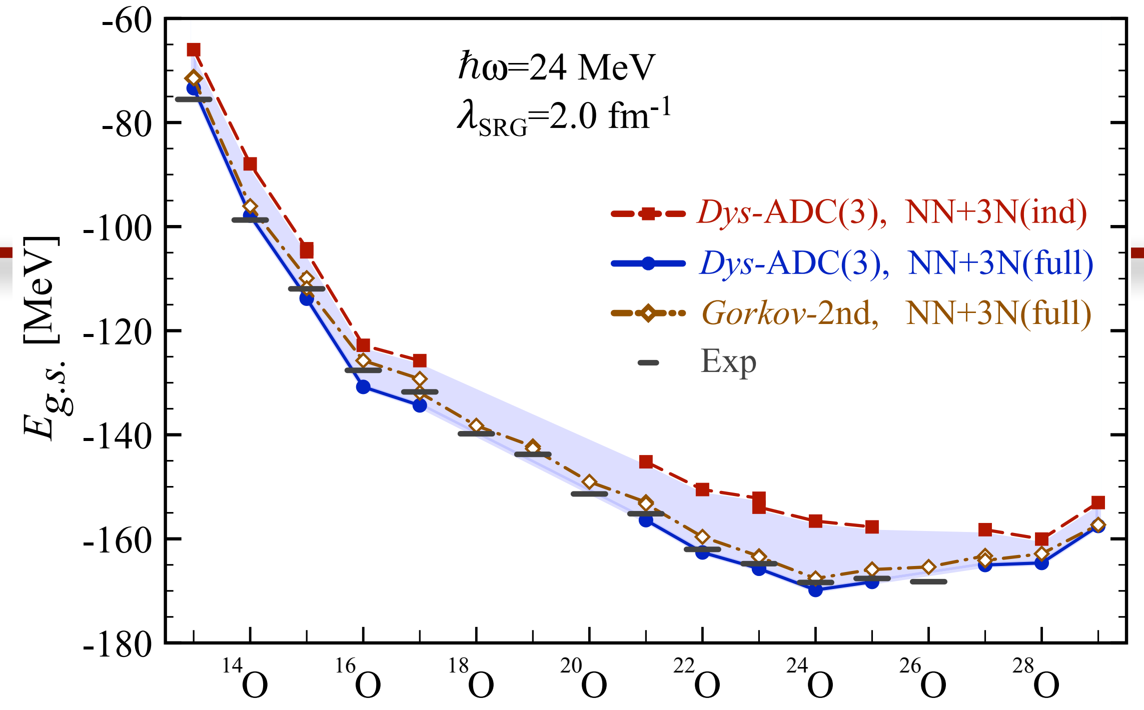
[Eur. Phys. J. A**43**, 137 (2010)]



Binding energies

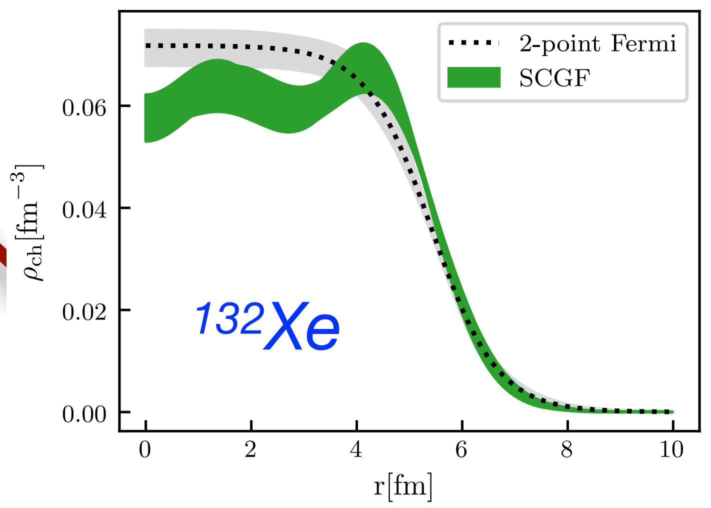
Oxygen drip line

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

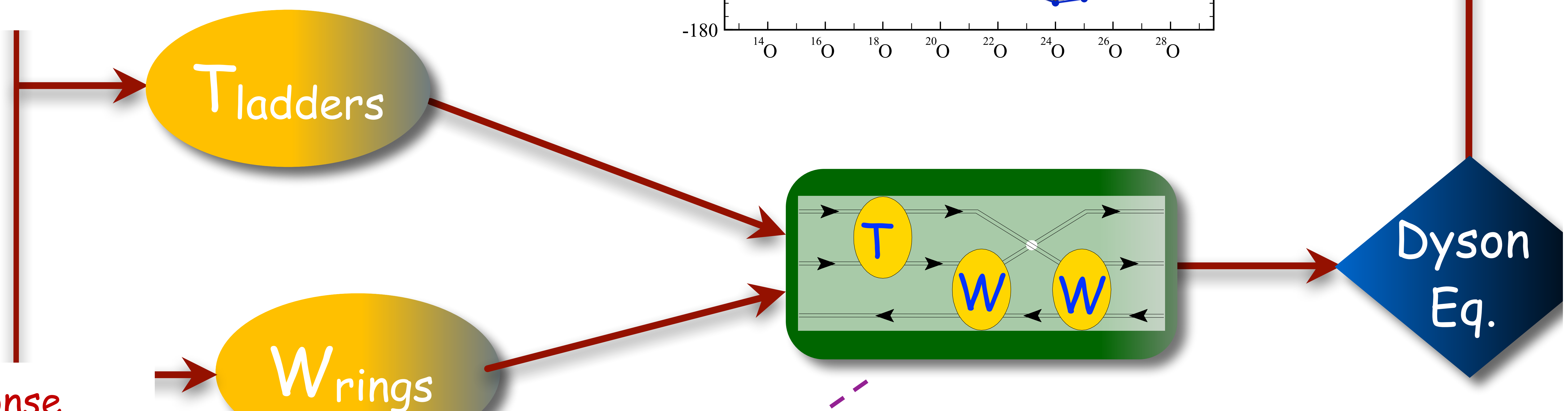


Charge & matter distribution

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

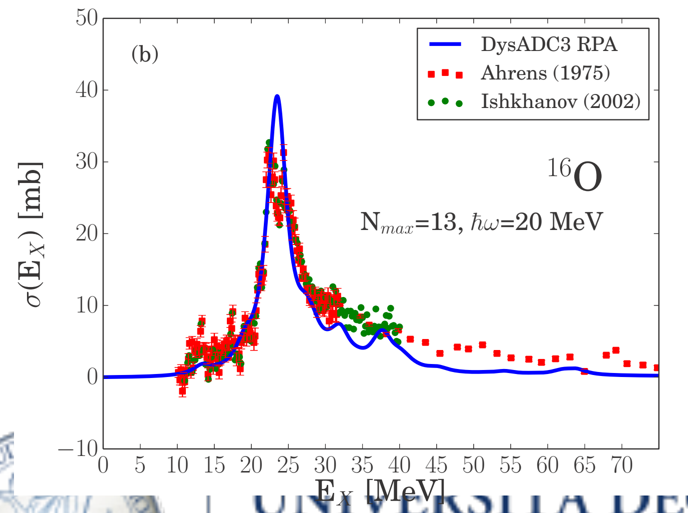
Ionisation energies and affinities for simple atoms and molecules

[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)]

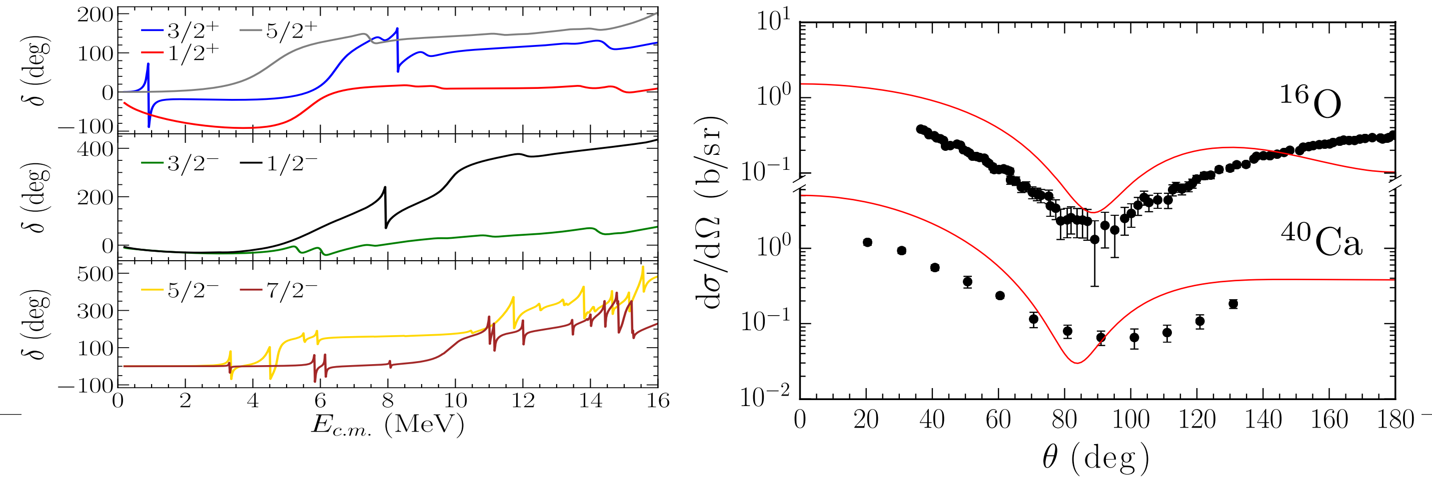


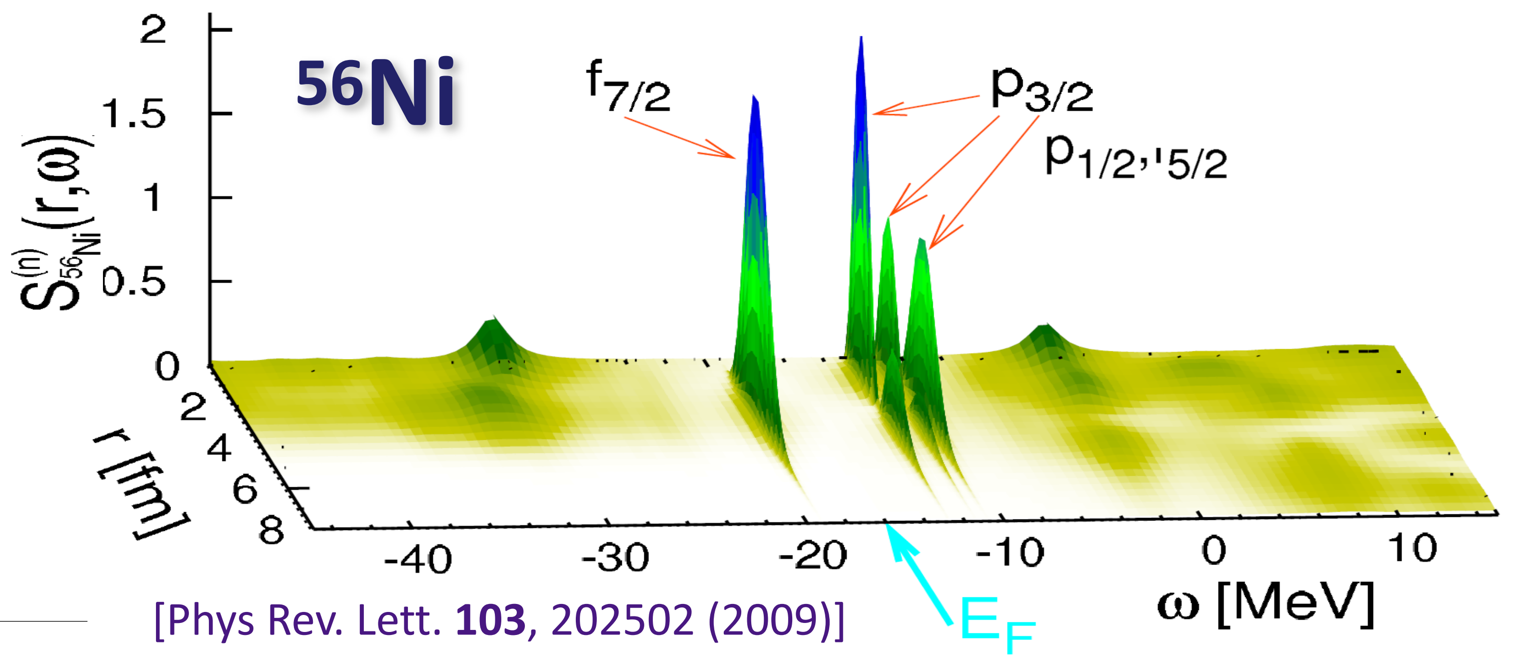
^{68}Ni:

	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)]

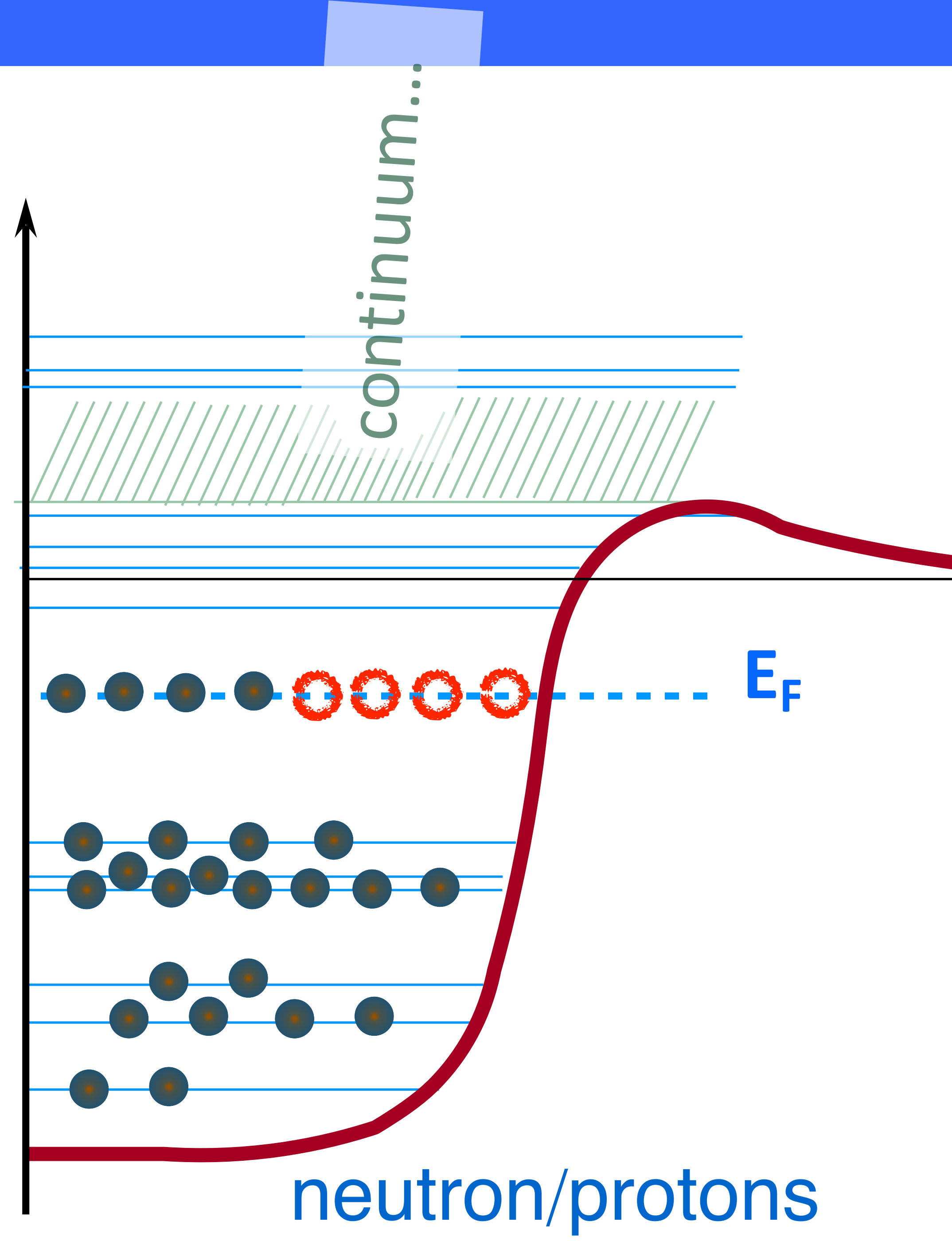
Gorkov ansatz… for atomic nuclei

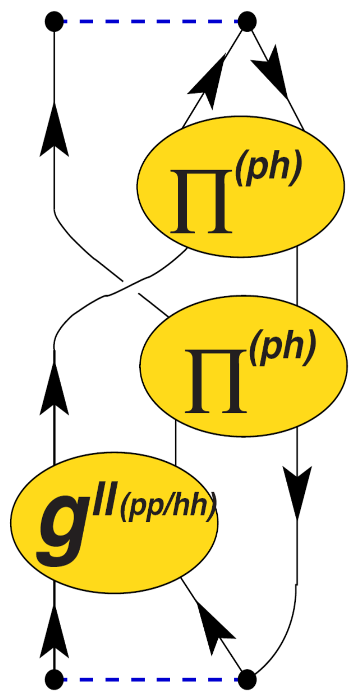
- ➢ In the presence of degenracies (vanishing ph- gaps), enforce (two nucleon) pairing to mitigate unstabilities:

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

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

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





- ➢ Generates a set of two normal and two anomalous propagators:

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

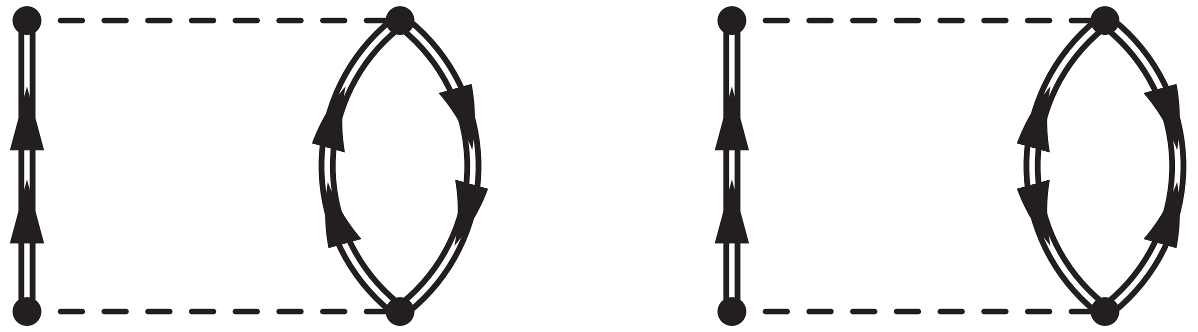
[Gorkov 1958]

V. Somà, T. Duguet, CB, Phys. Rev. C **84**, 064317 (2011)
V. Somà, CB, T. Duguet, Phys. Rev. C **89**, 024323 (2022)
CB, T. Duguet, V. Somà, Phys. Rev. C **105**, 044330 (2022)

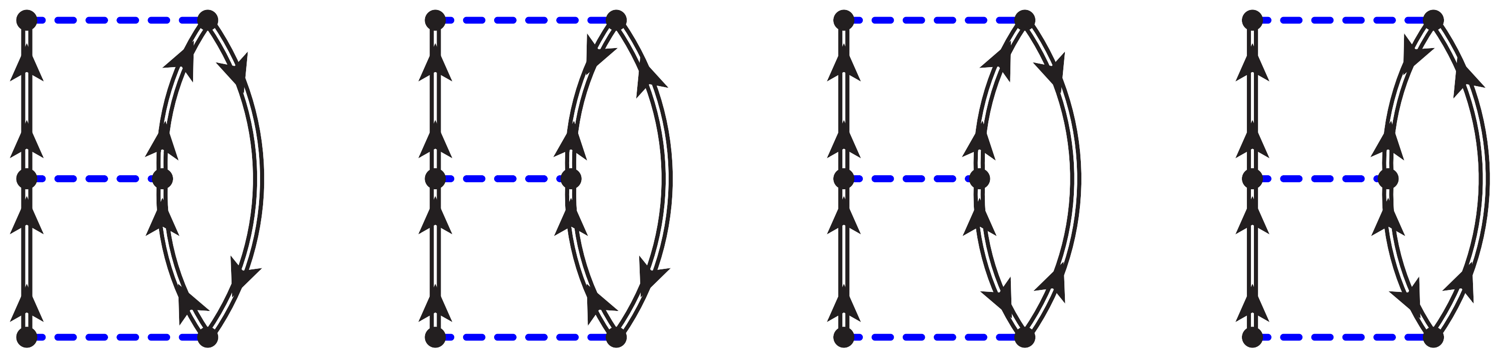
Nambu-Covariant approach to build (Gorkov) propagators

Gorkov at
2nd order:

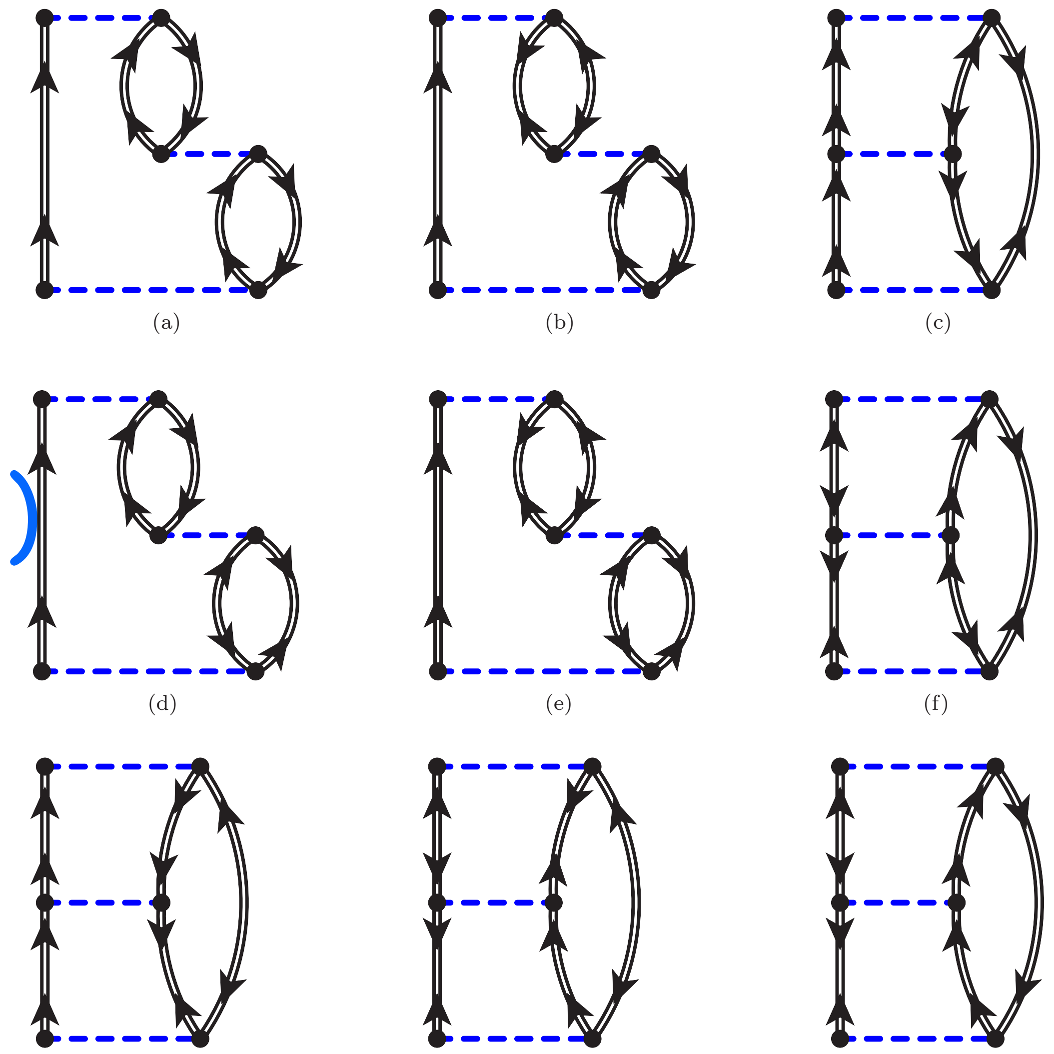
$$\Sigma^{11}_{\alpha\beta}(\omega) \; =$$



pp-ladders:

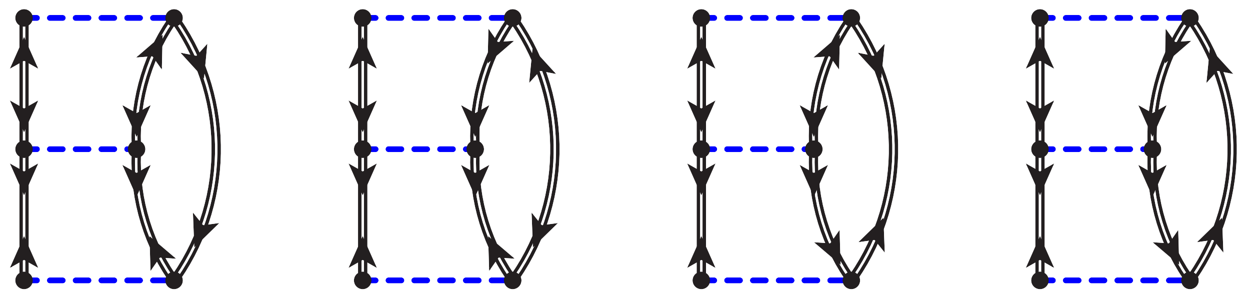


ph-rings:



Gorkov at
3rd order:
(ONLY NN forces)

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



(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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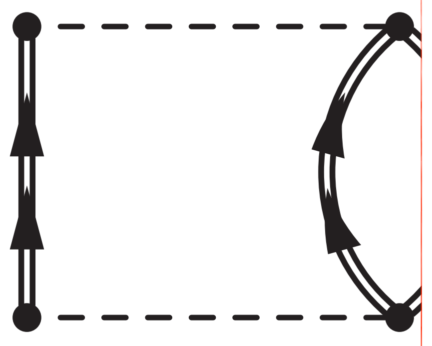
Gorkov at 2nd order:

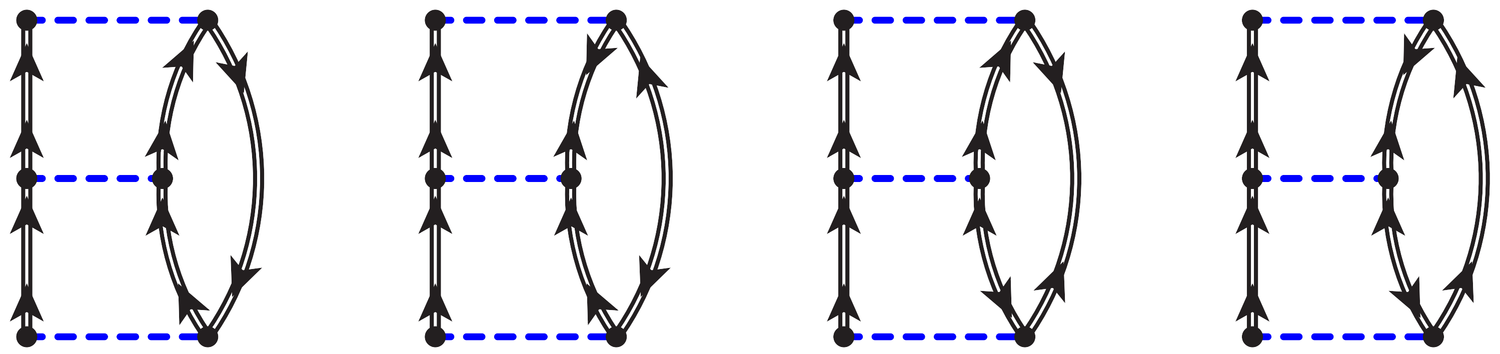
$$\Sigma^{11}_{\alpha\beta}(\omega) \; =$$



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

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

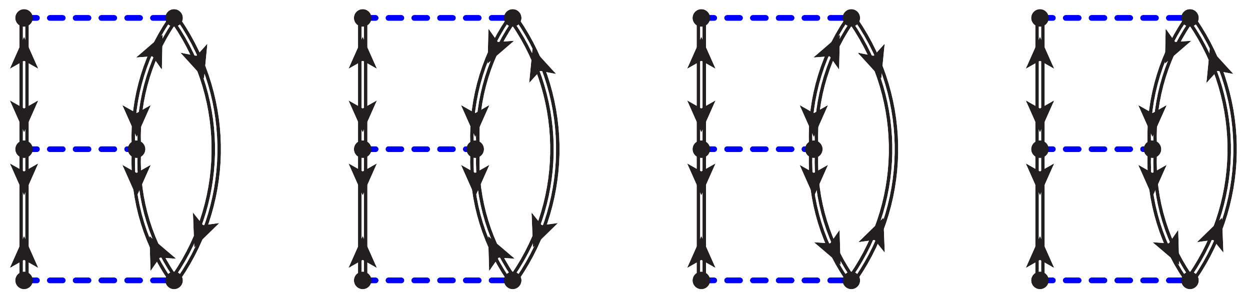
pp-ladders:



Gorkov at 3rd order:

(ONLY NN forces)

hh-interactions (hh int. among pp ladders



(NN ONLY forces)

$$\mathcal{C}^{(\mathrm{IIa})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{P}_{123}\sum_{\substack{\mu\nu\lambda\\ k_4k_5}} \frac{v_{\alpha\lambda,\mu\nu}}{2}\left(\bar{\mathcal{V}}^{k_4}_{\mu}\bar{\mathcal{V}}^{k_5}_{\nu}\right)^{*} t^{k_1k_2}_{k_4k_5}\bar{\mathcal{V}}^{k_3}_{\lambda}, \quad (43a)$$

$$\mathcal{C}^{(\mathrm{IIb})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{P}_{123}\sum_{\substack{\mu\nu\lambda\\ k_4k_5}} v_{\alpha\lambda,\mu\nu}\left(\bar{\mathcal{V}}^{k_4}_{\nu}\mathcal{U}^{k_5}_{\lambda}\right)^{*} t^{k_1k_2}_{k_4k_5}\mathcal{U}^{k_3}_{\mu}, \quad (43b)$$

$$\mathcal{C}^{(\mathrm{IIc})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{P}_{123}\sum_{\substack{\mu\nu\lambda\\ k_4k_5}} \frac{v_{\alpha\lambda,\mu\nu}}{2}\left(\bar{\mathcal{V}}^{k_4}_{\mu}\bar{\mathcal{V}}^{k_5}_{\nu}\right)^{*} t^{k_4k_5}_{k_1k_2}\bar{\mathcal{V}}^{k_3}_{\lambda}, \quad (47a)$$

$$\mathcal{C}^{(\mathrm{IId})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{P}_{123}\sum_{\substack{\mu\nu\lambda\\ k_4k_5}} v_{\alpha\lambda,\mu\nu}\left(\bar{\mathcal{V}}^{k_4}_{\nu}\mathcal{U}^{k_5}_{\lambda}\right)^{*} t^{k_4k_5}_{k_1k_2}\mathcal{U}^{k_3}_{\mu}, \quad (47b)$$

$$\mathcal{E}^{(pp)}_{k_1k_2,k_4k_5} = \sum_{\alpha\beta\gamma\delta}\left(\mathcal{U}^{k_1}_{\alpha}\mathcal{U}^{k_2}_{\beta}\right)^{*} v_{\alpha\beta,\gamma\delta}\,\mathcal{U}^{k_4}_{\gamma}\mathcal{U}^{k_5}_{\delta}, \quad (45)$$

$$\mathcal{E}^{(hh)}_{k_1k_2,k_4k_5} = \sum_{\alpha\beta\gamma\delta}\bar{\mathcal{V}}^{k_1}_{\alpha}\bar{\mathcal{V}}^{k_2}_{\beta}\, v_{\alpha\beta,\gamma\delta}\left(\bar{\mathcal{V}}^{k_4}_{\gamma}\bar{\mathcal{V}}^{k_5}_{\delta}\right)^{*}. \quad (46)$$

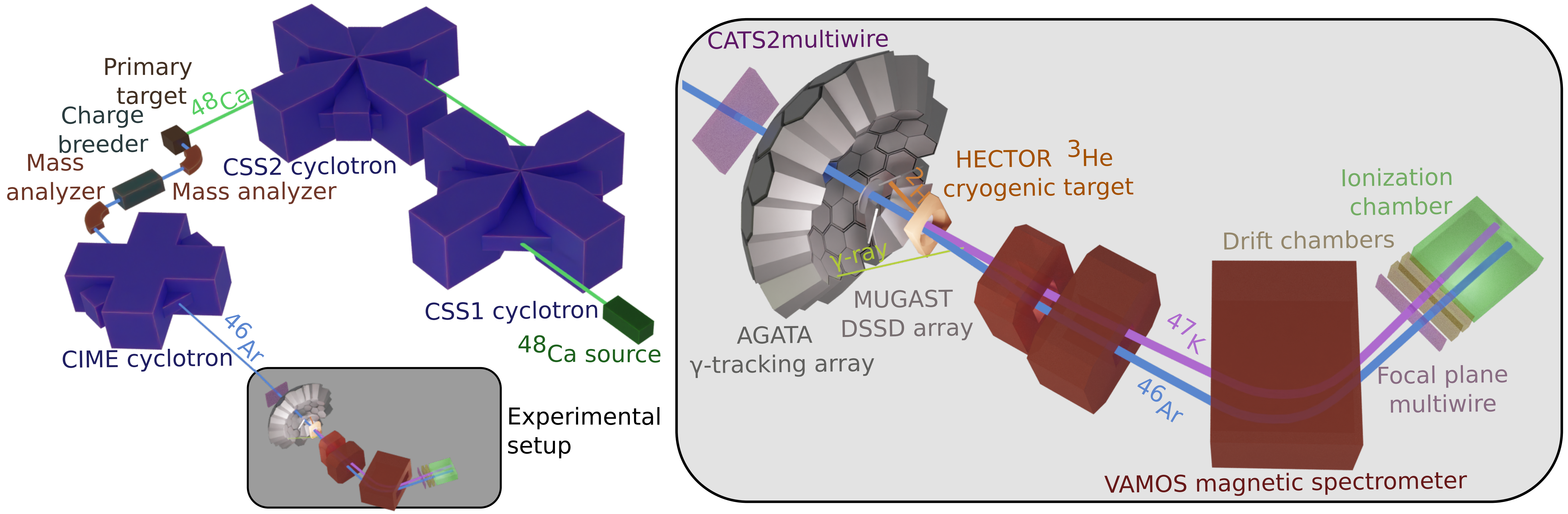
$$\mathcal{C}^{(\mathrm{IIe})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{A}_{123}\sum_{\substack{\mu\nu\lambda\\ k_7k_8}} v_{\alpha\lambda,\mu\nu}\left(\bar{\mathcal{V}}^{k_7}_{\nu}\mathcal{U}^{k_8}_{\lambda}\right)^{*}\mathcal{U}^{k_1}_{\mu}\, t^{k_8k_2}_{k_7k_3}, \quad (50a)$$

$$\mathcal{C}^{(\mathrm{IIf})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{A}_{123}\sum_{\substack{\mu\nu\lambda\\ k_7k_8}} v_{\alpha\lambda,\mu\nu}\left(\mathcal{U}^{k_7}_{\lambda}\bar{\mathcal{V}}^{k_8}_{\mu}\right)^{*}\mathcal{U}^{k_1}_{\nu}\, t^{k_8k_2}_{k_7k_3}, \quad (50b)$$

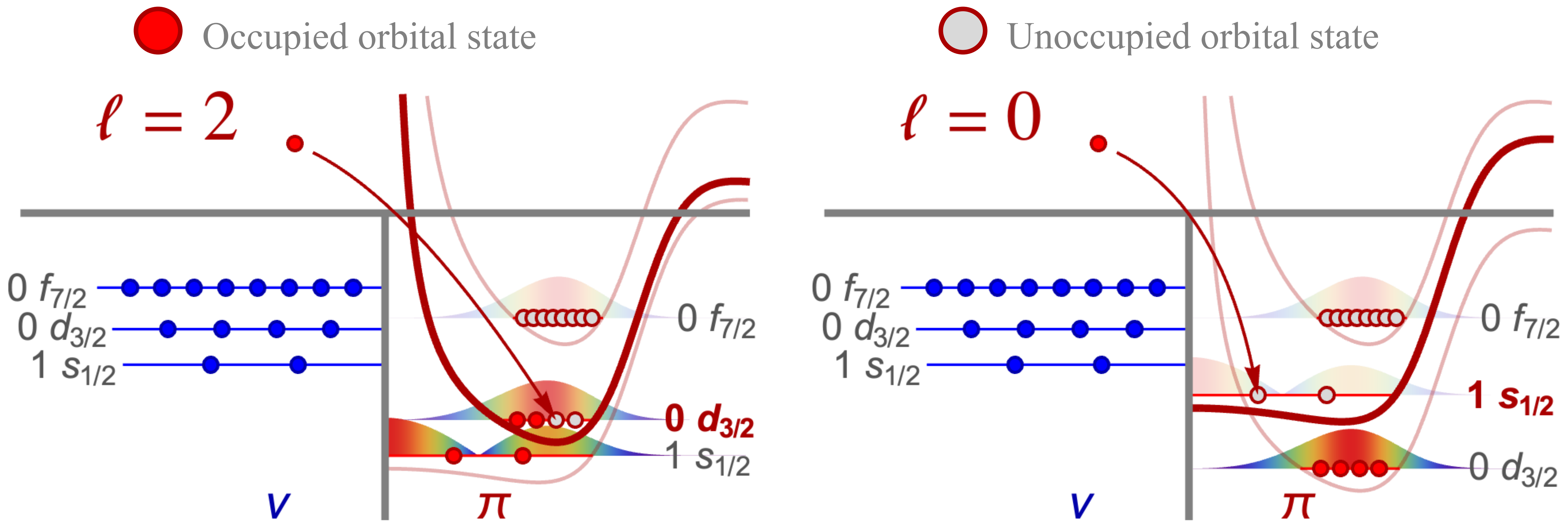
$$\mathcal{C}^{(\mathrm{IIg})}_{\alpha,r} = \frac{1}{\sqrt{6}}\mathcal{A}_{123}\sum_{\substack{\mu\nu\lambda\\ k_7k_8}} v_{\alpha\lambda,\mu\nu}\left(\bar{\mathcal{V}}^{k_7}_{\mu}\bar{\mathcal{V}}^{k_8}_{\nu}\right)^{*}\bar{\mathcal{V}}^{k_1}_{\lambda}\, t^{k_8k_2}_{k_7k_3}, \quad (50c)$$

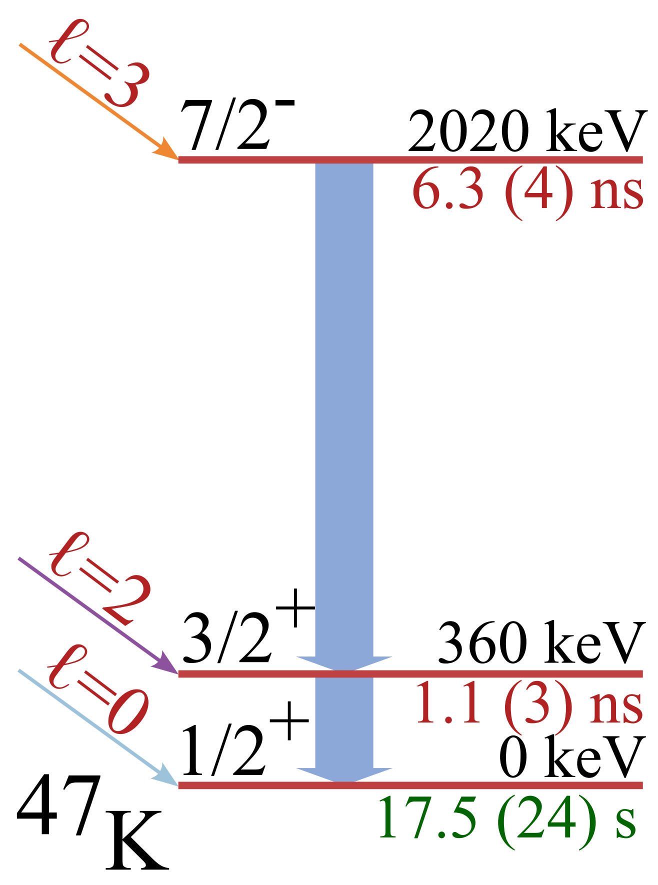
$$\mathcal{E}^{(\mathrm{Ic})}_{r,r'} = \tfrac{1}{6}\mathcal{A}_{123}\mathcal{A}_{456}\left(\delta_{k_1,k_4}\mathcal{E}^{(ph)}_{k_2k_3,k_5k_6}\right),$$

$^{46}Ar(^3He,d)^{47}K$ at GANIL



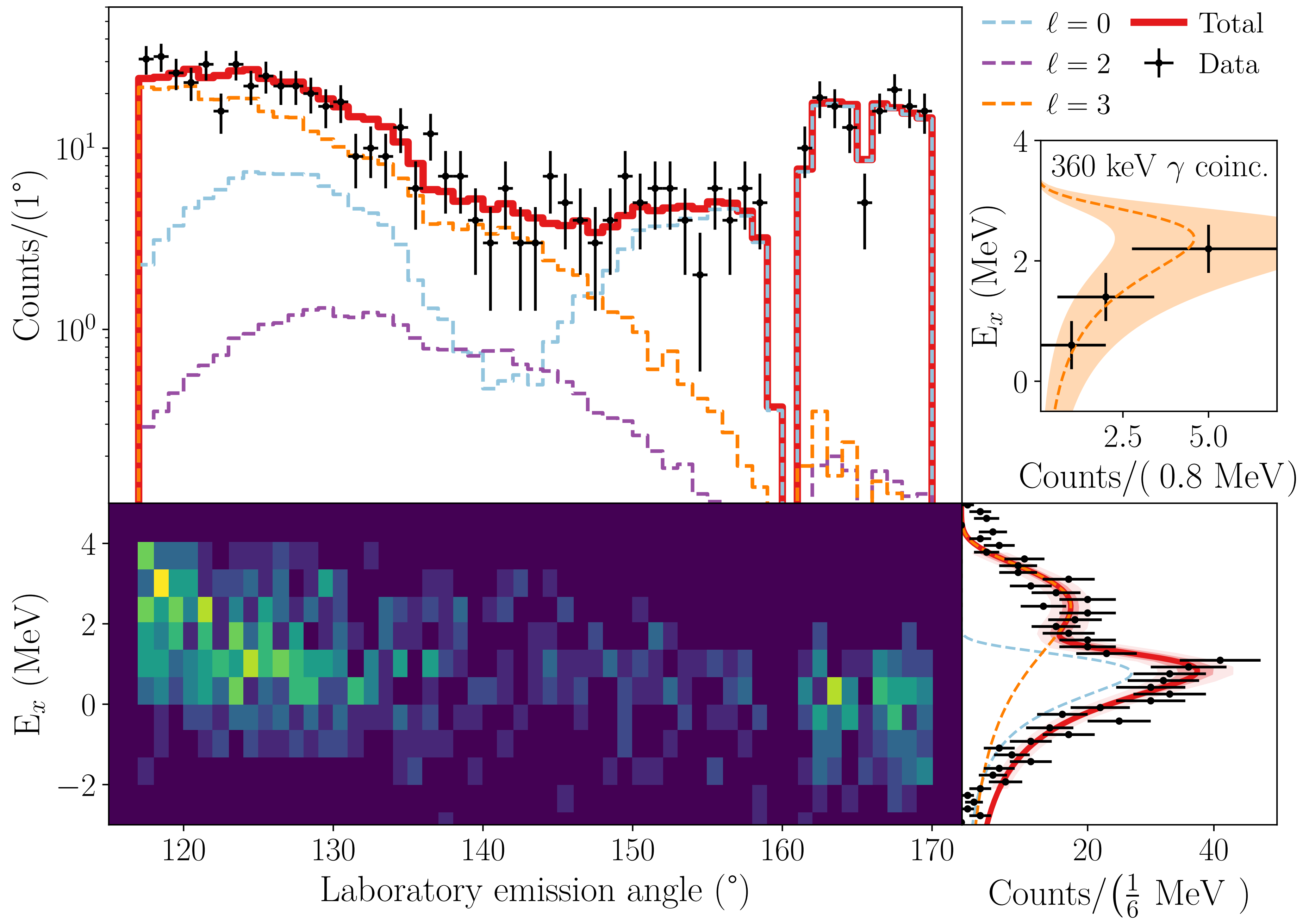
d3/2 - s1/2 inversion revisited from adding protons to ^{46}Ar

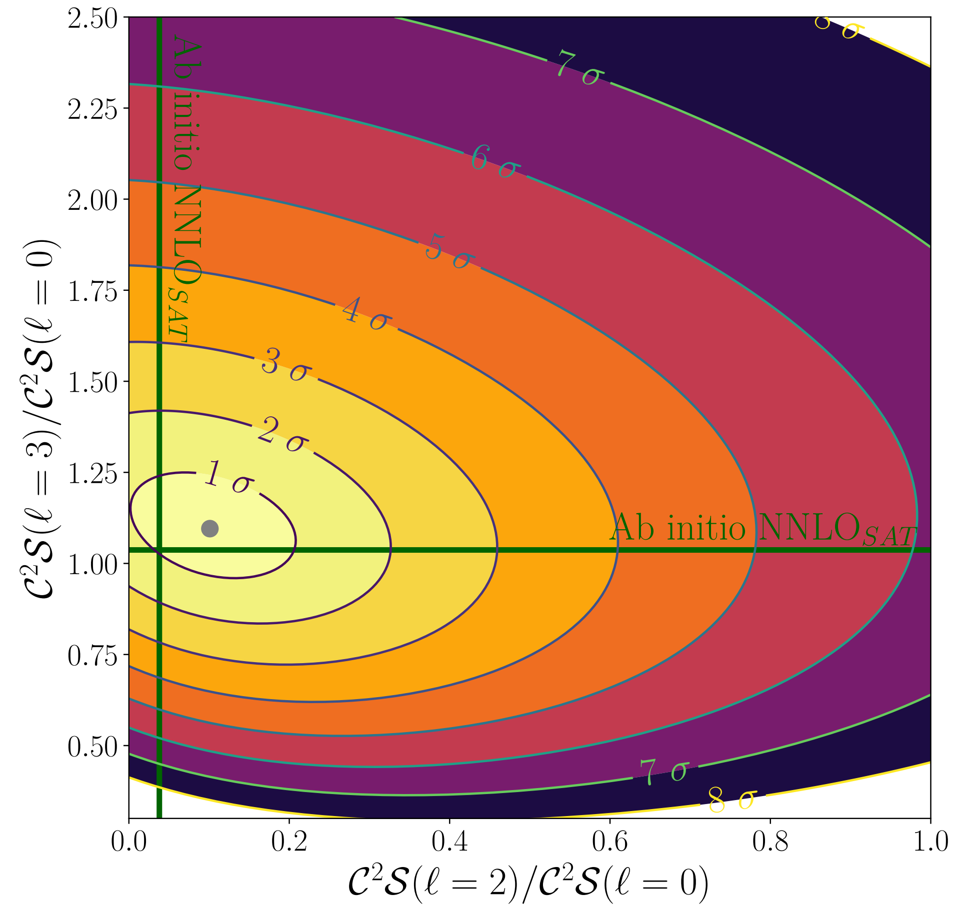




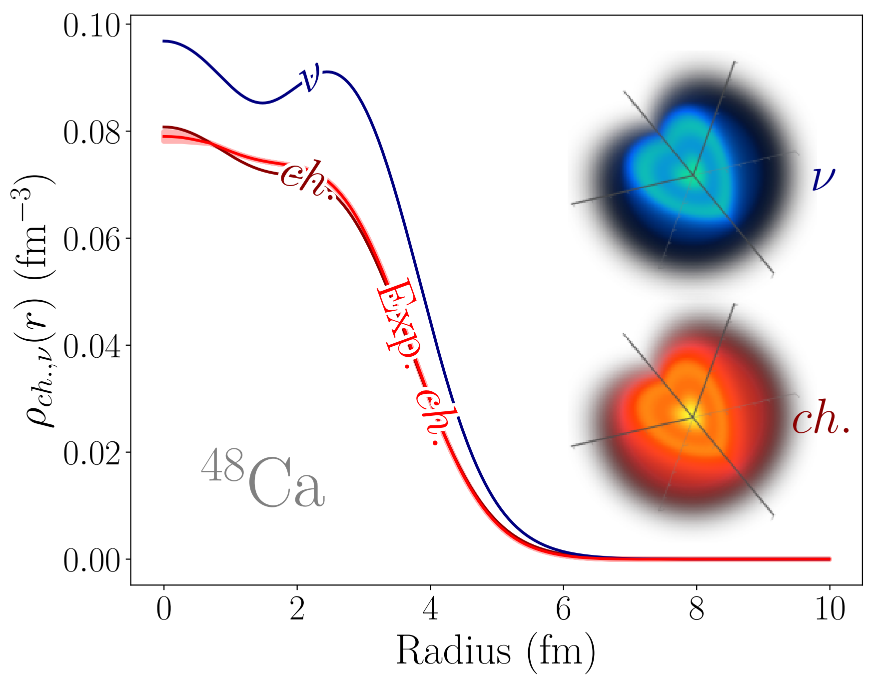
D. Brugnara, A. Gottardo, CB et al…

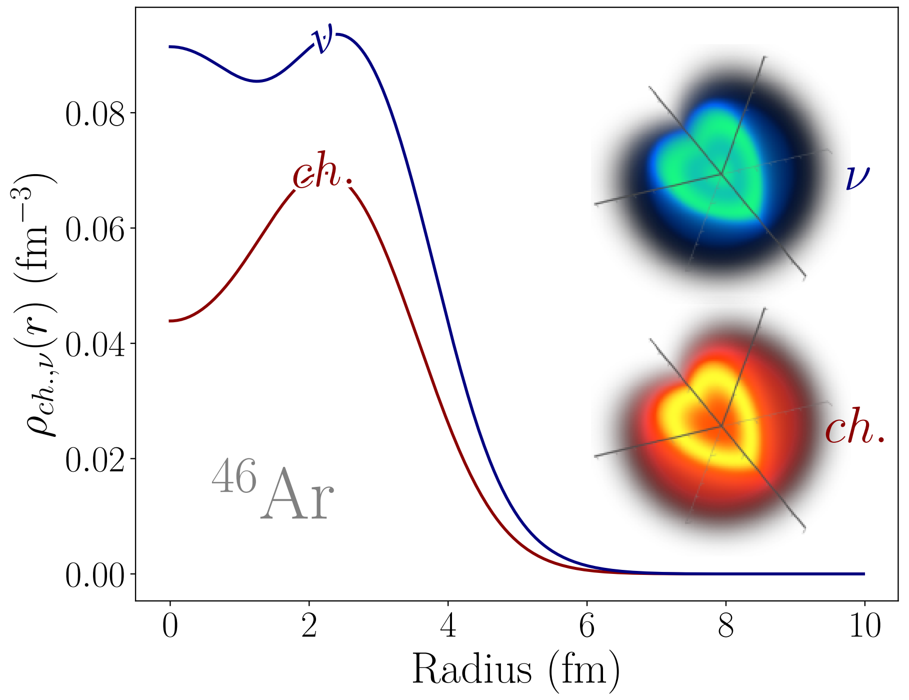
^{46}Ar(^{3}He,d)^{47}K at GANIL : New charge bobble in ^{46}Ar





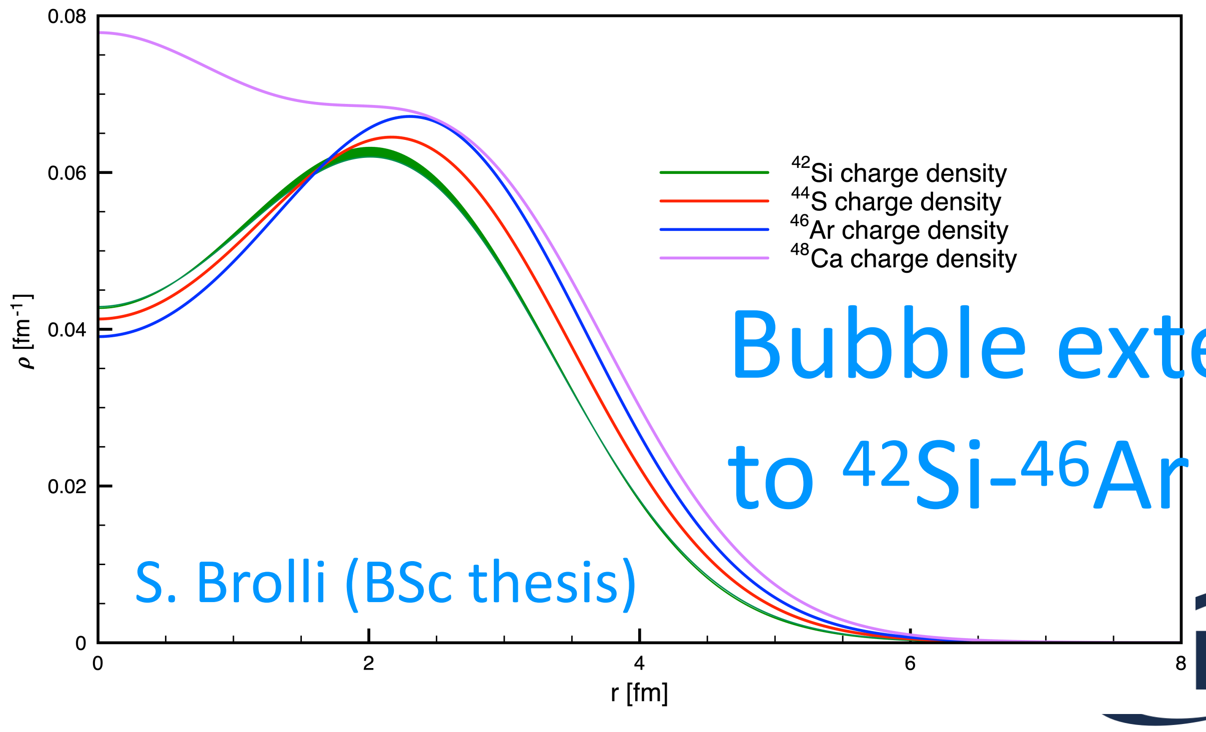
$$\frac{d\sigma}{d\Omega} = \sum_k g_k \, C^2 S_k \, \frac{d\sigma_k^{SP}}{d\Omega}$$





d3/2 - s1/2 inversion revisited from adding protons to ^{46}Ar

Theory & experiment for relative SFs agree within 1 sigma and confirms charge depletion in ^{46}Ar



Bubble extends to ^{42}Si-^{46}Ar ??

S. Brolli (BSc thesis)

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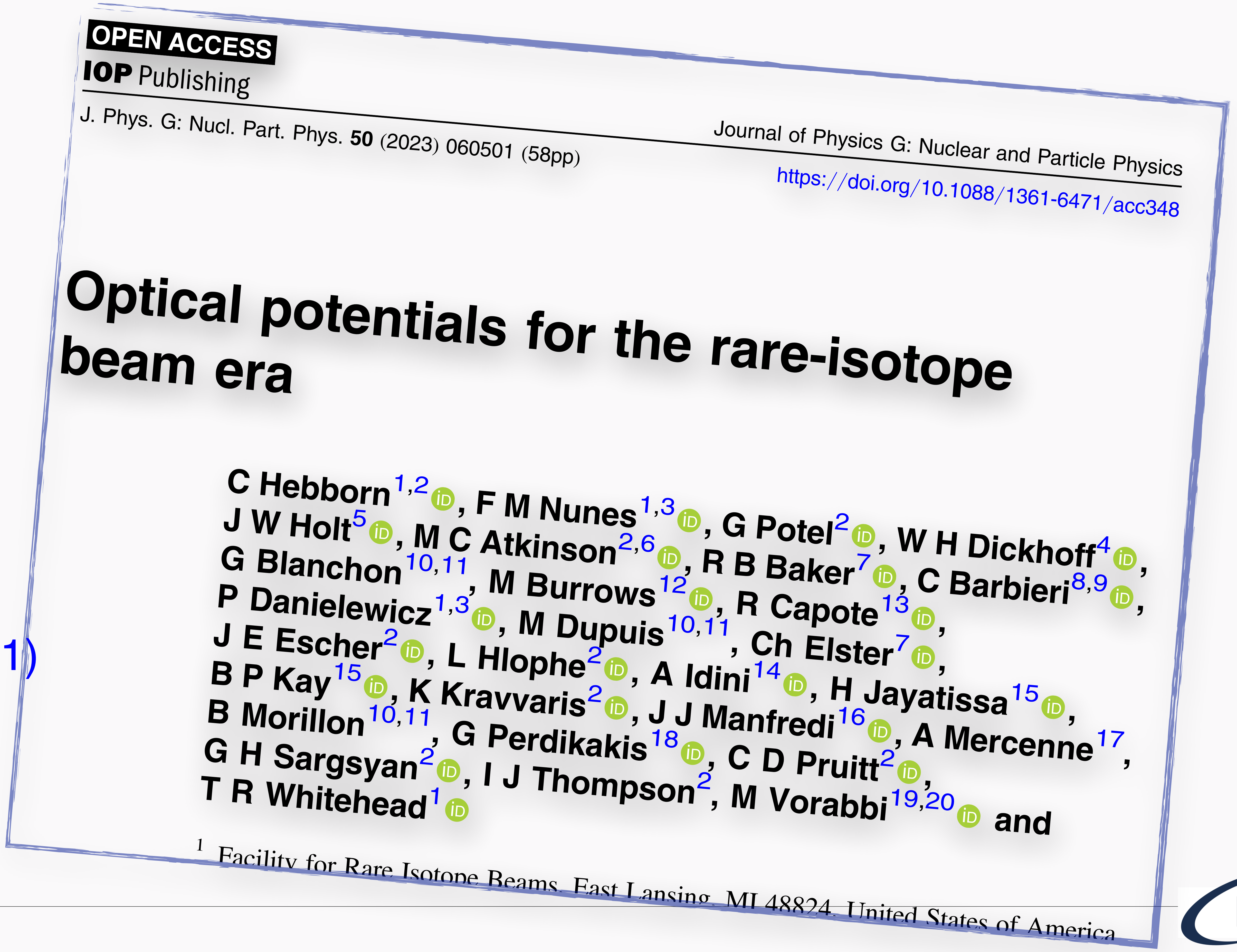
Ab initio optical potentials from propagator theory



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Journal of Physics G: Nuclear and Particle Physics
https://doi.org/10.1088/1361-6471/acc348

Optical potentials for the rare-isotope beam era

C Hebborn[1,2], F M Nunes[1,3], G Potel[2], W H Dickhoff[4], J W Holt[5], M C Atkinson[2,6], R B Baker[7], C Barbieri[8,9], G Blanchon[10,11], M Burrows[12], R Capote[13], P Danielewicz[1,3], M Dupuis[10,11], Ch Elster[7], J E Escher[2], L Hlophe[2], A Idini[14], H Jayatissa[15], B P Kay[15], K Kravvaris[2], J J Manfredi[16], A Mercenne[17], B Morillon[10,11], G Perdikakis[18], C D Pruitt[2], G H Sargsyan[2], I J Thompson[2], M Vorabbi[19,20] and T R Whitehead[1]

[1] Facility for Rare Isotope Beams, East Lansing, MI 48824, United States of America

Relation to Fesbach theory:

Mahaux & Sartor, Adv. Nucl. Phys. 20 (1991)

Escher & Jennings Phys. Rev. C**66**, 034313 (2002)

Previous SCGF work:

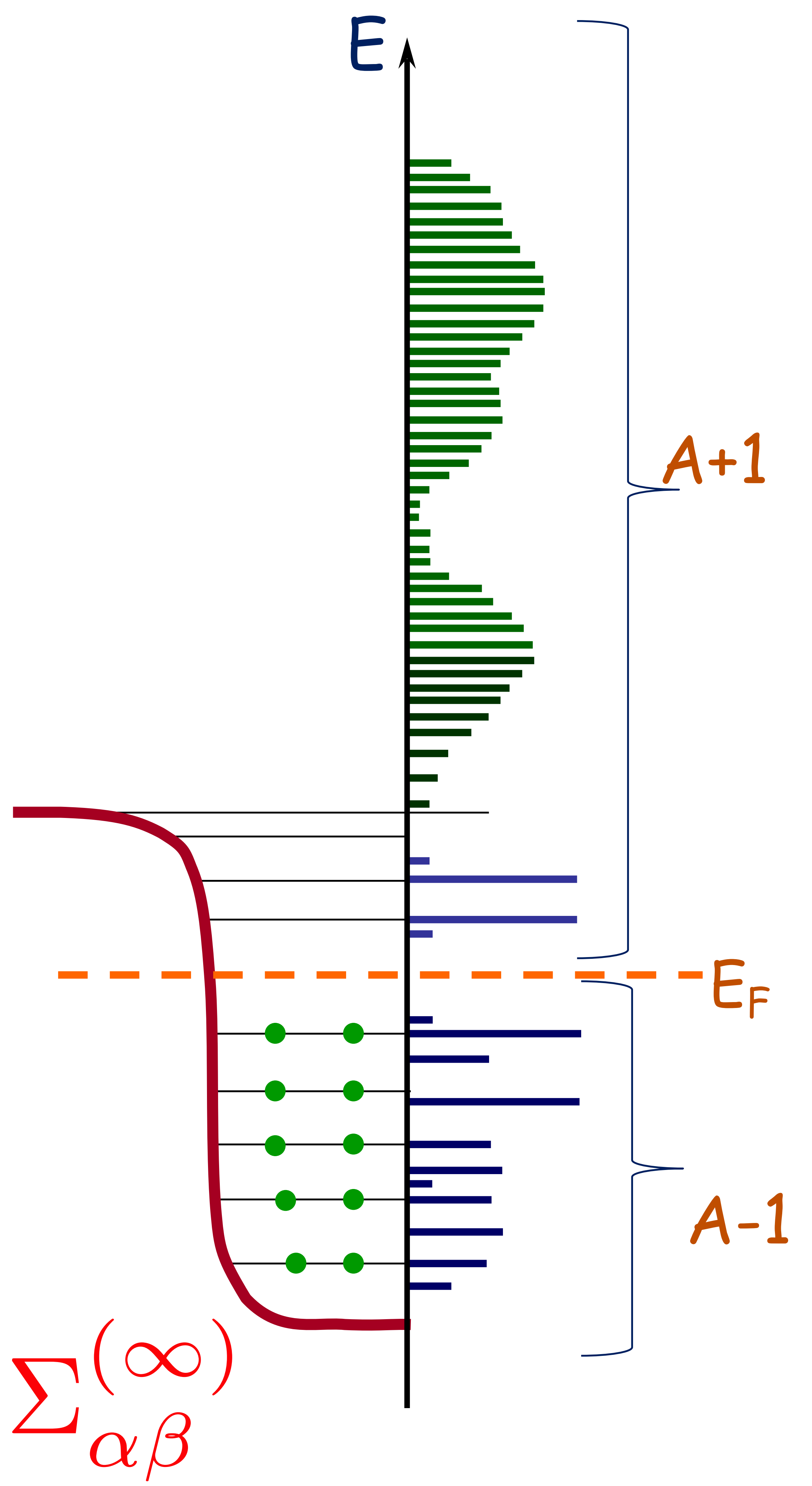
CB, B. Jennings, Phys. Rev. C**72**, 014613 (2005)

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

Microscopic optical potential



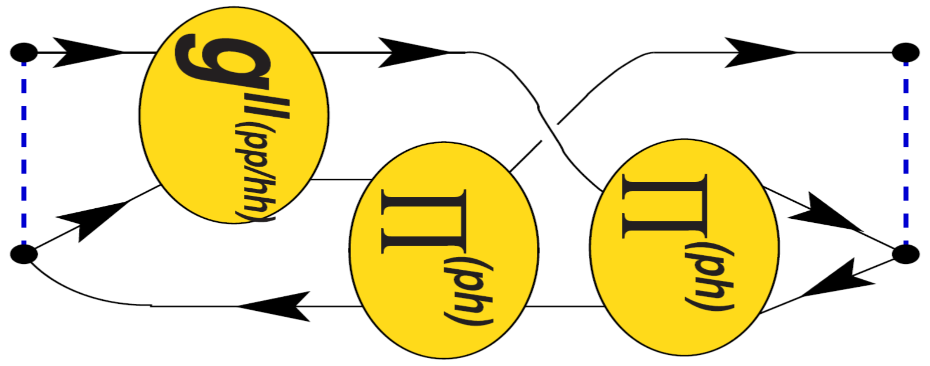
Nuclear self-energy $\Sigma^\star(\mathbf{r},\mathbf{r}';\varepsilon)$:

- 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:

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

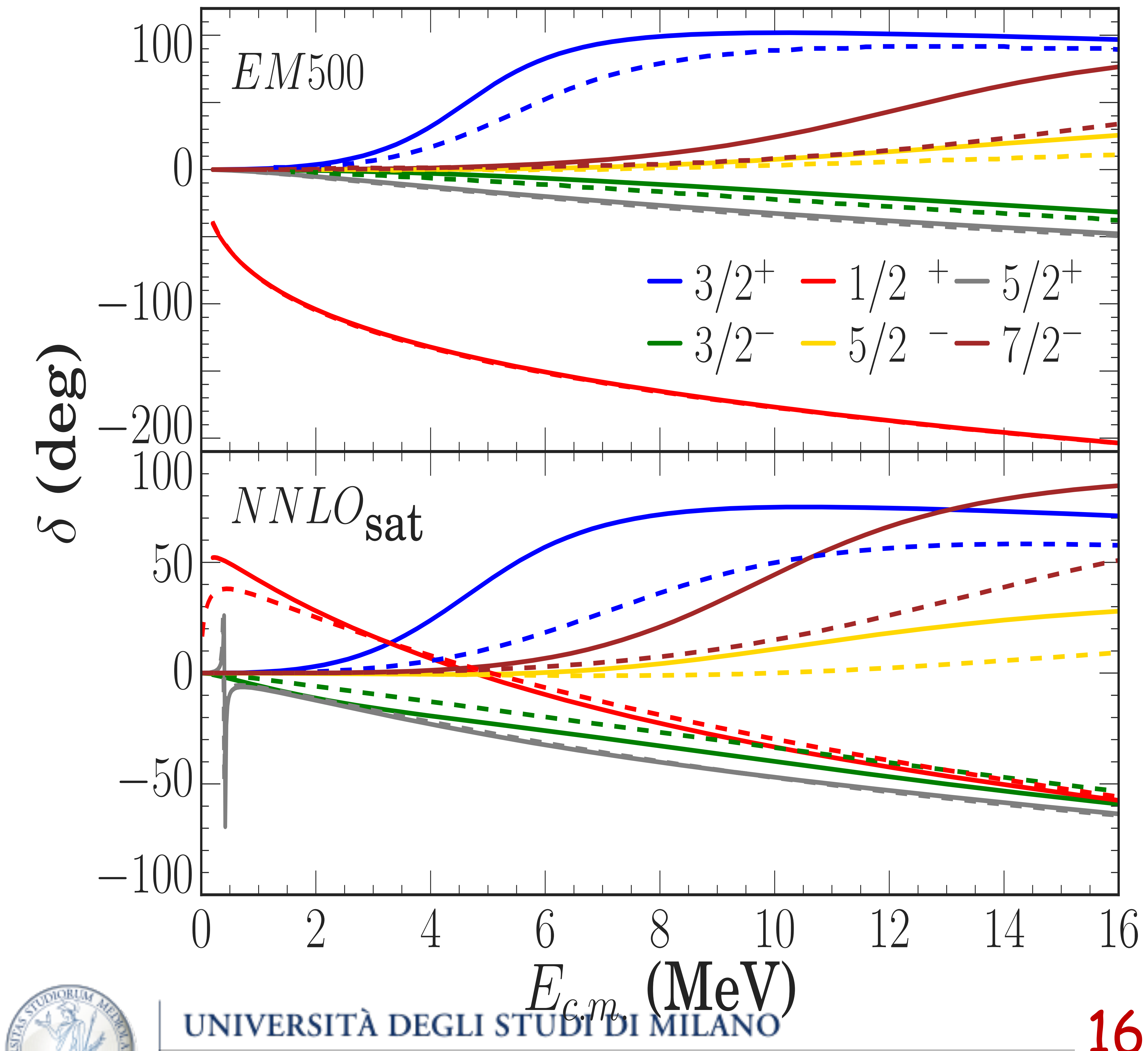
$$\frac{k^2}{2\mu}\psi_{l,j}(k) + \int \mathrm{d}k'\, k'^2\, \Sigma^{\star l,j}(k,k';E_{c.m.})\psi_{l,j}(k') = E_{c.m.}\psi_{l,j}(k)$$

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

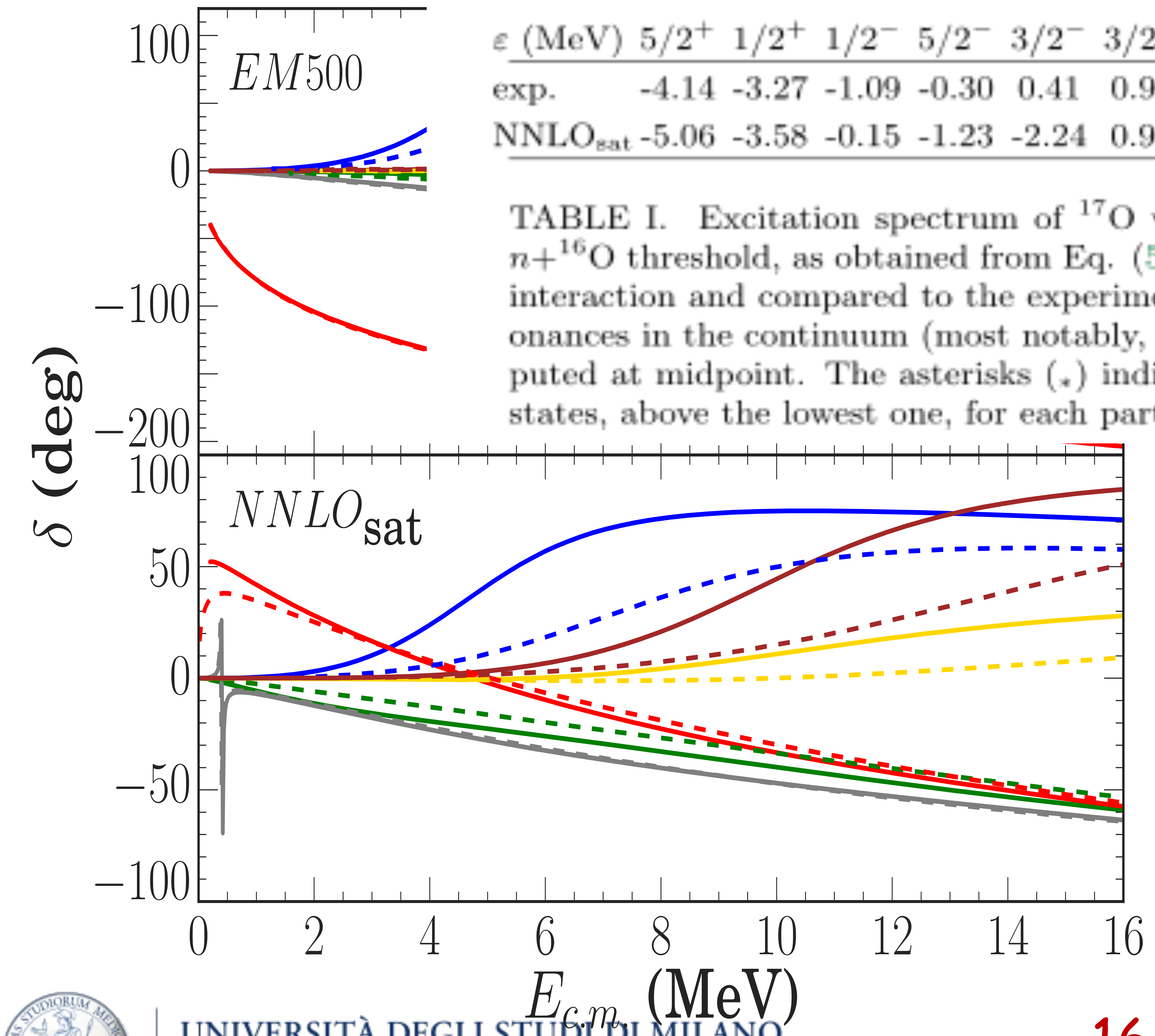
$^{16}O(n,n')^{16}O$

Low energy scattering - from SCGF

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

Benchmark with NCSM-based scattering.

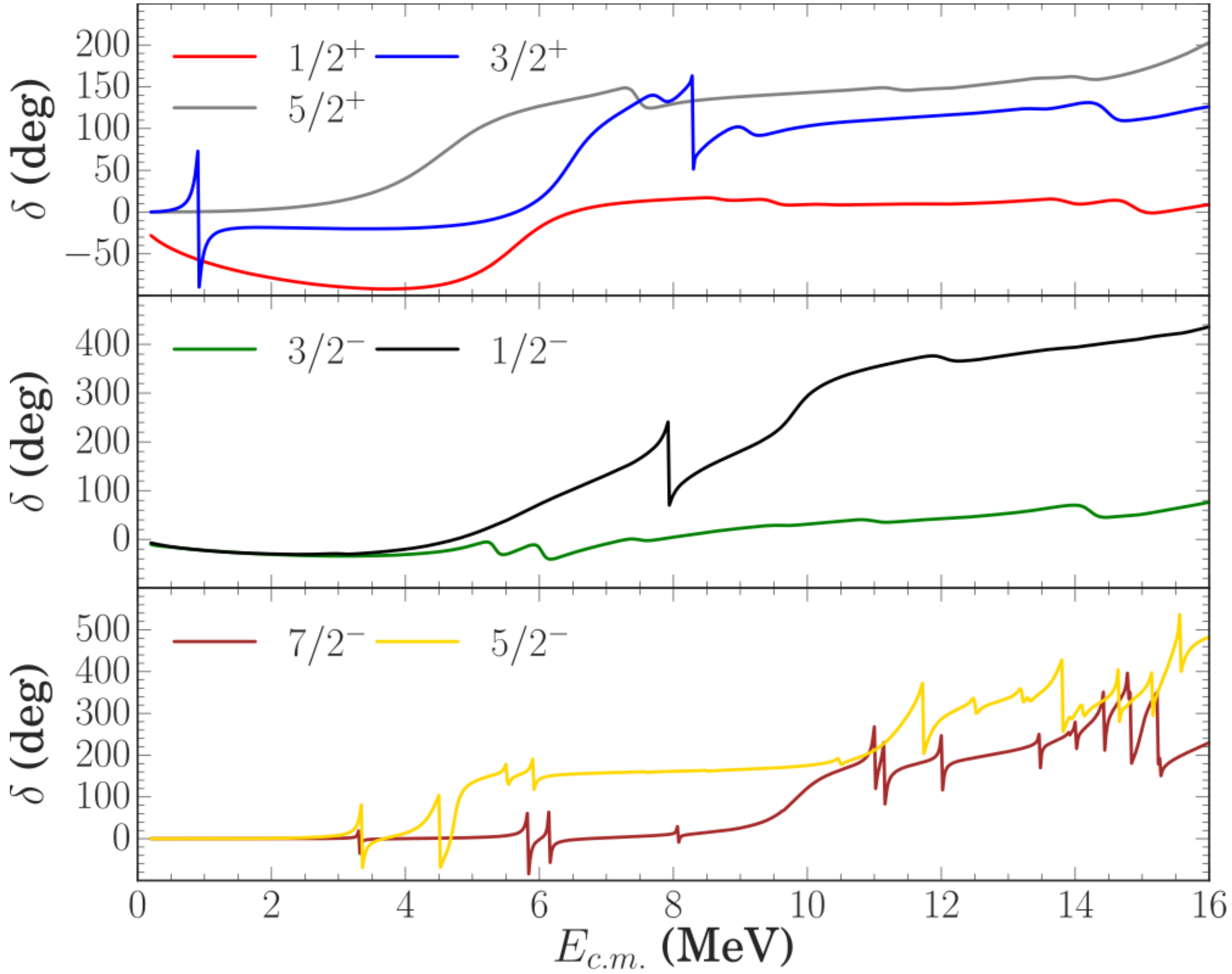
Scattering from mean-field only:



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
$\mathrm{NNLO_{sat}}$	-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 $\mathrm{NNLO_{sat}}$ 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:

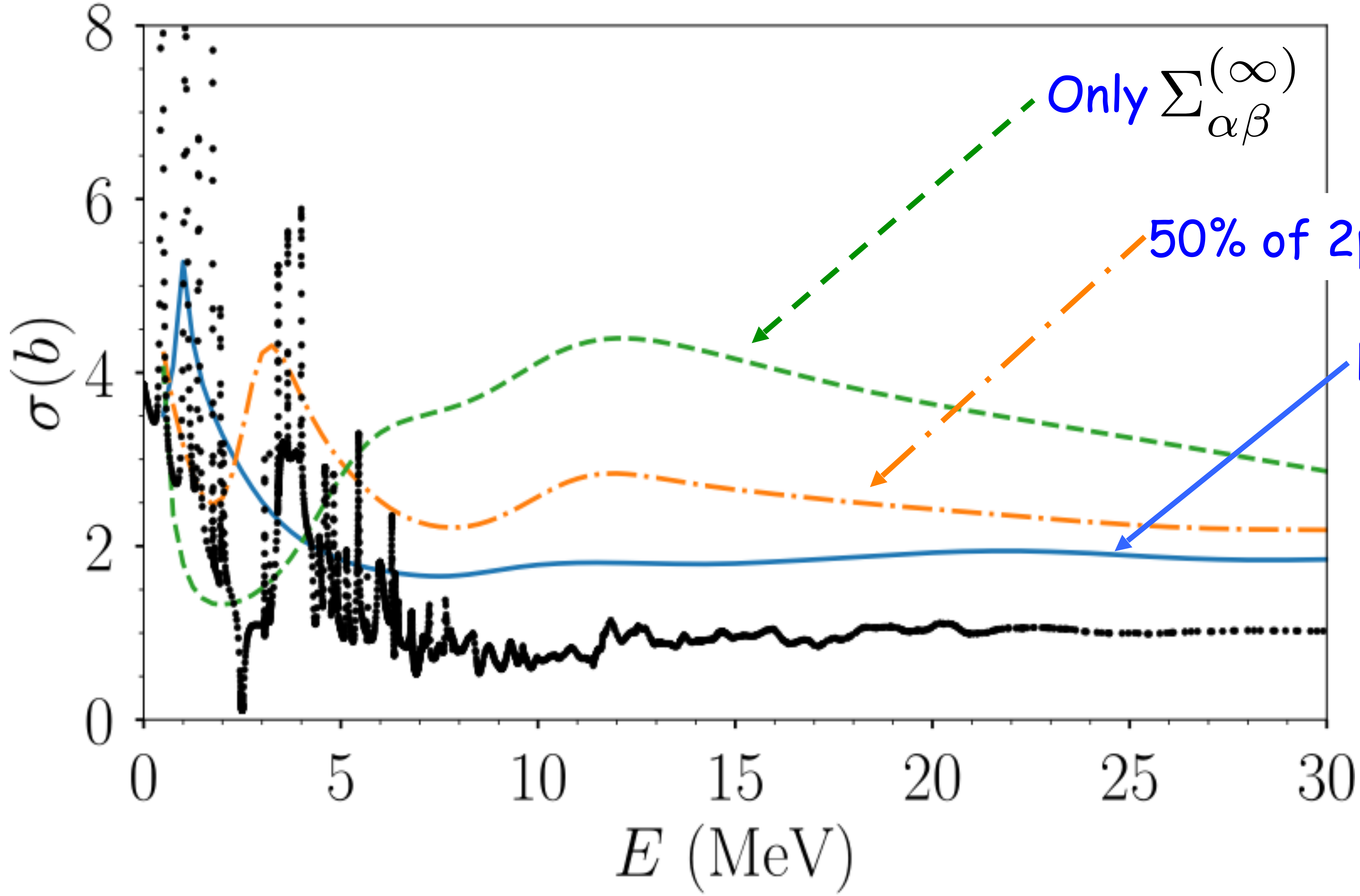


$^{16}O(n,n')^{16}O$

Role of intermediate state configurations (ISCs)

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

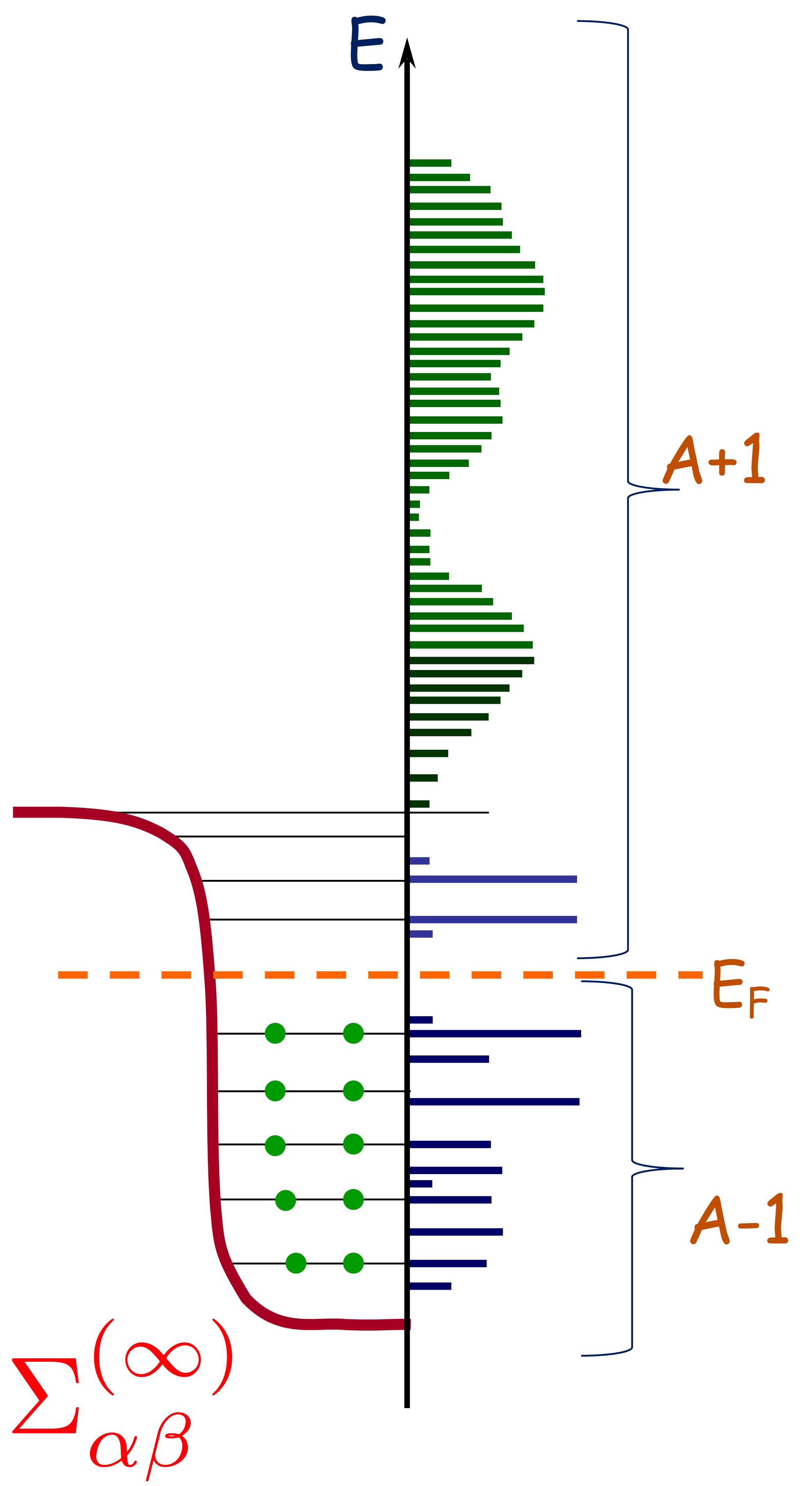
n-^{16}O, total elastic cross section



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

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

Microscopic optical potential



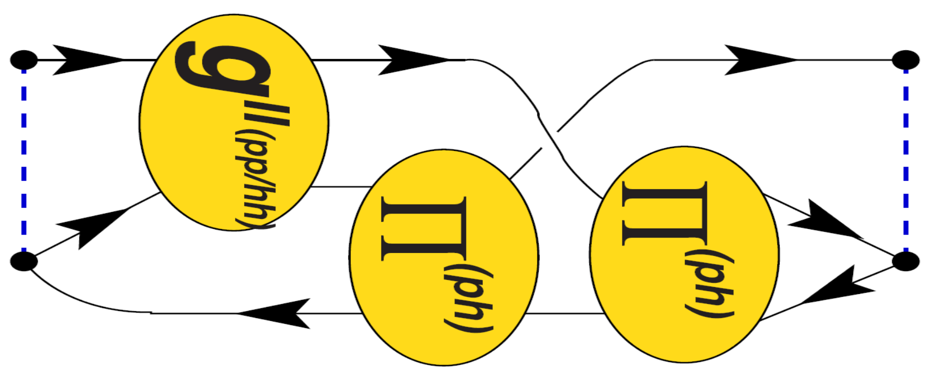
Nuclear self-energy $\Sigma^{\star}(\mathbf{r}, \mathbf{r}'; \varepsilon)$:

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

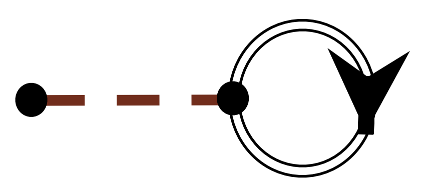
$$\Sigma^{\star}_{\alpha\beta}(\omega) = \Sigma^{(\infty)}_{\alpha\beta} + \sum_{i,j} \mathbf{M}^{\dagger}_{\alpha,i} \left(\frac{1}{E - (\mathbf{K}^{>} + \mathbf{C}) + i\Gamma} \right)_{i,j} \mathbf{M}_{j,\beta} + \sum_{r,s} \mathbf{N}_{\alpha,r} \left(\frac{1}{E - (\mathbf{K}^{<} + \mathbf{D}) - i\Gamma}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

mean-field

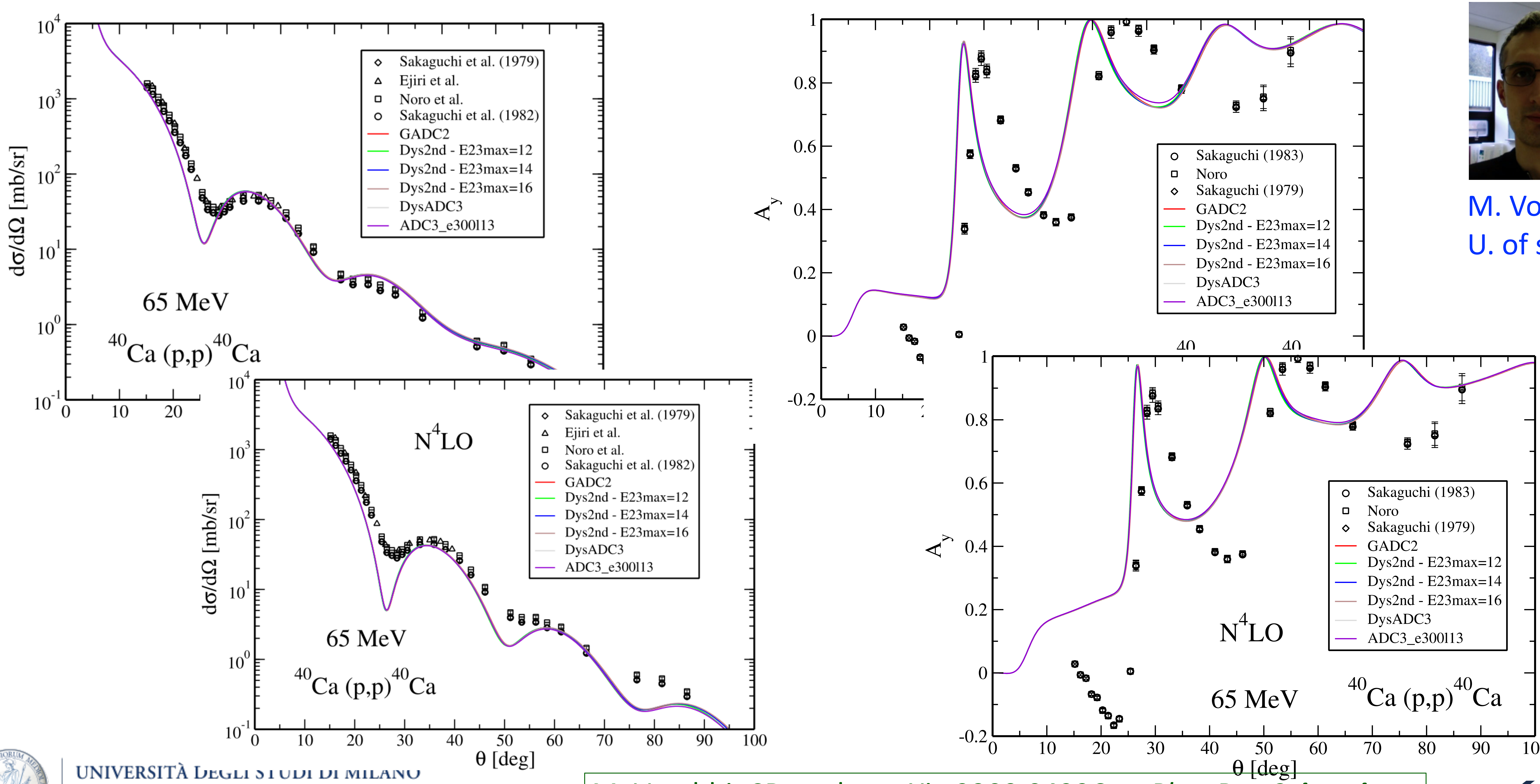
Particle-vibration couplings:



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



Elastic nucleon nucleus scattering



M. Vorabbi
U. of surrey

UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

M. Vorabbi, CB et al. – arXiv:2309.04226 — *Phys Rev C*, ***in print***.

INFN MILANO

(Ab Initio) Optical potentils workshop at the ECT*

TOWARDS A CONSISTENT APPROACH FOR NUCLEAR STRUCTURE AND REACTIONS: MICROSCOPIC OPTICAL POTENTIALS

June 17-24, 2024

17 June 2024 — 21 June 2024

Organizers

Carlo Barbieri (Università degli Studi di Milano)
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Charlotte Elster (Ohio University)
elster@ohio.edu
Chloë Hebborn (Facility of Rare Isotopes Beams (FRIB))
hebborn@frib.msu.edu
Alexandre Obertelli (TU Darmstadt)
aobertelli@ikp.tu-darmstadt.de

Direct nuclear reactions, processes such as nucleon transfer, knockout, anti-nucleon capture have been extensively exploited by experiments to learn about the structure of exotic isotopes far away from stability, to infer properties of the nuclear forces, to describe nucleosynthesis and to learn about the nuclear equation of state. In this respect, nucleon-nucleus optical potentials are of great importance since they are the fundamental building blocks needed to predict reaction observables to address such a wide range of Nuclear Physics facets. Traditional phenomenological optical potential parameterizations are fully reliable only in specific regions of the nuclear chart, near the stable isotopes they were fitted to. On the contrary, microscopically derived potentials can be systematically extended to isotopes far from stability that are the focus of modern experimental searches. This workshop will address the state-of-the-art of nuclear optical potentials to foster advances in their accuracy and handling of uncertainty propagation.

(Toward)
Diagrammatic Monte Carlo (DiagMC)
in finite systems

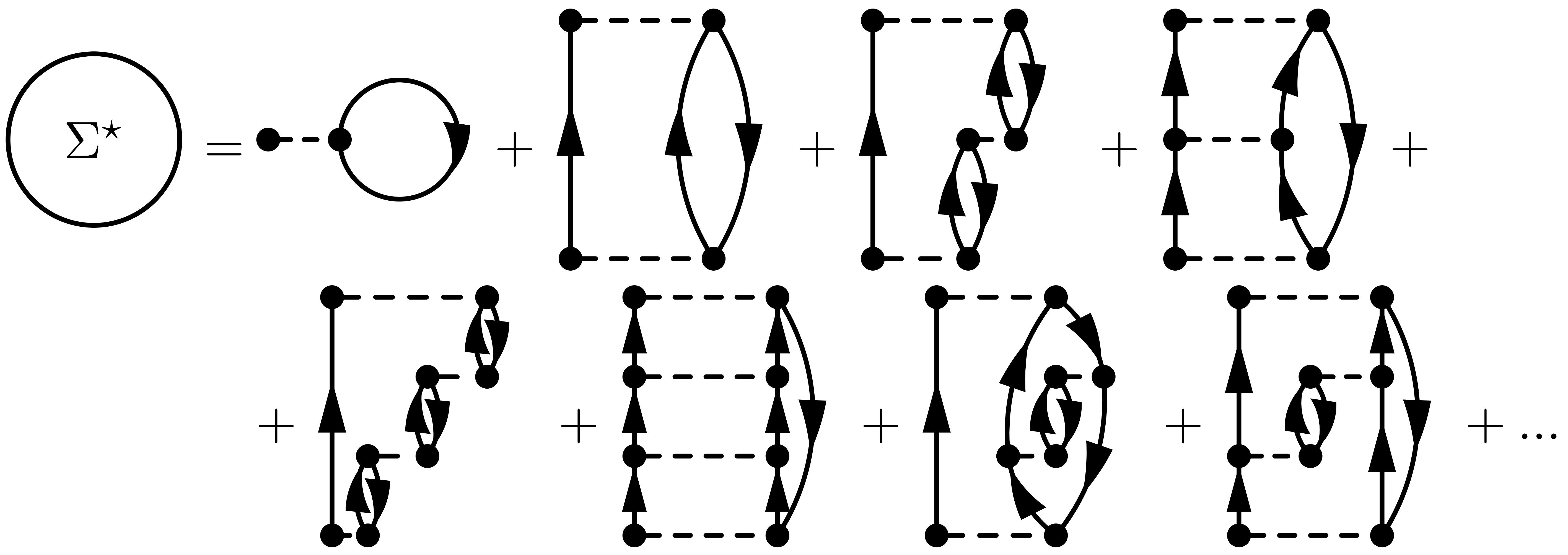
See also poster form S. Brolli (MSc Thesis)

Green's function theory beyond ADC(3)?

The Green's function is found as the exact solution of the Dyson equation:

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

It requires knowing the self-energy which is the sum of an *infinite series* of Feynman diagrams:

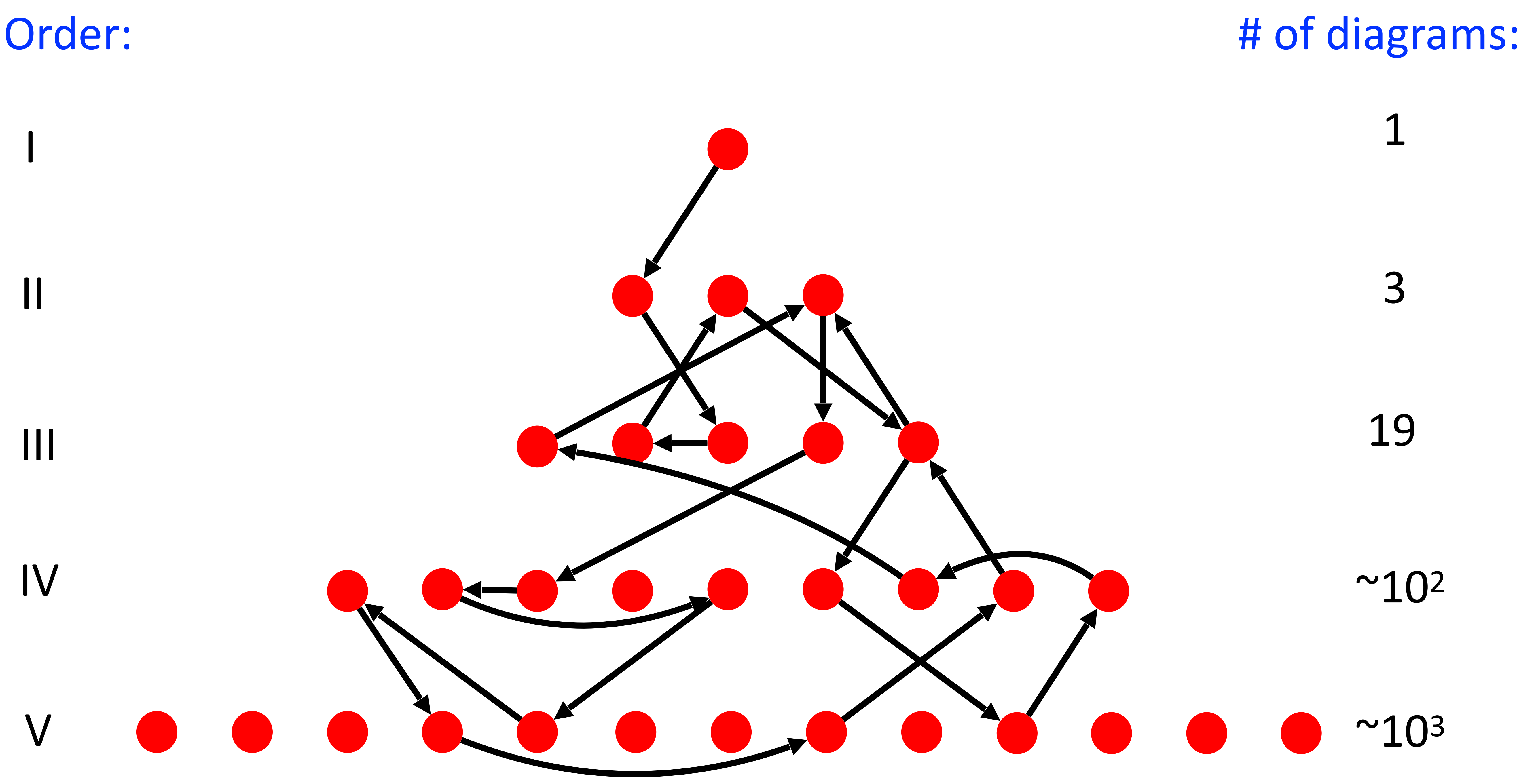


The number of required diagrams explodes (factorially!) with the order of the approximation…

Diagrams grow factorially (more than exponentially) with the order

S. Brolli (Masters thesis)

A direct calculation of all diagrams beyond order three is unfeasible.



Diagrammatic Monte Carlo (DiagMC) ***samples diagrams in their topological space*** using a Markov chain.

Diagrammatic Monte Carlo: overview

S. Brolli (Masters thesis)

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \sum_{\mathcal{T}} \sum_{\gamma_1 \dots \gamma_n} \int d\omega_1 \dots d\omega_m \, \mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{T};\gamma_1\dots\gamma_n;\omega_1\dots\omega_m)\, 1_{\mathcal{T}\in\mathcal{S}_{\Sigma^\star}}$$

We define $\mathcal{C} := (\mathcal{T};\gamma_1\dots\gamma_n;\omega_1\dots\omega_m)$

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \int d\mathcal{C}\, |\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})| e^{i\arg\left[\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})\right]} 1_{\mathcal{T}\in\mathcal{S}_{\Sigma^\star}}$$

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \mathcal{Z}^{\omega}_{\alpha\beta} \int d\mathcal{C}\, \frac{|\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})| W_o(N)}{\mathcal{Z}^{\omega}_{\alpha\beta}} \frac{e^{i\arg\left[\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})\right]}}{W_o(N)} 1_{\mathcal{T}\in\mathcal{S}_{\Sigma^\star}}$$

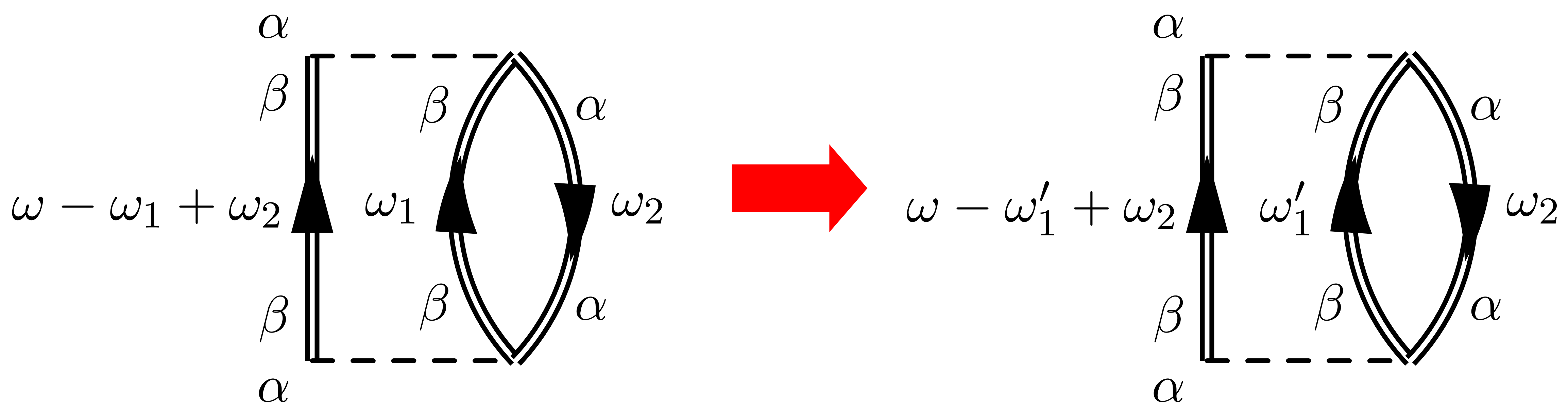
- $W_o(N)$ is an order dependent reweighting factor
- $\mathcal{Z}^{\omega}_{\alpha\beta} = \int d\mathcal{C}\, |\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})| W_o(N)$ is a normalization factor
- $w^{\omega}_{\alpha\beta}(\mathcal{C}) := \frac{|\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})| W_o(N)}{\mathcal{Z}^{\omega}_{\alpha\beta}}$ is a probability distribution function

The updates

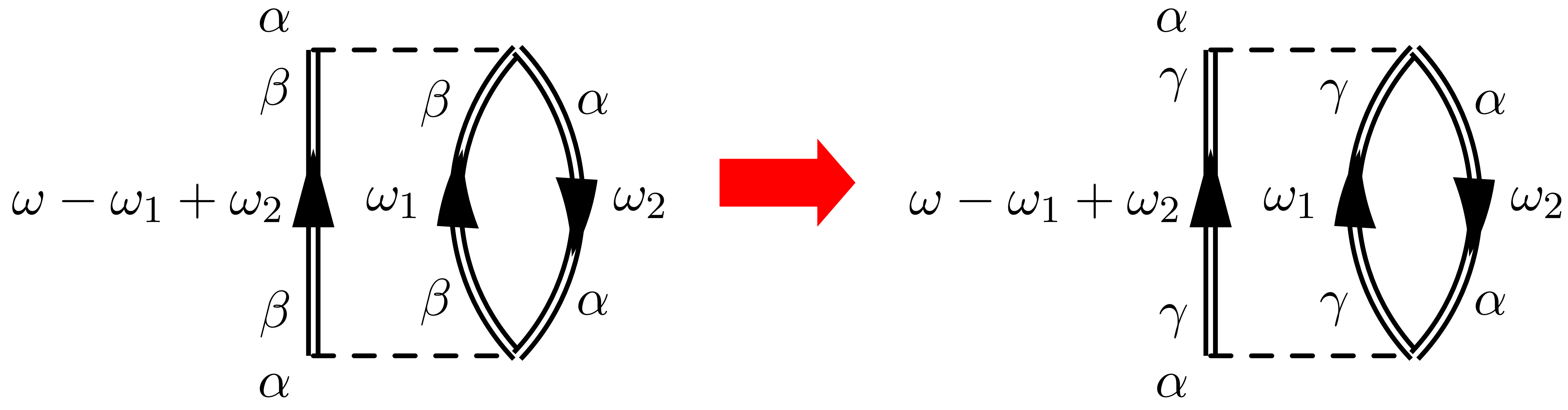
1. *Change Frequency*
2. *Change Single-Particle Quantum Numbers*

} Standard Monte Carlo

Change Frequency:



Change Single-Particle Quantum Numbers:



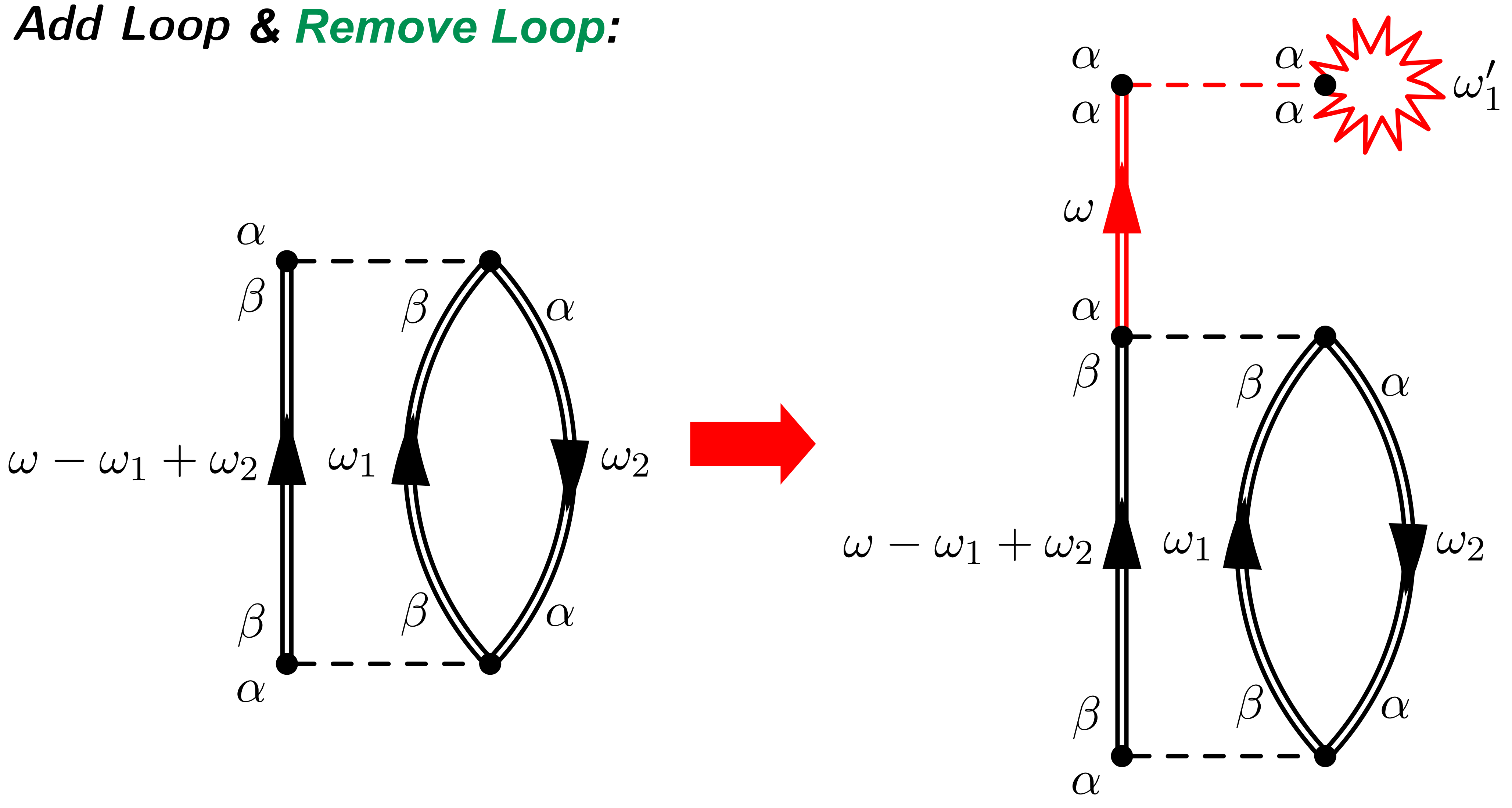
The updates

3. *Add Loop*
4. *Remove Loop*
5. *Reconnect*

} Monte Carlo on the topology

S. Brolli (Masters thesis)

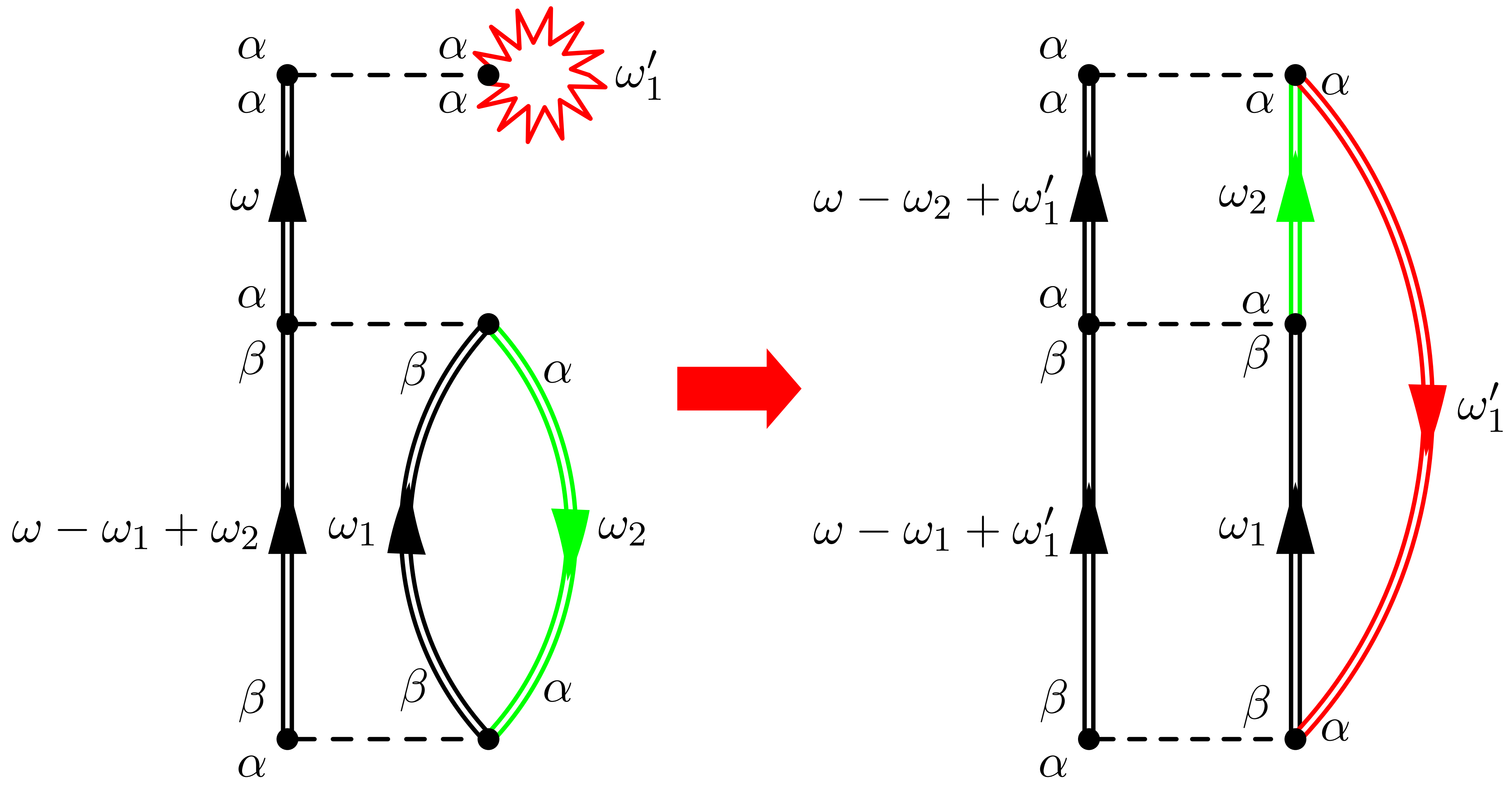
***Add Loop* & *Remove Loop*:**



ω'_1 is drawn from the probability distribution $W_f(\omega'_1)$.

$$q_{AL} = \frac{|g|}{4\pi} \frac{1}{W_f(\omega'_1)} e^{-k\omega_1'^2} |G_\alpha(\omega)| \frac{W_o(3)}{W_o(2)}$$

***Reconnect*:**

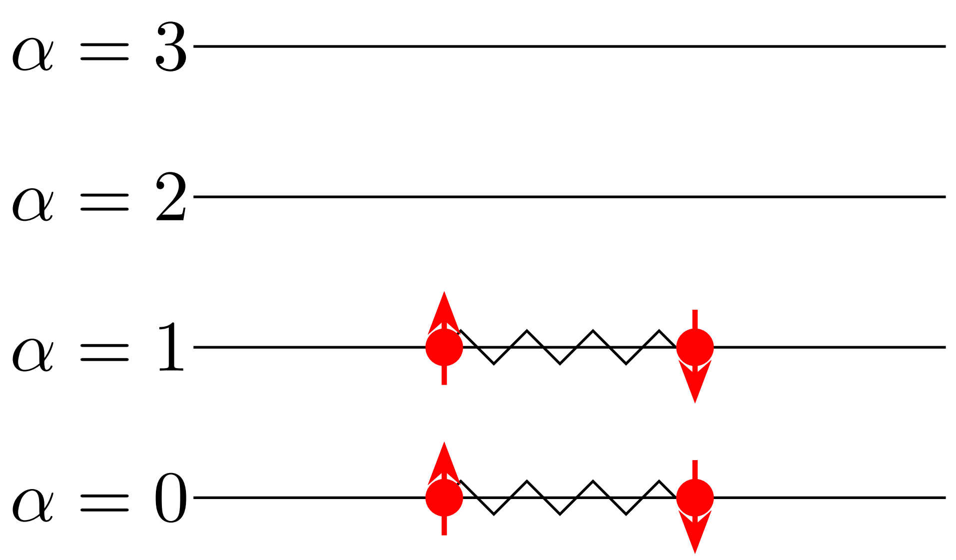


The unphysical propagators are turned into physical ones when reconnected.

Results of the simulation for D=4

Richardson pairing model with D states, half filled:

$$H = \xi \sum_{\alpha=0}^{D-1} \sum_{\sigma=+,-} \alpha c^{\dagger}_{\alpha\sigma} c_{\alpha\sigma} - \frac{g}{2} \sum_{\alpha,\beta=0}^{D-1} c^{\dagger}_{\alpha+} c^{\dagger}_{\alpha-} c_{\beta-} c_{\beta+}$$



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

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

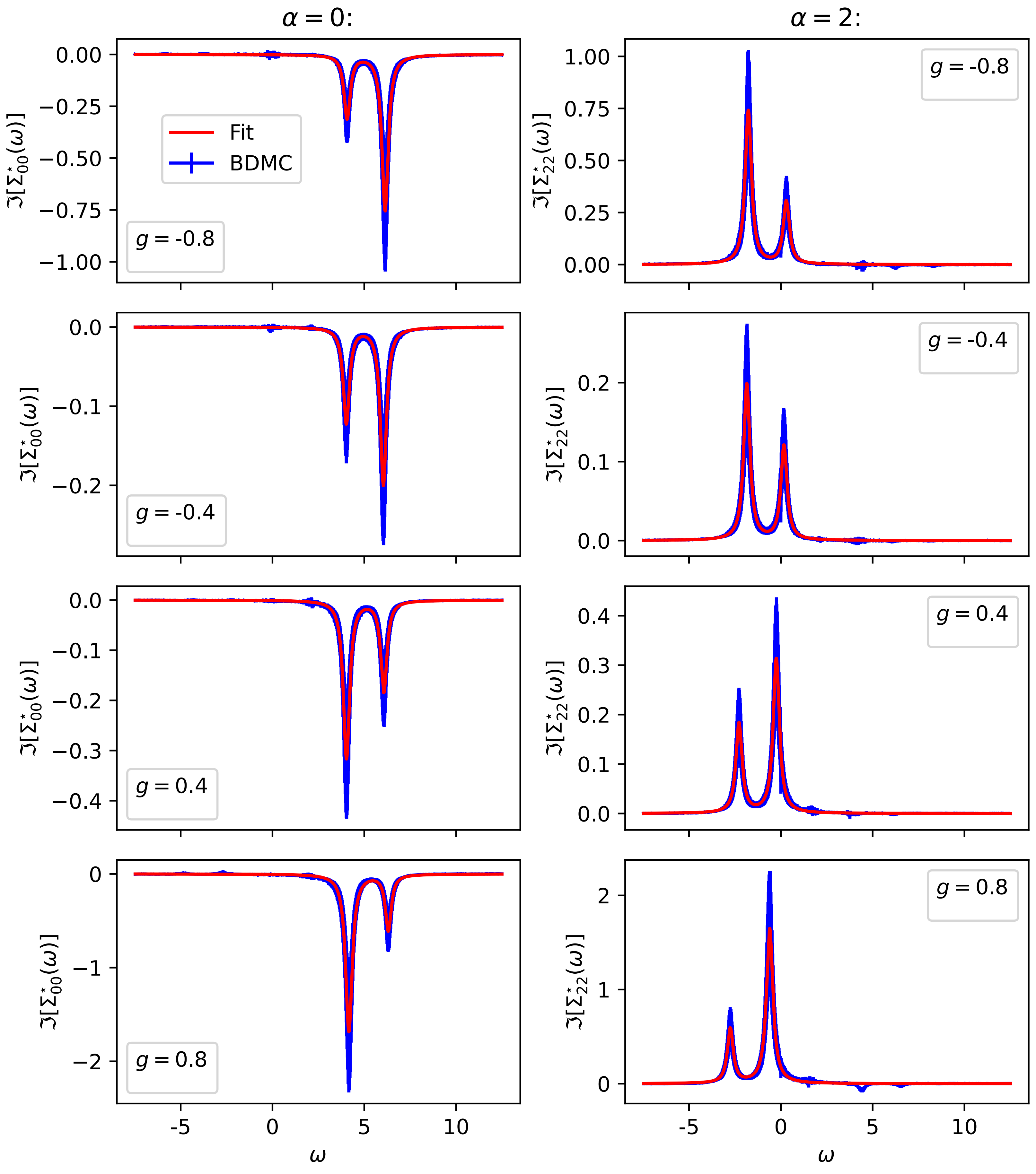
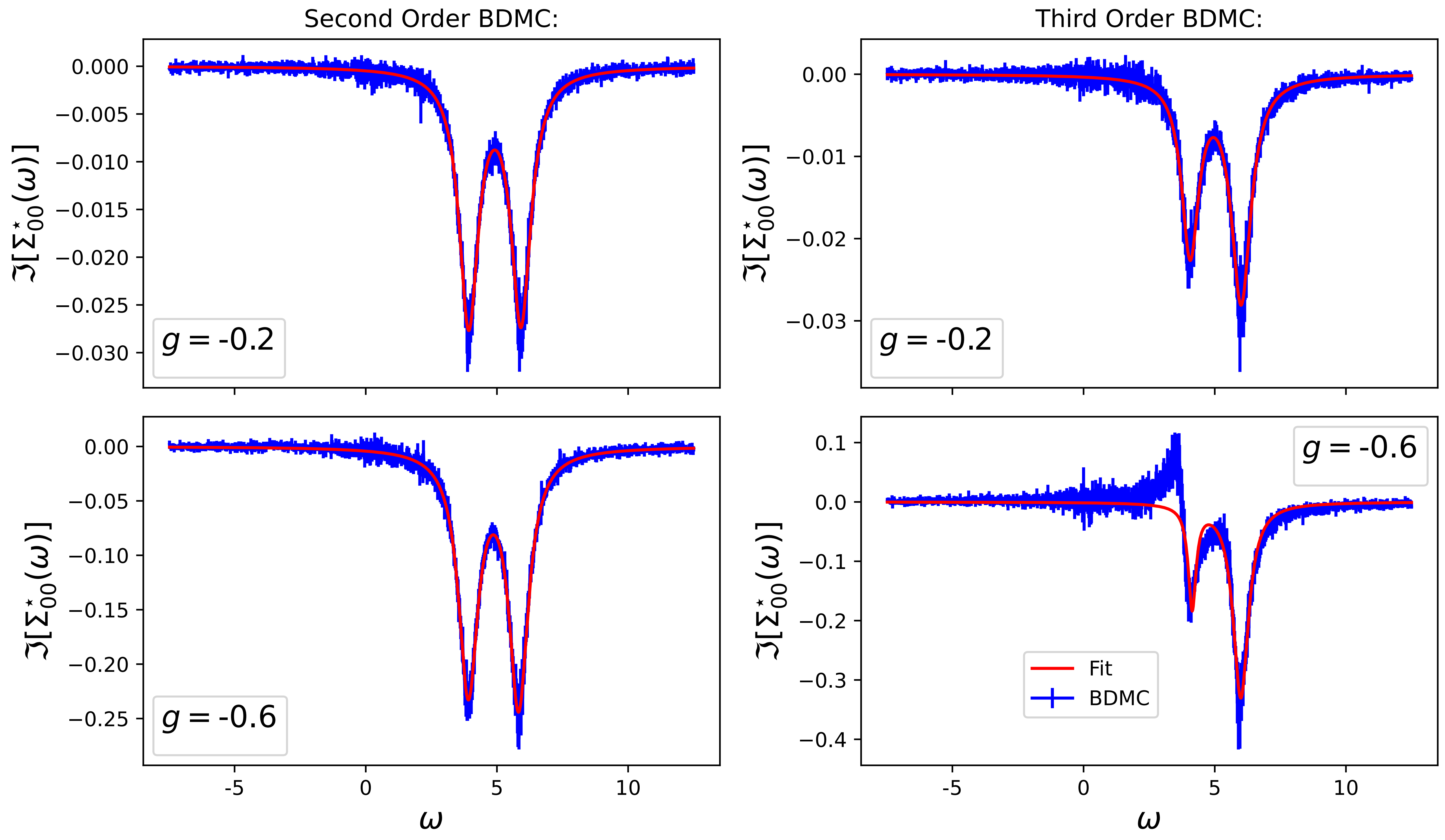


Figure 4.1: Components $\alpha = 0$ and $\alpha = 2$ of the imaginary part of the self-energy for different values of the coupling g. The blue line is the results obtained with the BDMC simulation, while the red line is the best fit as a sum of two Lorentzians. The results for the two values of $\alpha = 0, 2$ are displayed respectively on the left and on the right of the graph. The error bars are calculated as explained in the main text.

Results of the simulation for D=4

Imaginary part of the component $\alpha = 0$ of the diagonal self-energy for different values of the coupling:



$$H = \xi \sum_{\alpha=0}^{D-1} \sum_{\sigma=+,-} \alpha c^\dagger_{\alpha\sigma} c_{\alpha\sigma} - \frac{g}{2} \sum_{\alpha,\beta=0}^{D-1} c^\dagger_{\alpha+} c^\dagger_{\alpha-} c_{\beta-} c_{\beta+}$$

We fitted the imaginary part of the self-energy as a sum of Lorentzians.

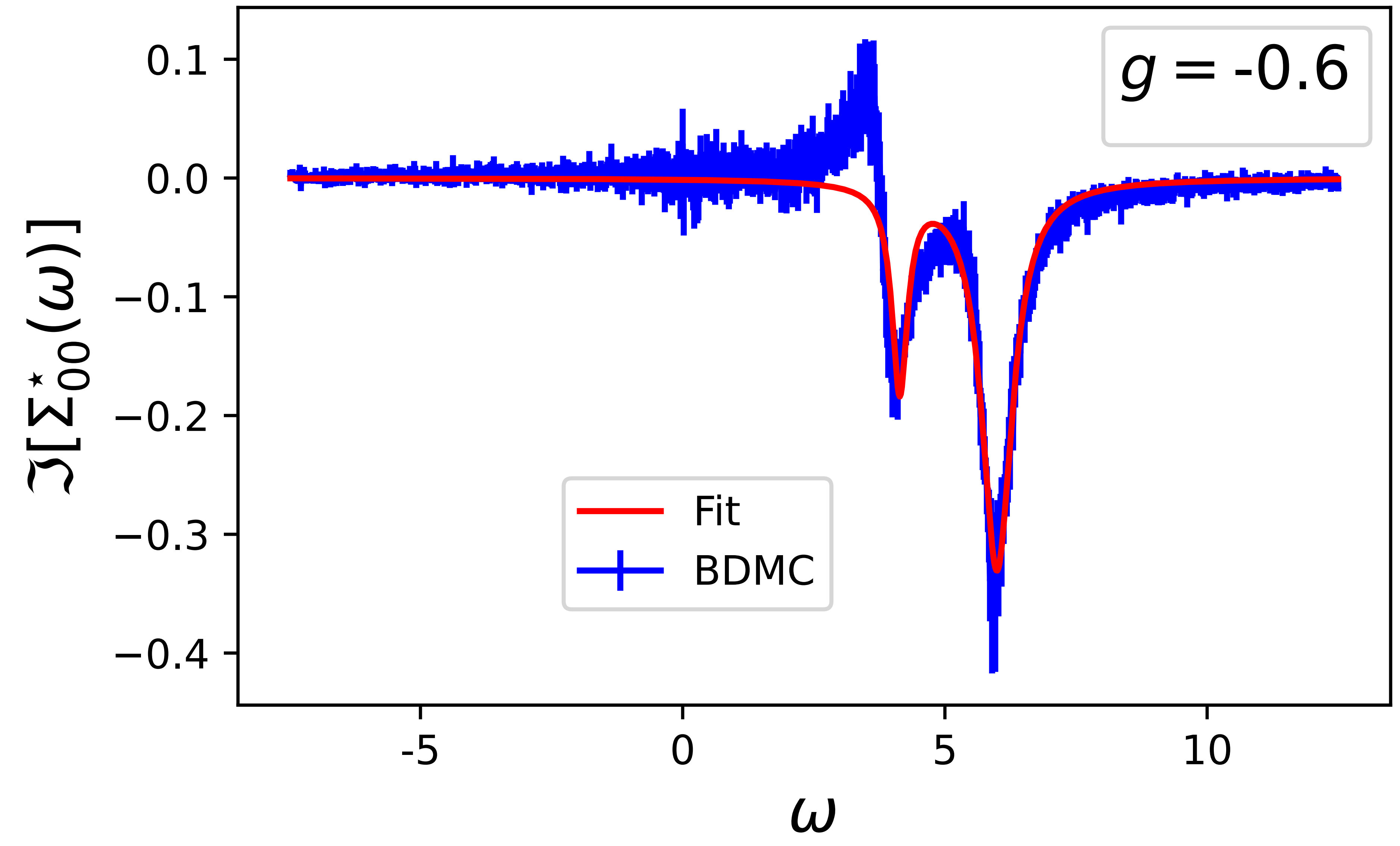
S. Brolli, CB, Vigezzi, in preparation

Reorganization in terms of ladders (Γ)

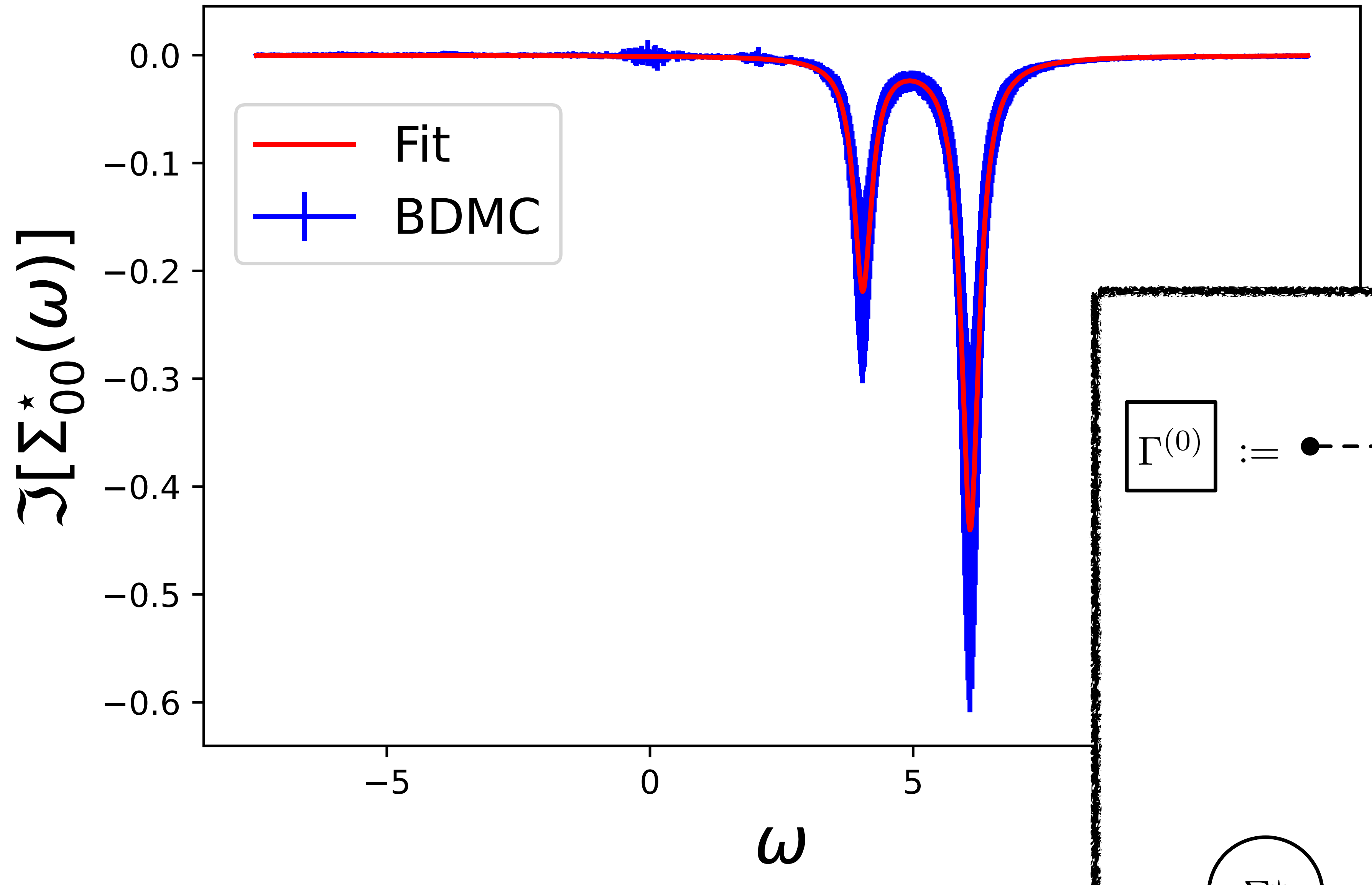
S. Brolli, CB, Vigezzi,
in preparation

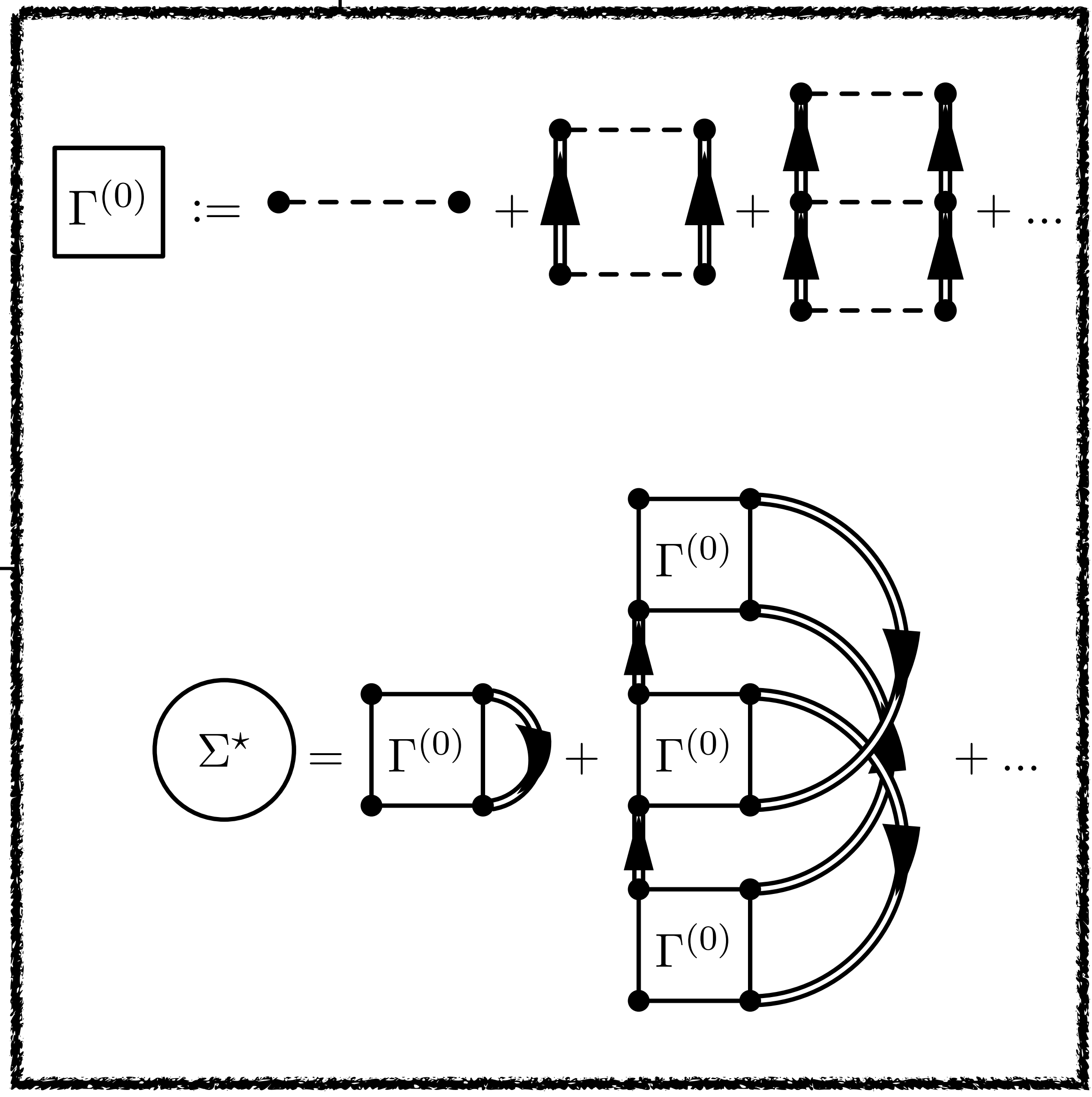
Imaginary part of the component α=0 of the diagonal self-energy (g=-0.6):

Old updating scheme:



New updating scheme:

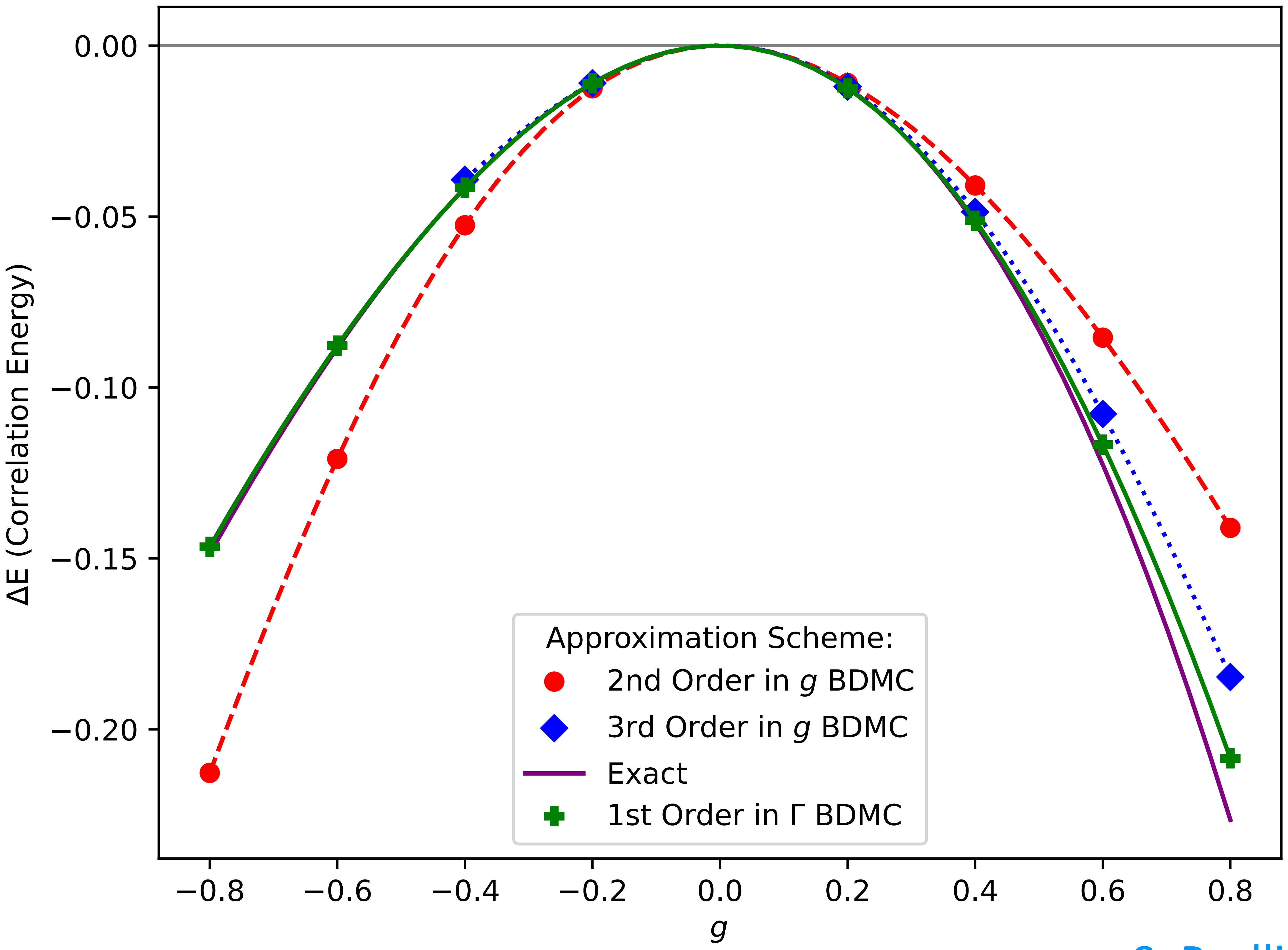




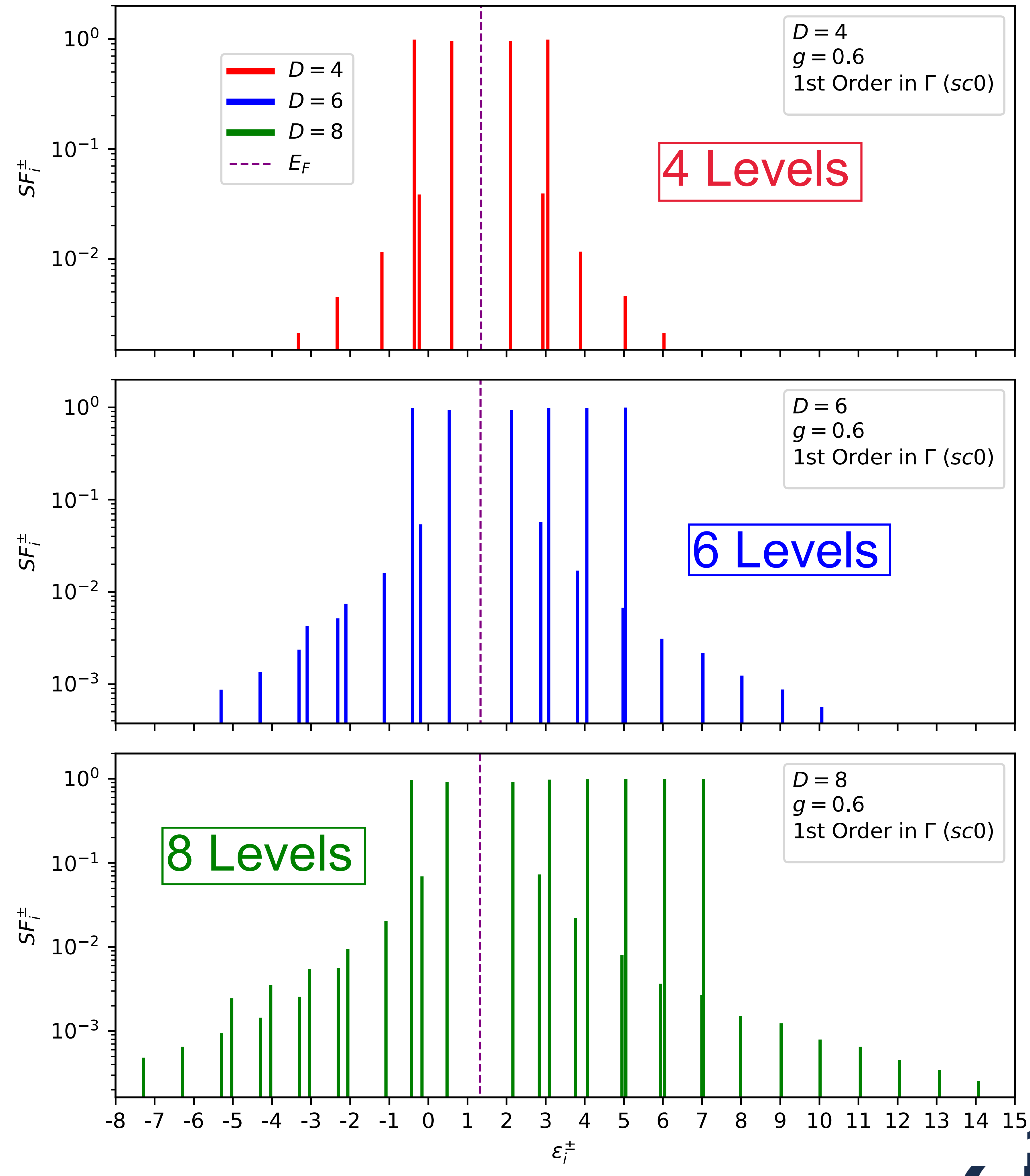
It restores the correct spectral representation also for g < −0.4!

Reorganization in terms of ladders (Γ)

Correlation energy $\Delta E = E - E_{HF}$ as a function of interaction strength (*g*):



Spectroscopic function for different dimensions of the model space (*D*):



S. Brolli, CB, Vigezzi, in preparation

SCGF computations of infinite matter

F. Marino (PhD Thesis)

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]

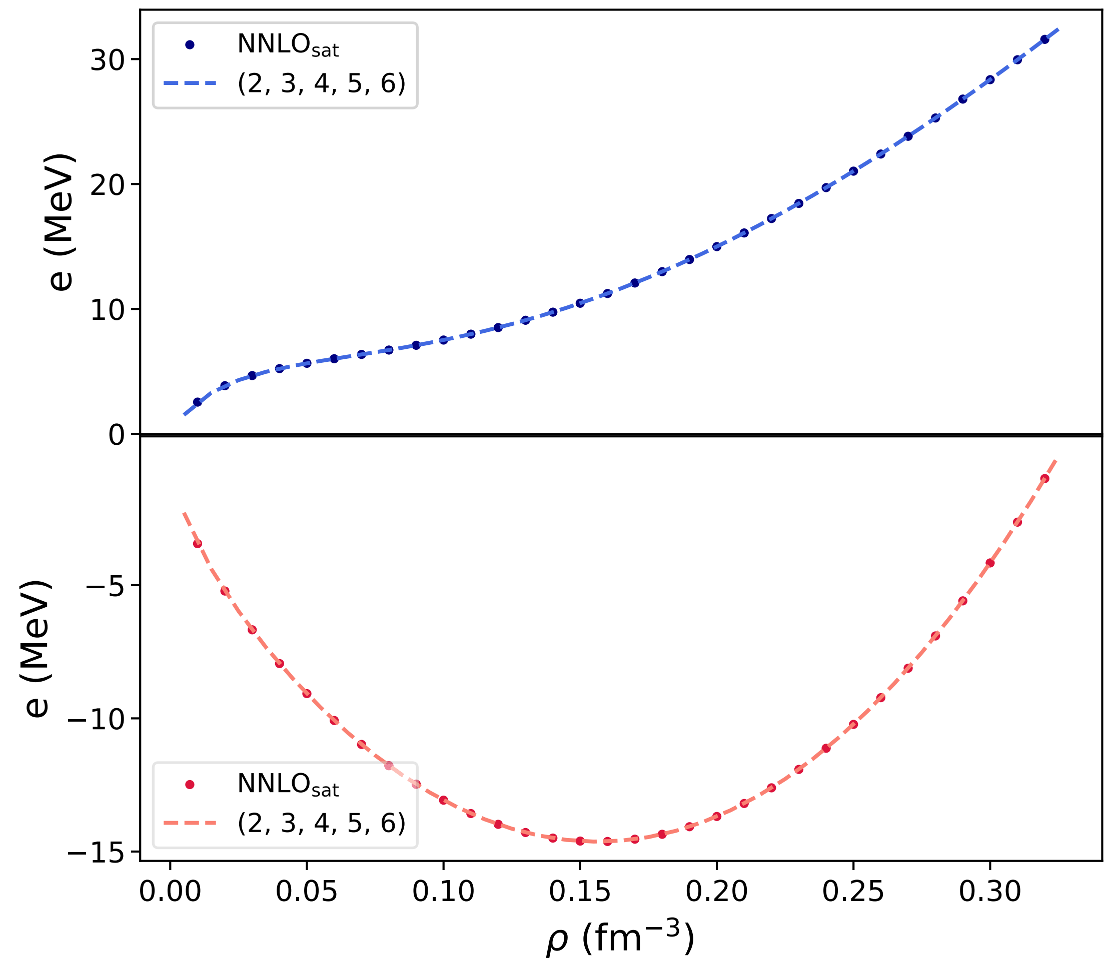
[1]*Dipartimento di Fisica "Aldo Pontremoli," Università degli Studi di Milano, 20133 Milano, Italy*

[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!



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

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

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

Machine-learn DFT functional on the nuclear equation of state

Jacob's ladder

+ approximate GA

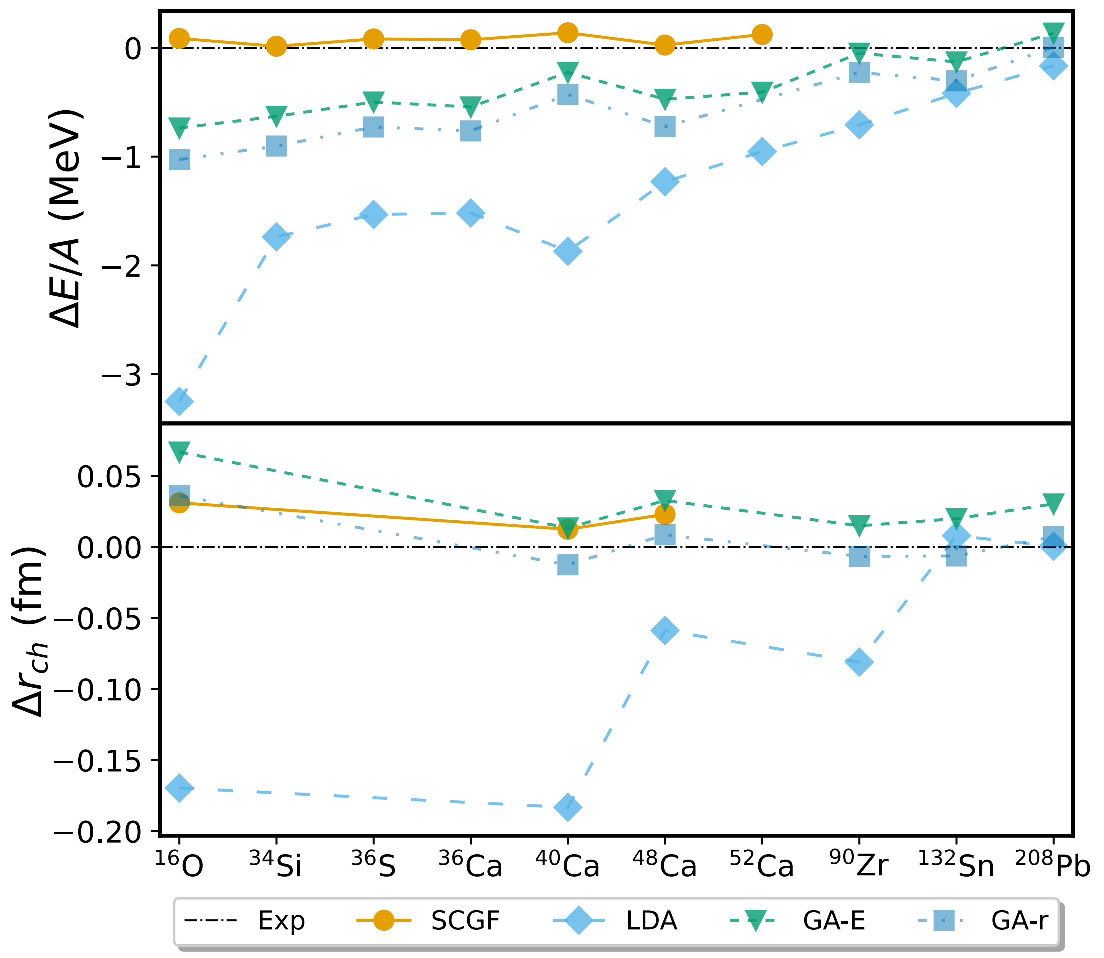
Benchmark in finite systems

Benchmark on finite systems

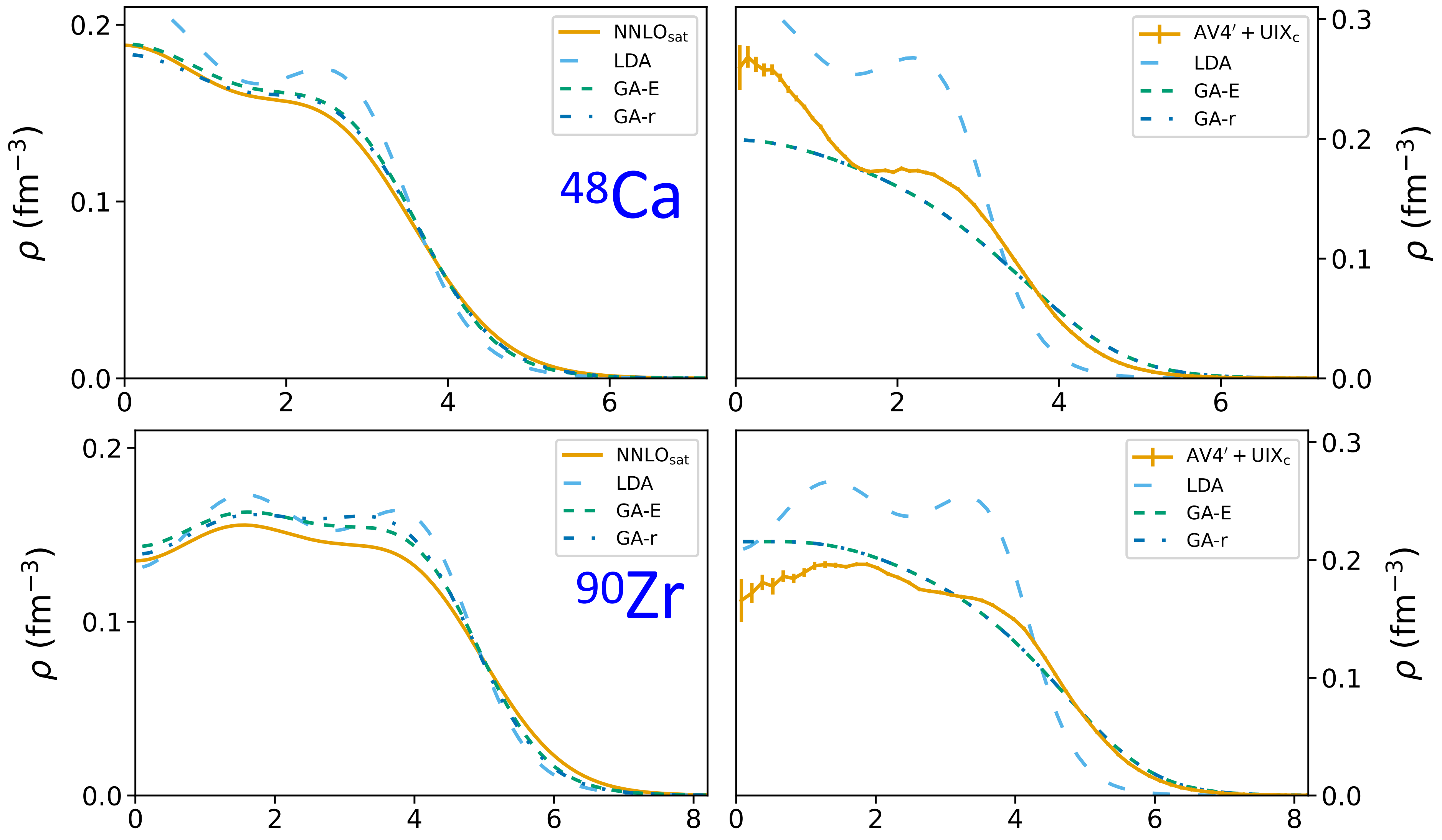
Jacob's ladder

Machine-learn DFT functional on the nuclear equation of state → *+ approximate GA* → *Benchmark in 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:

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

$$\phi(x+L,y,z) = \phi(x,y,z)$$

$$\dots$$

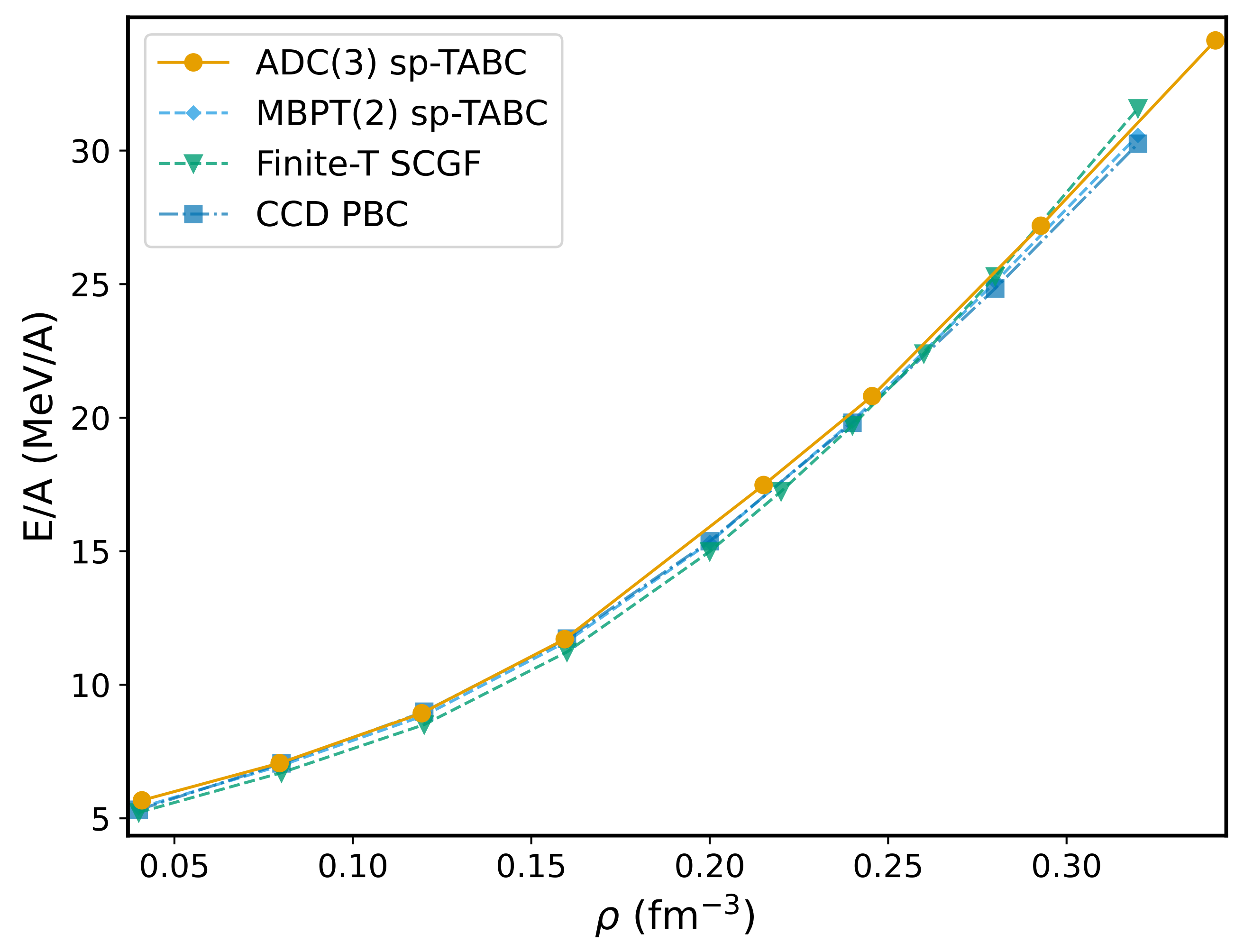
$$\widehat{H} = \sum_{\alpha} \varepsilon^0_\alpha\, a^\dagger_\alpha a_\alpha - \sum_{\alpha\beta} U_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \frac{1}{4}\sum_{\substack{\alpha\gamma\\ \beta\delta}} V_{\alpha\gamma,\beta\delta}\, a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta + \frac{1}{36}\sum_{\substack{\alpha\gamma\epsilon\\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

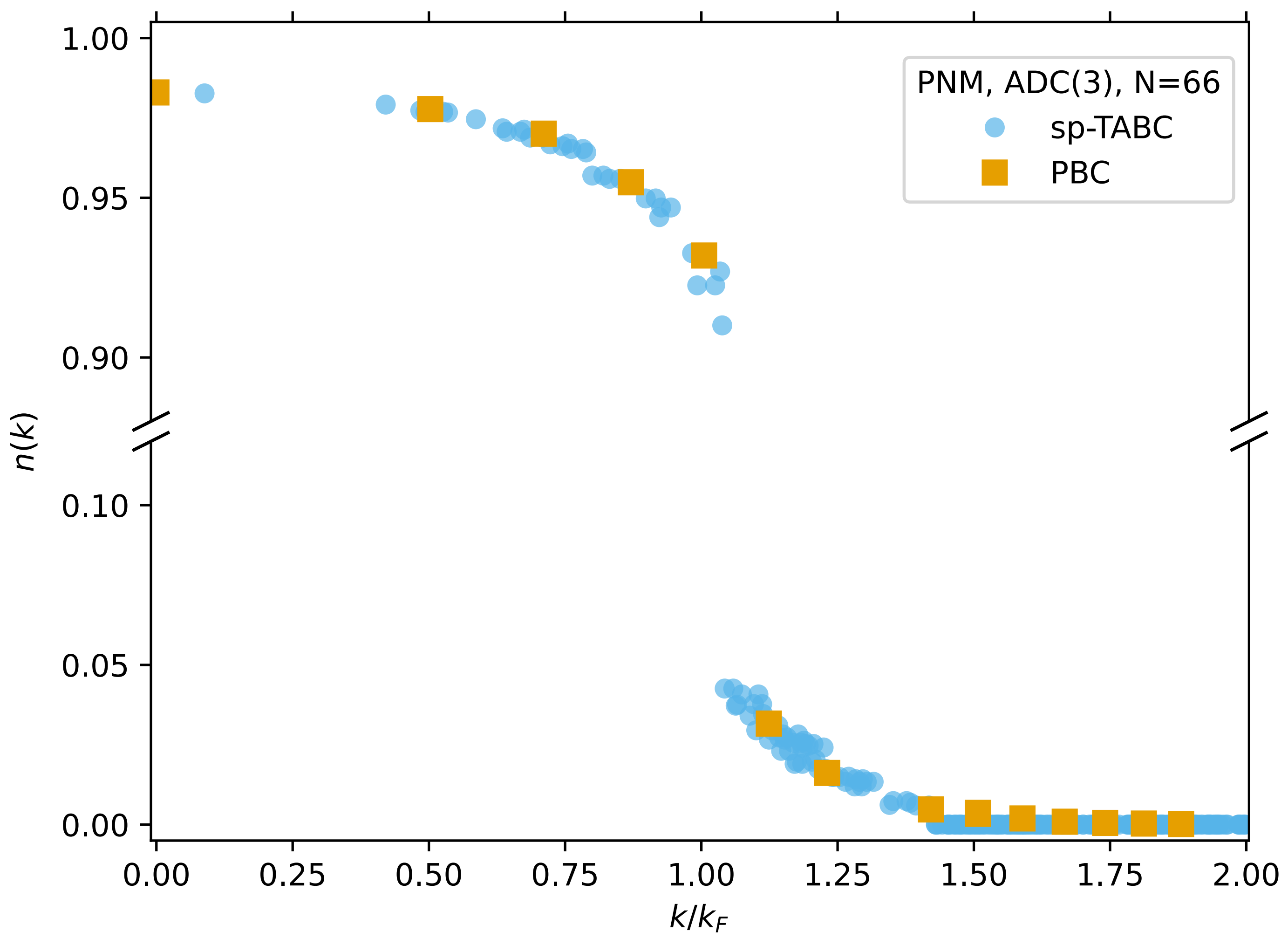
ADC(3) self energy:

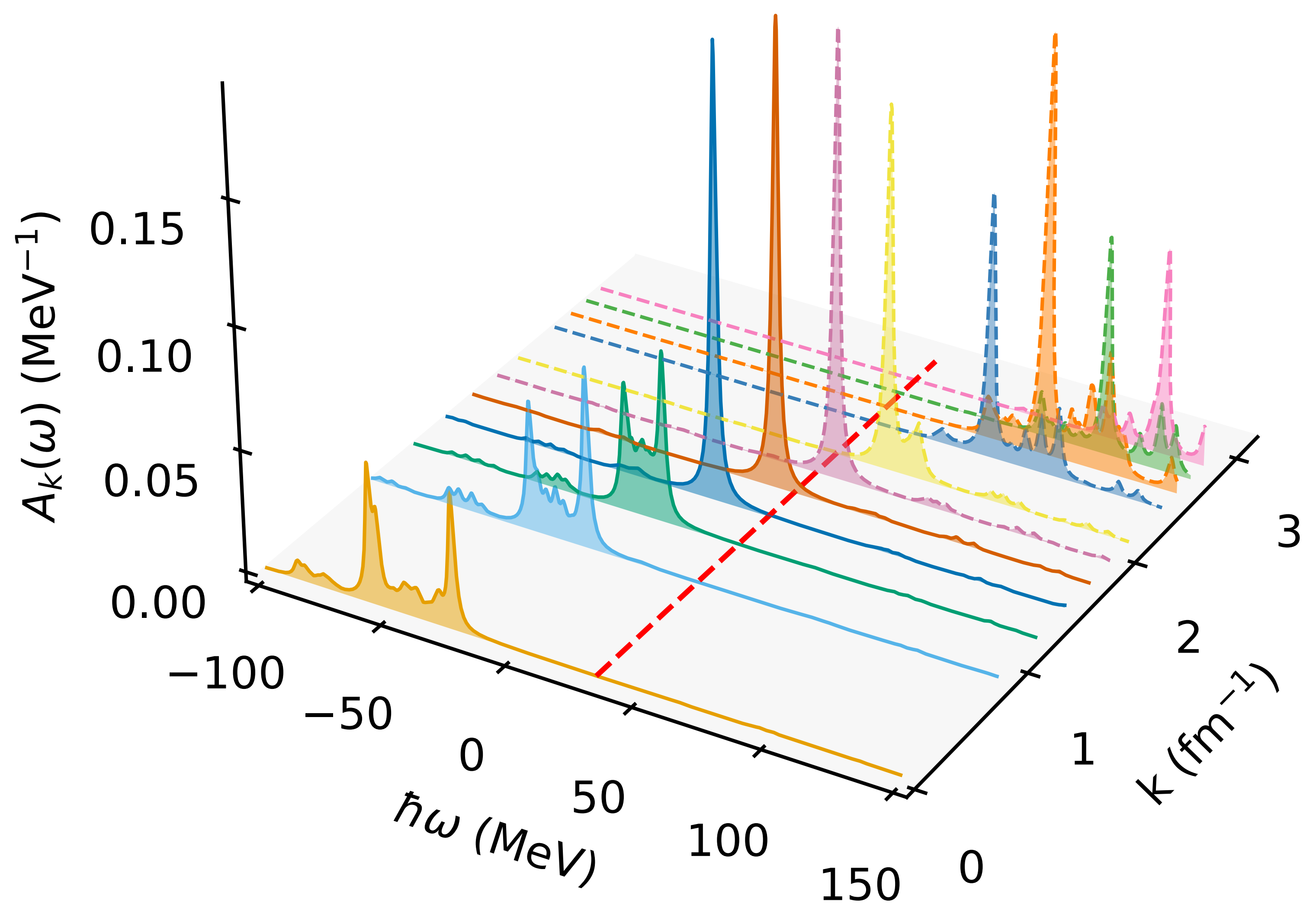
$$\Sigma^{(\star)}_{\alpha\beta}(\omega) = -U_{\alpha\beta} + \Sigma^{(\infty)}_{\alpha\beta} + M^\dagger_{\alpha,r}\left[\frac{1}{\omega - [E^> + C]_{r,r'} + i\eta}\right]_{r,r'} M_{r',\beta}$$

$$+N_{\alpha,s}\left[\frac{1}{\omega - (E^< + D) - i\eta}\right]_{s,s'} N^\dagger_{s',\beta}$$

A=66, 2+3 NF (NNLOsat)







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

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INFN MILANO

Combined Gkv-ADC(1) + Dys ADC(3)

- Self energy:

$$\Sigma^{\star\, g_1 g_2}_{\alpha\beta}(\omega) = \Sigma^{(\infty)\, g_1 g_2}_{\alpha\beta} + M^\dagger_\alpha \left[\frac{1}{\omega - E^{2p1h} + i\eta}\right] M_\beta + N_\alpha \left[\frac{1}{\omega - E^{2h1p} - i\eta}\right] N^\dagger_\beta$$

Gorkov-ADC(1)

Dyson-ADC(3)
(only normal part!)

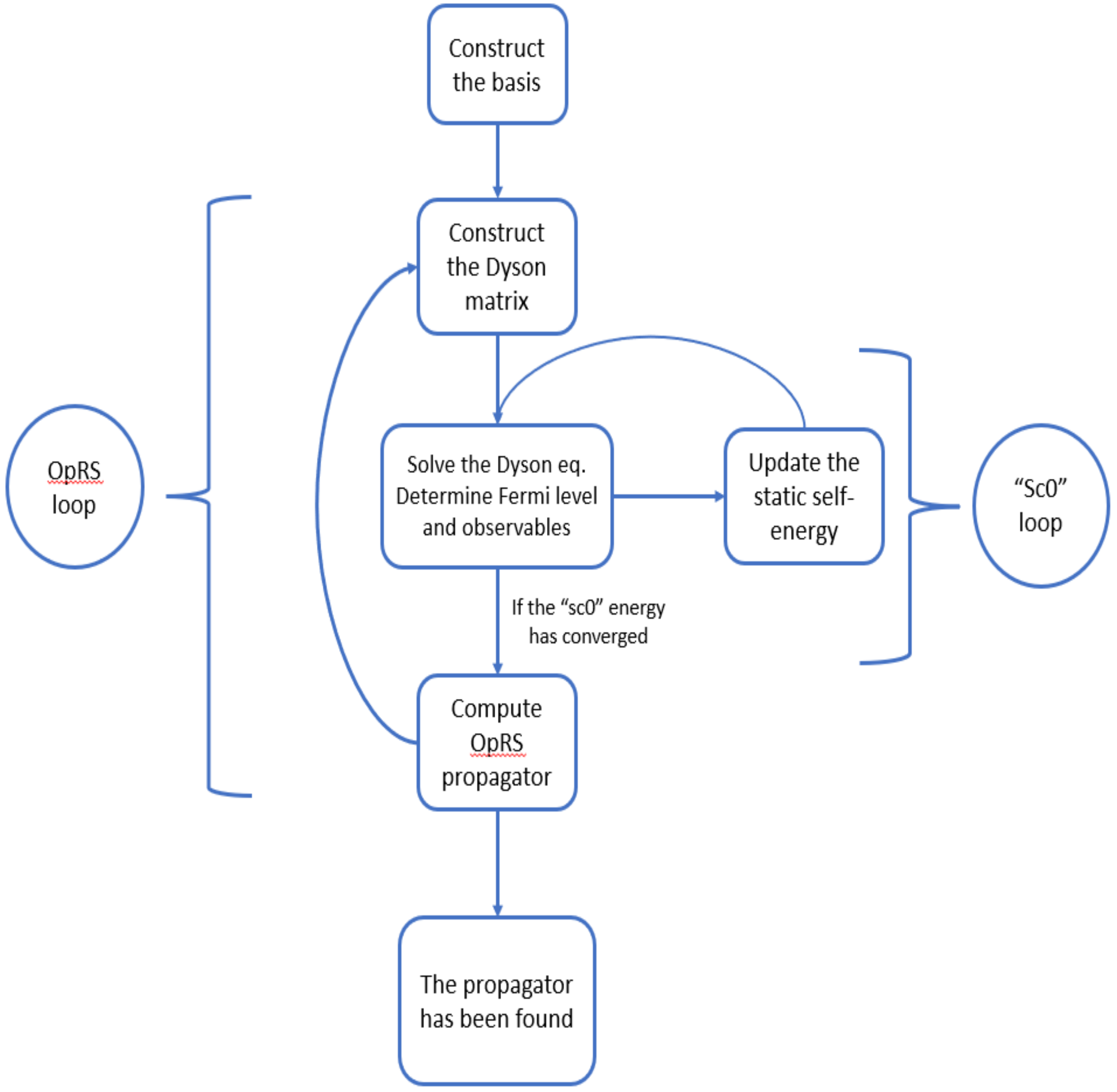
- Dyson ADC(3) needs s.p. energies: Optimized ref. states from Grkv

$$\mathcal{G}^{g_1 g_2}_{\alpha\beta}(\omega) = \mathcal{G}^{OpRS,\, g_1 g_2}_{\alpha\beta}(\omega) + \sum_{\dots} \mathcal{G}^{OpRS,\, g_1 g_3}_{\alpha\gamma}(\omega)\Sigma^{\star,\, g_3 g_4}_{\gamma\delta}(\omega)\mathcal{G}^{g_4 g_2}_{\alpha\delta}(\omega)$$

$$\mathcal{G}^{g_1 g_2}_{\alpha\beta}(\omega) \to \mathcal{G}^{OpRS,\, g_1 g_2}_{\alpha\beta}(\omega) \quad , \quad \omega^{OpRS}(k) \to \varepsilon^{OpRs}(k) = \mu \pm \omega^{OpRS}(k)$$

- Spectra function

$$S(k,\omega) = \mp\frac{1}{\pi}\,\Im m\, \mathcal{G}^{g_1=g_2=1}_{k=k'}(\omega)$$



Combined Gkv-ADC(1) + Dys ADC(3)

- Self energy:

$$\Sigma^{\star\, g_1 g_2}_{\alpha\beta}(\omega) = \Sigma^{(\infty)\, g_1 g_2}_{\alpha\beta} + M^{\dagger}_{\alpha}\left[\frac{1}{\omega - E^{2p1h} + i\eta}\right] M_{\beta} + N_{\alpha}\left[\frac{1}{\omega - E^{2h1p} - i\eta}\right] N^{\dagger}_{\beta}$$

Gorkov-ADC(1)

Dyson-ADC(3)
(only normal part!)

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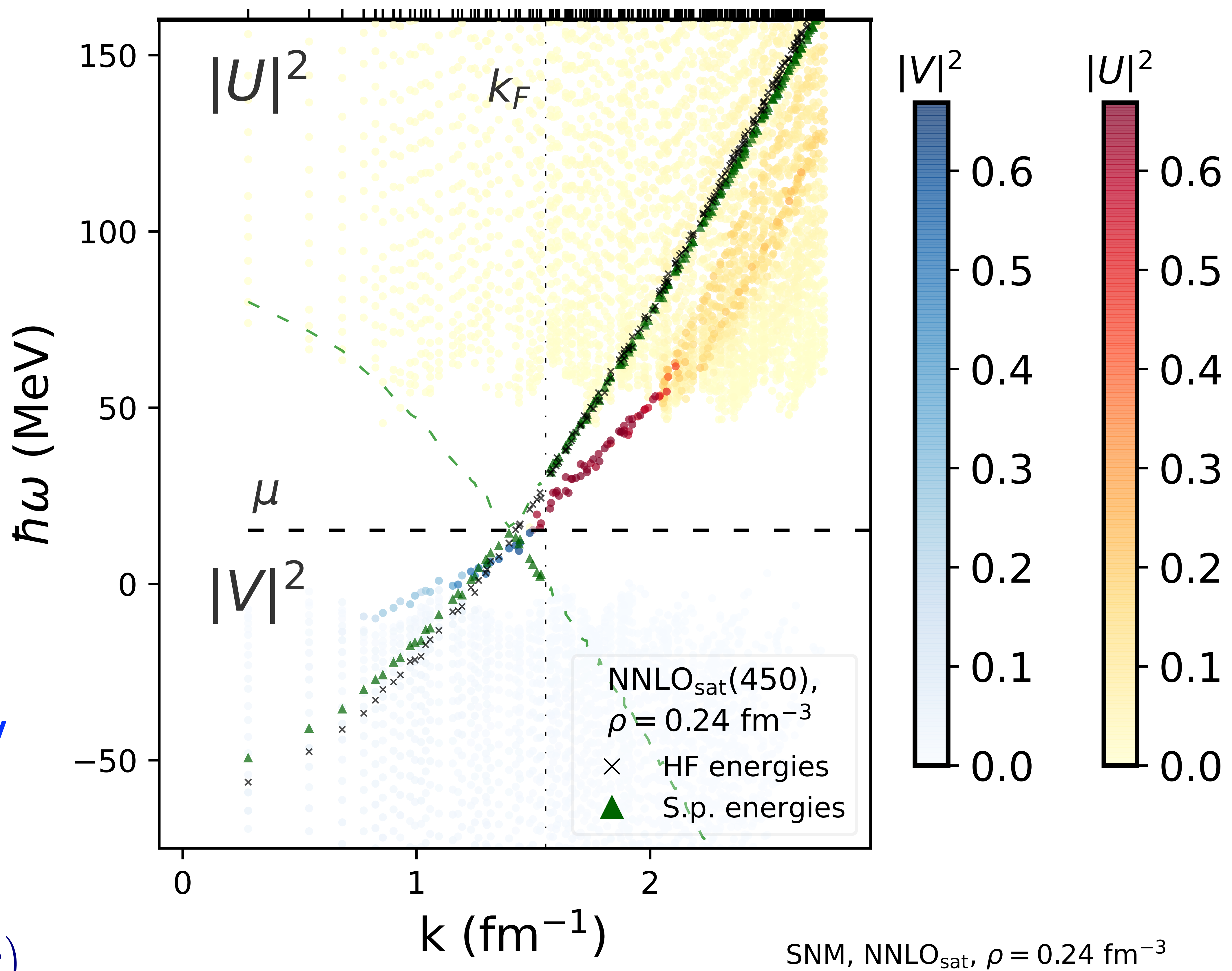
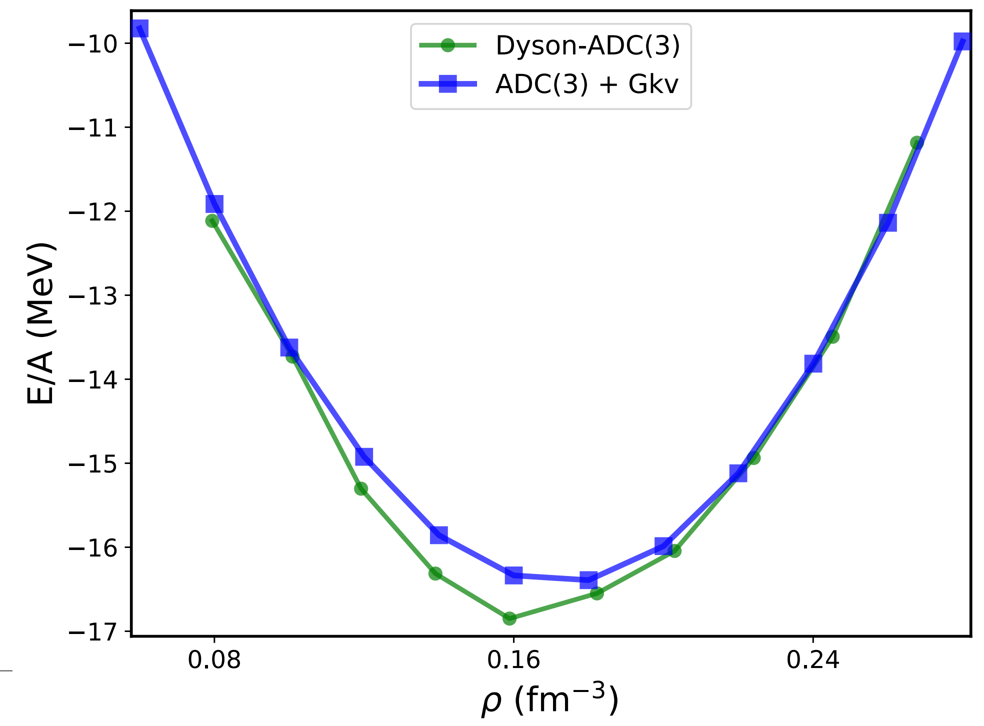
$$\mathcal{G}^{g_1 g_2}_{\alpha\beta}(\omega) = \mathcal{G}^{OpRS,\, g_1 g_2}_{\alpha\beta}(\omega) + \sum_{\cdots} \mathcal{G}^{OpRS,\, g_1 g_3}_{\alpha\gamma}(\omega)\Sigma^{\star,\, g_3 g_4}_{\gamma\delta}(\omega)\mathcal{G}^{g_4 g_2}_{\alpha\delta}(\omega)$$

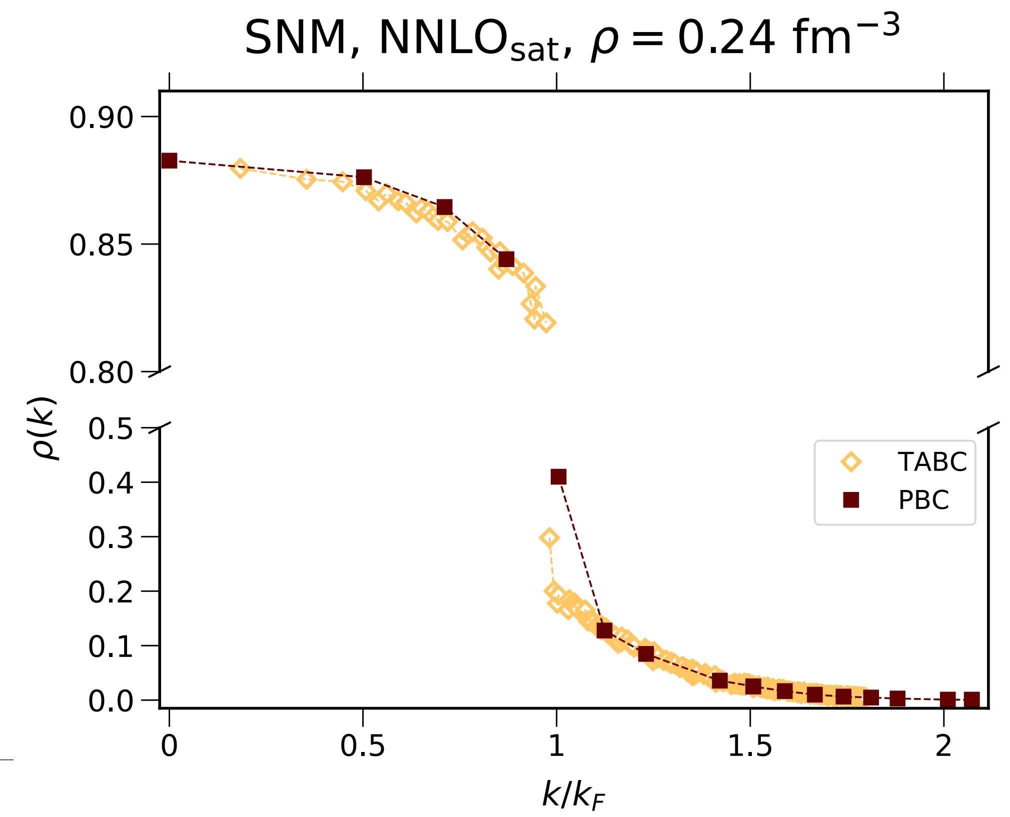
$$\mathcal{G}^{g_1 g_2}_{\alpha\beta}(\omega) \to \mathcal{G}^{OpRS,\, g_1 g_2}_{\alpha\beta}(\omega) \quad , \quad \omega^{OpRS}(k) \to \varepsilon^{OpRs}(k) = \mu \pm \omega^{OpRS}(k)$$

- Spectra function

$$S(k,\omega) = \mp\frac{1}{\pi}\,\Im m\,\mathcal{G}^{g_1=g_2=1}_{k=k'}(\omega)$$

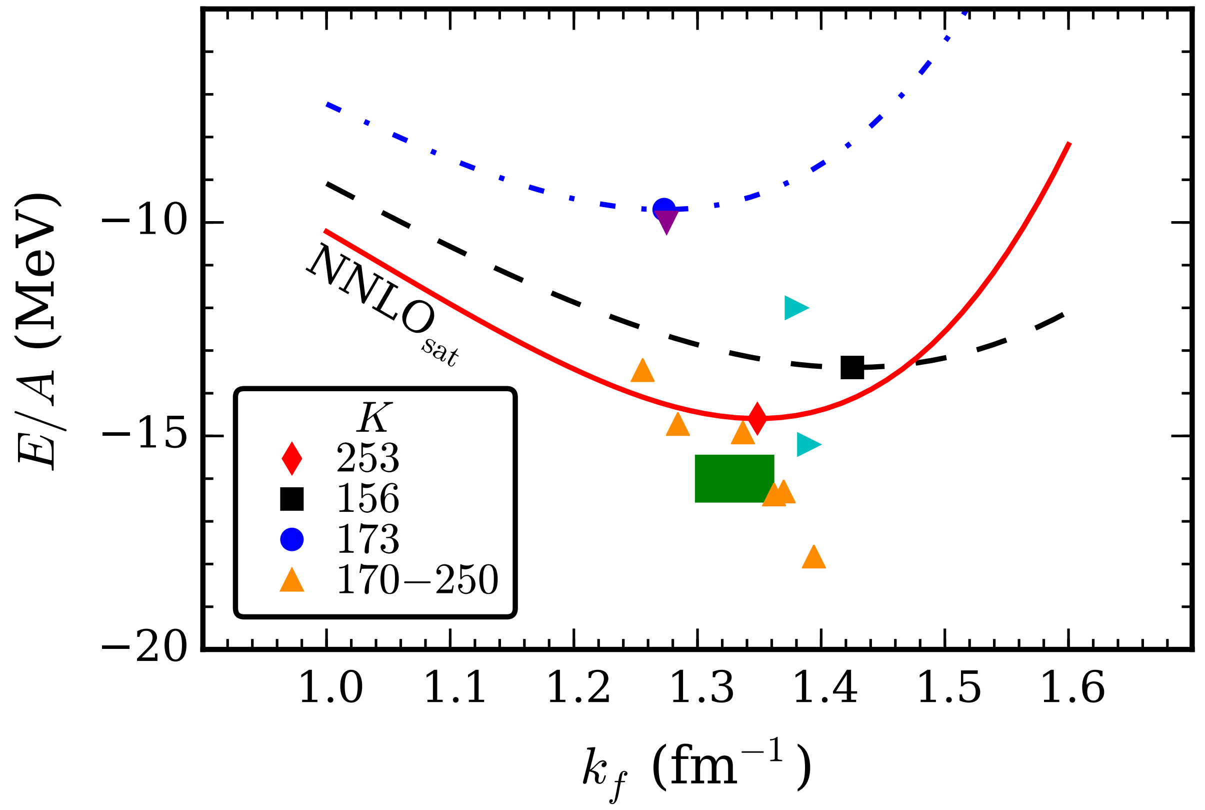






Benchmark to other methods

NNLOsat:
PRC 91, 051301(R) (2015)

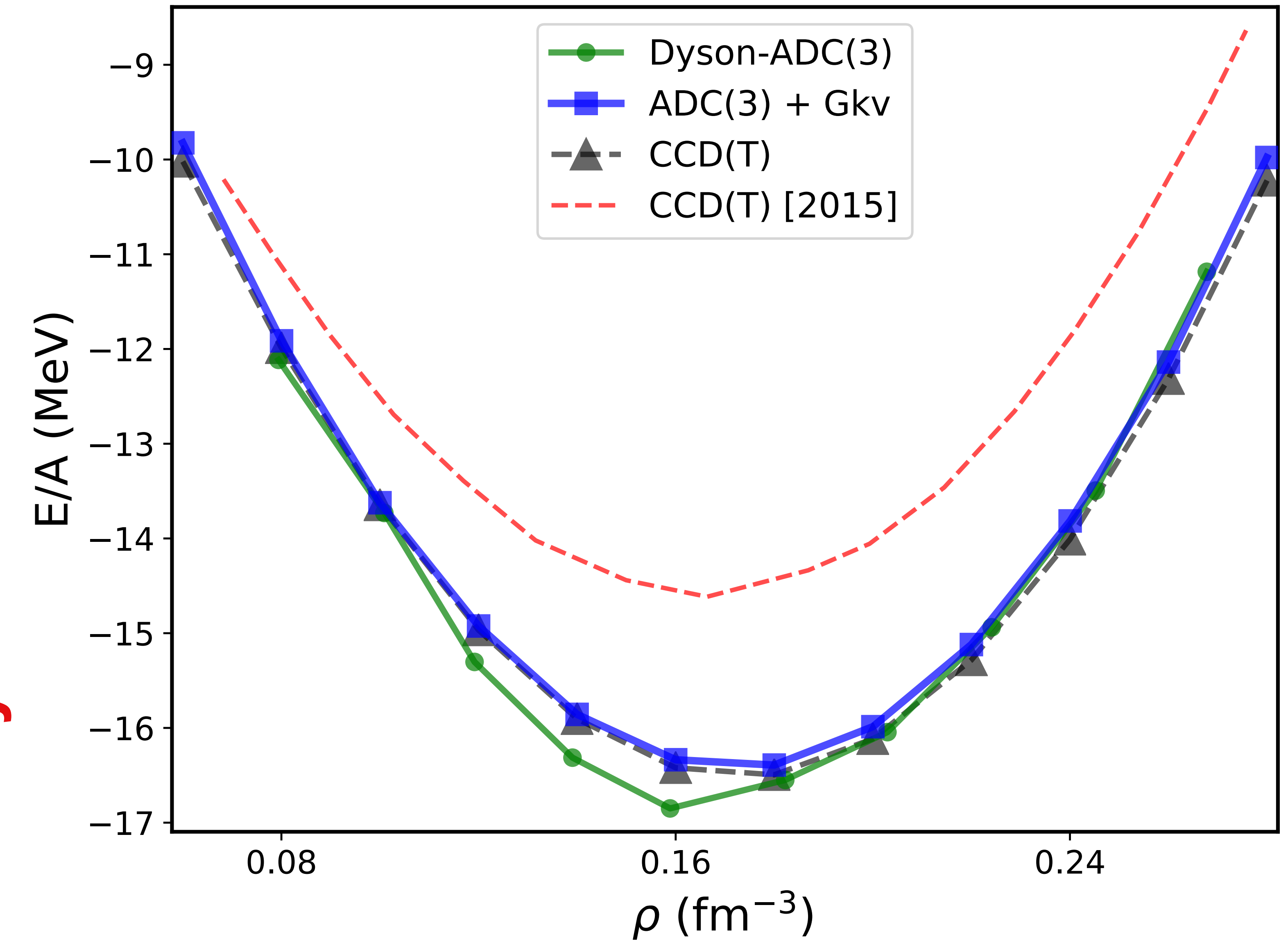


- Bug in ORNL CCM codes: $$V^{2N,eff} = V^{2N} + \sum_{k_h \leq k_F} (W^{3N})^* \rho(k_h)$$

- Dyson-ADC(3) instability at small p-h gaps and fully resolved in Gorkov(1) + ADC(3)

- Methods now agree — new NNLOsat saturation!

ALL Computations by F. Marino 2023-24



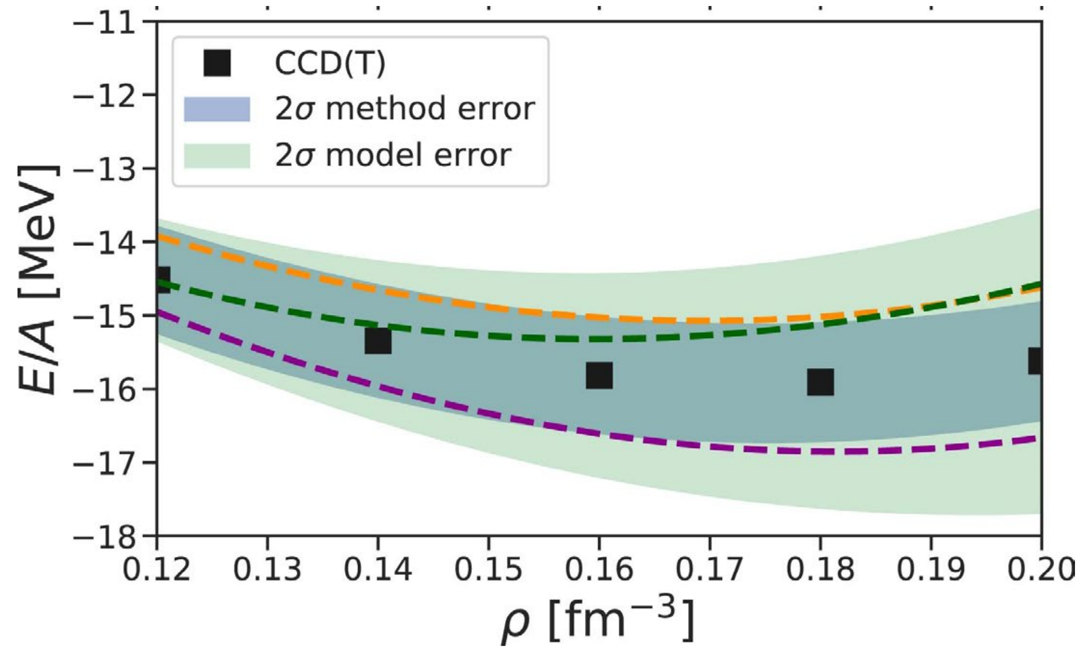
Author Correction: Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces

Correction to: *Nature Physics* https://doi.org/10.1038/s41567-022-01715-8, published online 22 August 2022.

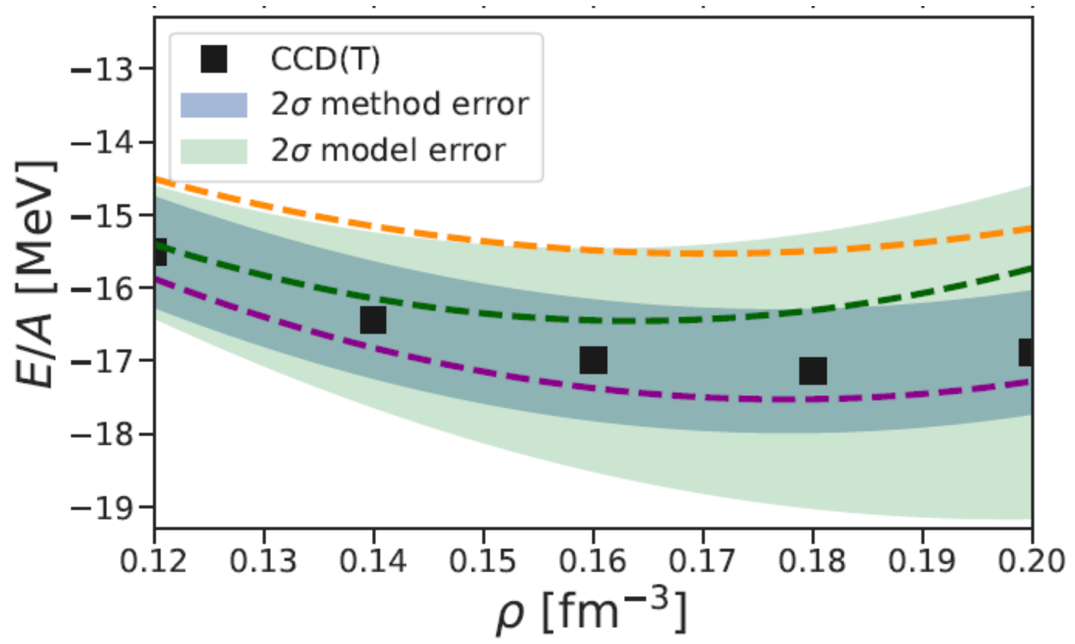
https://doi.org/10.1038/s41567-023-02324-9

Baishan Hu, Weiguang Jiang, Takayuki Miyagi, Zhonghao Sun, Andreas Ekström, Christian Forssén, Gaute Hagen, Jason D. Holt, Thomas Papenbrock, S. Ragnar Stroberg & Ian Vernon

The initially published version of the paper contained an error. Matrix elements in the



Original Extended Data Fig. 6



Revised Extended Data Fig. 6

Summary

Thank you for your attention!!!

→ Optical potentials: hold promise for solving structure reaction inconsistency (but still difficult)

→ Diagrammatic Monte Carlo is a promising method to go forward

→ SCGF Corkov/ASC(3) computations in nuclear matter in the way.

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

And thanks to my **collaborators** (over the years…):

*E. Vigezzi, **S. Brolli***

*M. Vorabbi, **P. Arthuis***

*V. Somà, T. Duguet, **A. Scalesi***

P. Navrártil

C. Giusti, P. Finelli

A. Idini

Backup slides

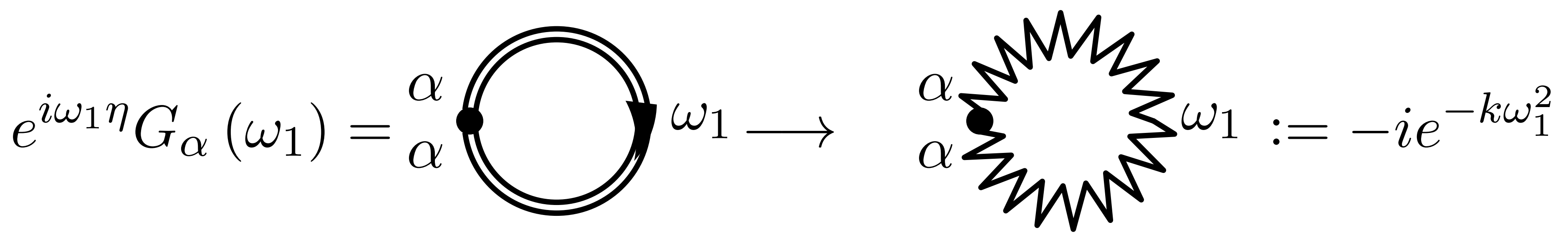
Diagrammatic Monte Carlo: normalization

The Markov chain must have the correct equilibrium distribution $w^{\omega}_{\alpha\beta}(\mathcal{C})$:

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \mathcal{Z}^{\omega}_{\alpha\beta}\left[\lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\frac{e^{i\arg\left[\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C}_i)\right]}}{W_o(N)}1_{\mathcal{T}_i\in\mathcal{S}_{\Sigma^\star}}\right]$$

where the normalization $\mathcal{Z}^{\omega}_{\alpha\beta}$ is unknown but it can be estimated.

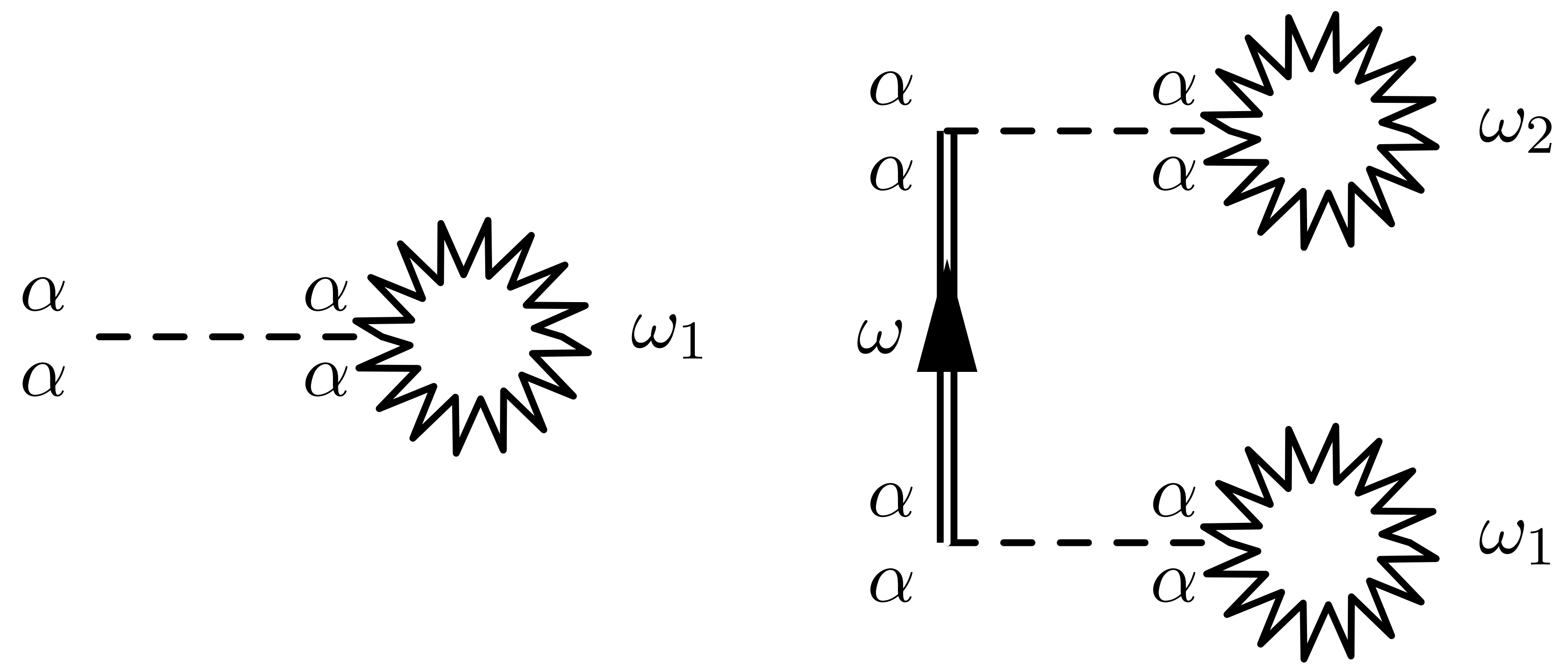
We turn propagators that close on themselves into zigzag lines with an arbitrary value



with *k* an arbitrary constant that can be used to optimize the convergence.

Diagrammatic Monte Carlo: normalization

Define the normalisation sector $\mathcal{S}_N$ to be made of ***both*** these diagrams:



- These diagrams belong to w_α^ω but not to $\mathcal{S}_{\Sigma^\star}$
- They are easy to integrate and to simulate with the Monte Carlo method

$\mathcal{S}_N$ has weight:

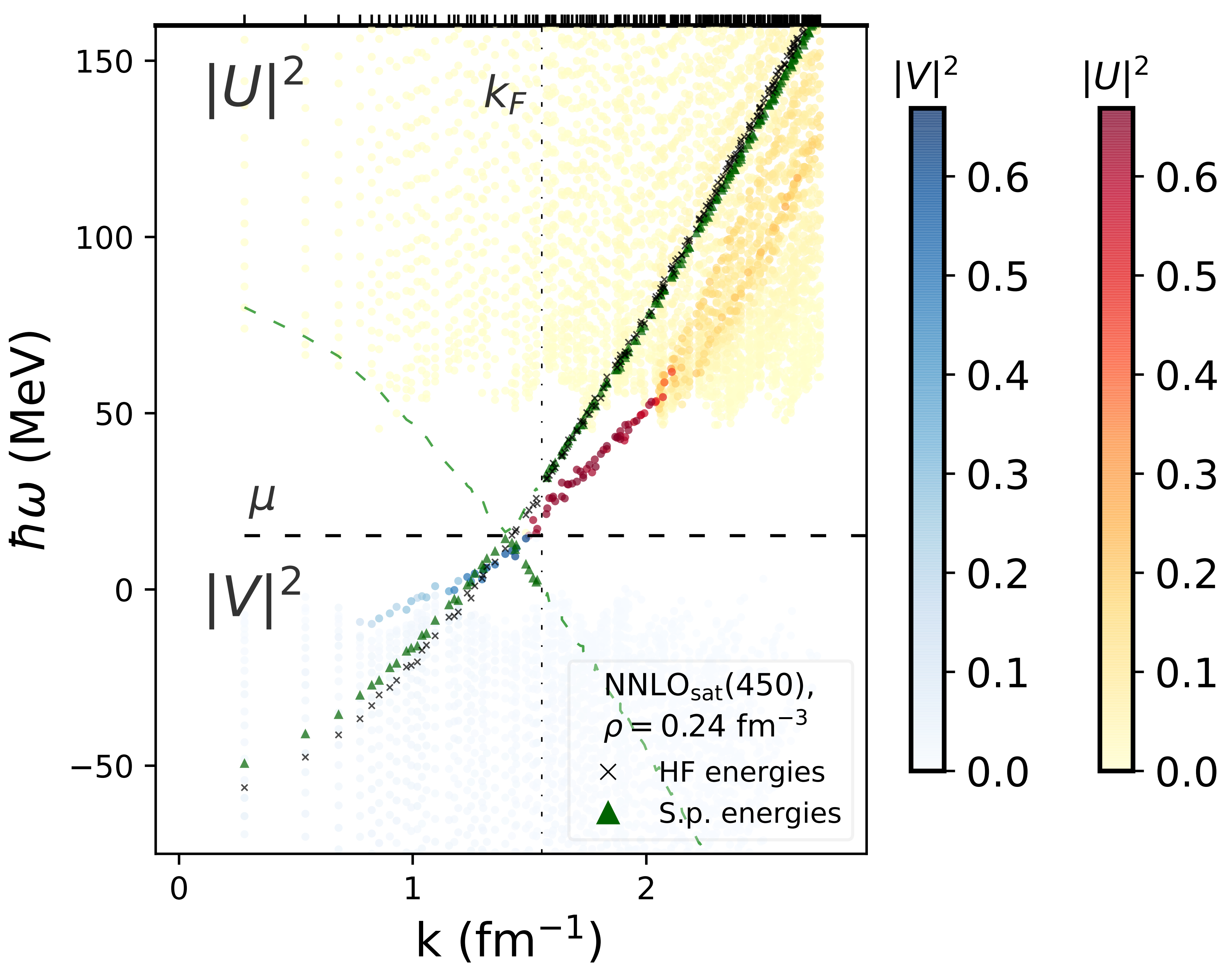
$$\mathcal{Z}_{N_\alpha}^{\omega} := \int_{\mathcal{S}_N} d\mathcal{C}\; w_\alpha^\omega = \frac{|g|}{4\sqrt{\pi k}} + \frac{g^2}{16\pi k}|G_\alpha(\omega)|W_o(2)$$

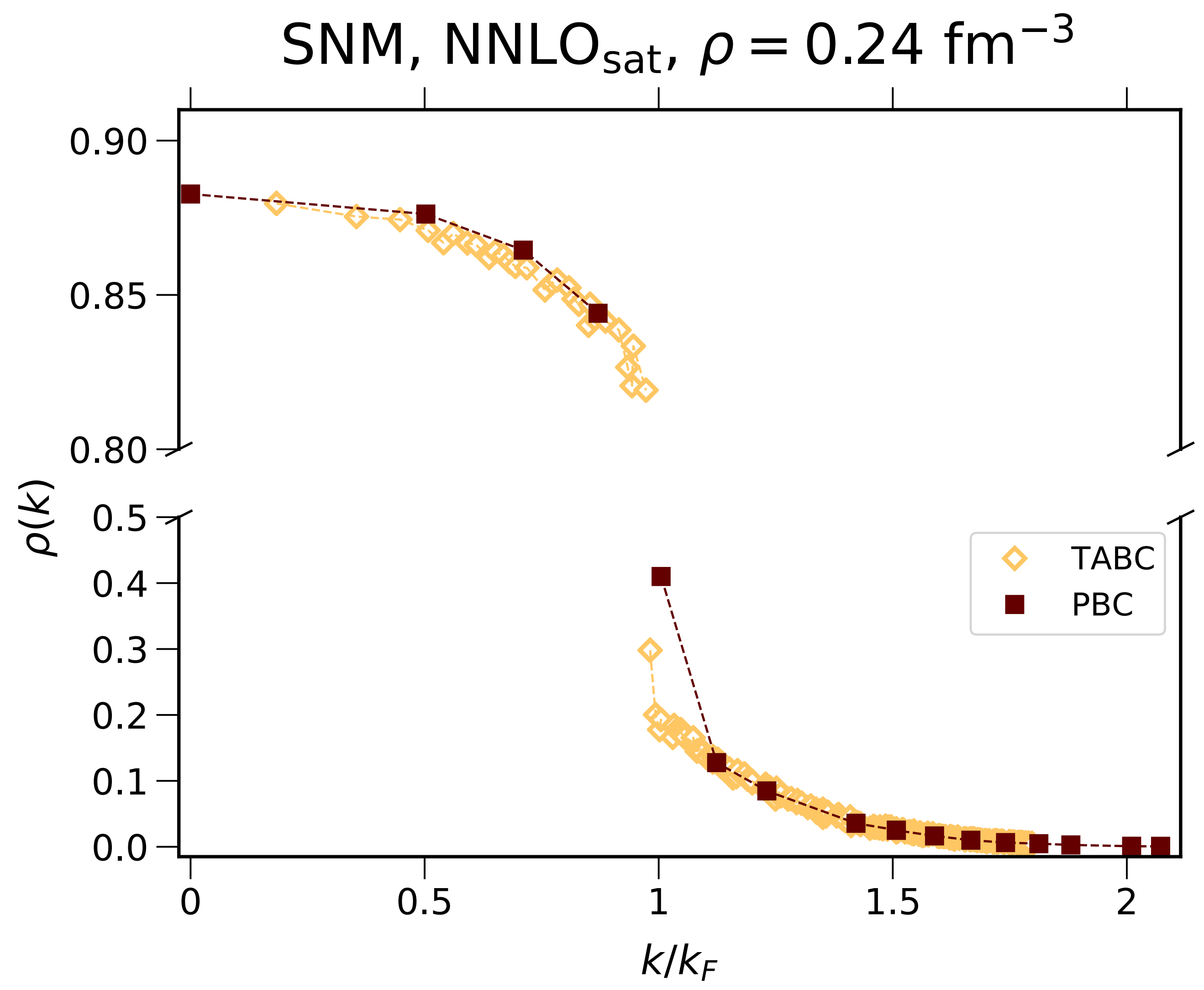
The expected number of times the normalization sector is visited ($\mathcal{N}$) gives the normalization $\mathcal{Z}_\alpha^\omega$:

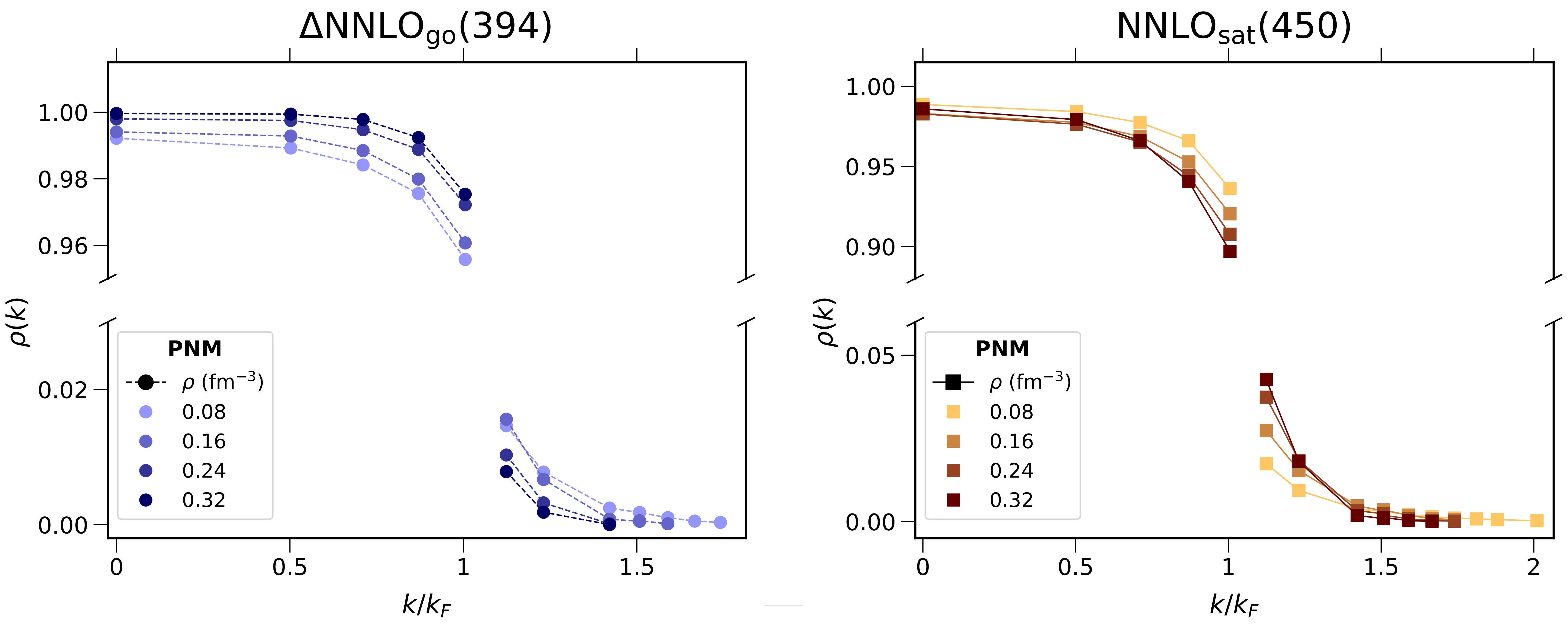
$$\frac{\mathcal{Z}_{N_\alpha}^{\omega}}{\mathcal{Z}_\alpha^\omega} = \lim_{n\to\infty}\frac{\mathcal{N}}{n}$$

Then, we get the fundamental equation of DiagMC: $\Sigma_\alpha^\star(\omega) = \mathcal{Z}_{N_\alpha}^{\omega} \lim_{n\to\infty}\frac{1}{\mathcal{N}}\sum_{i=1}^{n}\frac{e^{i\arg[\mathcal{D}_\alpha^\omega(\mathcal{C}_i)]}}{W_o(N)}1_{\mathcal{T}_i\in\mathcal{S}_{\Sigma^\star}}$

Combined Gkv-ADC(1) + Dys ADC(3)

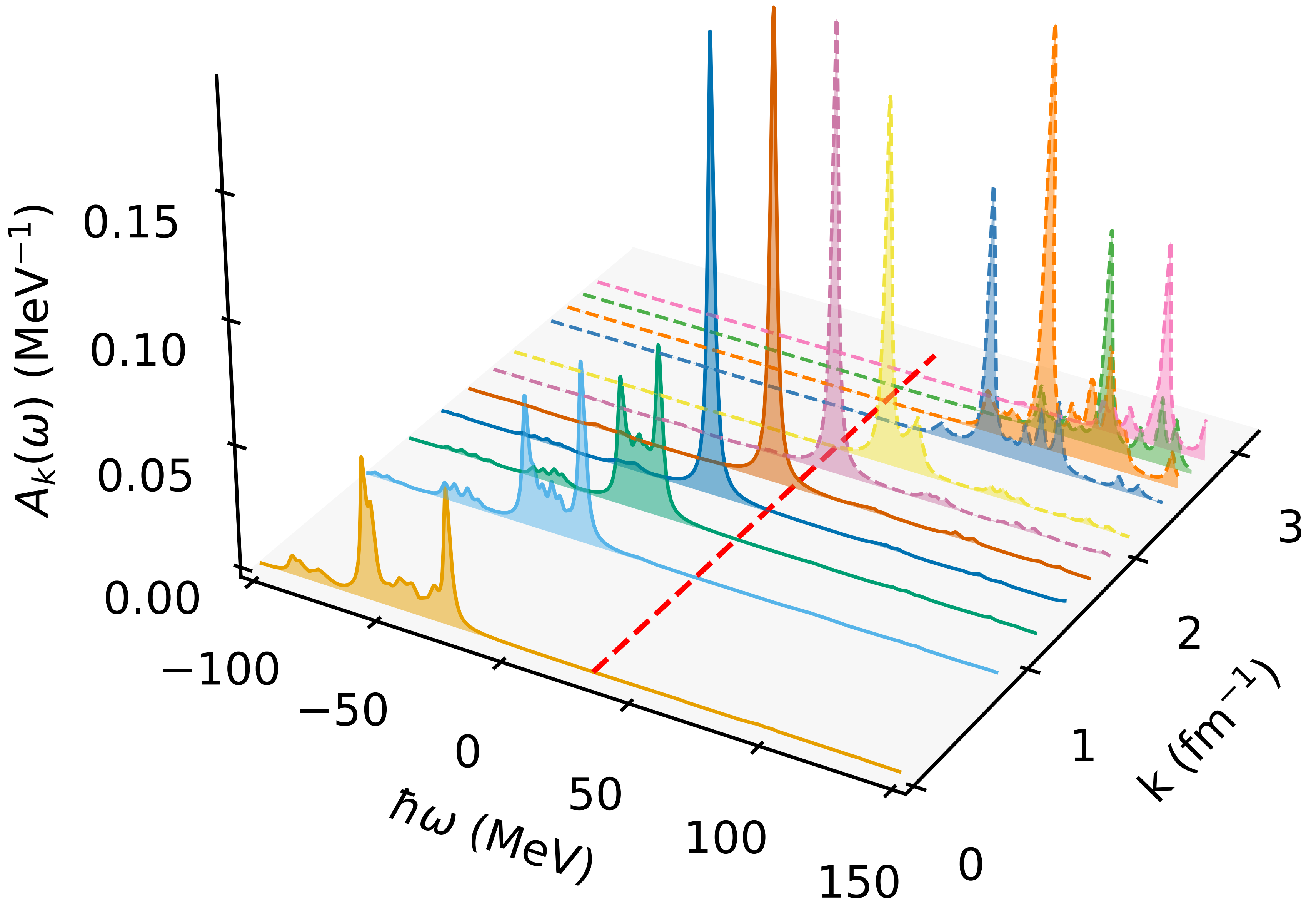




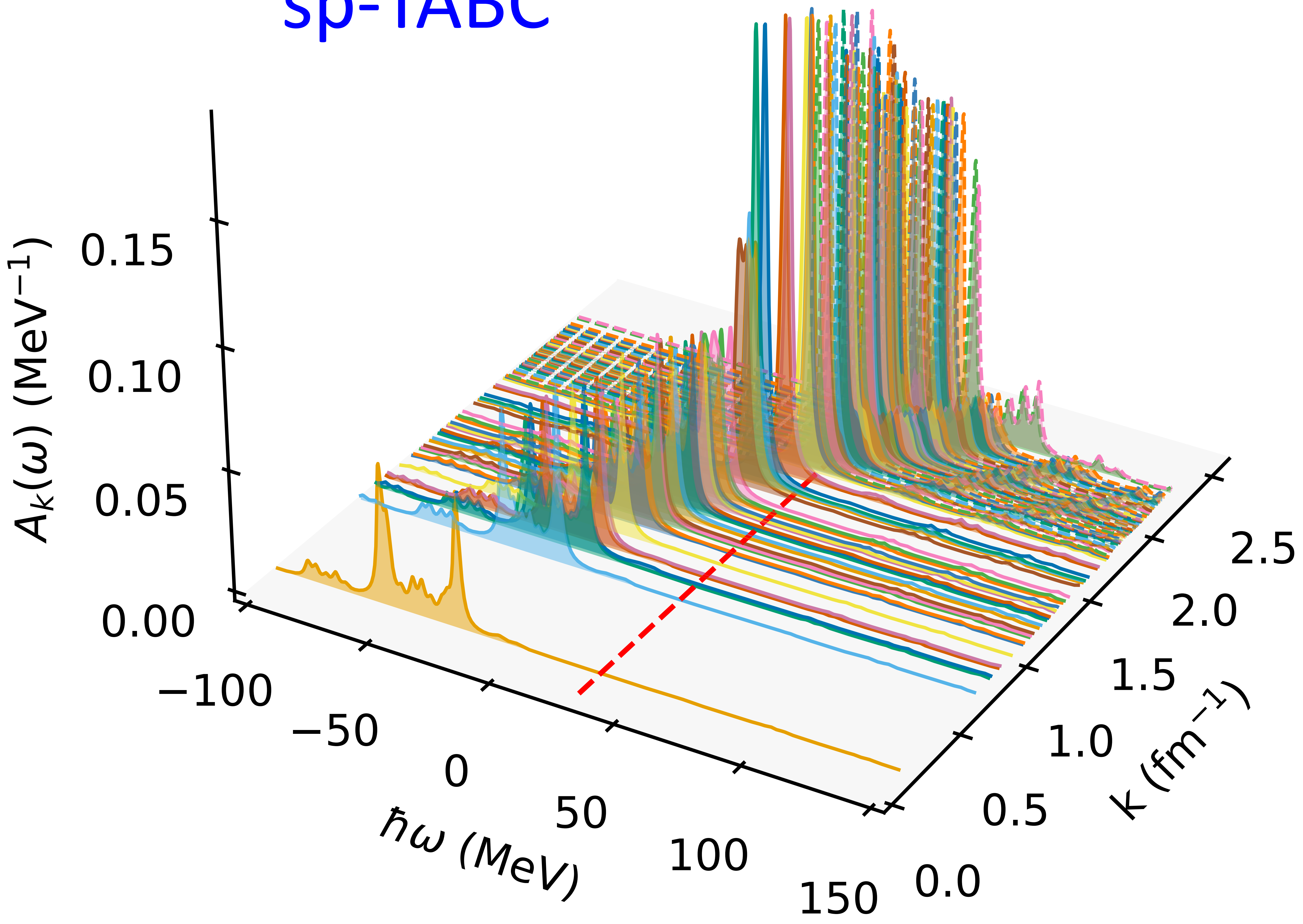


ADC(3) computations for infinite matter

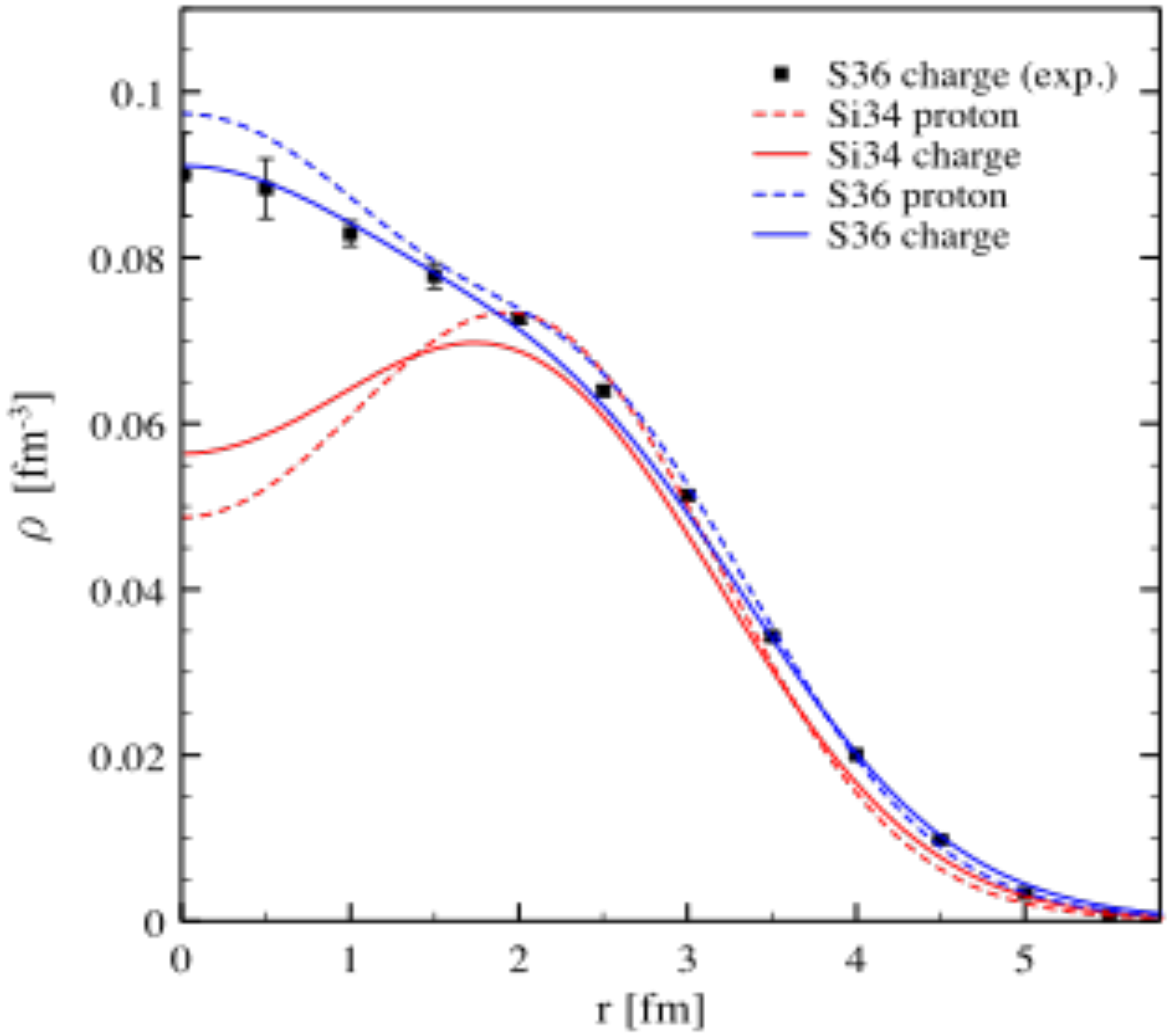
PBC



sp-TABC



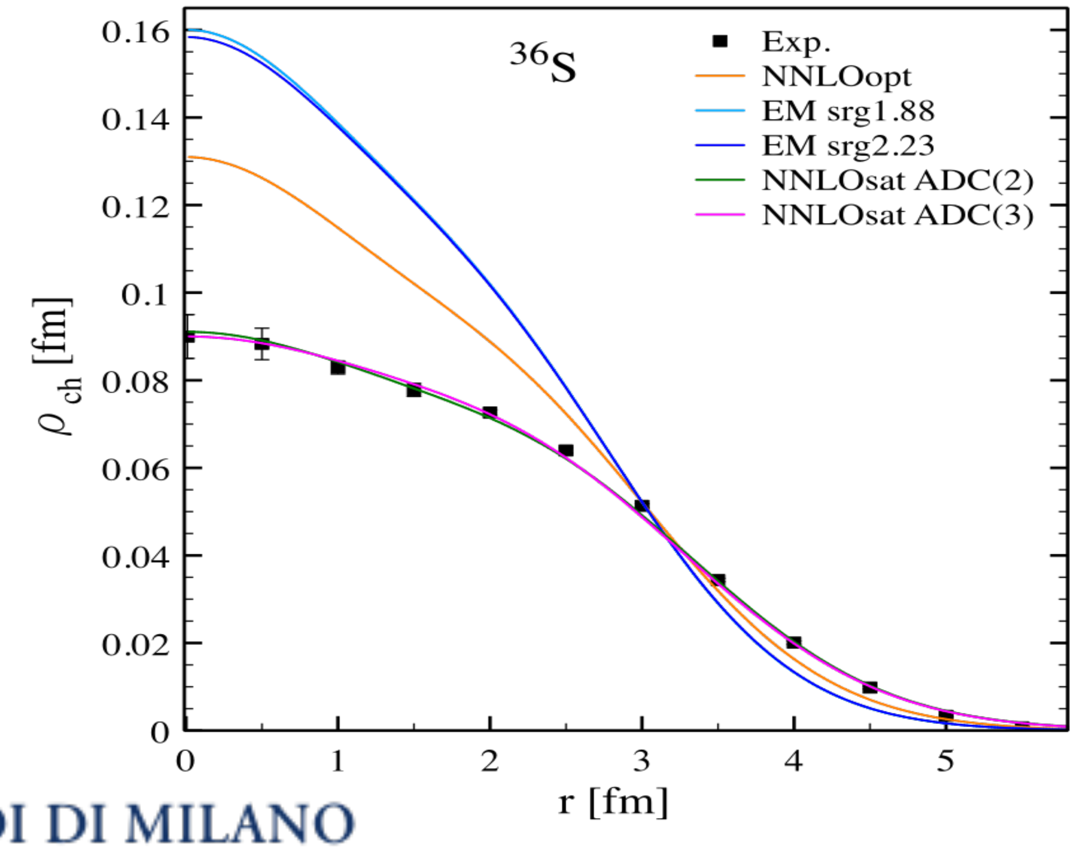
Bubble nuclei... ^{34}Si prediction

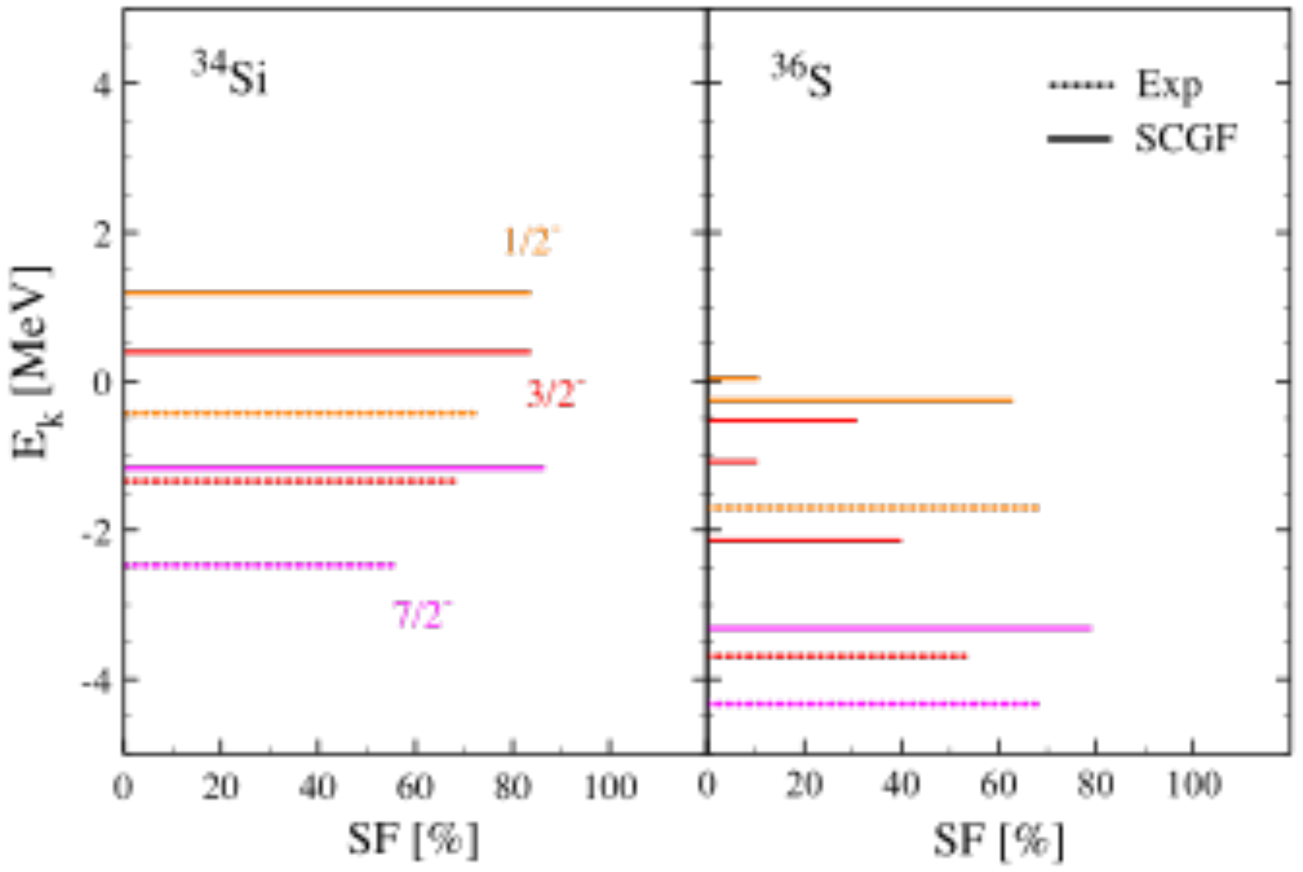


Duguet, Somà, Lecuse, CB, Navrátil,
Phys.Rev. C**95**, 034319 (2017)

- ^{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:

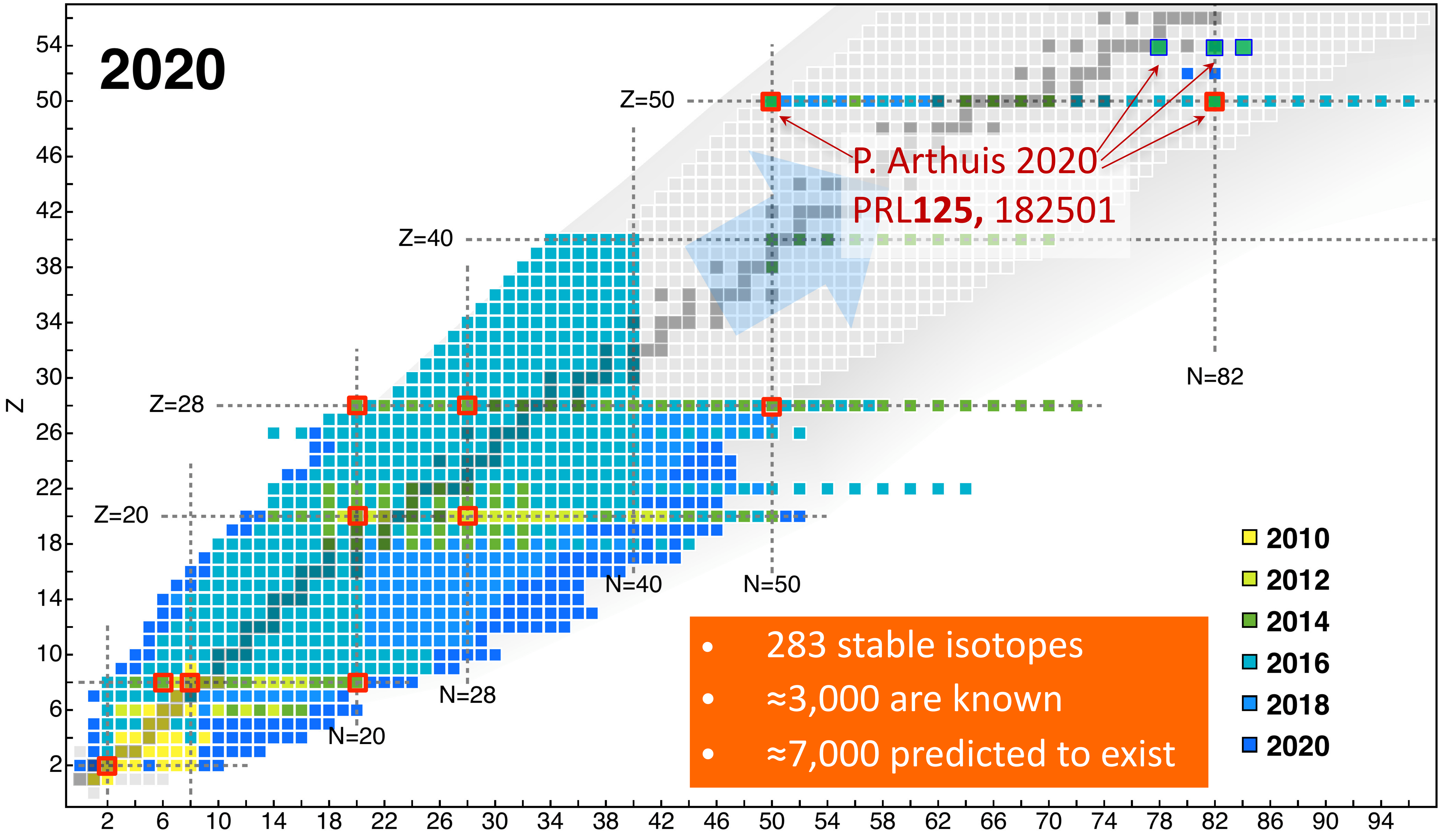




Reach of ab initio methods across the nuclear chart

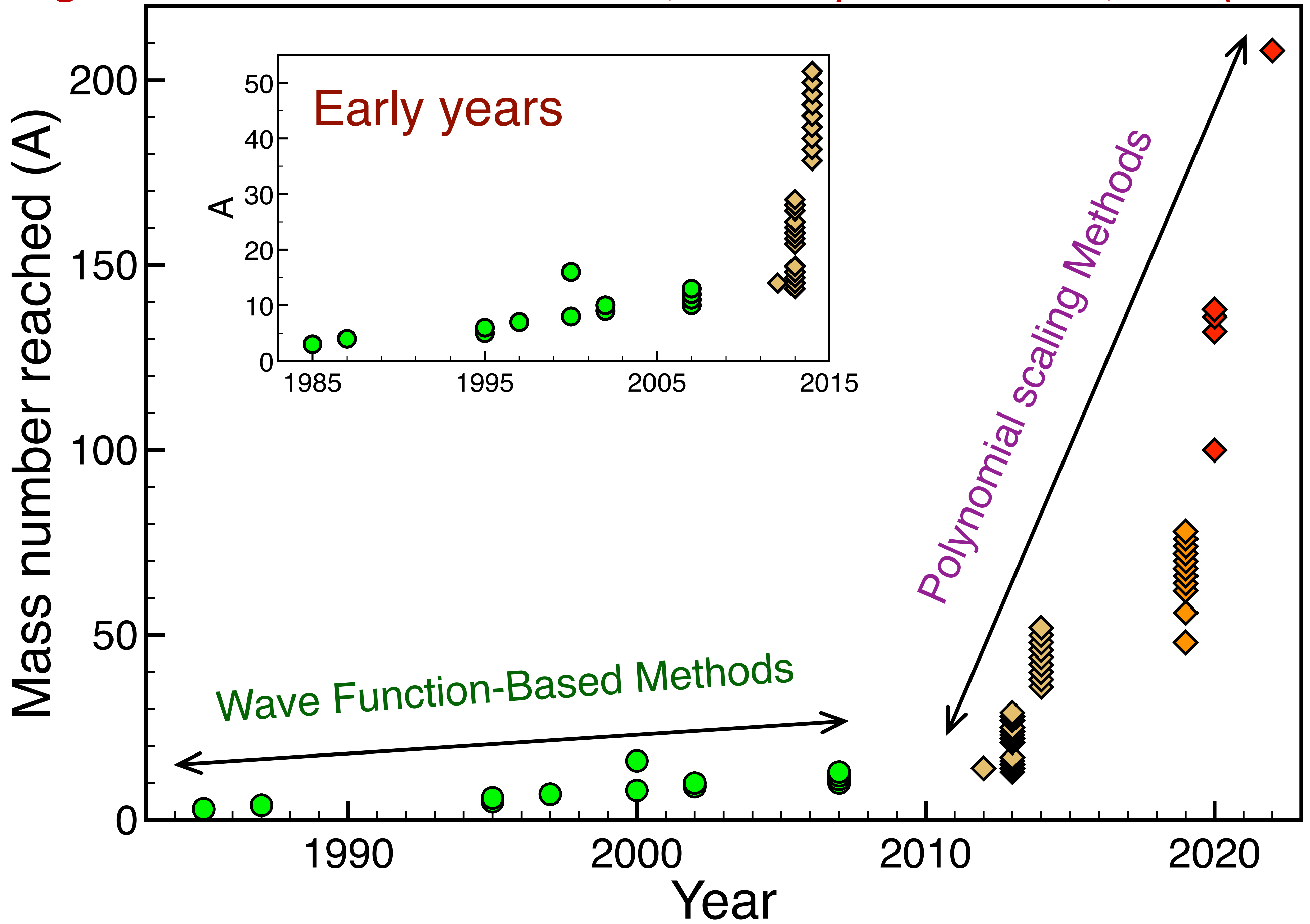
Extension beyond few-nucleons thanks to:

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



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

Legnaro Natl' Lab Mid Term Plan; Eur. Phys. J. Plus **138**, 709 (2023)



Open challenges:

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