

Self-Consistent Green's Function Theory for Atomic Nuclei

Many-Body Theory: Nuclear Physics Meets Quantum Chemistry

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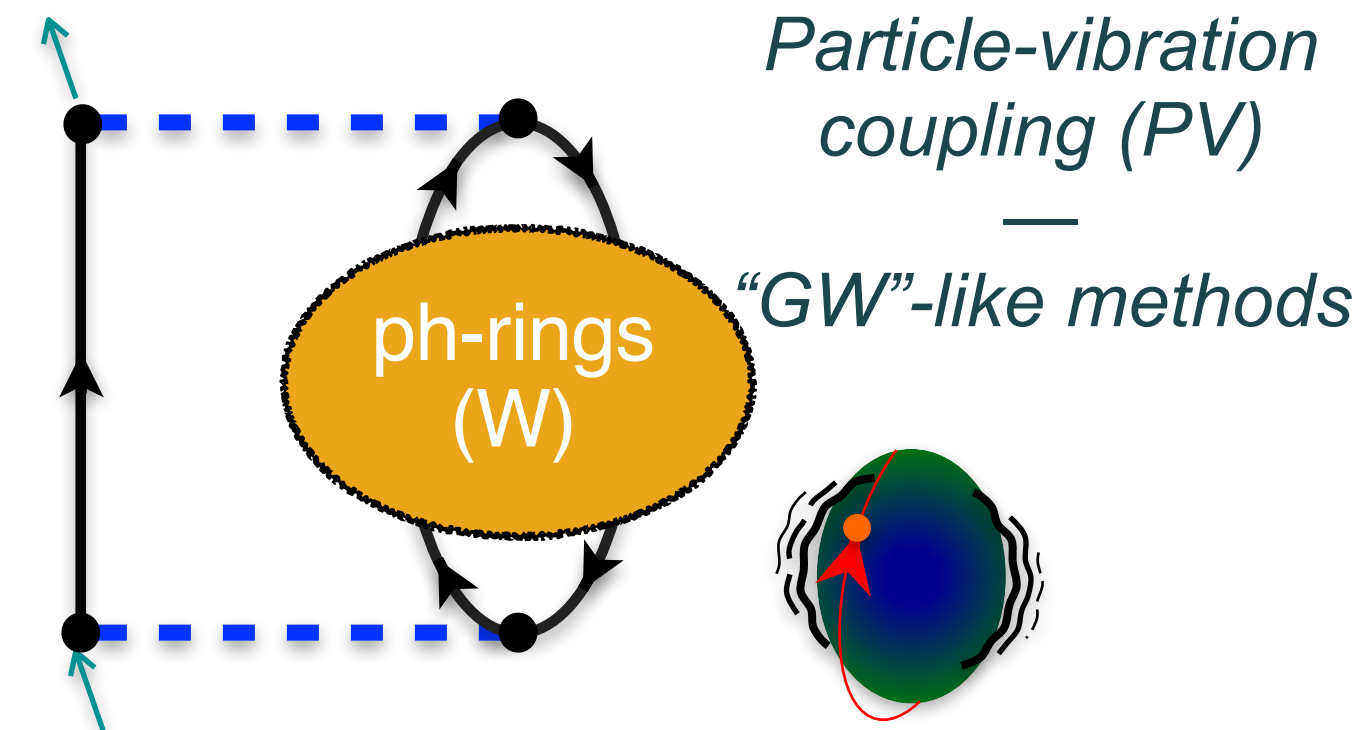
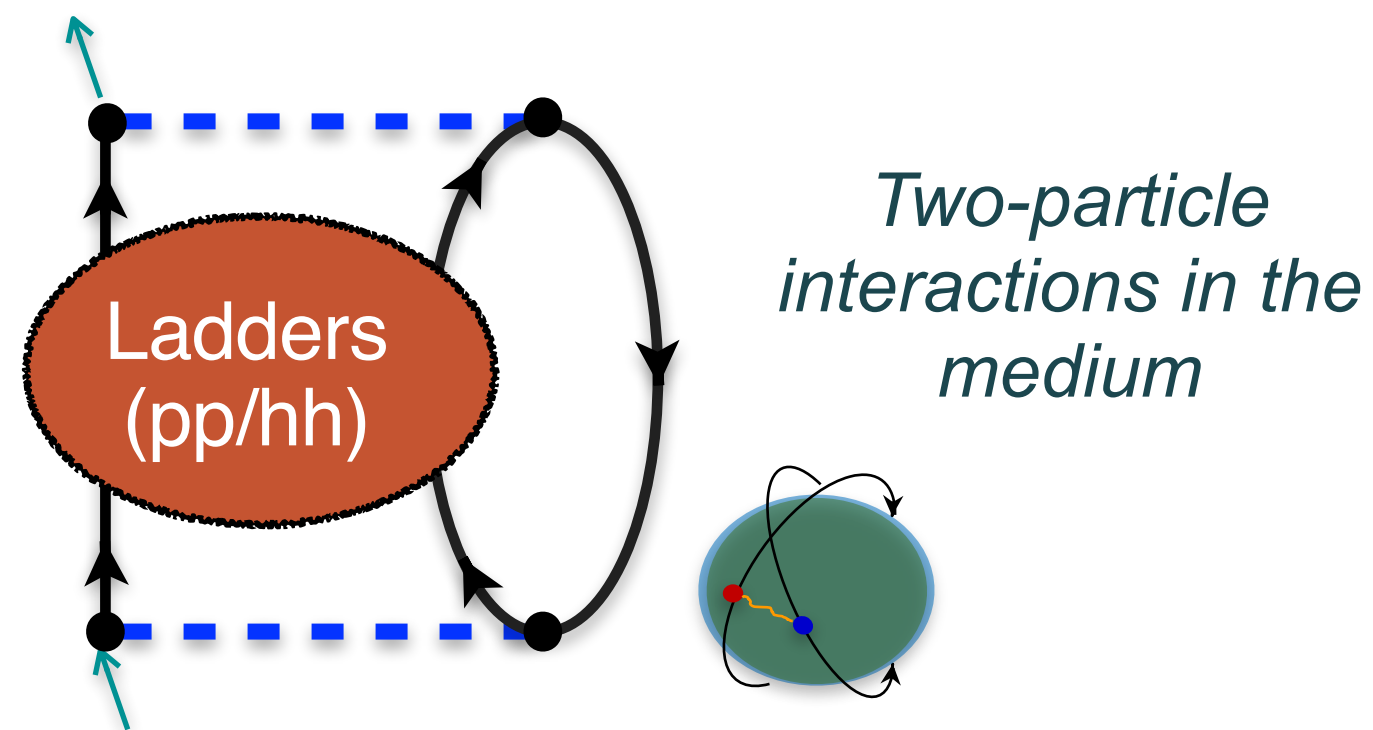


- A (partly historical) introduction to SCGF methods for nuclei...
...with some applications to Nuclear Physics, along the way
- Some other novel ideas:
 - Diagrammatic Monte Carlo
 - Emulators for SCGF
 - Physics Informed Neural Network

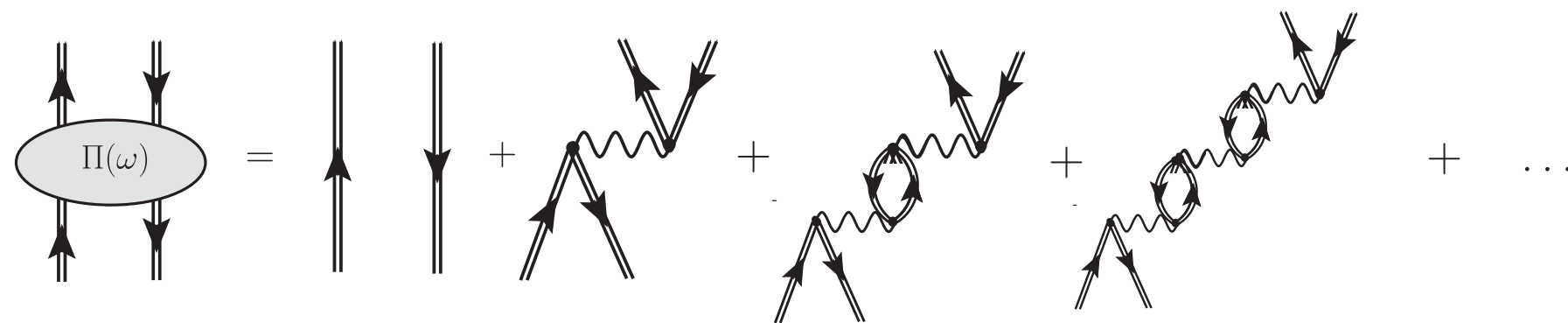


Basic many-body physics inside the self-energy

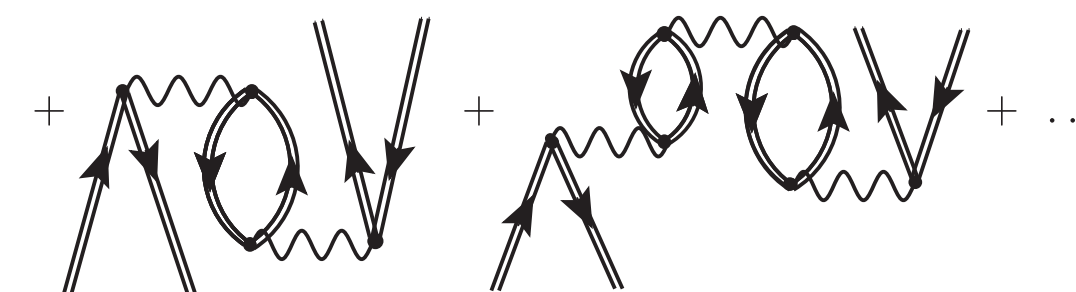
The *crudest* working approximations to many-body correlations (beyond HF/2nd order) are:



Where the blobs could be something like:



ph-configuration interaction (or TDA)



add 2p2h partial clusters

random phase approx. (RPA)

nuclei,
molecules,
solid state,
stars...
...they all need at
least some of this!

The physics contained in the **one-body** Green's function

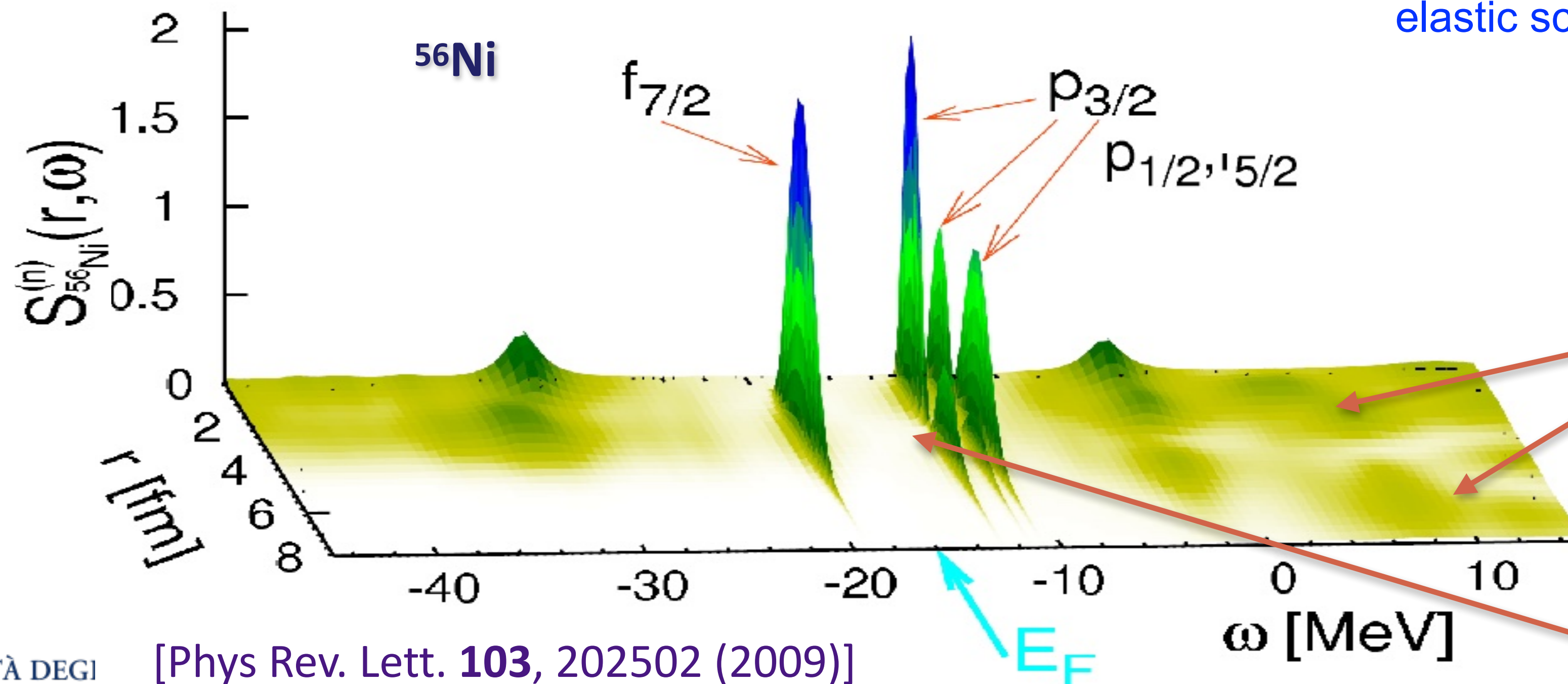
One-body propagator: $g_{\alpha\beta}(t - t') = -i/\hbar \langle \Psi_0^A | T[c_\alpha(t) c_\beta^\dagger(t')] | \Psi_0^A \rangle$

In frequency space:

$$g_{\alpha\beta}(\omega) = \int g_{\alpha\beta}(\tau) e^{i\omega\tau} d\tau = \sum_n \frac{\langle \Psi_0^A | c_\alpha | \Psi_n^{A+1} \rangle \langle \Psi_n^{A+1} | c_\beta^\dagger | \Psi_0^A \rangle}{\omega - (E_n^{A+1} - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c_\beta^\dagger | \Psi_k^{A-1} \rangle \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle}{\omega - (E_0^A - E_k^{A-1}) - i\eta}$$

(One-body) spectral function: $S(\alpha, \omega) := \pm \frac{1}{2\pi} \Im m \{ g_{\alpha\alpha}(\omega) \}$

The self-energy $\Sigma_{\alpha\beta}^*(\omega)$ determines both ground state observables and elastic scattering.

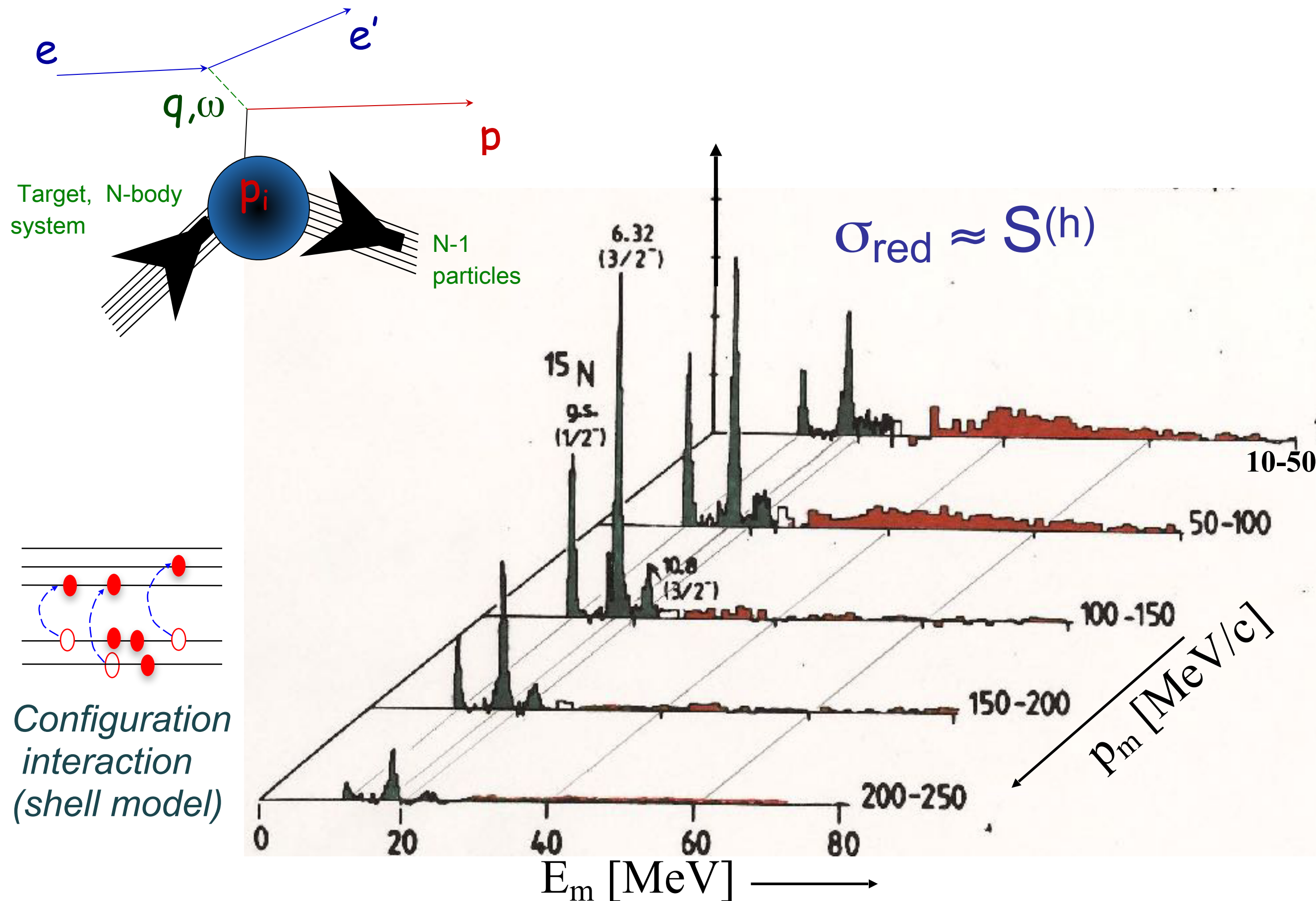


==> Consistent computation of structure and reactions !!

Elastic scattering states

Low-E spectroscopy

Experimental spectral function in fermi systems



Saclay data for $^{16}\text{O}(e,e'p)$
[Mougey et al., Nucl. Phys. A335, 35 (1980)]

An ARPES setup - spectroscopy at the Fermi surface

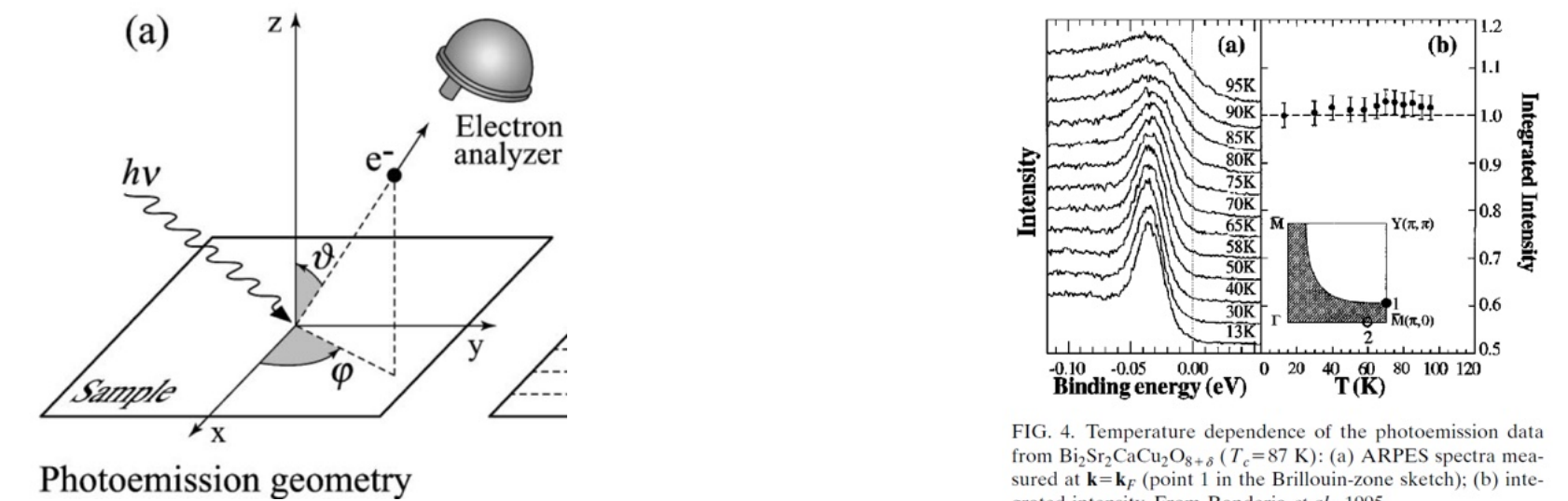


FIG. 4. Temperature dependence of the photoemission data from $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ ($T_c = 87$ K): (a) ARPES spectra measured at $k=k_F$ (point 1 in the Brillouin-zone sketch); (b) integrated intensity. From Damascelli et al., 1995

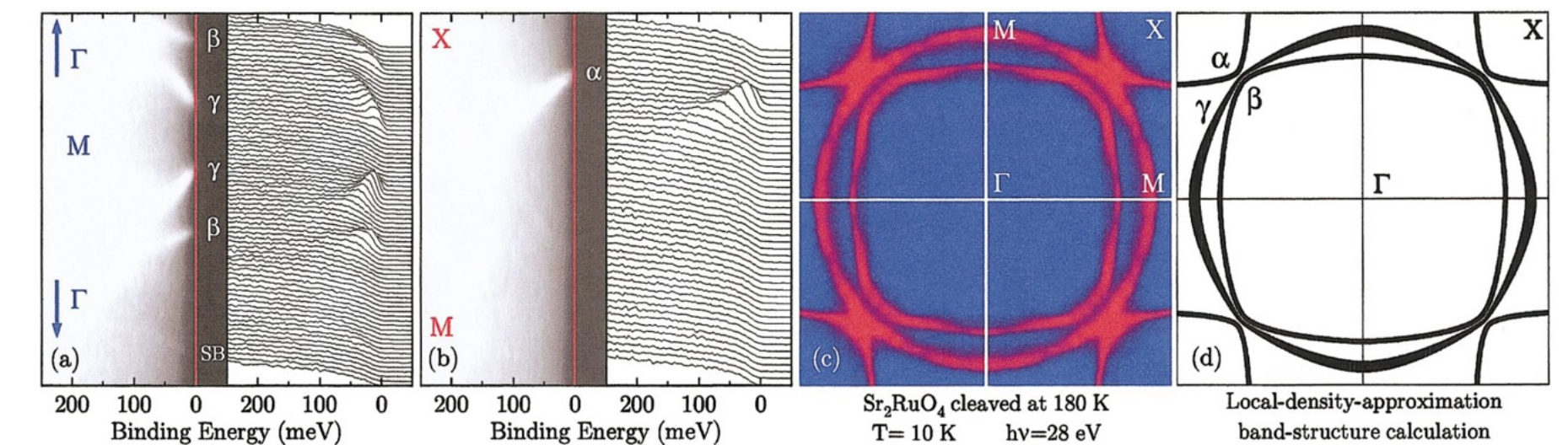


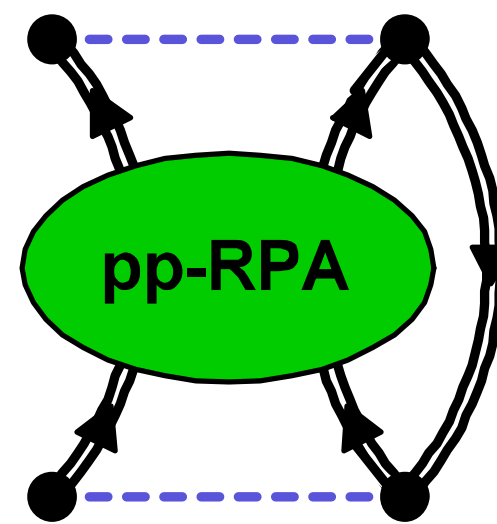
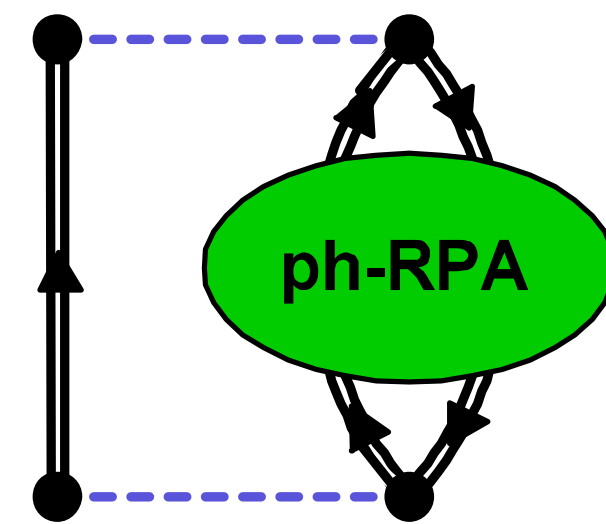
FIG. 9. Photoemission results from Sr_2RuO_4 : ARPES spectra and corresponding intensity plot along (a) Γ -M and (b) M-X; (c) measured Fermi surface; (d) calculated Fermi surface (Mazin and Singh, 1997). From Damascelli et al., 2000 (Color).

[A. Damascelli, et. al, Rev. Mod. Phys. **75**, 473 (2003)]

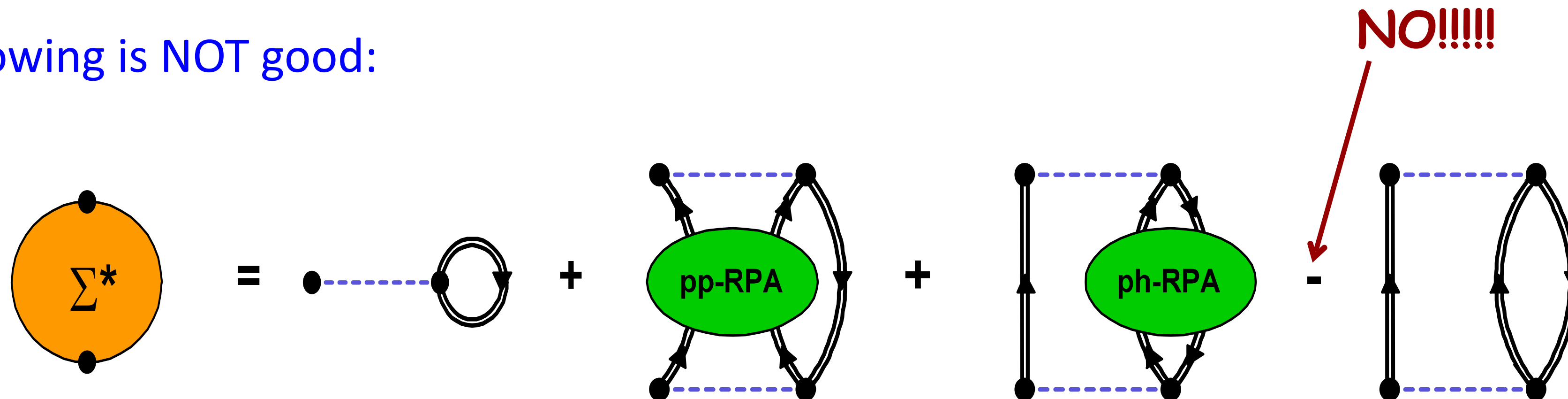
$$d\sigma \sim \sum_n \delta(E_{miss} - E_0^N + E_n^{N-1}) |\langle \Psi_n^{N-1} | a_{p_{miss}} | \Psi_0^N \rangle|^2$$

Faddeev RPA method

- The following two diagrams are be equally important. However, adding them does not work well:
 - They both contain $\Sigma_{\alpha\beta}^{2nd}(\omega)$, which would be over counted
 - They would not interfere...



- So, the following is NOT good:



Algebraic Diagrammatic Construction (ADC)

The proper Lehman representation of the self-energy (and propagators): *dictated by the causality principle!*

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

ADC(n):

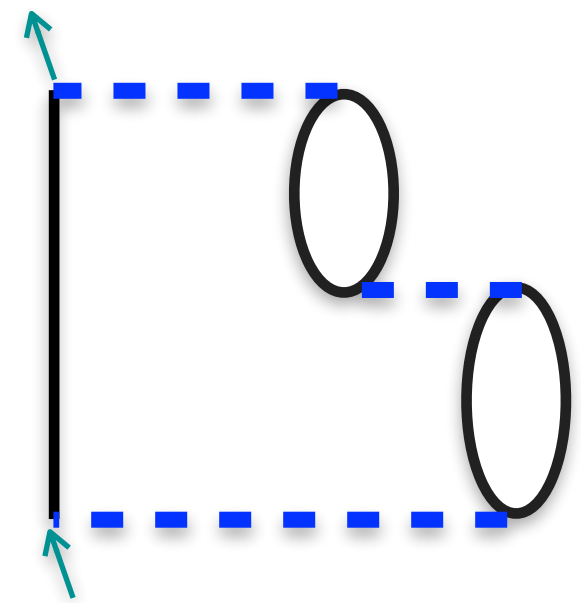
Shirmer et al. Phys Rev A 1982-1983

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

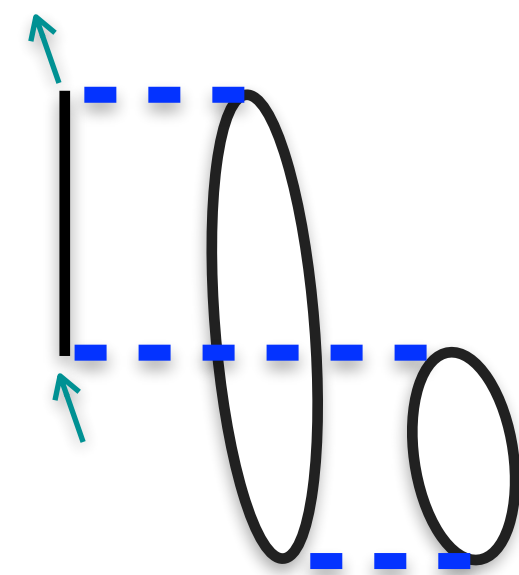


Algebraic Diagrammatic Construction (ADC)

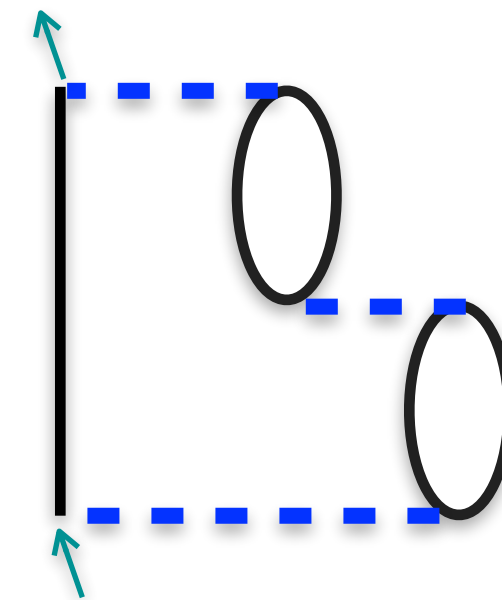
Implicit time orderings
(Feynman diagrams)



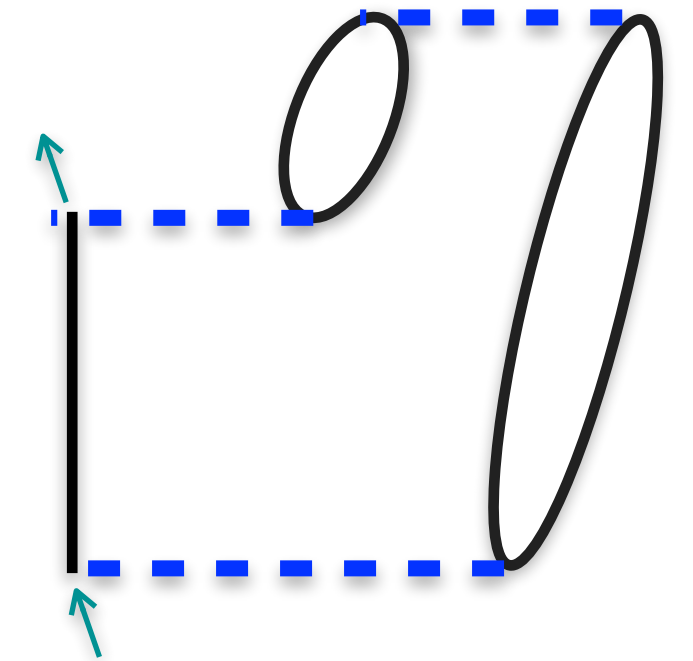
Time ordered diagrams
(Goldstone rep.)



$$M^{(1)\dagger} \frac{1}{\omega - E^> + i\eta} M^{(2)}$$



$$M^{(1)\dagger} \frac{1}{\omega - E^> + i\eta} C \frac{1}{\omega - E^> + i\eta} M^{(1)}$$



$$M^{(2)\dagger} \frac{1}{\omega - E^> + i\eta} M^{(1)}$$

$$\longrightarrow [M^{(1)} + M^{(2,ld)}]^\dagger \frac{1}{\omega - E^> - C^{(ld)} + i\eta} [M^{(1)} + M^{(2,ld)}]$$

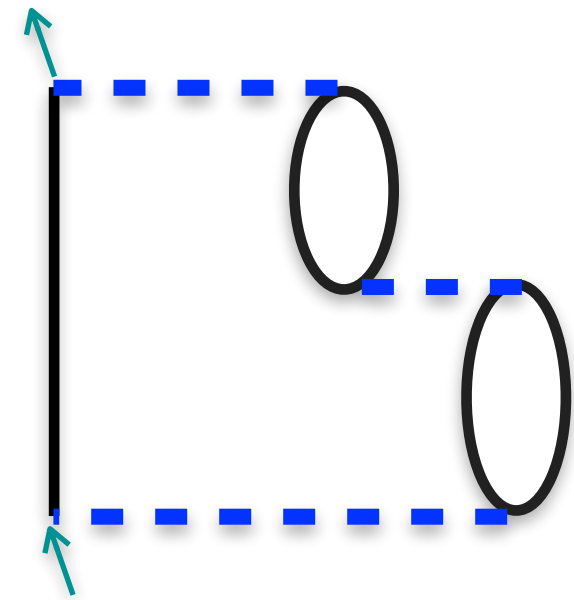
ADC(n):

Schirmer et al. Phys Rev A 1982-1983

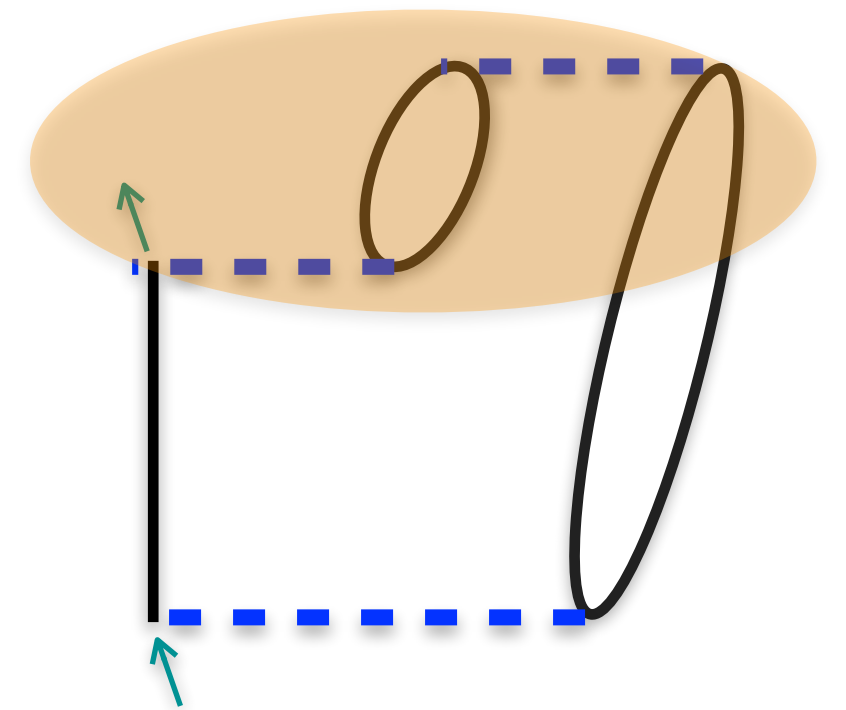
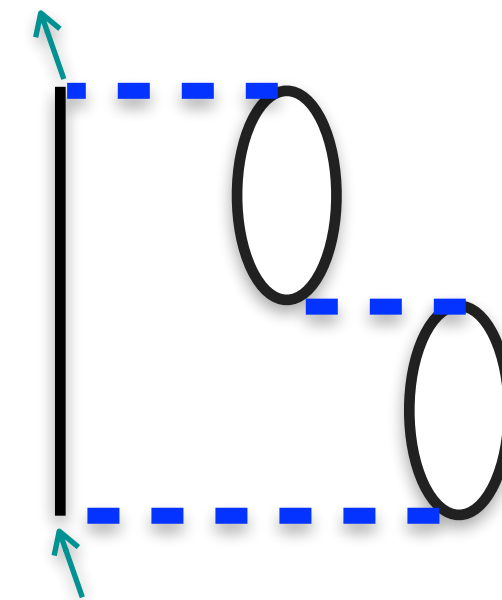
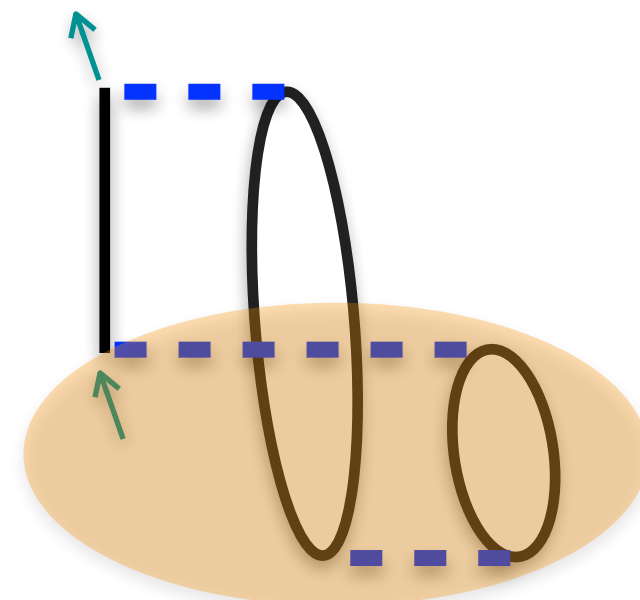
CB, A. Carbone, Lect. Notes in Phys **936** (2017)- Chapter 11.

Algebraic Diagrammatic Construction (ADC)

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Algebraic Diagrammatic Construction (ADC)

The proper Lehman representation of the self-energy (and propagators): *dictated by the causality principle!*

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

Expanding in powers of H_1 :

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

$$\Sigma^{\star}(\omega) = -\hat{U} + \Sigma^{(\infty)} + M^{(1)\dagger} \frac{1}{\omega - E^> + i\eta} C \frac{1}{\omega - E^> + i\eta} M^{(1)} + M^{(2)\dagger} \frac{1}{\omega - E^> + i\eta} M^{(1)} + M^{(1)\dagger} \frac{1}{\omega - E^> + i\eta} M^{(2)} + \mathcal{O}(\hat{H}_1^4)$$

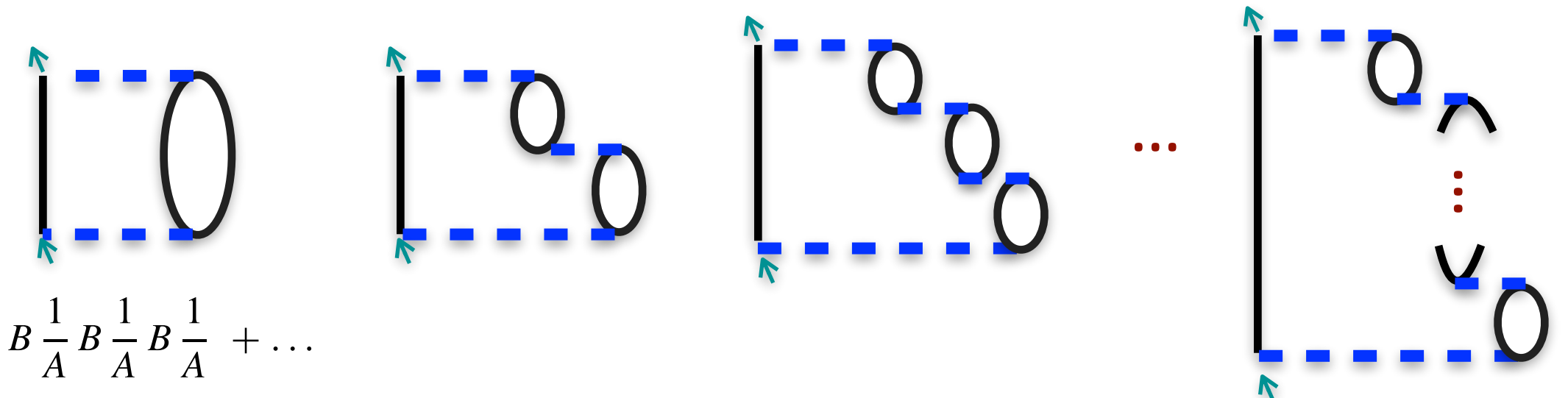
3rd order ADC:

$$\Sigma^{\star}(\omega) \longrightarrow [M^{(1)} + M^{(2,ld)}]^{\dagger} \frac{1}{\omega - E^> - C^{(ld)} + i\eta} [M^{(1)} + M^{(2,ld)}] = \Sigma^{(2)}(\omega) + \Sigma^{(3,ld)}(\omega) + \text{terms beyond } 3^{rd} \text{ order}$$

- **ADC(n)** can be done at any order n:
—> systematically improvable.

- **ADC(n≥3)** Implies infinite resummations:

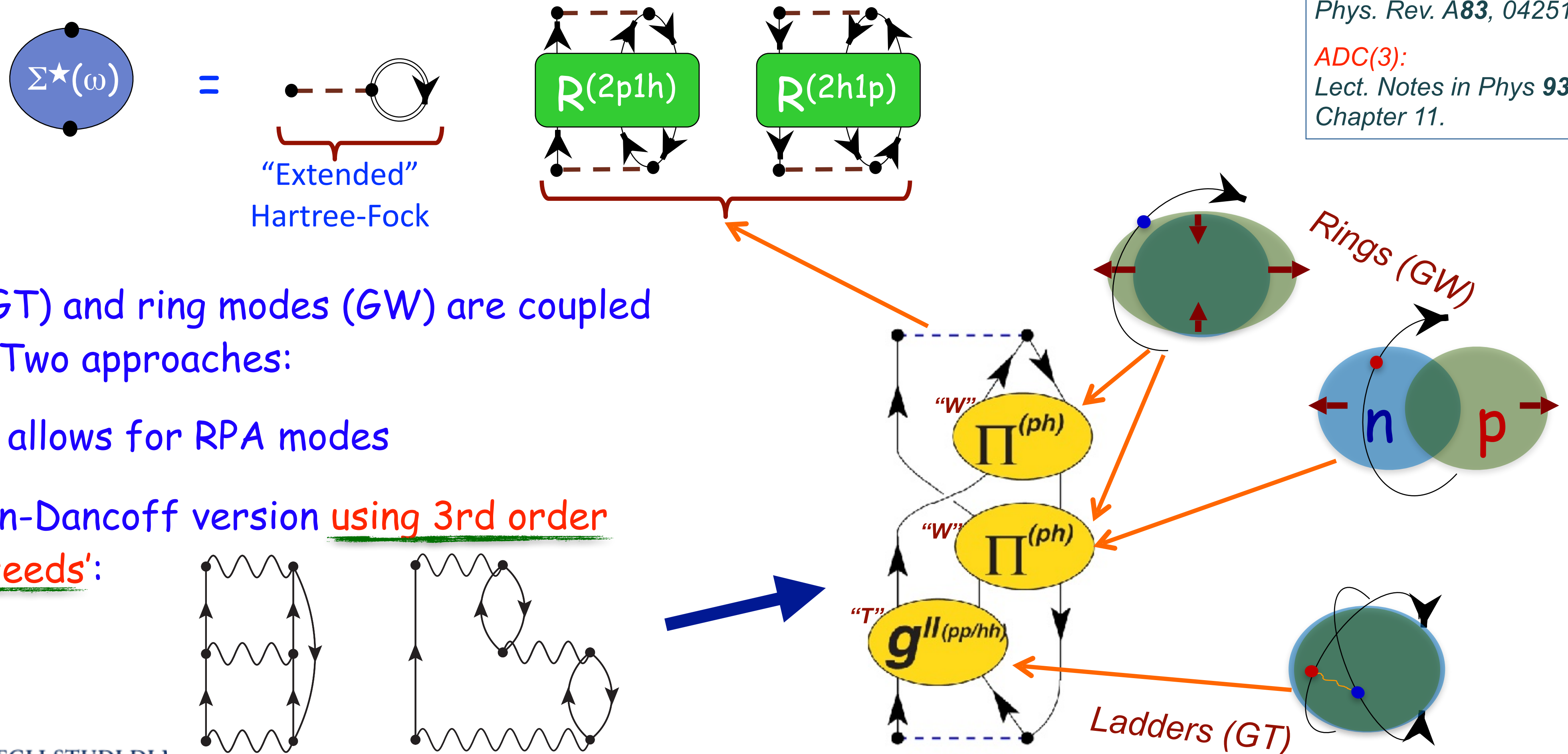
$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A} + \frac{1}{A} B \frac{1}{A} B \frac{1}{A} + \frac{1}{A} B \frac{1}{A} B \frac{1}{A} B \frac{1}{A} + \dots$$



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)

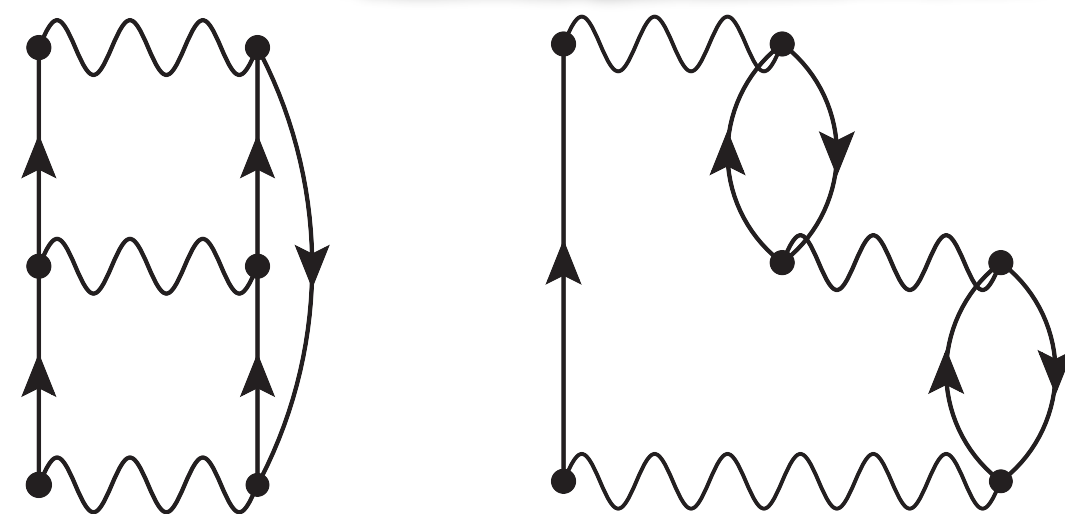
Phys. Rev. A **83**, 042517 (2011)

ADC(3):

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

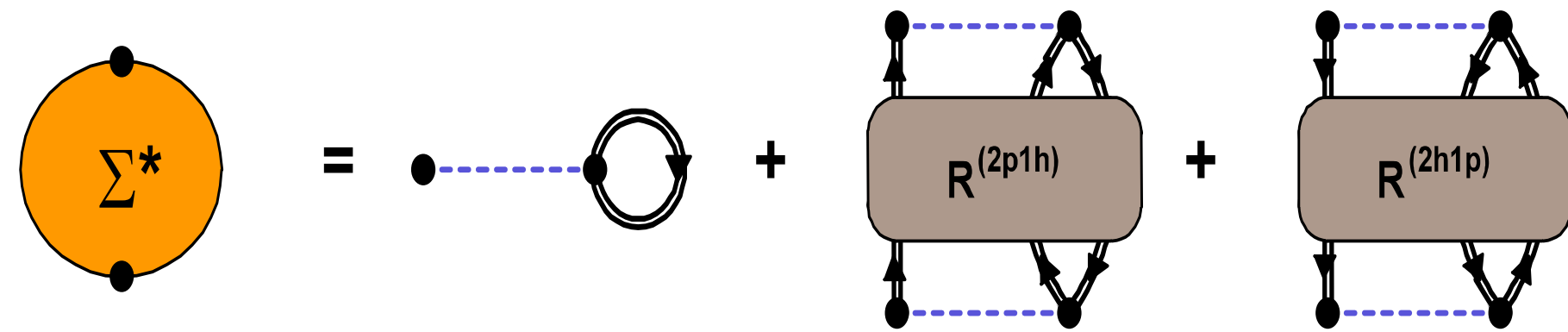
All Ladders (GT) and ring modes (GW) are coupled to all orders. Two approaches:

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



Dyson-Schwinger expansion of self-energy

Using the equation of motion *twice*, one finds again the Dyson equation, with the self-energy given in a symmetric form:

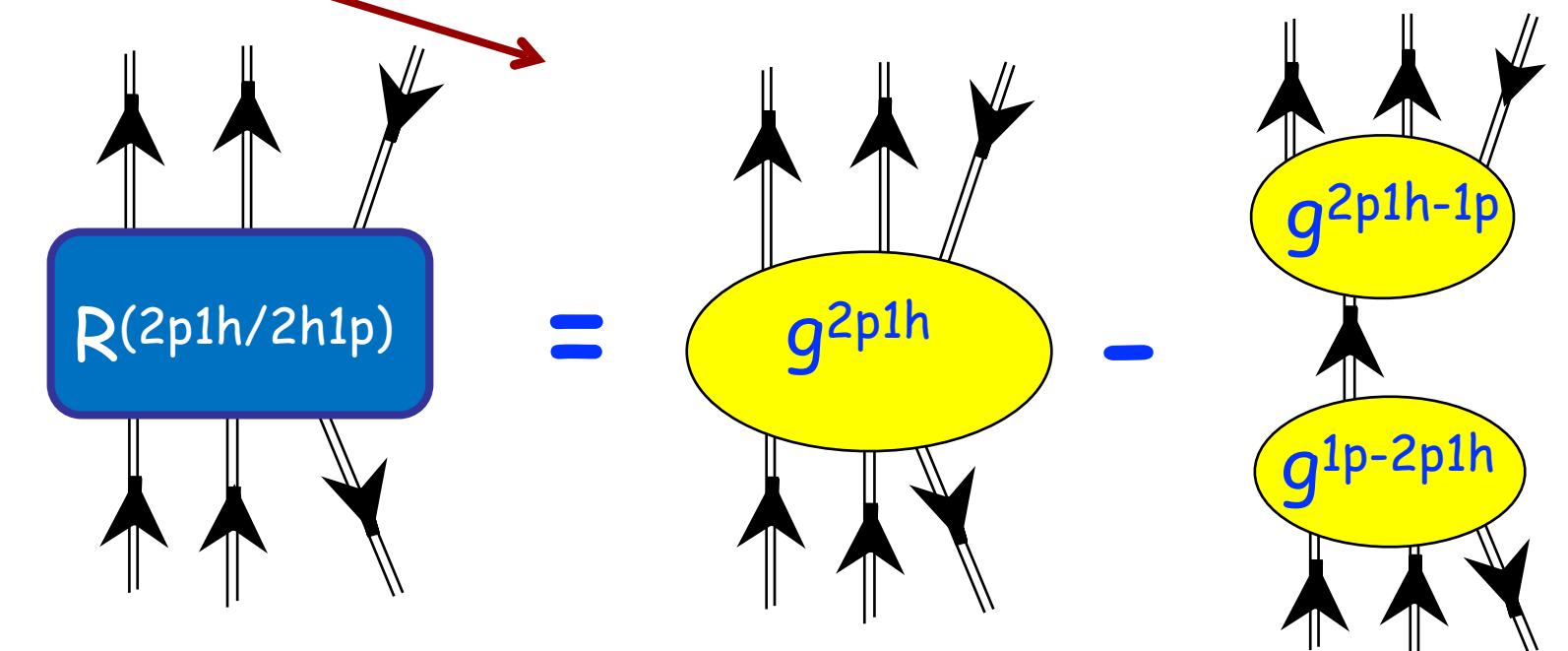


$$\Sigma_{\alpha\beta}^*(t - t') = \Sigma_{\alpha\beta}^{HF} + v_{\alpha\lambda,\mu\nu} R_{\mu\nu\lambda,\gamma\delta\zeta}(t, t') v_{\gamma\delta,\beta\zeta}$$

where:

$$R_{\mu\nu\lambda,\alpha\beta\gamma}(t; t') \equiv g_{\mu\nu\lambda,\alpha\beta\gamma}^{2p1h}(t; t') - g_{\mu\nu\lambda,\eta}^{2p1h-1p}(t, t_1) g_{\eta\sigma}^{-1}(t_1 - t_2) g_{\sigma,\alpha\beta\gamma}^{1p-2p1h}(t_2, t')$$

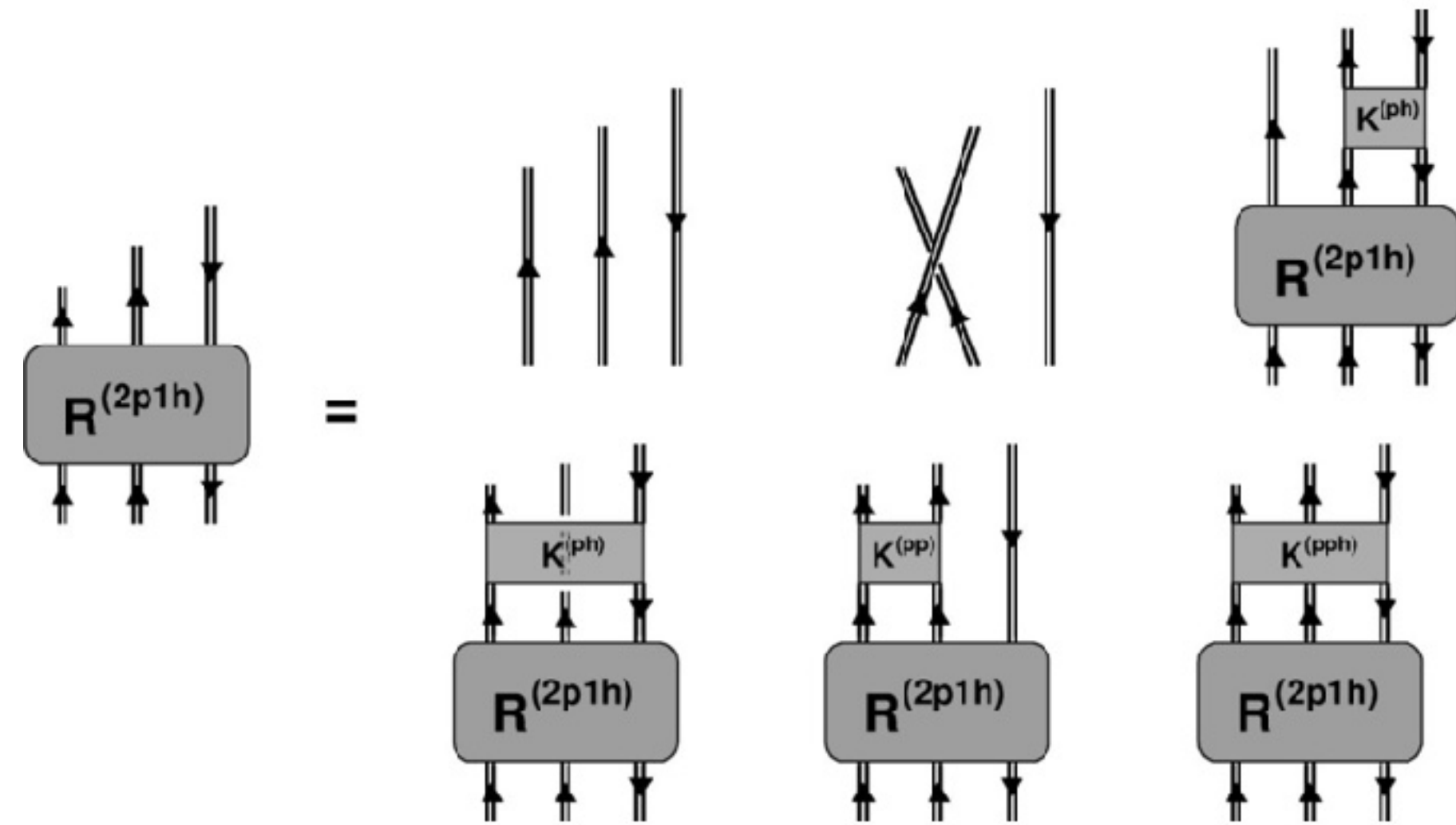
Irreducible
2p1h/2h1p
propagator



$$g_{\alpha,\mu\nu\lambda}^{1p-2p1h}(t - t') \equiv -\frac{i}{\hbar} \langle \Psi_0^N | T[c_\alpha(t) c_\mu^\dagger(t') c_\nu^\dagger(t') c_\lambda(t')] | \Psi_0^N \rangle$$

Faddeev RPA method

- The full 2p1h/2h1p polarization propagator also satisfies a Bethe-Salpeter-like equation:



$$R_{\alpha\beta\gamma,\mu\nu\lambda}(\omega_1, \omega_2, \omega_3) = [g_{\alpha\mu}(\omega_1)g_{\beta\nu}(\omega_2) - g_{\beta\mu}(\omega_2)g_{\alpha\nu}(\omega_1)]g_{\lambda\gamma}(-\omega_3) \\ + \left(g_{\beta\beta_1}(\omega_2)g_{\gamma_1\gamma}(-\omega_3)V_{\beta_1\sigma,\gamma_1\rho} \int \frac{ds}{2\pi i} R_{\alpha\rho\sigma,\mu\nu\lambda}(\omega_1, s, \omega_2 + \omega_3 - s) \right. \\ + g_{\alpha\alpha_1}(\omega_1)g_{\gamma_1\gamma}(-\omega_3)V_{\alpha_1\sigma,\gamma_1\rho} \int \frac{ds}{2\pi i} R_{\rho\beta\sigma,\mu\nu\lambda}(s, \omega_2, \omega_1 + \omega_3 - s) \\ \left. + \frac{1}{2}g_{\alpha\alpha_1}(\omega_1)g_{\beta\beta_1}(\omega_2)V_{\alpha_1\beta_1,\rho\sigma} \int \frac{ds}{-2\pi i} R_{\rho\sigma\gamma,\mu\nu\lambda}(s, \omega_1 + \omega_2 - s, \omega_3) \right)$$

- However, this depends on 4-times (3 frequencies) and it is much more complicated than the ph Bethe-Salpeter.
- Strategy:** solve each “pp” and “ph” channel separately, by solving the (simpler) DRPA equations. Then couple to a third line and mix the corresponding amplitudes → **Faddeev equations**

Faddeev equations for the 2h1p motion

Strategy: solve each “pp” and “ph” channel separately, by solving the (simpler) DRPA equations.
Then couple to a third line and mix the corresponding amplitudes → Faddeev equations

$$R^{2h1p}(\omega) = \text{diagram} + R^1(\omega) + R^2(\omega) + R^3(\omega) \quad \text{Faddeev components}$$

The diagram shows three vertical lines with arrows pointing down, followed by a minus sign and a crossed-out diagram of three vertical lines with arrows pointing down.

Faddeev eqns.

$$\begin{pmatrix} R^1 \\ R^2 \\ R^3 \end{pmatrix} = \begin{pmatrix} \text{diagram} \\ \text{diagram} \\ \text{diagram} \end{pmatrix} + \begin{pmatrix} 0 & \text{diagram} & \text{diagram} \\ \text{diagram} & 0 & \text{diagram} \\ \text{diagram} & \text{diagram} & 0 \end{pmatrix} \begin{pmatrix} R^1 \\ R^2 \\ R^3 \end{pmatrix}$$

The diagrams in the matrix are labeled with Γ and π . A label "TDA/RPA phonons" with an arrow points to the Γ diagrams in the matrix.

Benchmarking FRPA on molecules:

Molecule		FTDA	FTDA(c)	FRPA	FRPA(c)	CCSD(T)	FCI	Expt.
H ₂	E_0	-1.170	-1.161	-1.170	-1.161	-1.164	-1.164	-1.175
	$r_{\text{H-H}}$	0.769	0.757	0.770	0.757	0.761		0.741
	I	16.16	16.03	16.16	16.03	16.12		16.08
HF	E_0	-100.175	-100.224	-100.173	-100.228	-100.228	-100.231	
	$r_{\text{H-F}}$	0.904	0.916	0.897	0.913	0.920		0.917
	I	15.70	15.70	15.56	15.54	15.42		16.12
HCl	E_0	-460.295	-460.256	-460.293	-460.255	-460.254		
	$r_{\text{H-Cl}}$	1.314	1.297	1.314	1.293	1.290		1.275
	I	12.44	12.24	12.44	12.24	12.26		
H ₂ O	E_0	-76.248	-76.240	-76.243	-76.236	-76.241		
	$r_{\text{H-O}}$	0.986	0.964	0.981	0.962	0.967		0.958
	$\Lambda_{\text{O-H-O}}$	101	102	100	102	102		104
	I	12.07	12.15	12.25	12.21	11.94		12.61
N ₂	E_0		-109.258		-109.272	-109.276		
	$r_{\text{N-N}}$		1.104		1.106	1.119		1.098
	I		15.37		14.80	15.05		15.58
CO	E_0	-113.096	-113.037	-113.100	-113.048	-113.055		
	$r_{\text{C-O}}$	1.140	1.130	1.133	1.123	1.145		1.128
	I	14.39	13.69	14.23	14.44	13.64		14.01
CO ₂	E_0		-188.139		-188.134	-188.148		
	$r_{\text{C-O}}$		1.162		1.162	1.175		1.162
	I		13.25		13.42	13.26		13.78
C ₂ H ₂	E_0		-77.102		-77.093	-77.111		
	$r_{\text{C-C}}$		1.298		1.298	1.232		1.203
	$r_{\text{C-H}}$		1.083		1.080	1.081		1.063
	I		11.26		11.14	11.08		11.49

HF	Level	HF	FTDA	FTDA(c)	ADC(3)	FRPA	FRPA(c)	Expt.
HF	1π	17.17	16.22	16.46	16.48	16.05	16.35	16.05
	3σ	20.98	20.14	20.33	20.36	20.03	20.24	20.0
N ₂	$3\sigma_g$	17.25	16.14	15.65	15.72	15.76	15.18	15.60
	$1\pi_u$	16.73	17.20	16.82	16.85	17.71	17.14	16.98
	$2\sigma_u$	21.25	19.35	18.99	19.06	18.29	17.90	18.78
H ₂ O	$1b_1$	13.86	12.80	12.83	12.86	12.62	12.67	12.62
	$3a_1$	15.93	15.06	15.11	15.15	14.91	14.98	14.74
	$1b_2$	19.56	19.15	19.19	19.21	19.06	19.13	18.51
	$\bar{\Delta}$ (eV)	1.26(1.14)	0.34(0.31)	0.27(0.28)	0.30(0.30)	0.25(0.23)	0.31(0.26)	
	Δ_{max} (eV)	2.47(2.27)	0.64(0.64)	0.68(0.68)	0.70(0.70)	0.73(0.73)	0.88(0.62)	

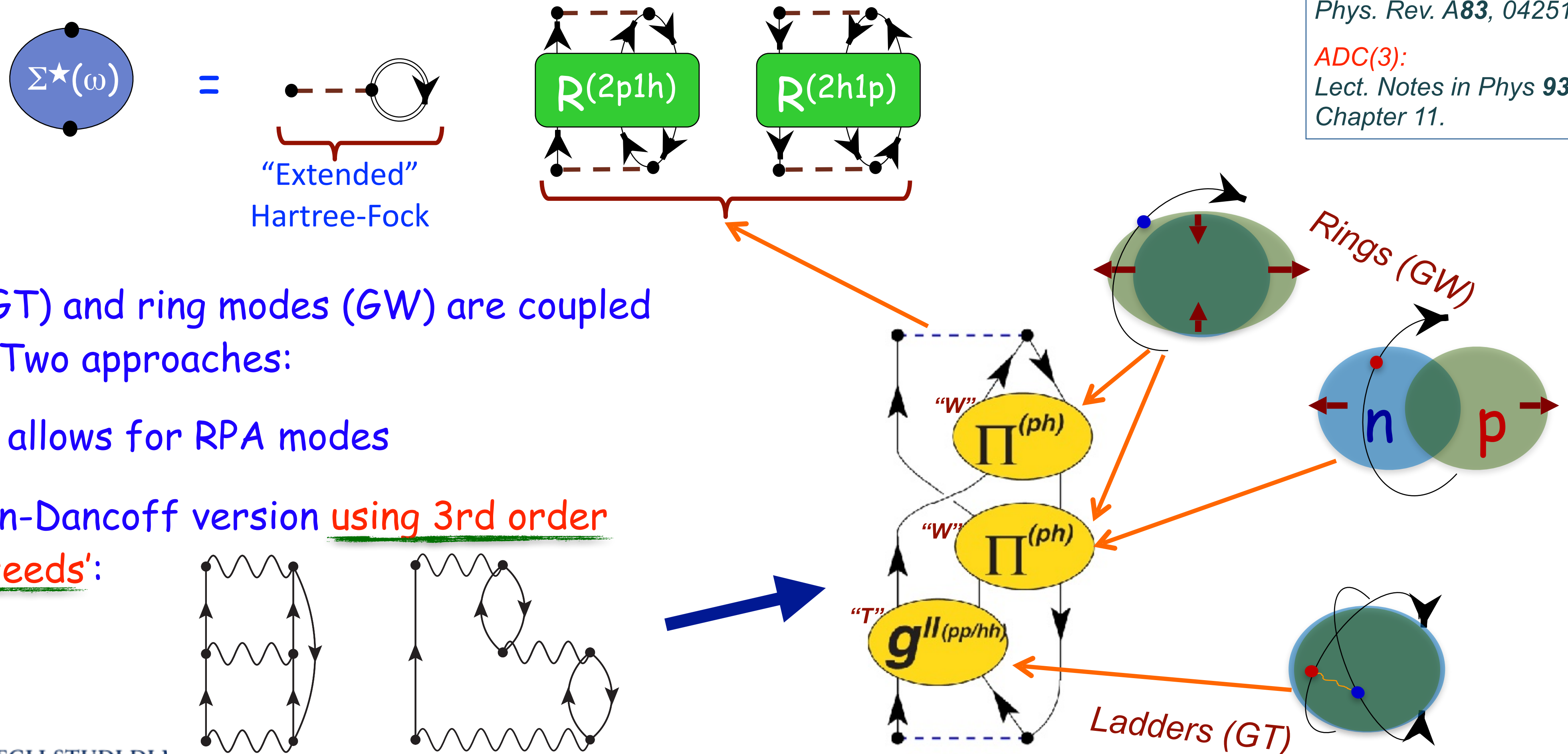
TABLE I. FRPA results for a set of small molecules in a cc-pVDZ basis set. The ground-state energy E_0 is given in hartree, the ionization energy I in electronvolt, equilibrium bond distances are in Angstrom, and the equilibrium angles in degrees. FRPA and FTDA refer to the calculations after the first iteration, while FRPA(c) and FTDA(c) refer to the calculations where consistency at the Hartree-Fock level was applied. The calculated data are compared to the coupled-cluster method at the level of CCSD(T) and to experimental data or exact calculations taken from Ref. [27]. The FCI energies were calculated at the FRPA(c) geometry.



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)

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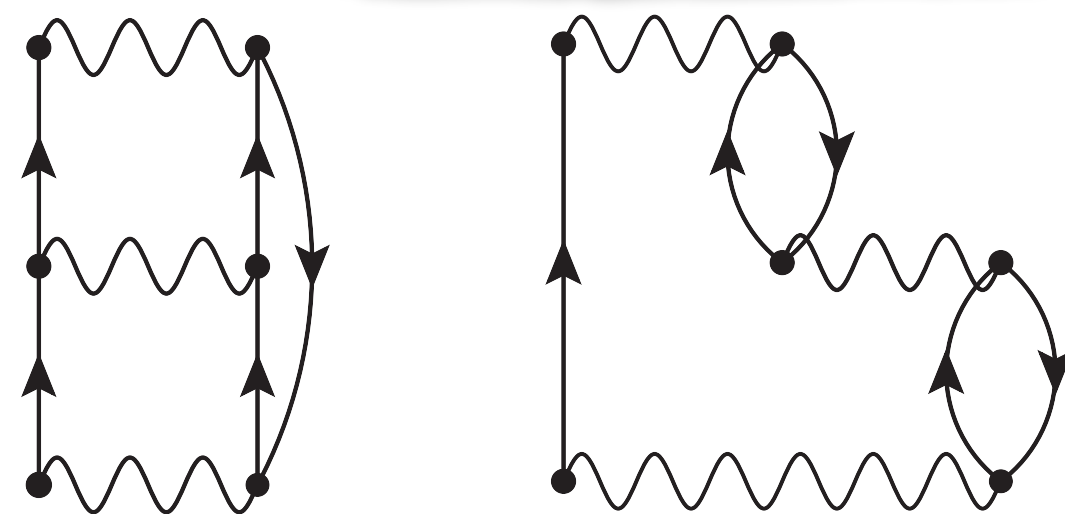
Phys. Rev. A **83**, 042517 (2011)

ADC(3):

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

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

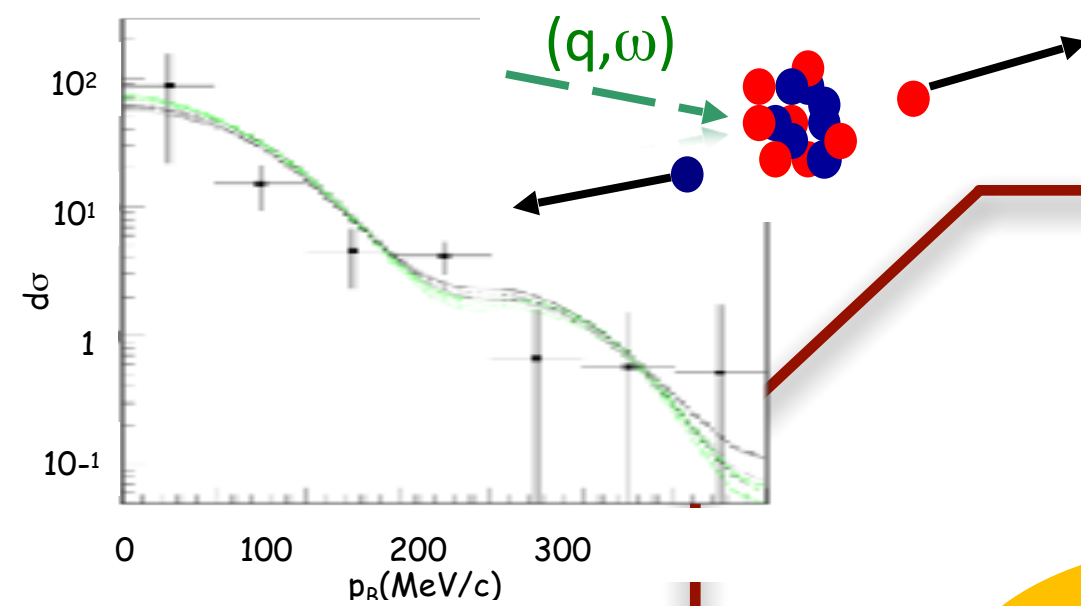
- Faddev-RPA allows for RPA modes
- ADC(3) Tamn-Dancoff version using 3rd order diagrams as 'seeds':



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

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

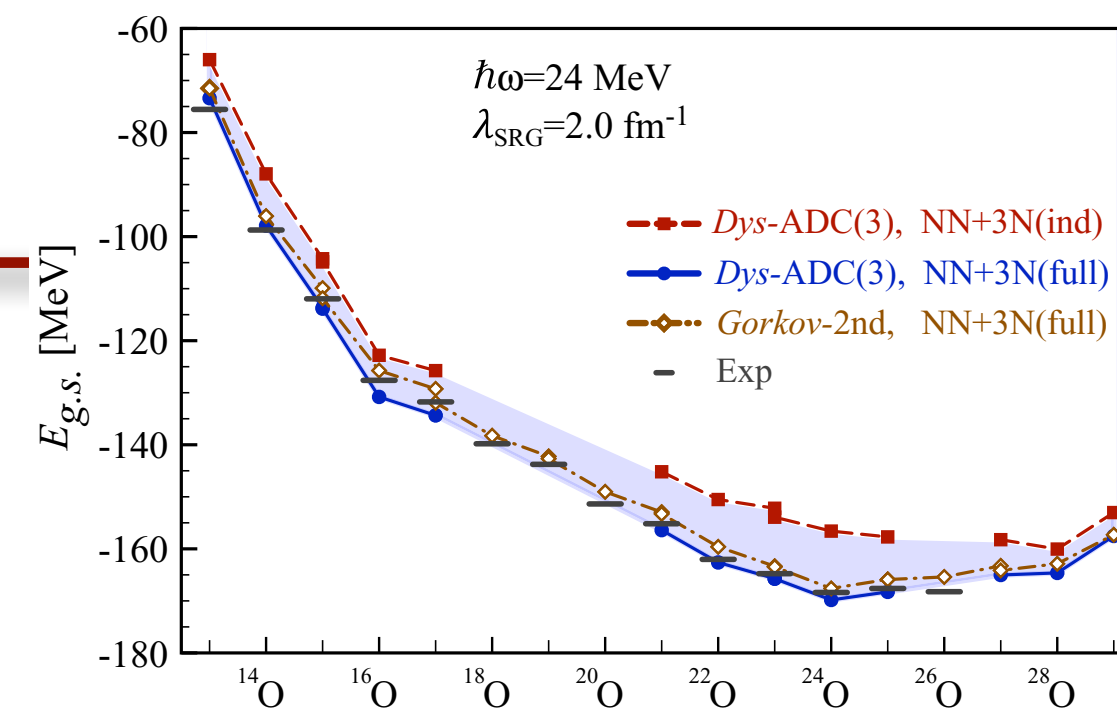
[Eur. Phys. J. A43, 137 (2010)]



Binding energies

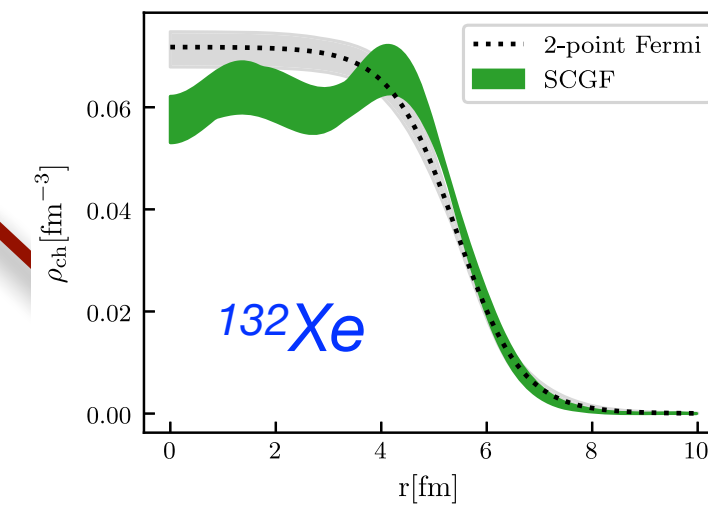
Oxygen drip line

[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

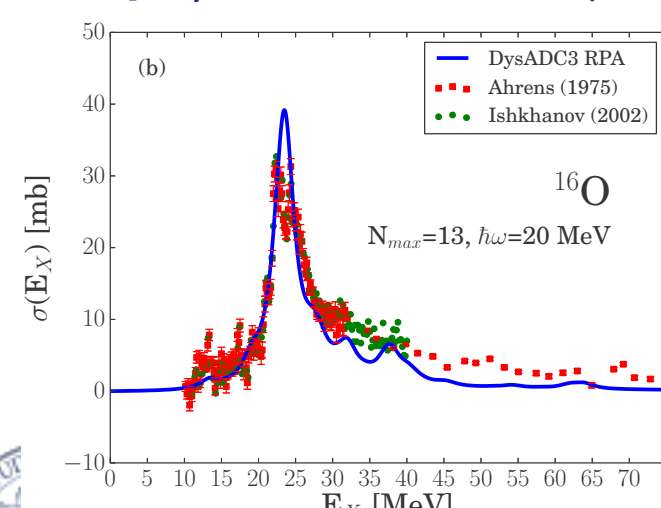
Ionisation energies and affinities for simple atoms and molecules

[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
H_2O	4σ	20.19	19.46	19.59	19.72
	$1b_1$	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)]

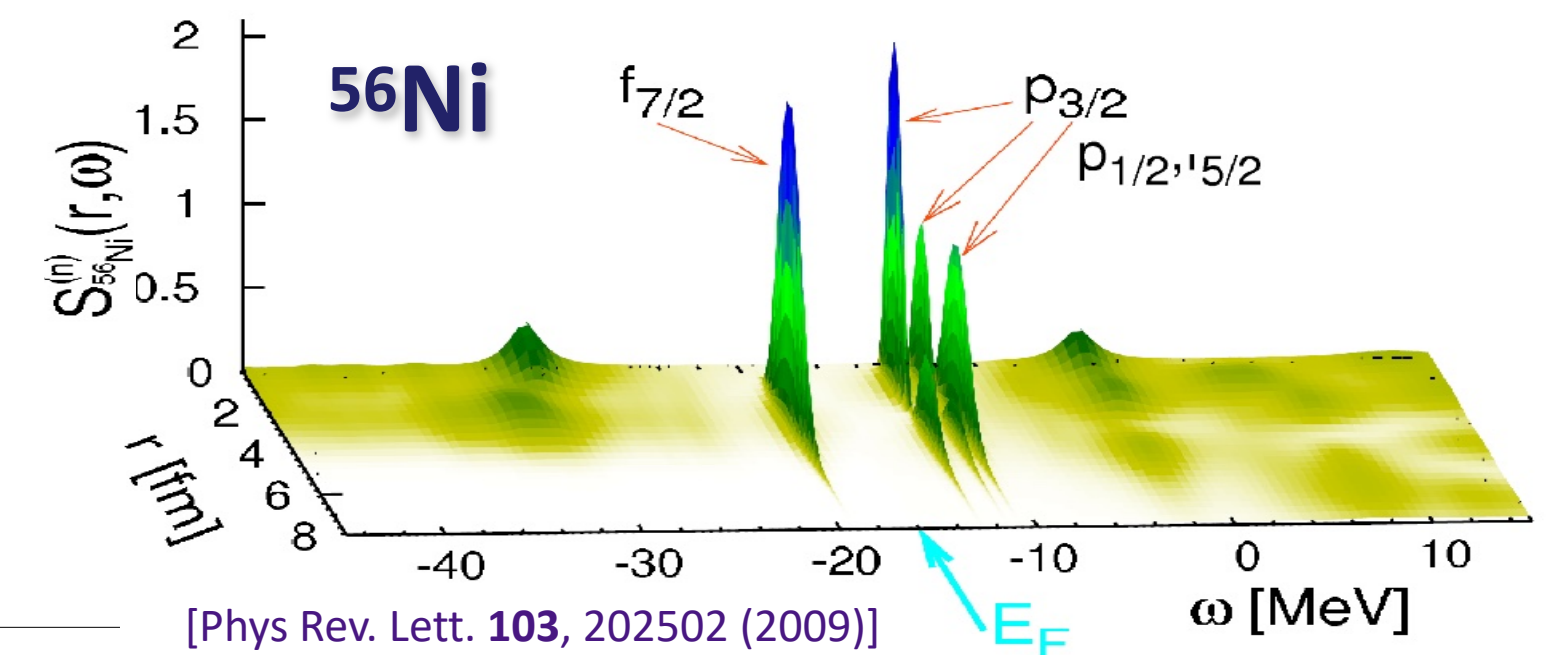
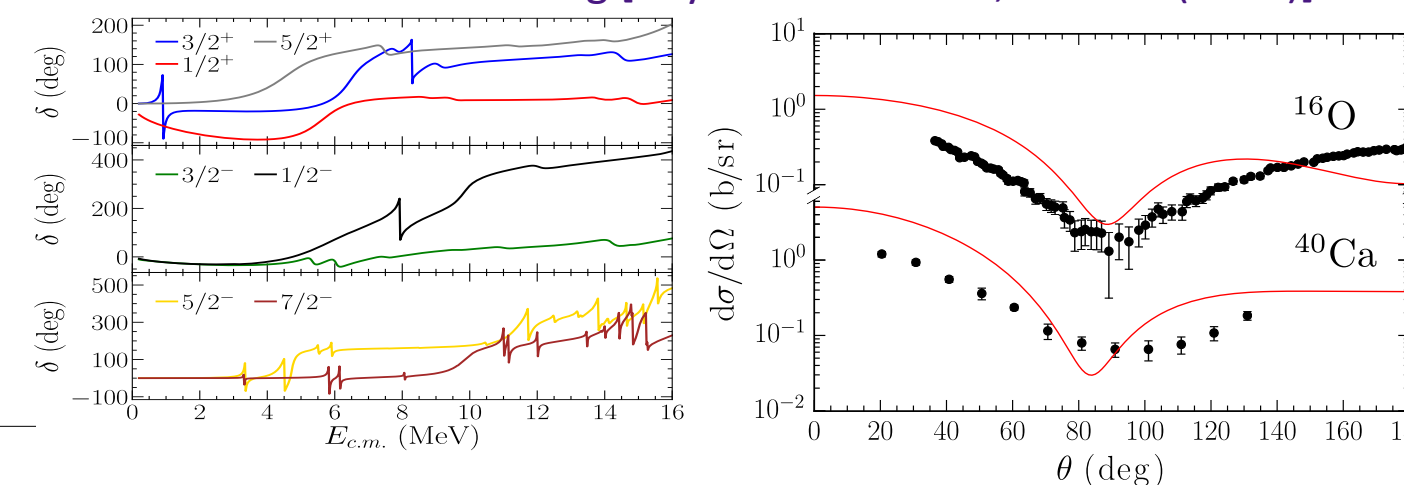


^{68}Ni :

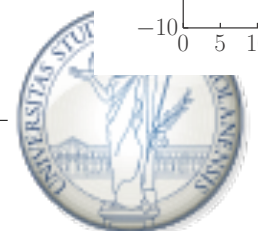
	SCGF	Exp
E_{PDR} (MeV)	10.68	9.55(17)
	10.92	
E_{GDR} (MeV)	18.1	17.1(2)
α_D (fm ³)	3.60	3.40(23)
		3.88(31)

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

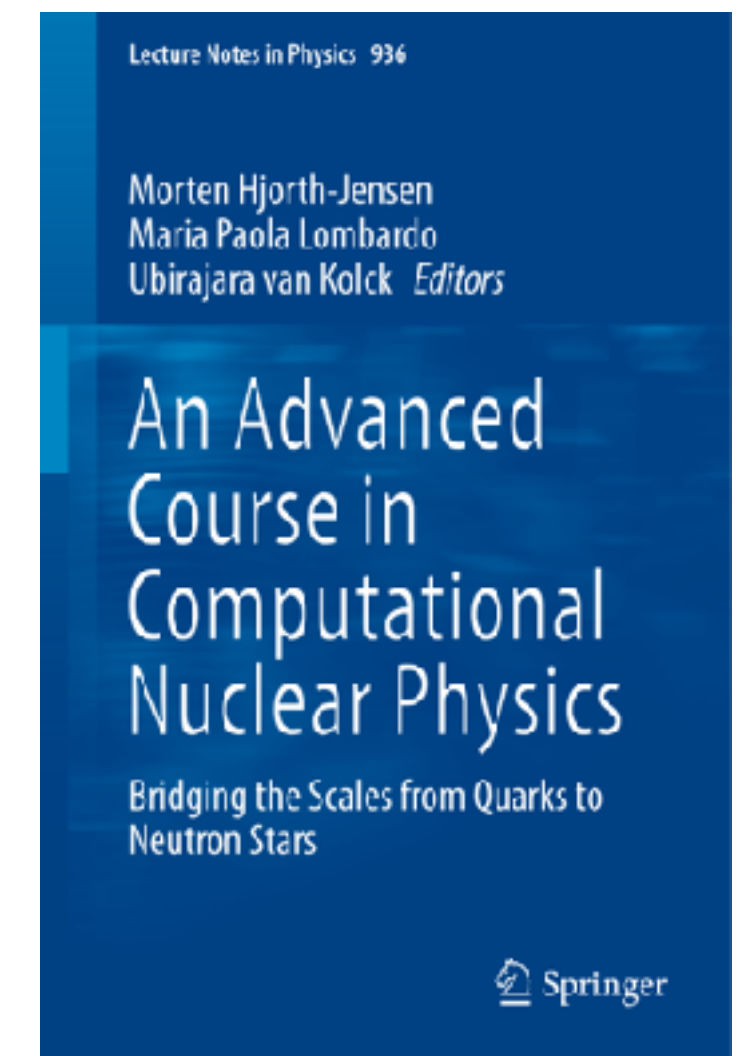
Gorkov at 3rd order (will become massively parallel...)

2022

applications →



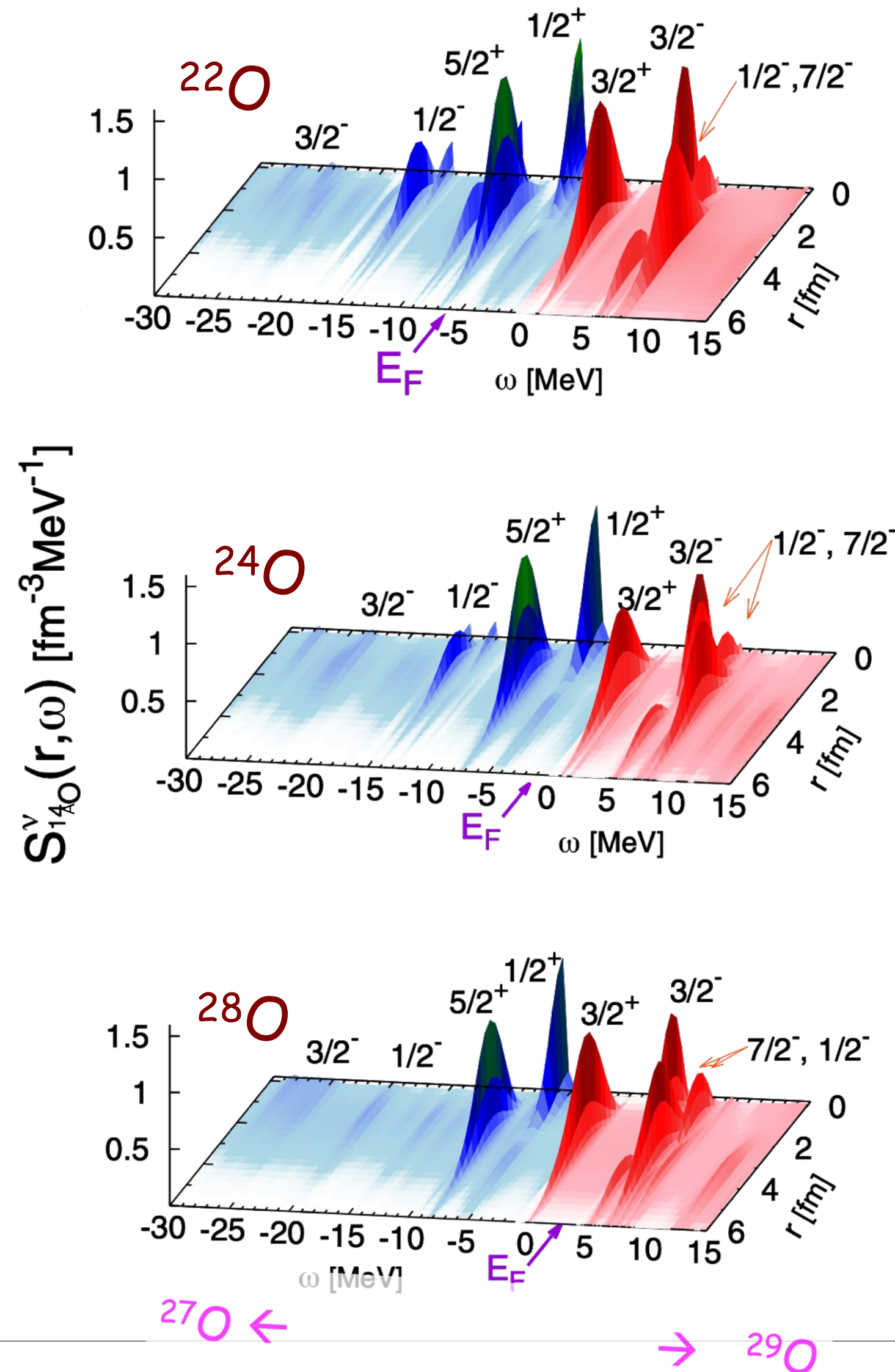
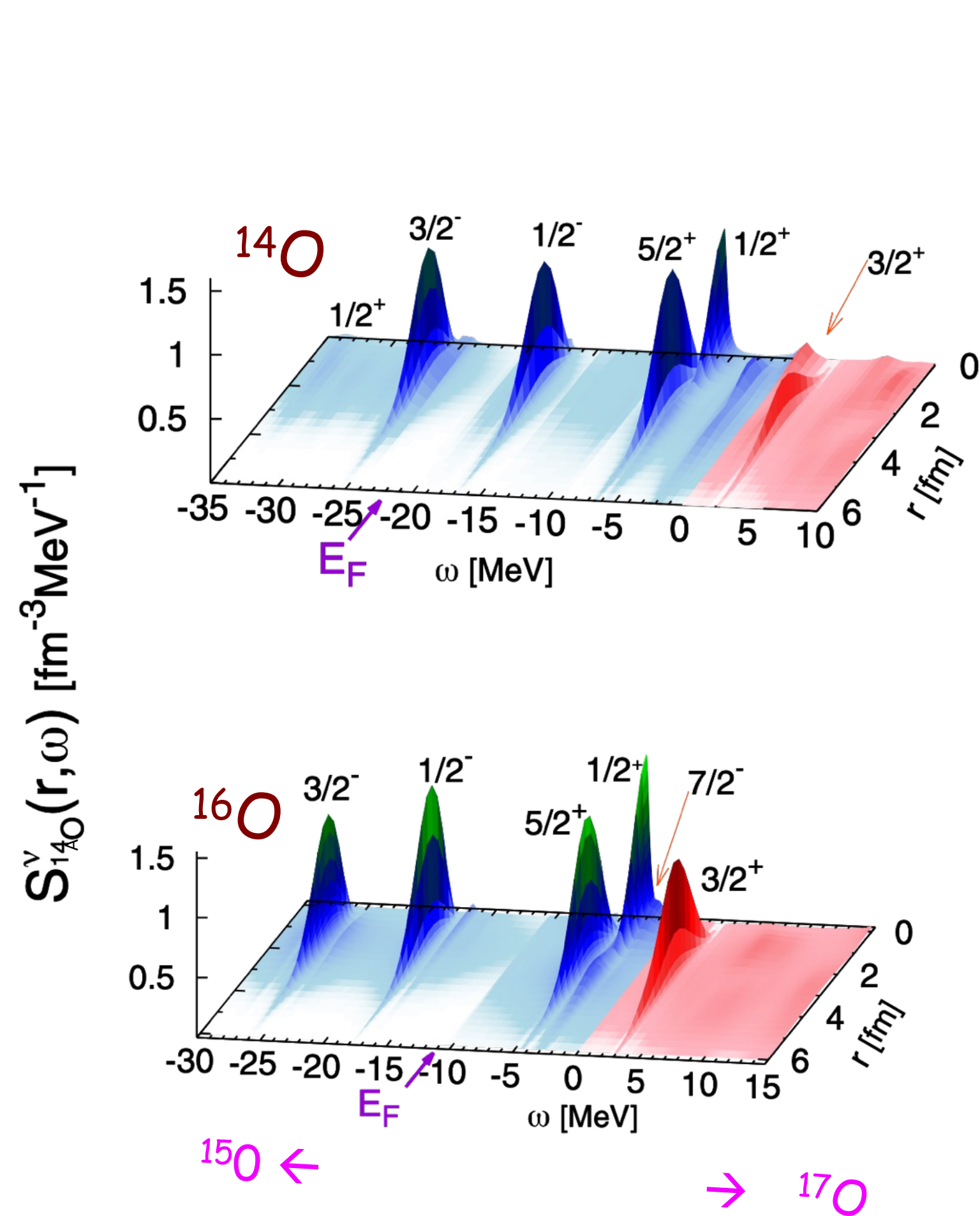
UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA



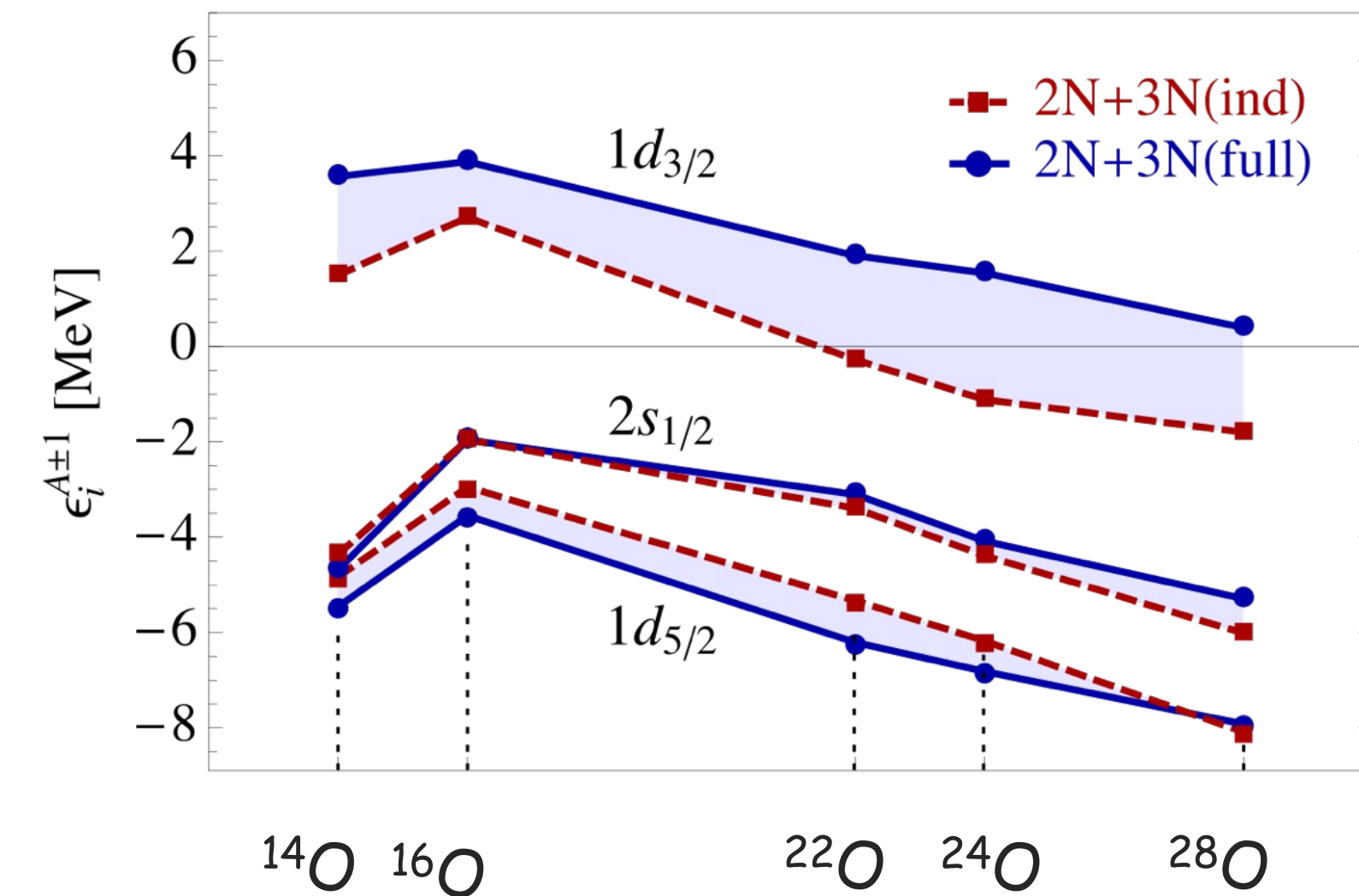
Self-consistent Green's function formalism and methods for Nuclear Physics

Neutron spectral function for oxygen isotopes

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

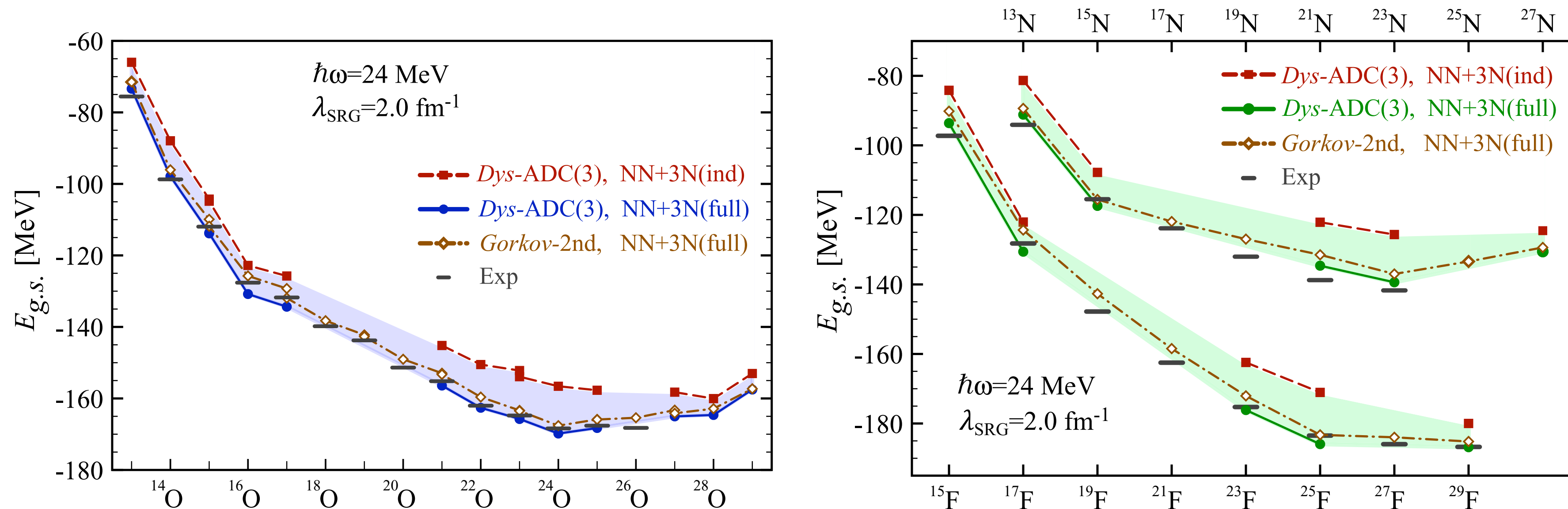


Neutron quasiparticle energies



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).]



Gorkov ansatz... for atomic nuclei

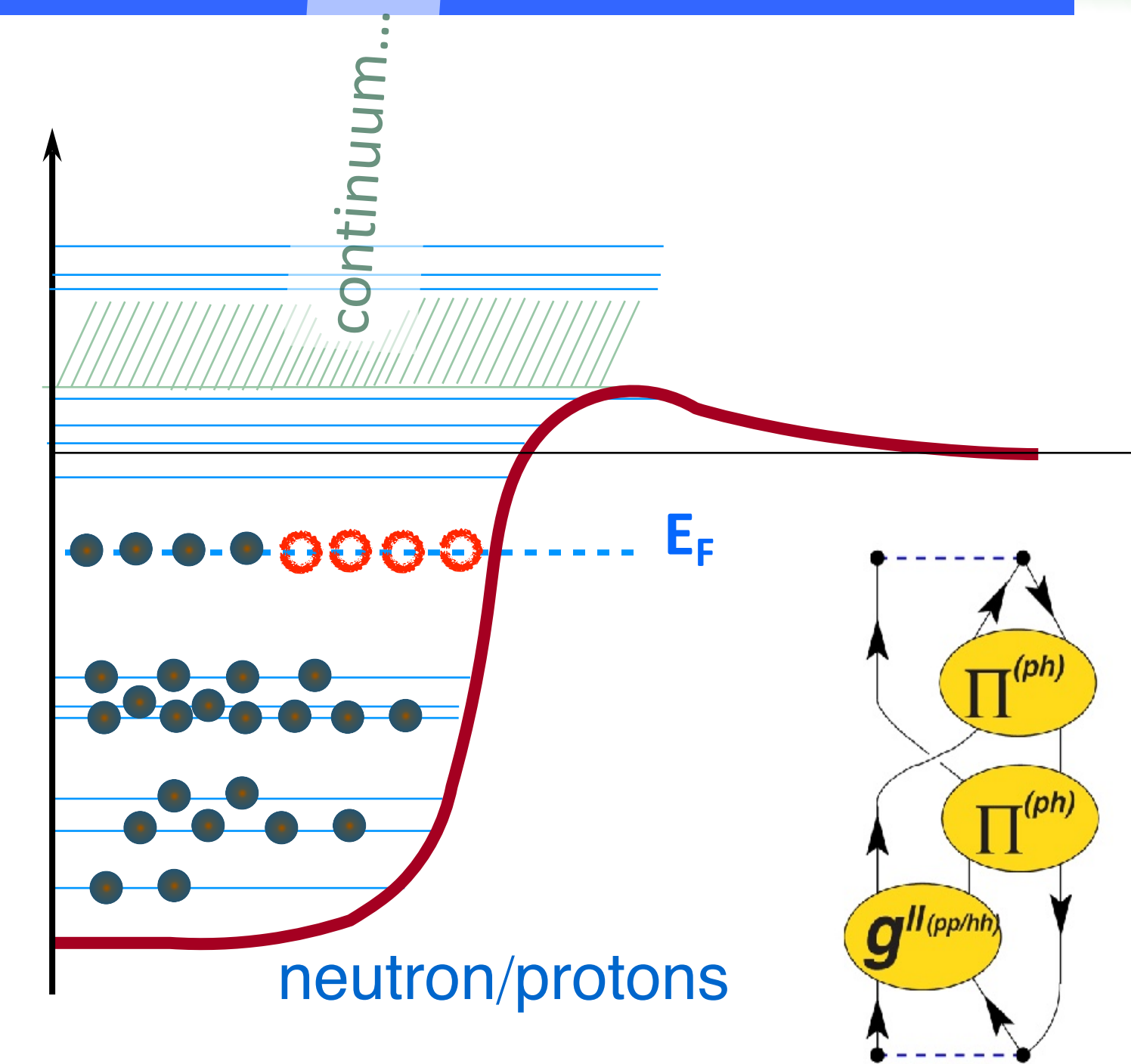
- In the presence of degeneracies (vanishing ph- gaps), enforce (two nucleon) pairing to mitigate instabilities:

- 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 $N = \langle \Psi_0 | N | \Psi_0 \rangle$

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



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

[Gorkov 1958]



unperturbed ones, i.e.,

$$G_{ab}^{11}(\omega) \equiv \begin{array}{c} a \\ \uparrow \omega \\ b \end{array}, \quad (B5a)$$

$$G_{ab}^{12}(\omega) \equiv \begin{array}{c} a \\ \uparrow \omega \\ \bar{b} \end{array}, \quad (B5b)$$

propagator one obtains

$$\Sigma_{ab}^{11(1)}(\omega) = -i \int_{C^+} \frac{d\omega'}{2\pi} \sum_{cd,k} \bar{V}_{acbd} \frac{\mathcal{U}_d^k \mathcal{U}_c^{k*}}{\omega' - \omega_k + i\eta} - i \int_{C^+} \frac{d\omega'}{2\pi} \sum_{cd,k} \bar{V}_{acbd} \frac{\mathcal{V}_d^{k*} \mathcal{V}_c^k}{\omega' + \omega_k - i\eta} = \sum_{cd,k} \bar{V}_{acbd} \mathcal{V}_d^{k*} \mathcal{V}_c^k,$$

where the residue theorem has been used, i.e., the first with $+i\eta$ in the denominator, contains no pole in the u plane and thus cancels out. As in the standard case the Hartree-Fock self-energy is energy independent.

Similarly, one computes the other normal self-energy

$$\Sigma_{ab}^{22(1)}(\omega) = \begin{array}{c} \bar{a} \\ \bullet \text{---} \bar{c} \text{---} \bar{b} \\ \downarrow \omega' \end{array},$$

Ab INITIO SELF-CONSISTENT GORKOV-GREEN'S ...

PHYSICAL REVIEW C **84**, 064317 (2011)

5. Block-diagonal structure of self-energies

a. First order

The goal of this subsection is to discuss how the block-diagonal form of the propagators and interaction matrix reflects in the various self-energy contributions, starting with the first-order normal self-energy $\Sigma^{11(1)}$. Substituting Eq. (C19) into Eq. (B7), and introducing the factor

$$f_{a\beta\gamma\delta}^{n_a n_b n_c n_d} \equiv \sqrt{1 + \delta_{a\beta} \delta_{n_a n_b}} \sqrt{1 + \delta_{\gamma\delta} \delta_{n_c n_d}},$$

one obtains

$$\begin{aligned} \Sigma_{ab}^{11(1)} &= \sum_{cd,k} \bar{V}_{acbd} \mathcal{V}_d^{k*} \mathcal{V}_c^k \\ &= \sum_{n_a n_b} \sum_{\gamma} \sum_{m_c} \sum_{JM} \sum_{J'M'} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} C_{j_a m_a j_b -m_b}^{JM} C_{j_c m_c j_d -m_d}^{J'M'} \bar{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \delta_{a\beta} \delta_{m_a m_b} \sum_{n_c n_d} \sum_{\gamma} \sum_J \sum_{J'} f_{a\gamma a\gamma}^{n_a n_b n_c n_d} \frac{2J+1}{2J_a+1} \bar{V}_{n_a n_b n_c n_d}^J \rho_{n_d[\gamma]}^{[J]} \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \Sigma_{n_a n_b}^{11[a](1)} \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \Lambda_{n_a n_b}^{[a]}. \end{aligned}$$

where the block-diagonal normal density matrix is introduced through $\rho_{ab} \equiv \delta_{a\beta} \delta_{m_a m_b} \rho_{n_a n_b}^{[a]}$, such that

$$\rho_{n_a n_b}^{[a]} = \sum_{n_d} \mathcal{V}_{n_b[a]}^{n_d} \mathcal{V}_{n_d[a]}^{n_a*},$$

and properties of Clebsch-Gordan coefficients has been used. The fact that the interaction conserves parity and charge, leading to $\delta_{a\beta} = \delta_{j_a j_b} \delta_{m_a m_b} \delta_{n_a n_b}$. Similarly, for $\Sigma^{22(1)}$,

$$\begin{aligned} \Sigma_{ab}^{22(1)} &= - \sum_{cd,k} \bar{V}_{bcad} \mathcal{V}_c^k \mathcal{V}_d^{k*} \\ &= -\delta_{a\beta} \delta_{m_a m_b} \sum_{n_c n_d} \sum_{\gamma} \sum_J \sum_{J'} f_{a\gamma a\gamma}^{n_a n_b n_c n_d} \frac{2J+1}{2J_a+1} \bar{V}_{n_a n_b n_c n_d}^J \rho_{n_d[\gamma]}^{[J]} \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \Sigma_{n_a n_b}^{22[a](1)} \\ &= -\delta_{a\beta} \delta_{m_a m_b} \Lambda_{n_a n_b}^{[a]} \\ &= -\delta_{a\beta} \delta_{m_a m_b} [\Lambda_{n_a n_b}^{[a]}]^*. \end{aligned}$$

Let us consider the anomalous contributions to the first-order self-energy. Substituting Eqs. (C27b) and (C19) into Eq. (B7), one derives

$$\begin{aligned} \Sigma_{ab}^{12(1)} &= \frac{1}{2} \sum_{cd,k} \bar{V}_{abcd} \mathcal{V}_c^{k*} \mathcal{U}_d^k \\ &= -\frac{1}{2} \sum_{n_a n_b} \sum_{\gamma} \sum_{m_c} \sum_{JM} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \eta_b \eta_c C_{j_a m_a j_b -m_b}^{JM} C_{j_c m_c j_d -m_d}^{JM} \bar{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{U}_{n_c[\gamma]}^{m_b} \\ &= -\frac{1}{2} \sum_{n_a n_b} \sum_{\gamma} \sum_{m_c} \sum_J f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \eta_b \eta_c C_{j_a m_a j_b -m_b}^{J0} C_{j_c m_c j_d -m_d}^{J0} \bar{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{U}_{n_c[\gamma]}^{m_b} \\ &= -\frac{1}{2} \sum_{n_a n_b} \sum_{\gamma} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \eta_b \pi_c (-1)^{2j_b} C_{j_a m_a j_b -m_b}^{00} \sqrt{2j_c+1} \bar{V}_{n_a n_b n_c n_d}^J \rho_{n_d[\gamma]}^{[J]} \\ &= \delta_{a\beta} \delta_{m_a m_b} \frac{1}{2} \sum_{n_c n_d} \sum_{\gamma} f_{a\gamma a\gamma}^{n_a n_b n_c n_d} \pi_a \pi_c (-1)^{2j_b} \frac{\sqrt{2j_c+1}}{\sqrt{2j_a+1}} \bar{V}_{n_a n_b n_c n_d}^J \rho_{n_d[\gamma]}^{[J]} \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \Sigma_{n_a n_b}^{12[a](1)} \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \tilde{H}_{n_a n_b}^{[a]}, \end{aligned}$$

where the block-diagonal anomalous density matrix is introduced through $\tilde{\rho}_{ab} \equiv \delta_{a\beta} \delta_{m_a m_b} \tilde{\rho}_{n_a n_b}^{[a]}$, such that

$$\tilde{\rho}_{n_a n_b}^{[a]} = \sum_{n_d} \mathcal{U}_{n_b[a]}^{n_d} \mathcal{V}_{n_d[a]}^{n_a*}.$$

on with (Gorkov) SCGF

Ab INITIO SELF-CONSISTENT GORKOV-GREEN'S ...

PHYSICAL REVIEW C **84**, 064317 (2011)

V. SOMÀ, T. DUGUET, AND C. BARBIERI

It is interesting to note that the first-order anomaly with a $J = 0$ many-body state. The other anomaly

$$\begin{aligned} \Sigma_{ab}^{21(1)} &= \frac{1}{2} \sum_{cd,k} \bar{V}_{cdab} \mathcal{V}_c^{k*} \mathcal{V}_d^k \\ &= -\frac{1}{2} \sum_{n_a n_b} \sum_{\gamma} \sum_{m_c} \sum_{JM} \bar{V}_{acbd} \mathcal{V}_d^{k*} \mathcal{V}_c^k \\ &= \delta_{a\beta} \delta_{m_a m_b} \frac{1}{2} \sum_{n_c n_d} \sum_{\gamma} \bar{V}_{acbd} \mathcal{V}_d^{k*} \mathcal{V}_c^k \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \Sigma_{n_a n_b}^{21[a](1)} \\ &= \delta_{a\beta} \delta_{m_a m_b} \tilde{H}_{n_a n_b}^{[a]}. \end{aligned}$$

Block-diagonal forms of second-order self-energy angular momentum couplings of the three quasiparticle, $\mathcal{Q}$, $\mathcal{R}$, and $\mathcal{S}$. One proceeds first coupling particle give J_{tot} . The recoupled $\mathcal{M}$ term is computed as follows

$$\begin{aligned} \mathcal{M}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \sum_{m_1 m_2 m_3 M_c} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} \mathcal{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \sum_{m_1 m_2 m_3 M_c} \sum_{rst} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} C_{j_5 m_5 j_6 m_6}^{J_d M_d} \mathcal{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \sum_{m_1 m_2 m_3 M_c} \sum_{rst} \sum_{J_d M_d} \delta_{k_1, \rho} \delta_{m_1, m_r} \delta_{k_2, \sigma} \delta_{m_2, m_s} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} C_{j_5 m_5 j_6 m_6}^{J_d M_d} \mathcal{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \sum_{m_1 m_2 m_3 M_c} \sum_{rst} \sum_{J_d M_d} \eta_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} C_{j_1 m_1 j_2 m_2}^{J_c M_c} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \sum_{m_1 m_2 m_3 M_c} \sum_{rst} \sum_{J_d M_d} \eta_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \frac{\sqrt{2J_c+1}}{\sqrt{2J_a+1}} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= -\delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \sum_{\gamma} \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \sqrt{\frac{2J_c+1}{2J_a+1}} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &\equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{M}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \end{aligned}$$

where general properties of Clebsch-Gordan coefficients

$$\begin{aligned} \mathcal{N}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &\equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{N}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \end{aligned}$$

One can show that the same result is obtained by

$$\begin{aligned} \mathcal{N}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \sum_{m_1 m_2 m_3 M_c} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} \mathcal{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \sum_{m_1 m_2 m_3 M_c} \sum_{rst} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} C_{j_5 m_5 j_6 m_6}^{J_d M_d} \mathcal{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \sum_{m_1 m_2 m_3 M_c} \sum_{rst} \sum_{J_d M_d} \delta_{k_1, \rho} \delta_{m_1, m_r} \delta_{k_2, \sigma} \delta_{m_2, m_s} \delta_{k_3, \tau} \delta_{m_3, m_t} \eta_a \eta_t f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} C_{j_5 m_5 j_6 m_6}^{J_d M_d} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \mathcal{U}_{n_t[\tau]}^{m_s} \mathcal{U}_{n_r[\rho]}^{m_t} \end{aligned}$$

064317-28

(C33)

Ab INITIO SELF-CONSISTENT GORKOV-GREEN'S ...

PHYSICAL REVIEW C **84**, 064317 (2011)

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

$$\begin{aligned} &= \sum_{m_1 m_2 m_3 M_c} \sum_{n_c n_d} \sum_{\gamma} \eta_a \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} C_{j_5 m_5 j_6 m_6}^{J_d M_d} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \sum_{\gamma} \eta_a \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \frac{\sqrt{2J_c+1}}{\sqrt{2J_a+1}} (-1)^{J_c+J_3-J_2} C_{j_1 m_1 j_2 m_2}^{J_c M_c} C_{j_3 m_3 j_4 m_4}^{J_{tot} M_{tot}} C_{j_5 m_5 j_6 m_6}^{J_d M_d} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ &= -\delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \eta_a \mathcal{N}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \end{aligned}$$

which recovers relation (72a). The remaining quantities [see Eqs. (69) and (70)] are related to $\{k_1, k_2, k_3\}$ indices and can be obtained from Eqs. (C35) and (C36) by taking into account the dependence on J_{tot} and J_c as follows:

$$\begin{aligned} \mathcal{P}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \sum_{J_d} (-1)^{J_c+J_d+J_3+J_2} \sqrt{2J_c+1} \sqrt{2J_d+1} \begin{Bmatrix} j_{k_1} & j_{k_2} & J_c \\ j_{k_3} & J_{tot} & J_d \end{Bmatrix} \mathcal{M}_{a(J,J_{tot})}^{k_1 k_2 k_3} \\ &= -\delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \sum_{\gamma} \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \frac{\sqrt{2J_c+1}}{\sqrt{2J_a+1}} (2J_d+1) (-1)^{J_c+J_3+J_2} \\ &\quad \times \bar{V}_{n_a n_b n_c n_d}^J \mathcal{U}_{n_c[\gamma]}^{m_c} \mathcal{U}_{n_d[\gamma]}^{m_b} \mathcal{V}_{n_t[\tau]}^{m_s} \\ &\equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{P}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ \mathcal{Q}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \sum_{J_d} (-1)^{J_c+J_d+J_3+J_2} \sqrt{2J_c+1} \sqrt{2J_d+1} \begin{Bmatrix} j_{k_1} & j_{k_2} & J_c \\ j_{k_3} & J_{tot} & J_d \end{Bmatrix} \mathcal{N}_{a(J,J_{tot})}^{k_1 k_2 k_3} \\ &= \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \sum_{\gamma} \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \frac{\sqrt{2J_c+1}}{\sqrt{2J_a+1}} (2J_d+1) (-1)^{J_c+J_3+J_2} \\ &\quad \times \bar{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_c[\gamma]}^{m_b} \mathcal{V}_{n_d[\gamma]}^{m_c} \mathcal{U}_{n_t[\tau]}^{m_s} \\ &\equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{Q}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ \mathcal{R}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \sum_{J_d} (-1)^{2J_1+2J_d} \sqrt{2J_c+1} \sqrt{2J_d+1} \begin{Bmatrix} j_{k_1} & j_{k_2} & J_c \\ j_{k_3} & J_{tot} & J_d \end{Bmatrix} \mathcal{M}_{a(J,J_{tot})}^{k_1 k_2 k_3} \\ &= -\delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \sum_{\gamma} \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \frac{\sqrt{2J_c+1}}{\sqrt{2J_a+1}} (2J_d+1) (-1)^{J_c+J_3+J_2} \\ &\quad \times \bar{V}_{n_a n_b n_c n_d}^J \mathcal{U}_{n_c[\gamma]}^{m_c} \mathcal{U}_{n_d[\gamma]}^{m_b} \mathcal{V}_{n_t[\tau]}^{m_s} \\ &\equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{R}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \\ \mathcal{S}_{a(J,J_{tot})}^{k_1 k_2 k_3} &= \sum_{J_d} (-1)^{2J_1+2J_d} \sqrt{2J_c+1} \sqrt{2J_d+1} \begin{Bmatrix} j_{k_1} & j_{k_2} & J_c \\ j_{k_3} & J_{tot} & J_d \end{Bmatrix} \mathcal{N}_{a(J,J_{tot})}^{k_1 k_2 k_3} \\ &= \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \sum_{n_c n_d} \sum_{\gamma} \pi_{k_1} f_{a\beta\gamma\gamma}^{n_a n_b n_c n_d} \frac{\sqrt{2J_c+1}}{\sqrt{2J_a+1}} (2J_d+1) (-1)^{J_c+J_3+J_2} \\ &\quad \times \bar{V}_{n_a n_b n_c n_d}^J \mathcal{V}_{n_c[\gamma]}^{m_b} \mathcal{V}_{n_d[\gamma]}^{m_c} \mathcal{U}_{n_t[\tau]}^{m_s} \\ &\equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{S}_{n_a n_b n_c n_d}^{k_1 k_2 k_3} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b} \end{aligned}$$

These terms are finally put together to form the different contributions to second-order self-energy, as an example [see Eq. (75)]. By inserting Eqs. (C35) and (C36) and summing over all possible total and intermediate angular momenta, one has

$$\Sigma_{ab}^{11(2)} = \frac{1}{2} \sum_{J_{tot}, M_{tot}} \sum_{k_1 k_2 k_3} \left\{ \frac{\mathcal{M}_{a(J,J_{tot})}^{k_1 k_2 k_3} (\mathcal{M}_{b(J,J_{tot})}^{k_1 k_2 k_3})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{\mathcal{N}_{a(J,J_{tot})}^{k_1 k_2 k_3} (\mathcal{N}_{b(J,J_{tot})}^{k_1 k_2 k_3})^*}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}$$

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$$\begin{aligned} &= \delta_{a\beta} \delta_{m_a m_b} \frac{1}{2} \sum_J \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{c_1 c_2 c_3} \left\{ \frac{\mathcal{M}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} (\mathcal{M}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{\mathcal{N}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} (\mathcal{N}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^*}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\} \\ &\equiv \delta_{a\beta} \delta_{m_a m_b} \Sigma_{n_a n_b}^{11[a](2)}. \end{aligned} \quad (C42)$$

Proceeding similarly for the other terms and defining

$$\mathcal{C}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \equiv \frac{1}{\sqrt{6}} [\mathcal{M}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} - \mathcal{P}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} - \mathcal{R}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}}], \quad (C43a)$$

$$\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \equiv \frac{1}{\sqrt{6}} [\mathcal{M}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} + \mathcal{P}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} + \mathcal{R}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}}], \quad (C43b)$$

$$\Sigma_{n_a n_b}^{11[a](2)} = \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{J_c} \sum_{c_1 c_2 c_3} \left\{ \frac{\mathcal{C}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} (\mathcal{C}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{D}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}}}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44a)$$

$$\Sigma_{n_a n_b}^{12[a](2)} = \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{J_c} \sum_{c_1 c_2 c_3} \left\{ \frac{\mathcal{C}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} (\mathcal{D}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{C}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}}}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44b)$$

$$\Sigma_{n_a n_b}^{21[a](2)} = \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{J_c} \sum_{c_1 c_2 c_3} \left\{ \frac{\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} (\mathcal{C}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{C}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{D}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}}}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}, \quad (C44c)$$

$$\Sigma_{n_a n_b}^{22[a](2)} = \sum_{n_{k_1} n_{k_2} n_{k_3}} \sum_{J_c} \sum_{c_1 c_2 c_3} \left\{ \frac{\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} (\mathcal{D}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^*}{\omega - (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) + i\eta} + \frac{(\mathcal{C}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{C}_{n_b n_a n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}}}{\omega + (\omega_{k_1} + \omega_{k_2} + \omega_{k_3}) - i\eta} \right\}. \quad (C44d)$$

6. Block-diagonal structure of Gorkov's equations

In the previous subsections it has been proven that all single-particle Green's functions and all self-energy contributions entering Gorkov's equations display the same block-diagonal structure if the systems is in a $\bar{0}^+$ state. Defining

$$T_{ab} - \mu \delta_{ab} \equiv \delta_{a\beta} \delta_{m_a m_b} [T_{n_a n_b}^{[a]} - \mu^{[a]} \delta_{n_a n_b}], \quad (C45)$$

introducing block-diagonal forms for amplitudes $\mathcal{W}$ and $\mathcal{Z}$ through

$$\mathcal{W}_{k(J,J_{tot})}^{k_1 k_2 k_3} \equiv \delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \mathcal{W}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b}, \quad (C46a)$$

$$\mathcal{Z}_{k(J,J_{tot})}^{k_1 k_2 k_3} \equiv -\delta_{J_{tot}, J_a} \delta_{M_{tot}, M_a} \eta_k \mathcal{Z}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \mathcal{V}_{n_d[\gamma]}^{m_c*} \mathcal{V}_{n_c[\gamma]}^{m_b}, \quad (C46b)$$

with

$$(\omega_k - E_{k_1 k_2 k_3}) \mathcal{W}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \equiv \sum_{n_d} [(C_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{U}_{n_d[a]}^{n_{k_1}} + (\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{V}_{n_d[a]}^{n_{k_1}}], \quad (C47a)$$

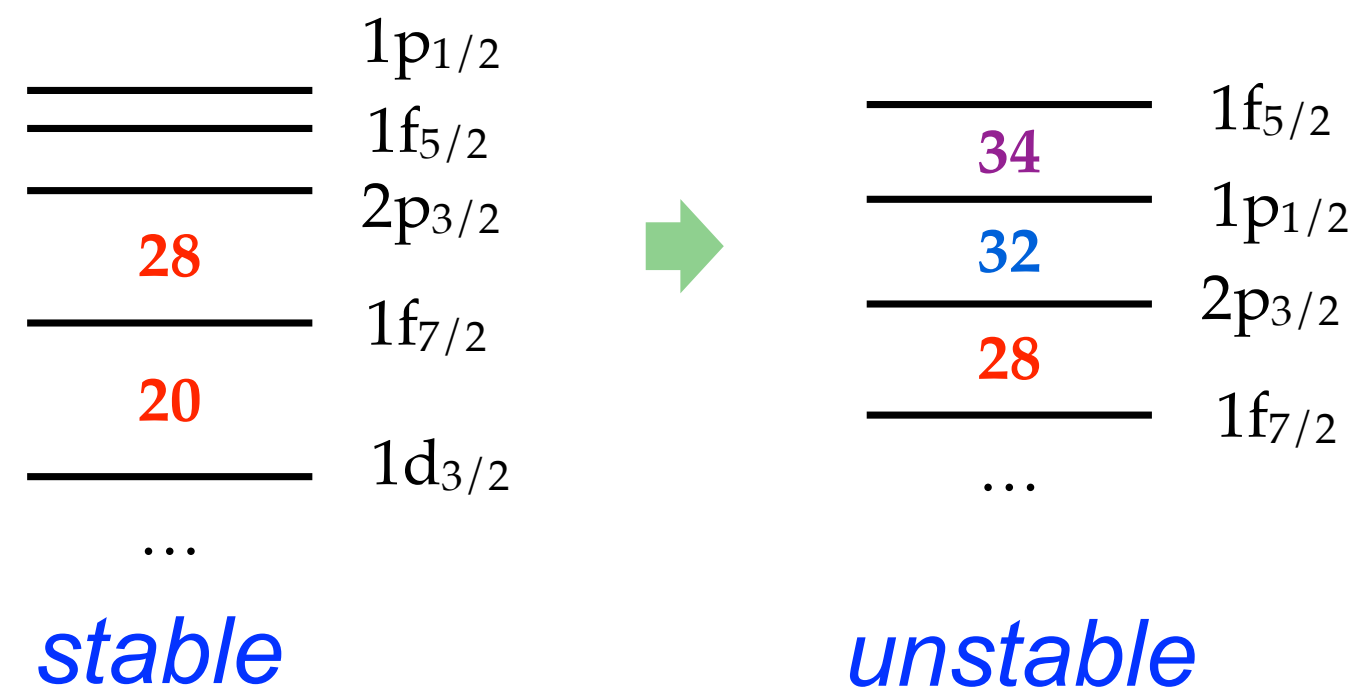
$$(\omega_k + E_{k_1 k_2 k_3}) \mathcal{Z}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \equiv \sum_{n_d} [\mathcal{D}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}} \mathcal{U}_{n_d[a]}^{n_{k_1}} + (\mathcal{C}_{n_a n_b n_c n_d}^{n_{k_1} n_{k_2} n_{k_3}})^* \mathcal{V}_{n_d[a]}^{n_{k_1}}], \quad (C47b)$$

and using Eqs. (C29), (C31), (C32), (C34), and (C44), one finally writes Eqs. (81) as

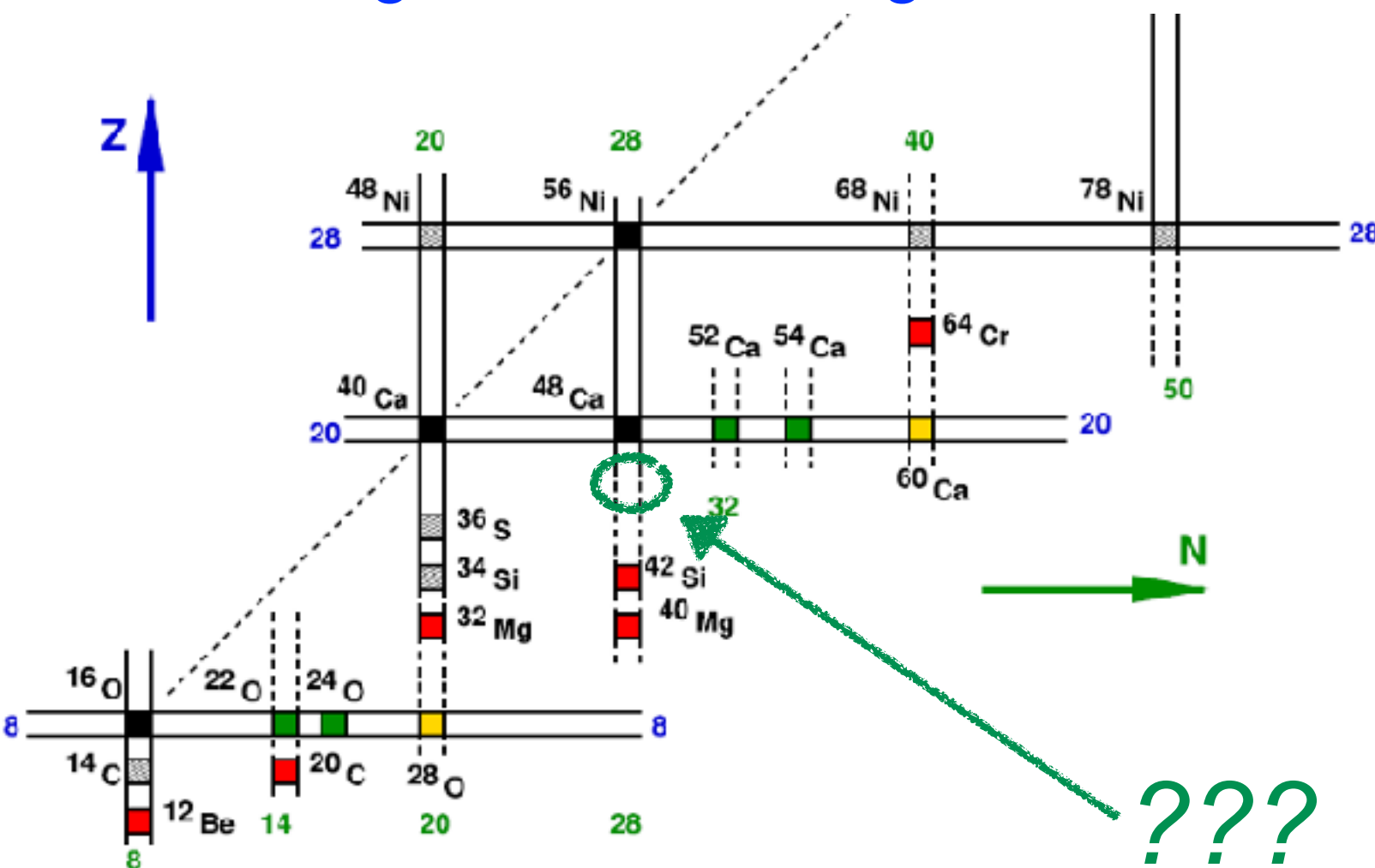
$$\begin{aligned} \omega_k \mathcal{U}_{n_a[a]}^{n_{k_1}} &= \sum_{n_b} [(T_{n_a n_b}^{[a]} - \mu^{[a]} \delta_{n_a n_b} + \Lambda_{n_a n_b}^{[a]}) \mathcal{U}_{n_b[a]}^{n_{k_1}} + \tilde{H}_{n_a n_b}^{[a]} \mathcal{V}_{n_b[a]}^{n_{k_1}}] \\ &\quad + \sum_{n_{k_2} n_{k_3}} \sum_{c_1 c_2 c_3} [\mathcal{C}_{n_a n_b n_c$$

Magic numbers

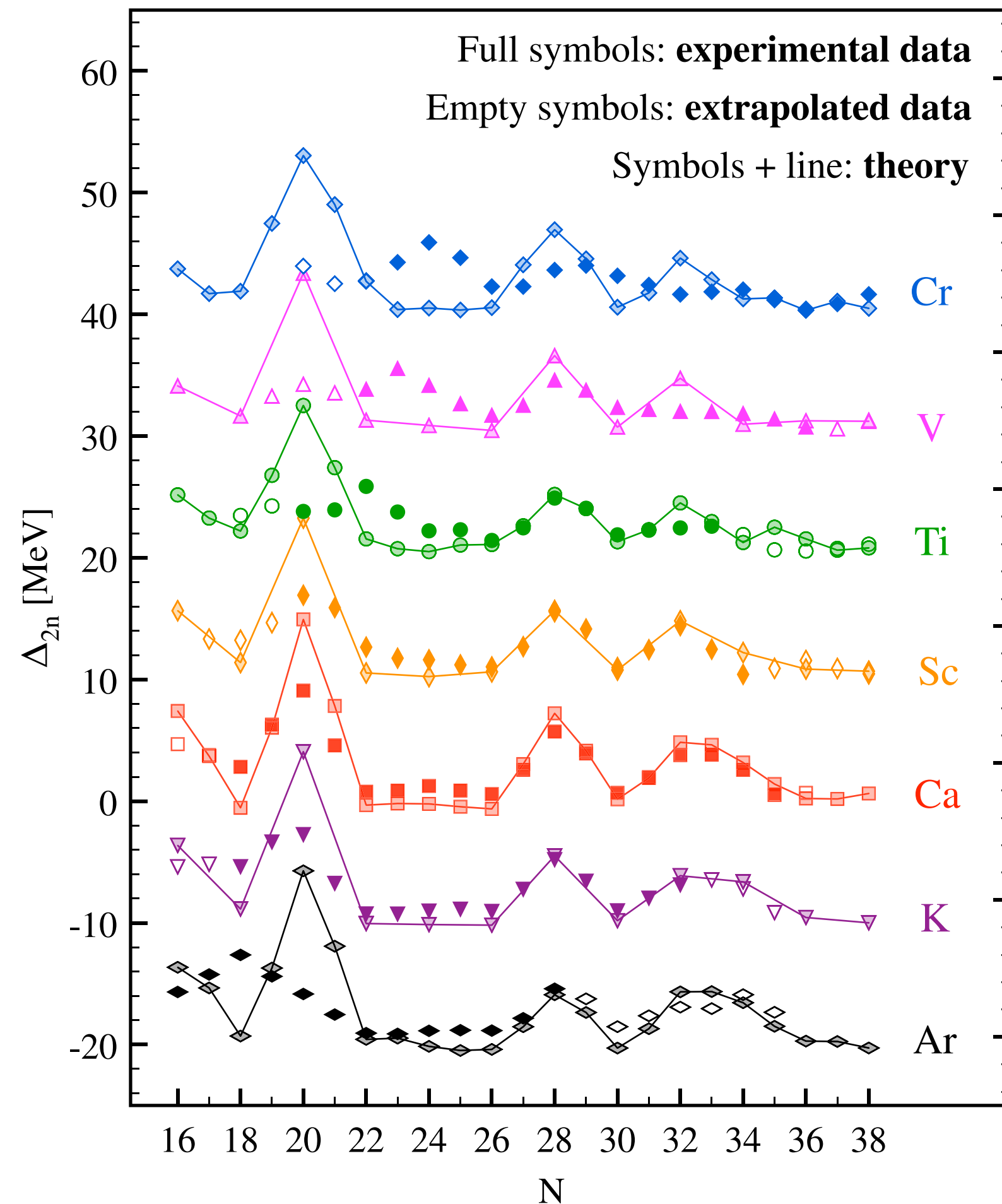
- Magic numbers: extra-stable combinations of N & Z



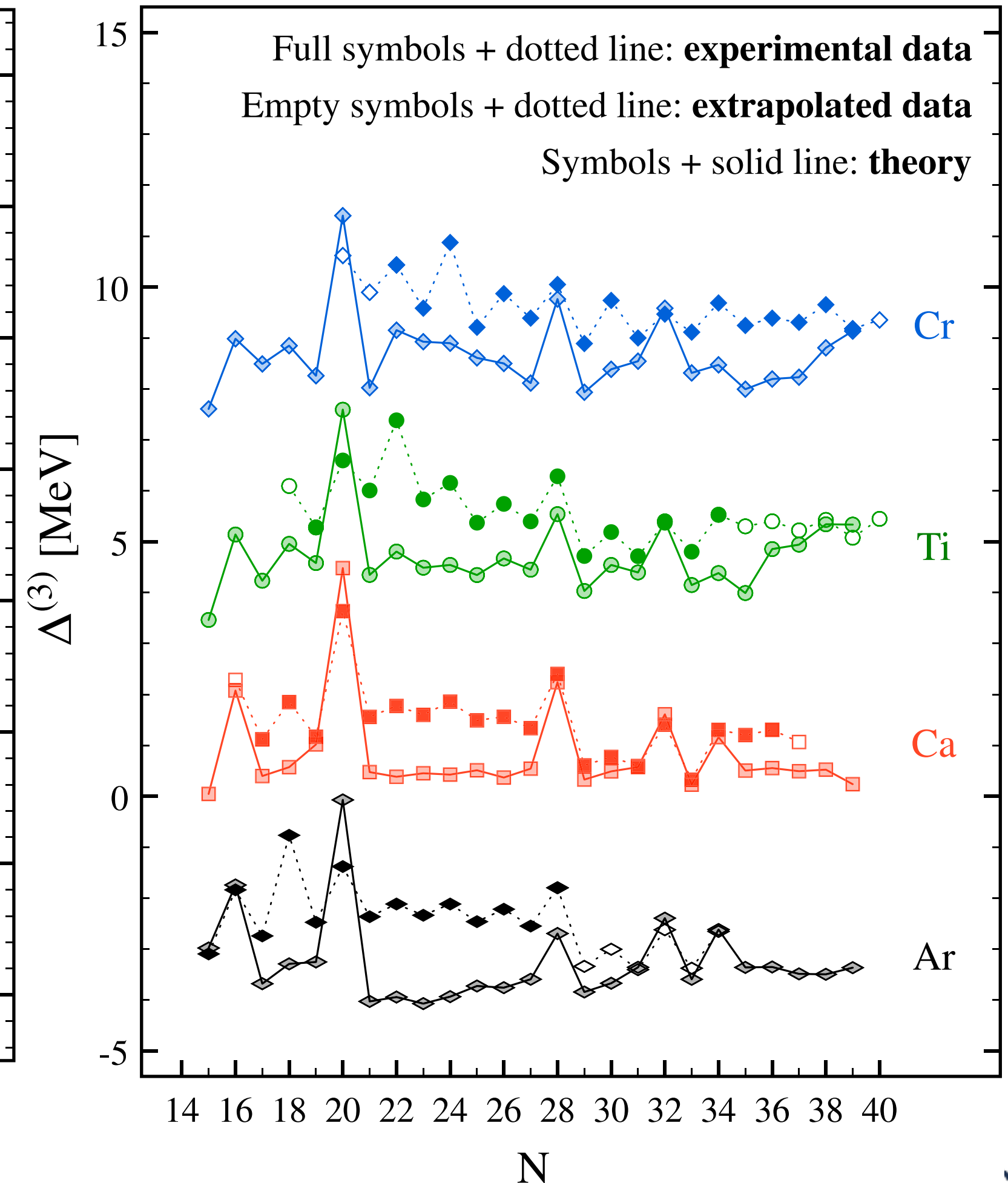
Known magic and semimagic nuclei:



$$\Delta_{2n}(N, Z) \equiv S_{2n}(N, Z) - S_{2n}(N + 2, Z)$$



$$\Delta^{(3)}(N, Z) \equiv \frac{(-1)^N}{2} [E(N - 1, Z) - 2E(N, Z) + E(N + 1, Z)]$$



[Somà, CB et al. Eur. Phys. J. A **57**, 135 (2021)]

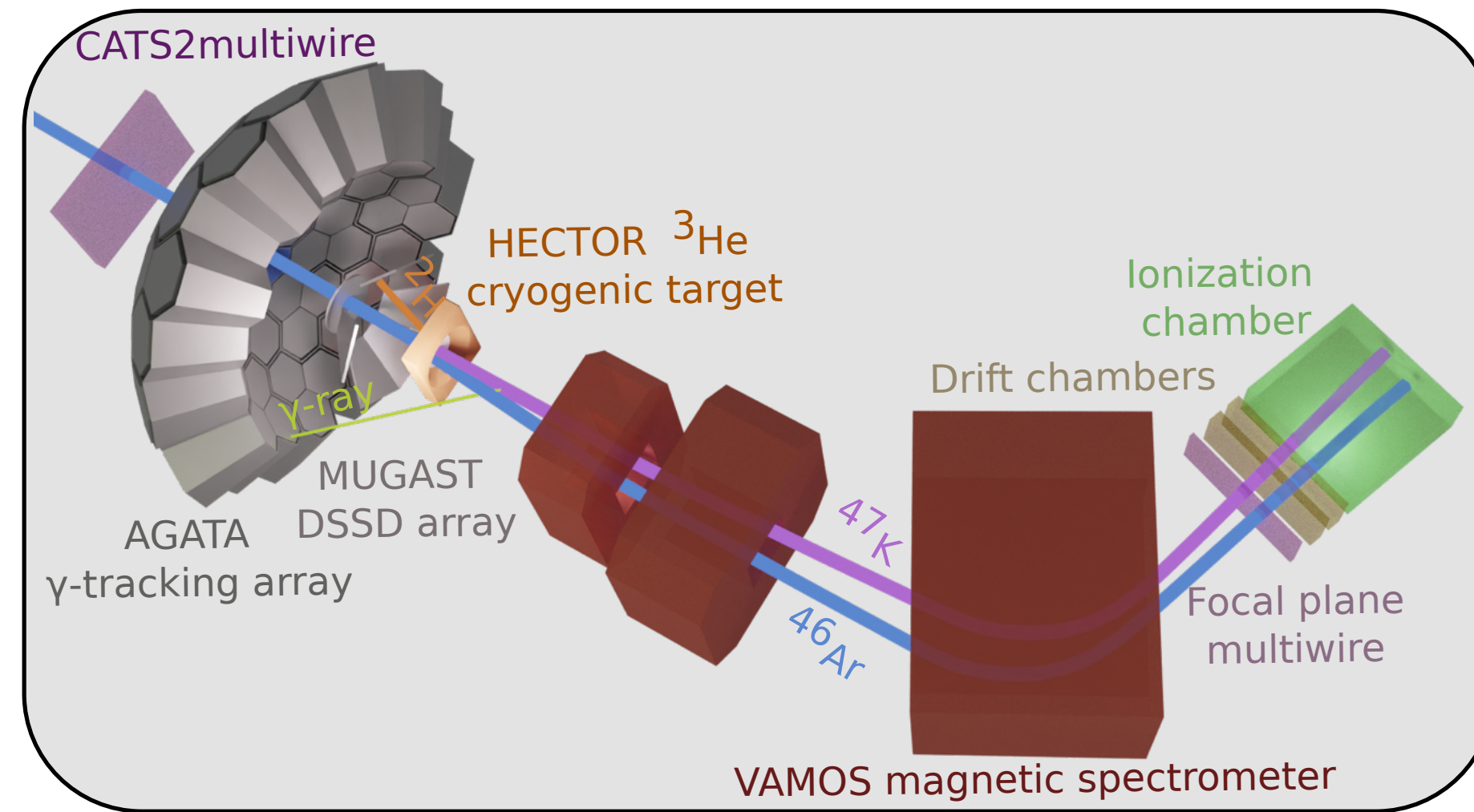
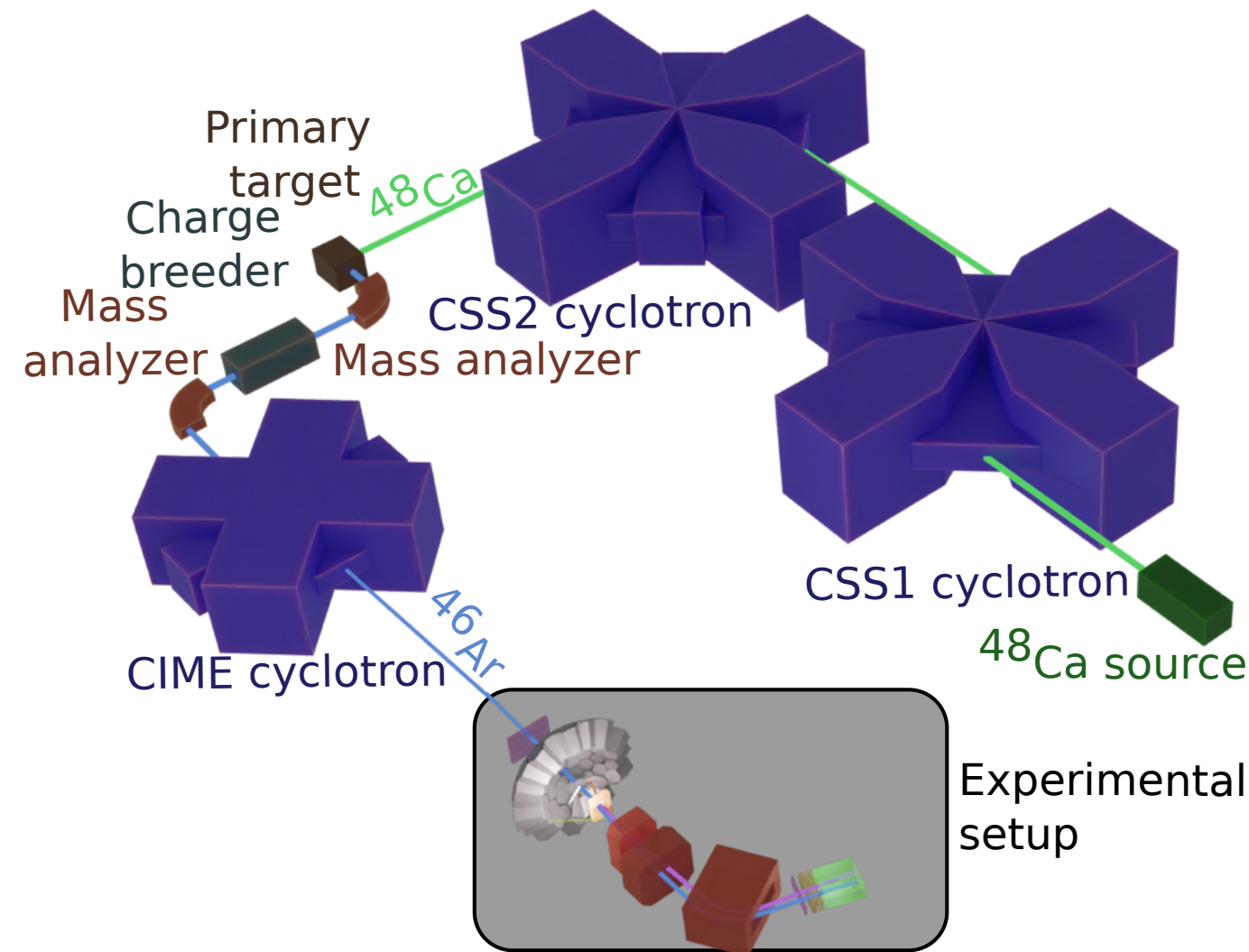
[Nowacki, Obertelli, Poves, PPNP 120, 103866 (2021)]



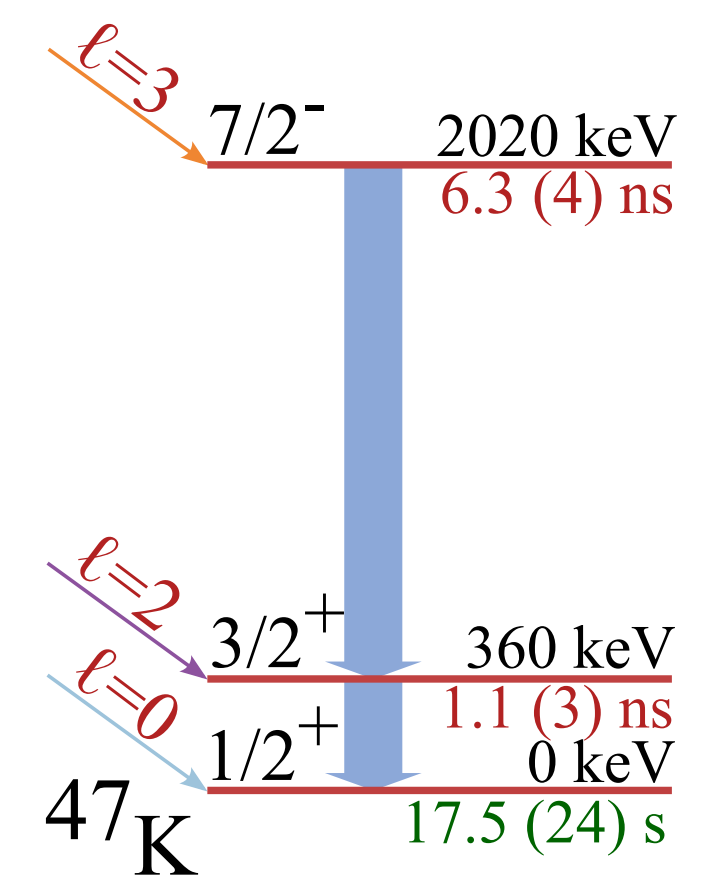
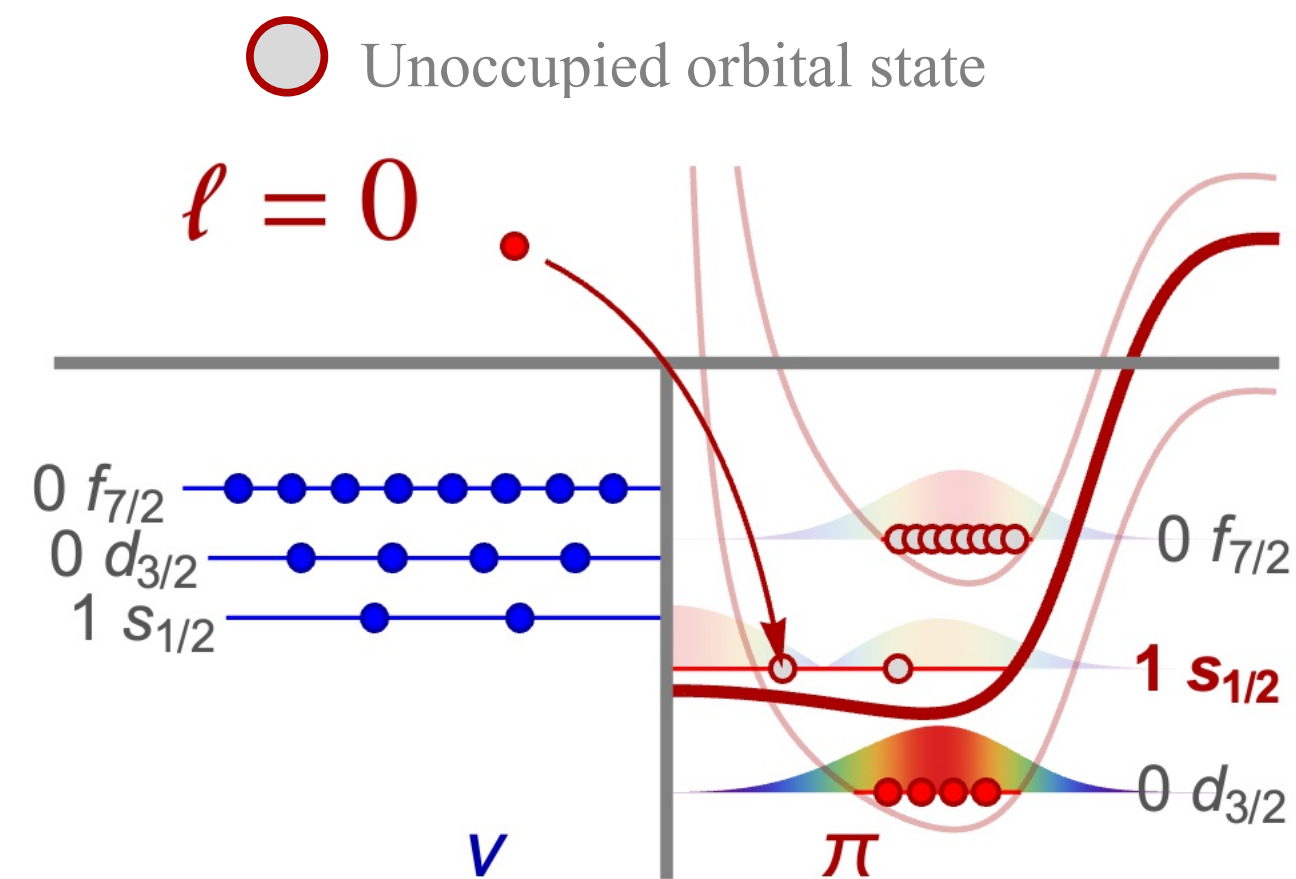
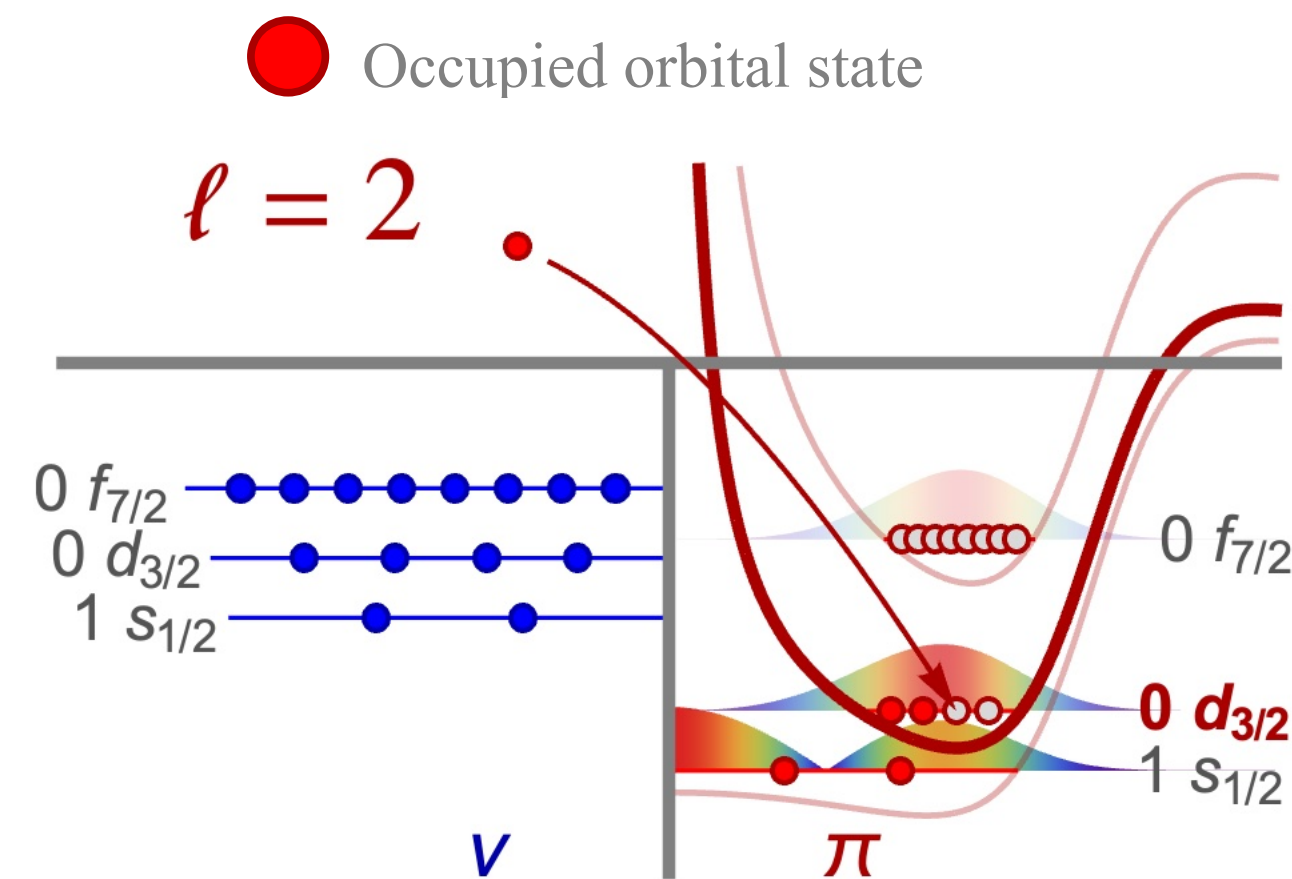
DIPARTIMENTO DI FISICA



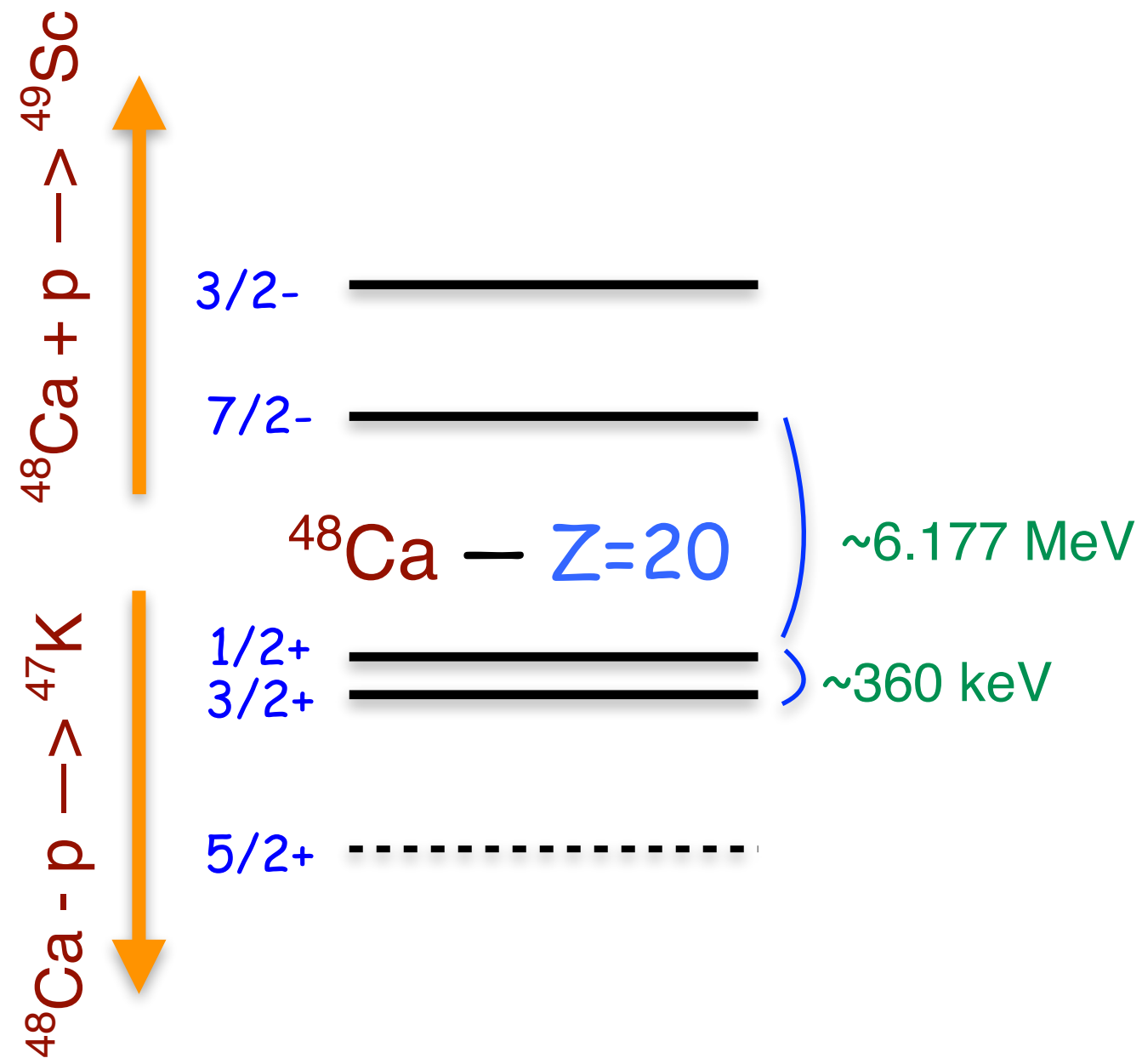
$^{46}\text{Ar}(^3\text{He},d)^{47}\text{K}$ at GANIL



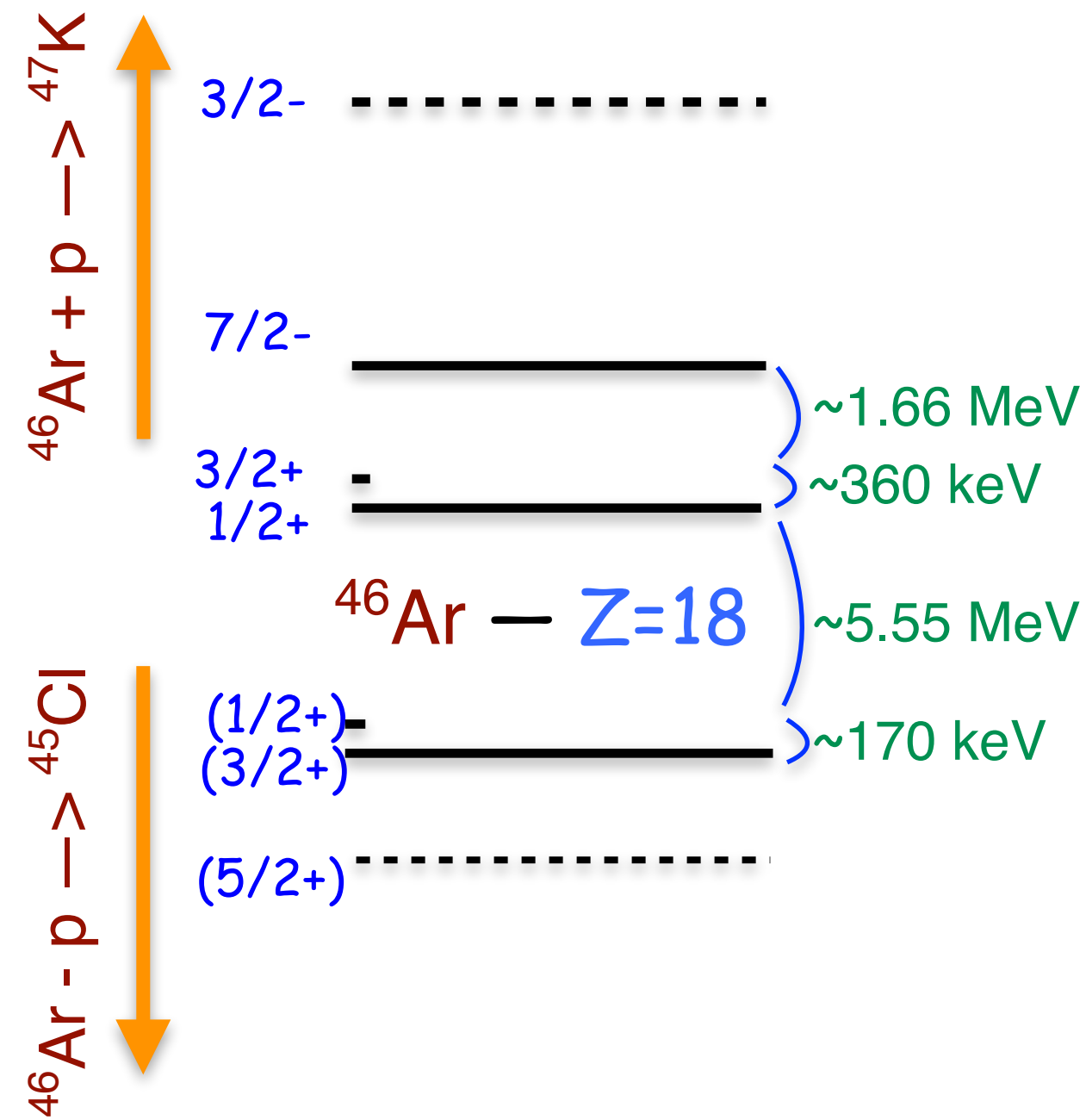
d3/2 - s1/2 inversion
revisited from adding
protons to ^{46}Ar



$^{46}\text{Ar}(^3\text{He},d)^{47}\text{K}$ at GANIL : shell closure & charge bubble in ^{46}Ar



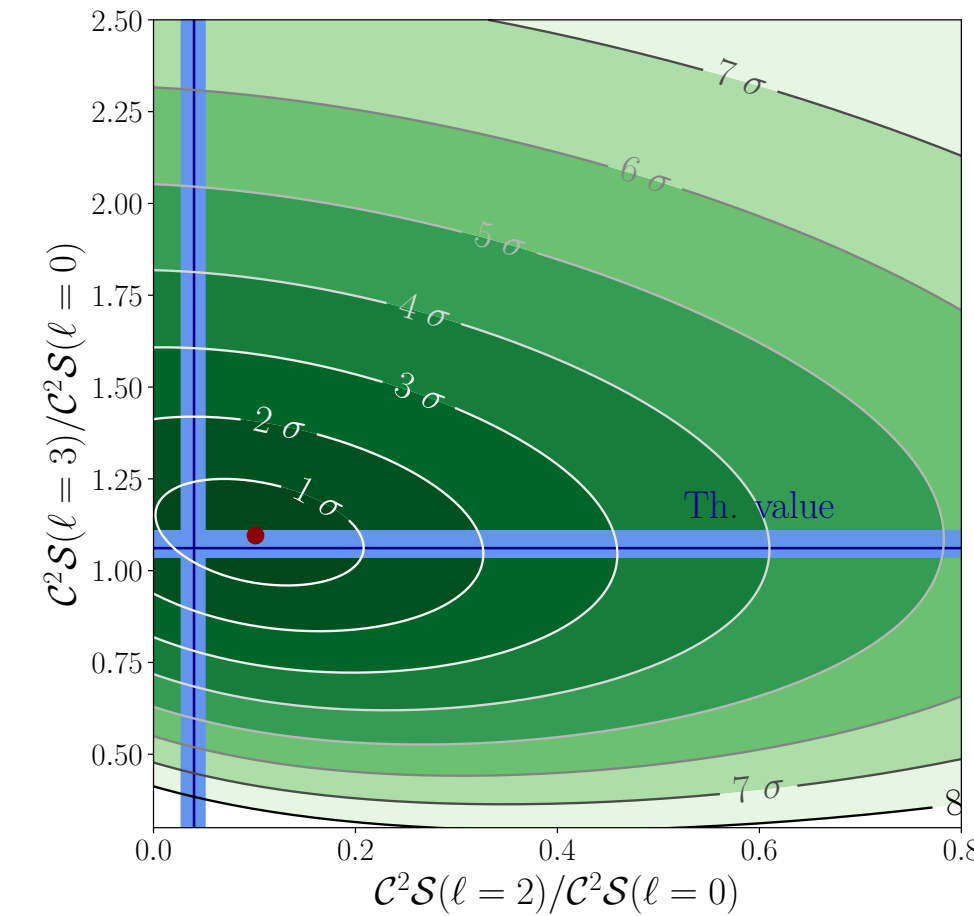
$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 360 \text{ keV}$$



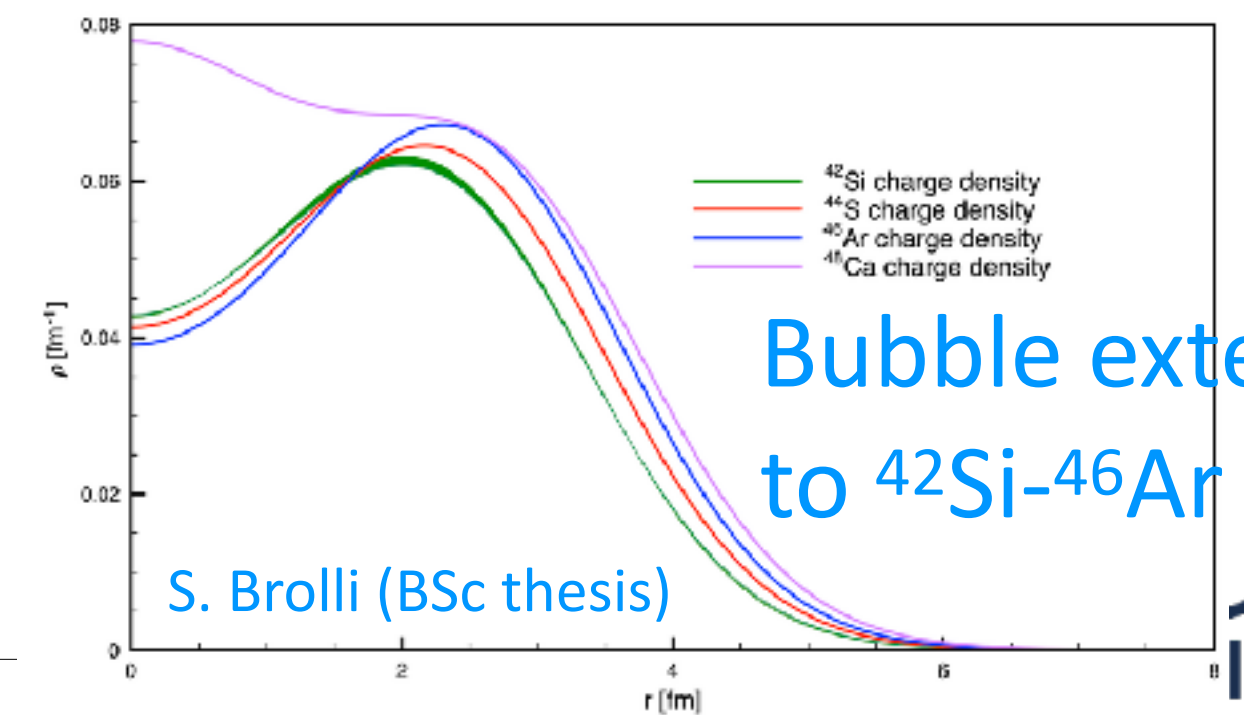
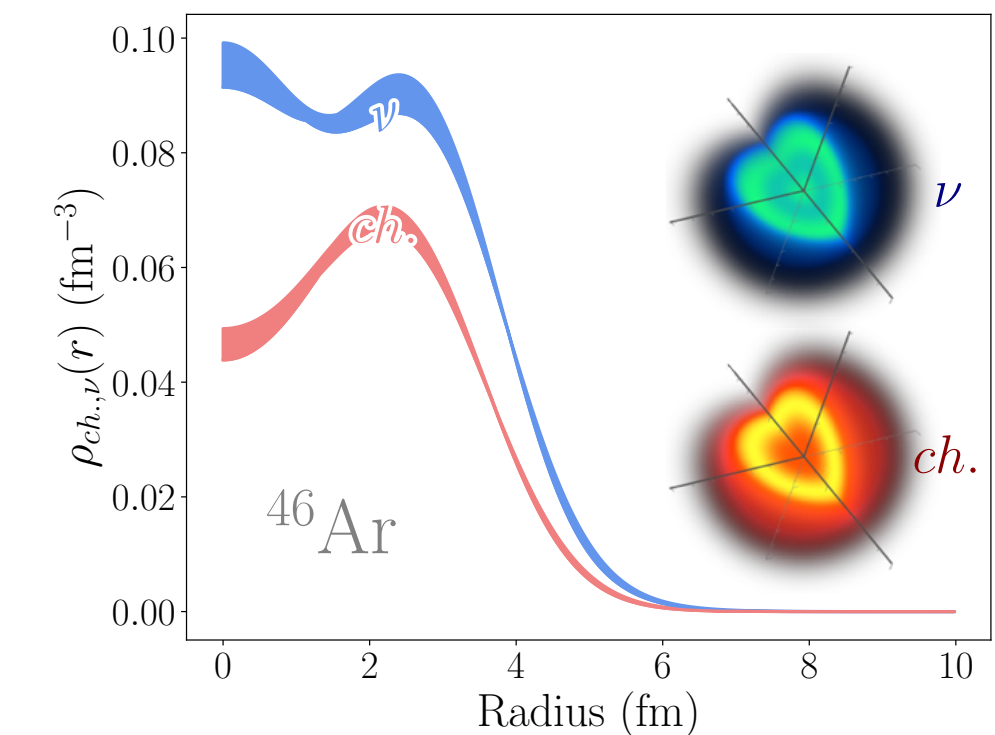
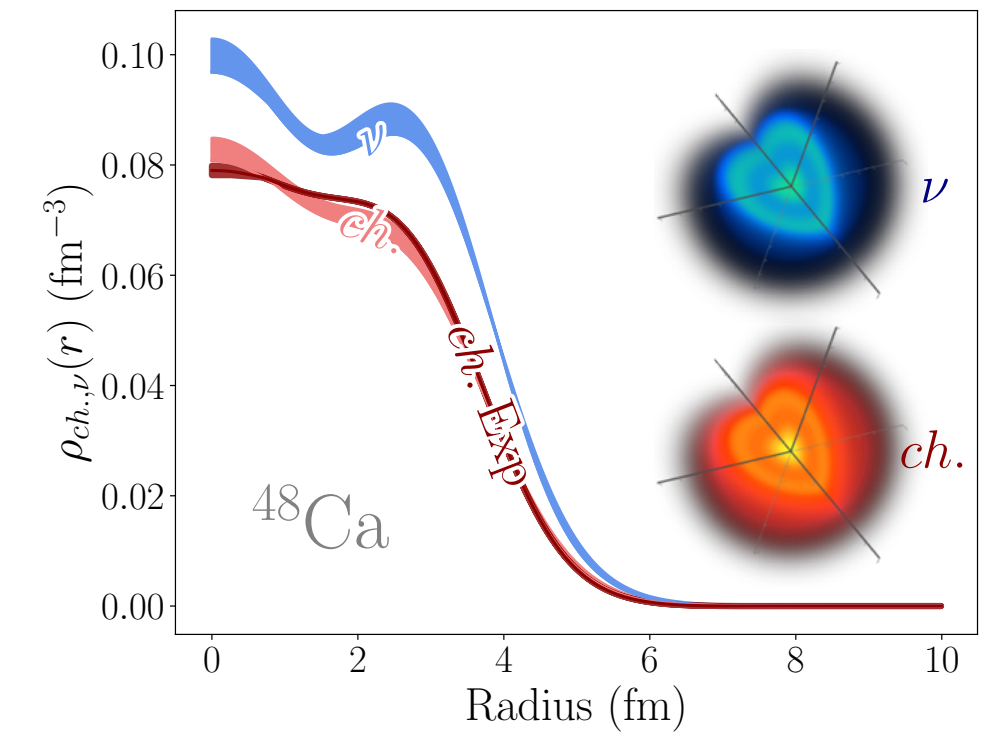
$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 5,55 \text{ MeV}$$

$$(\text{theo}) = 2,59 \text{ MeV}$$

The d3/2 - s1/2 gap opening and new shell closure at Z=18 !!



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

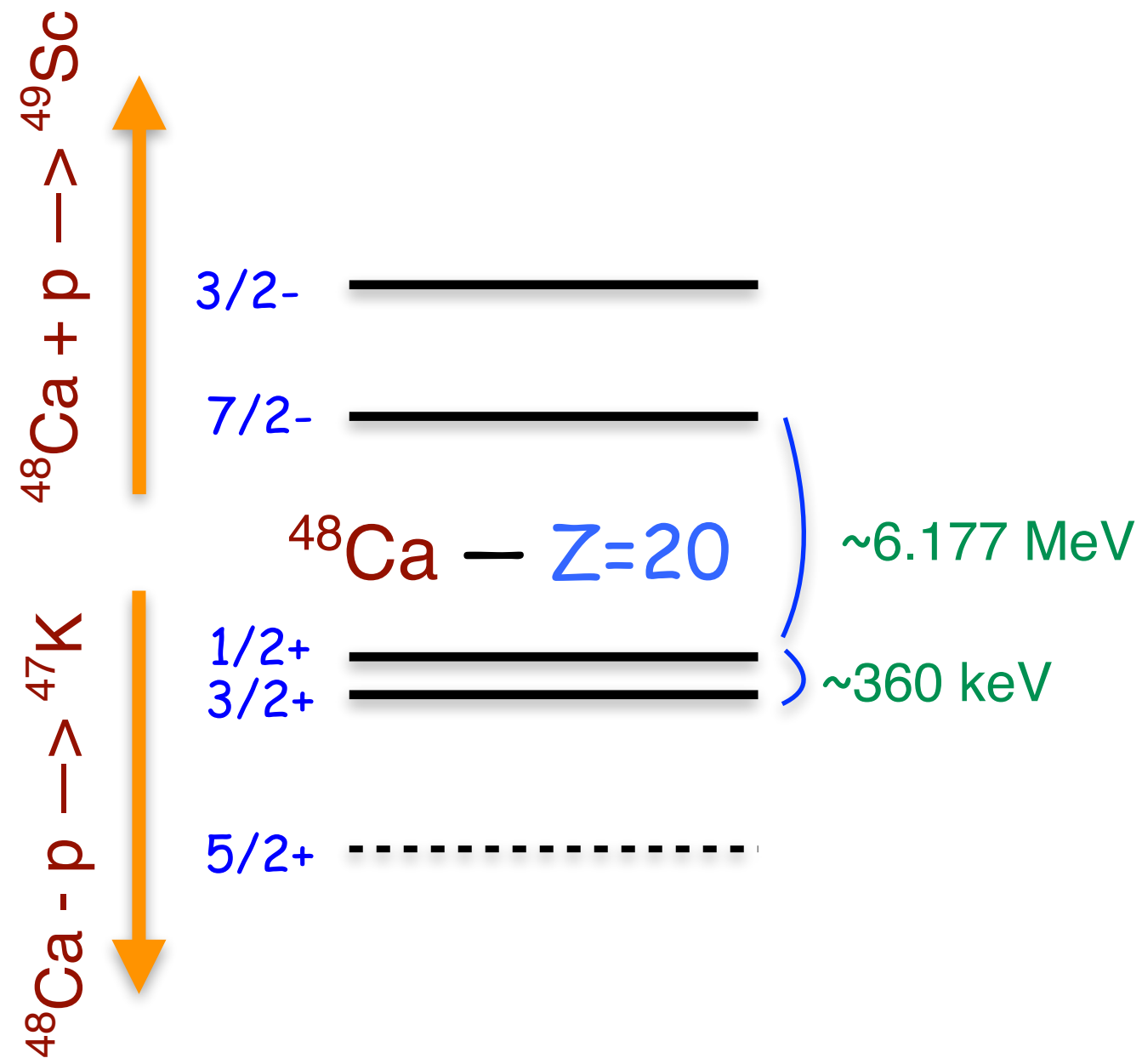


Bubble extends to ^{42}Si - ^{46}Ar ??

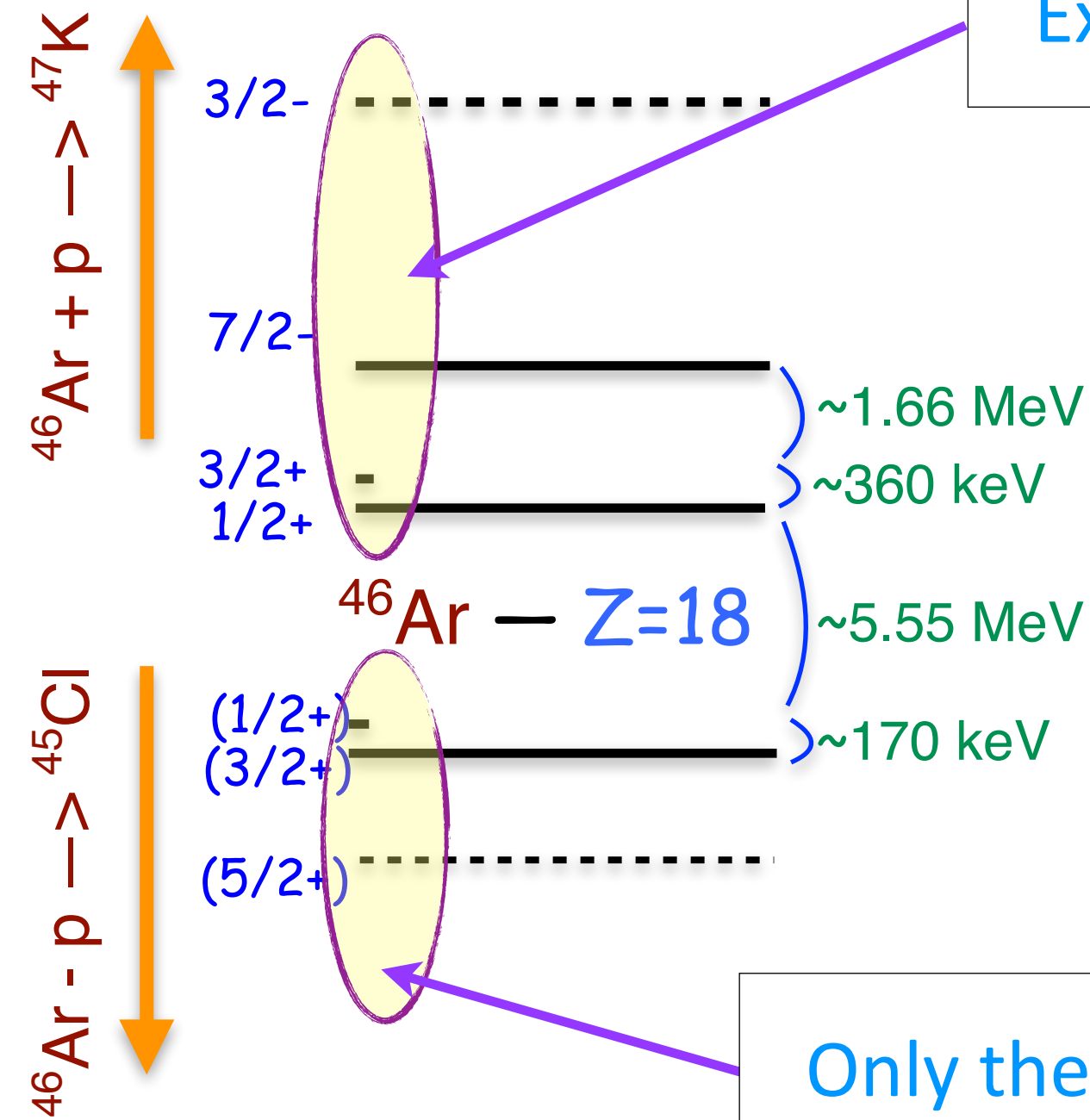
S. Brolli (BSc thesis)



$^{46}\text{Ar}(^3\text{He},d)^{47}\text{K}$ at GANIL : shell closure & charge bubble in ^{46}Ar



$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 360 \text{ keV}$$

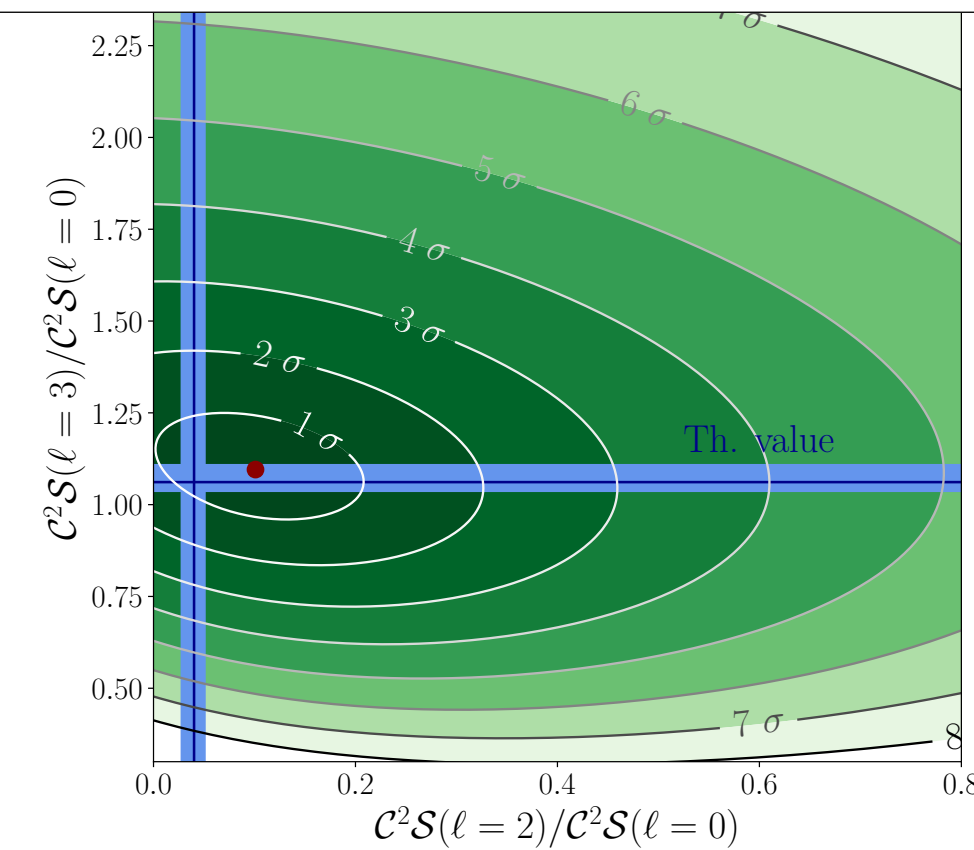


$$\Delta E_{1/2+ - 3/2+} (\text{exp}) = 5,55 \text{ MeV}$$

$$(\text{theo}) = 2,59 \text{ MeV}$$

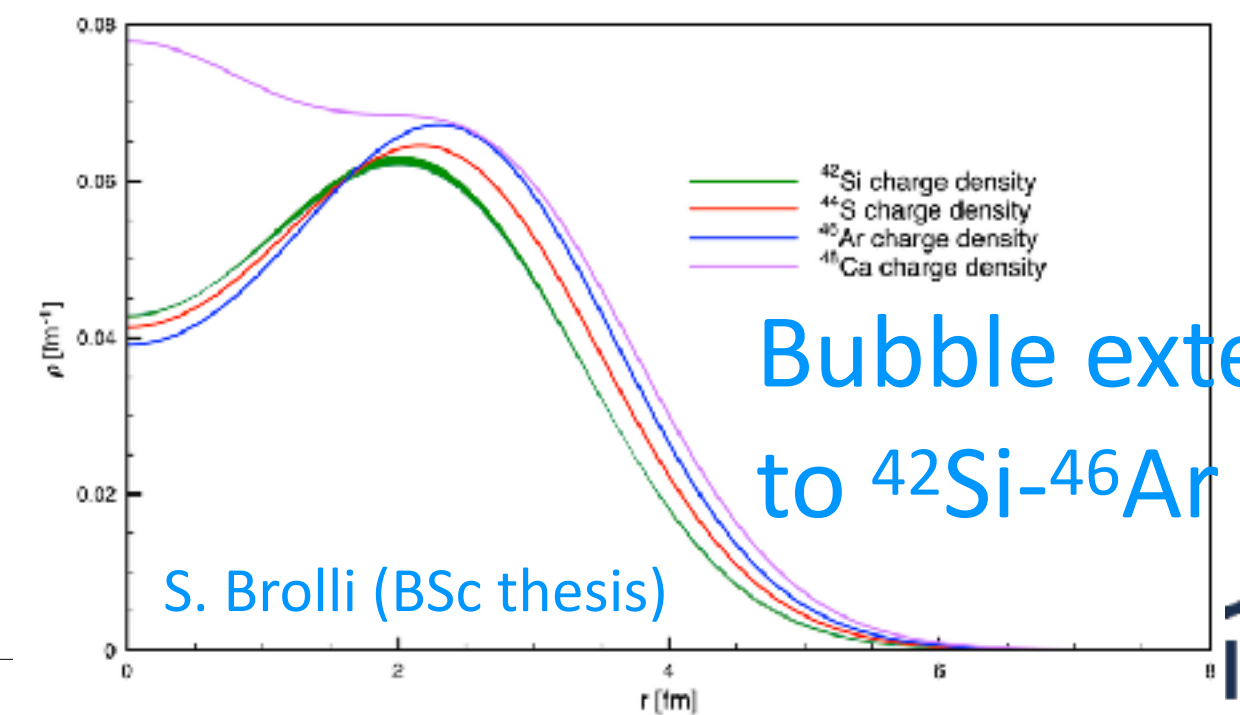
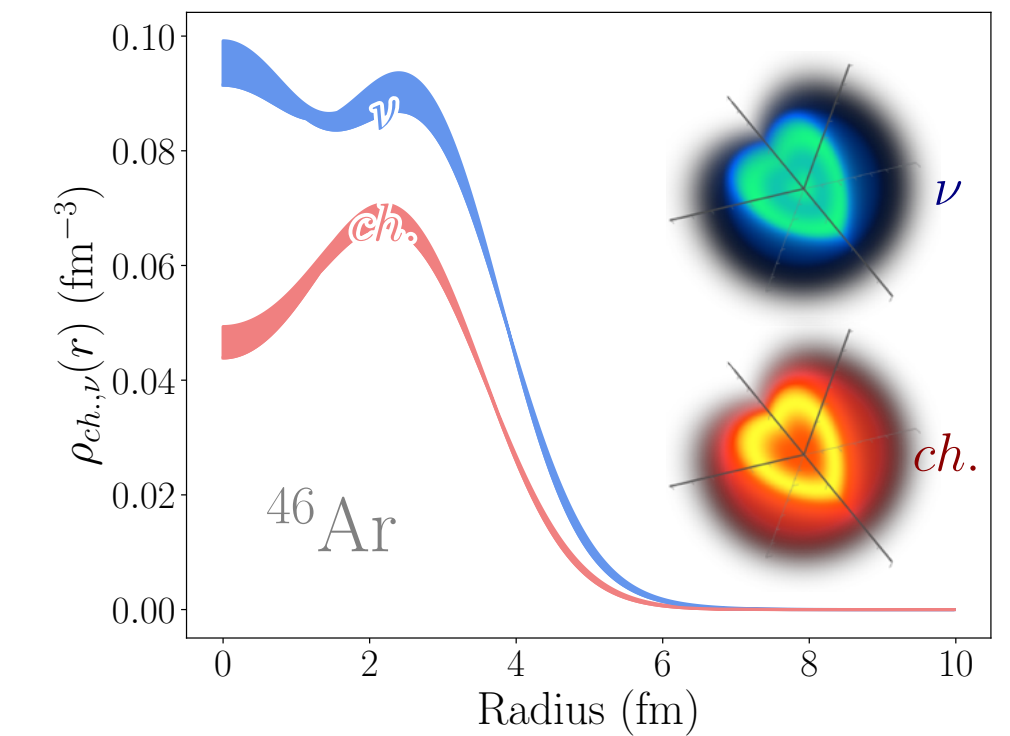
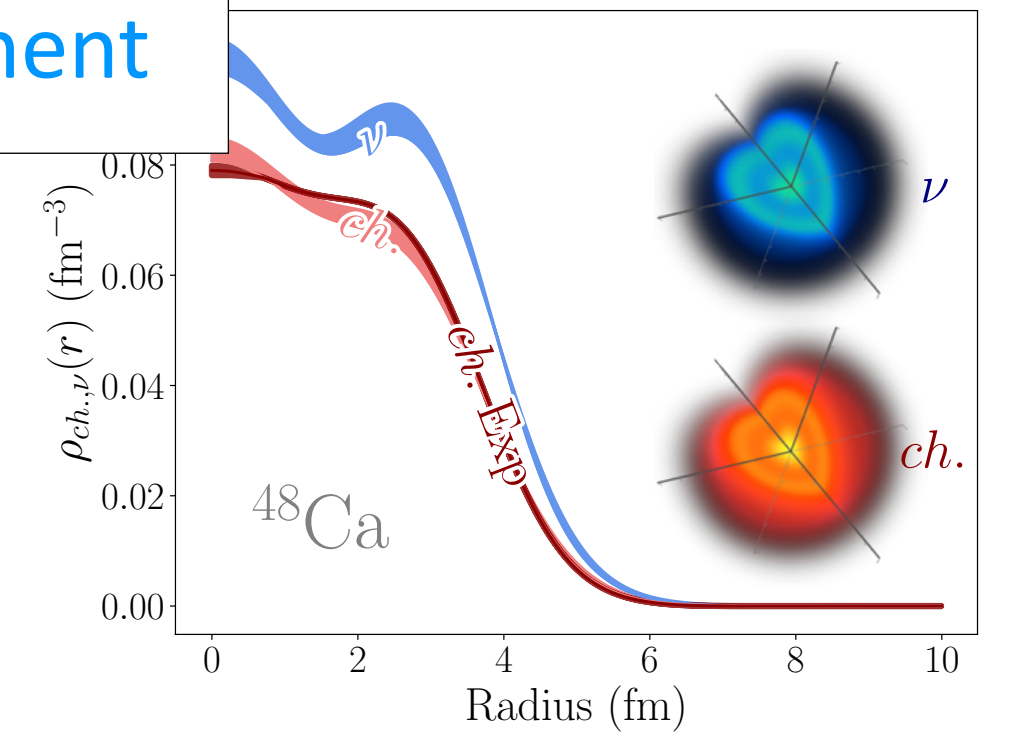
The d3/2 - s1/2 gap opening and new shell closure at Z=18 !!

Experiment & theory in agreement



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

Only theory prediction is available



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

S. Brolli (BSc thesis)



Electron-Ion Trap colliders...

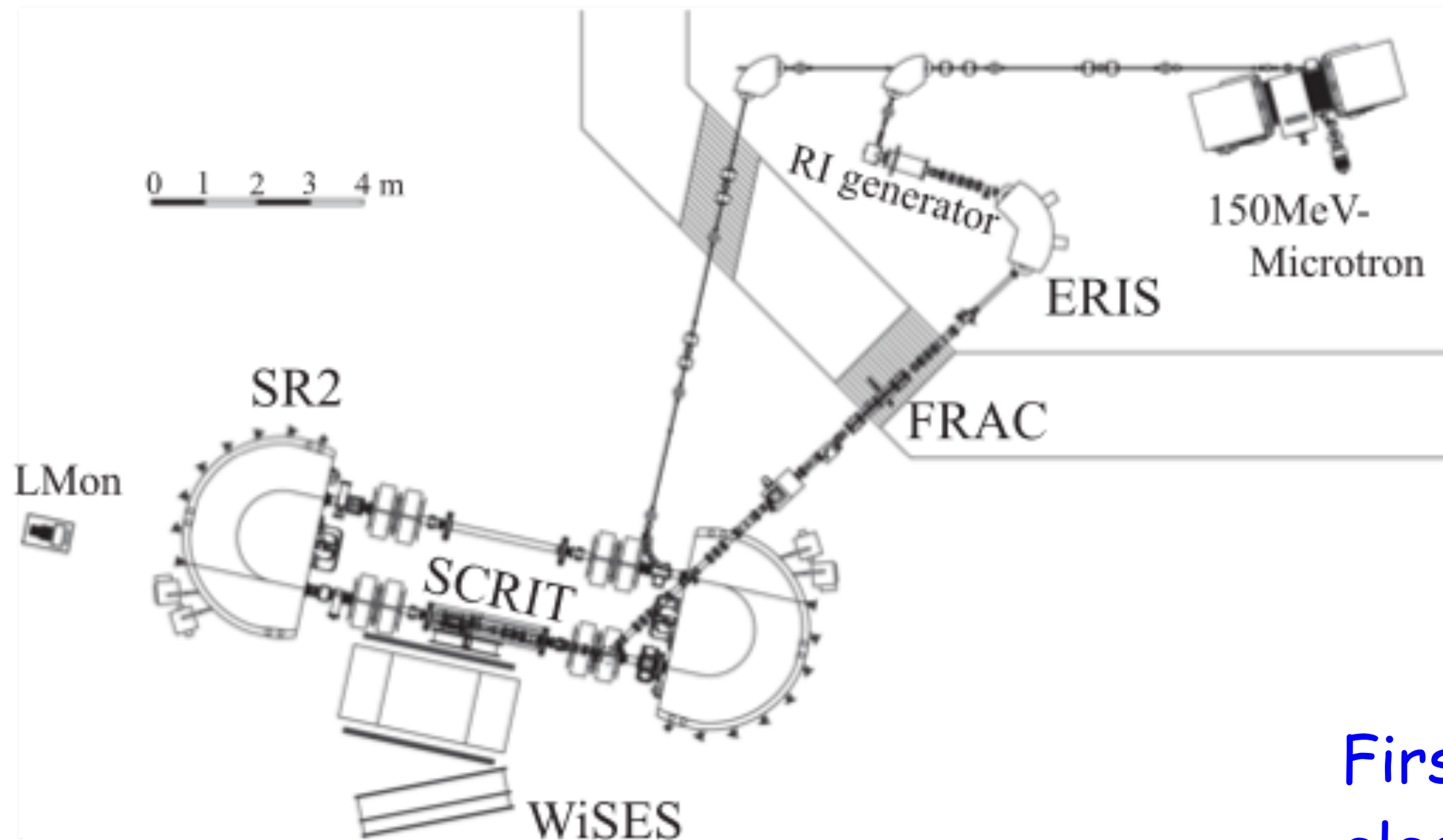


FIG. 1. Overview of the SCRIT electron scattering facility.

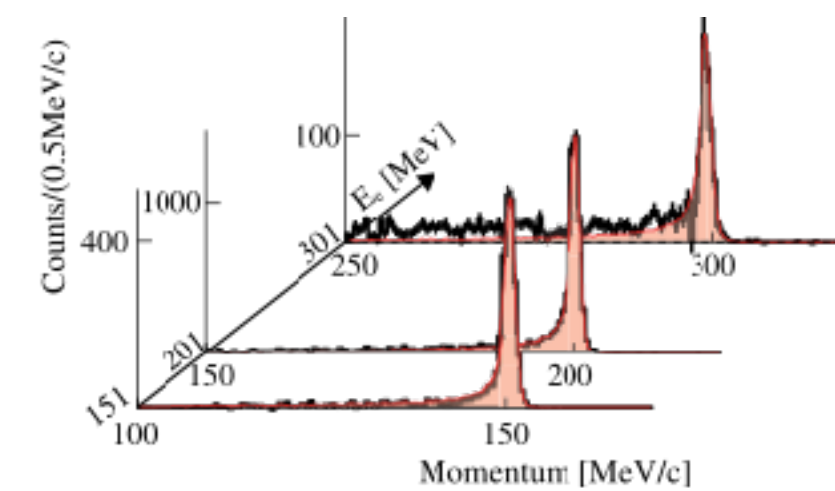
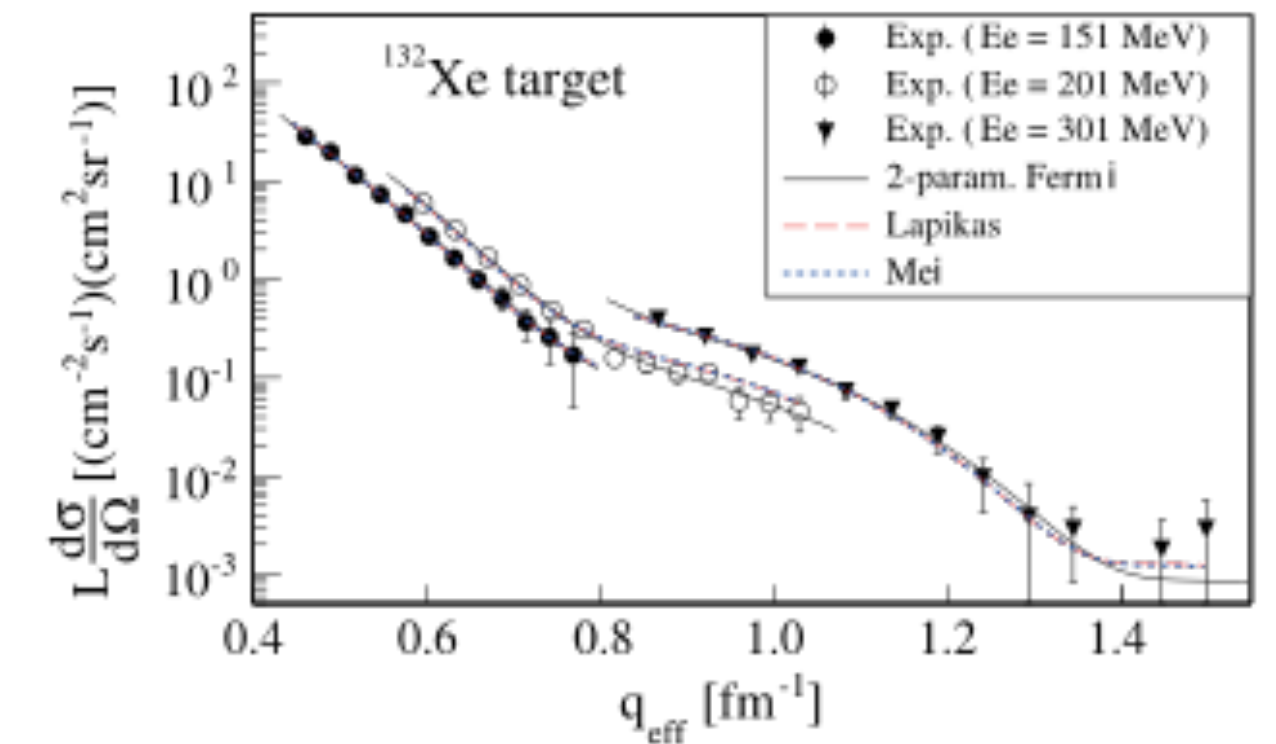


FIG. 3. Reconstructed momentum spectra of ^{132}Xe target after background subtraction. Red shaded lines are the simulated radiation tails following the elastic peaks.

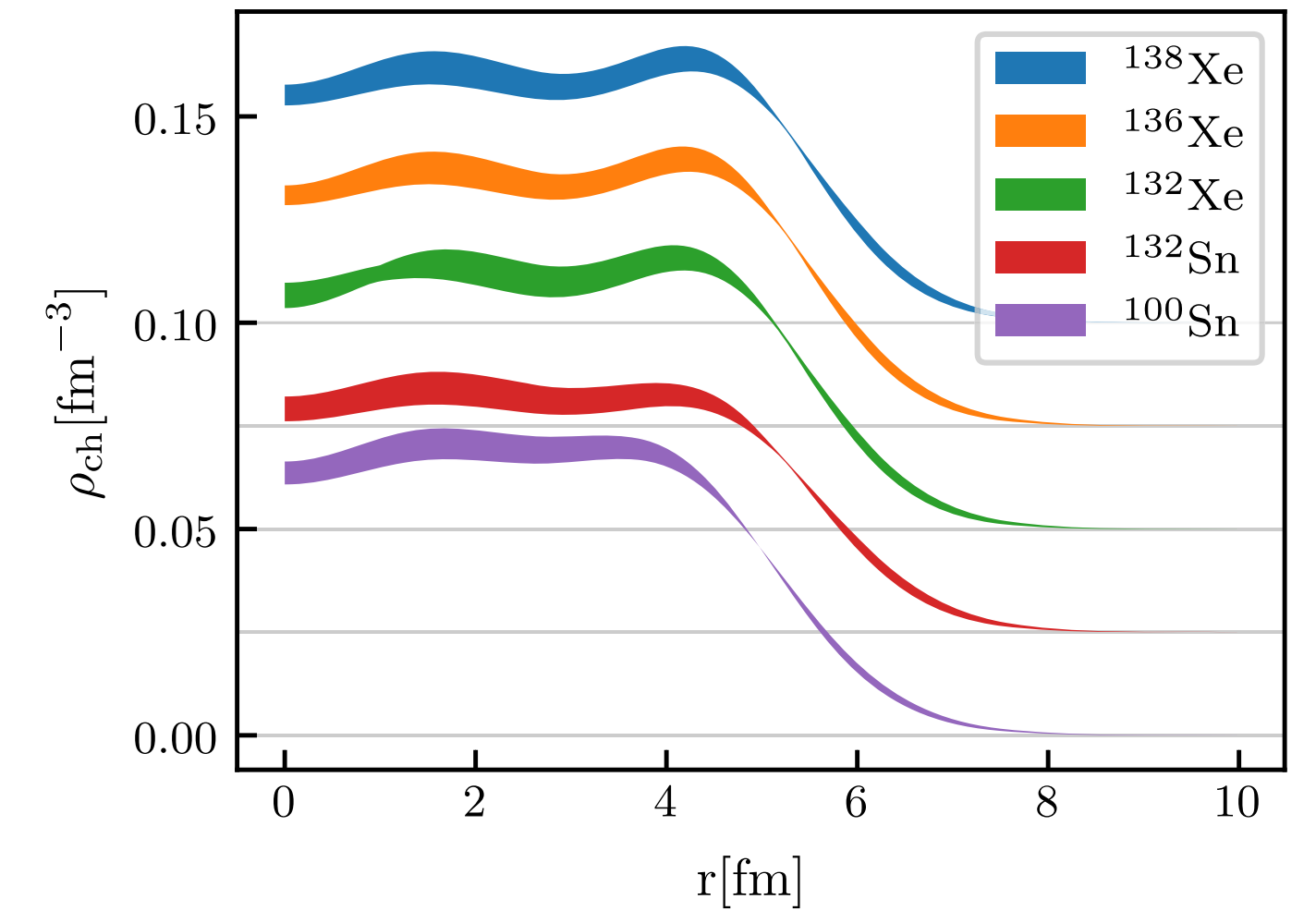
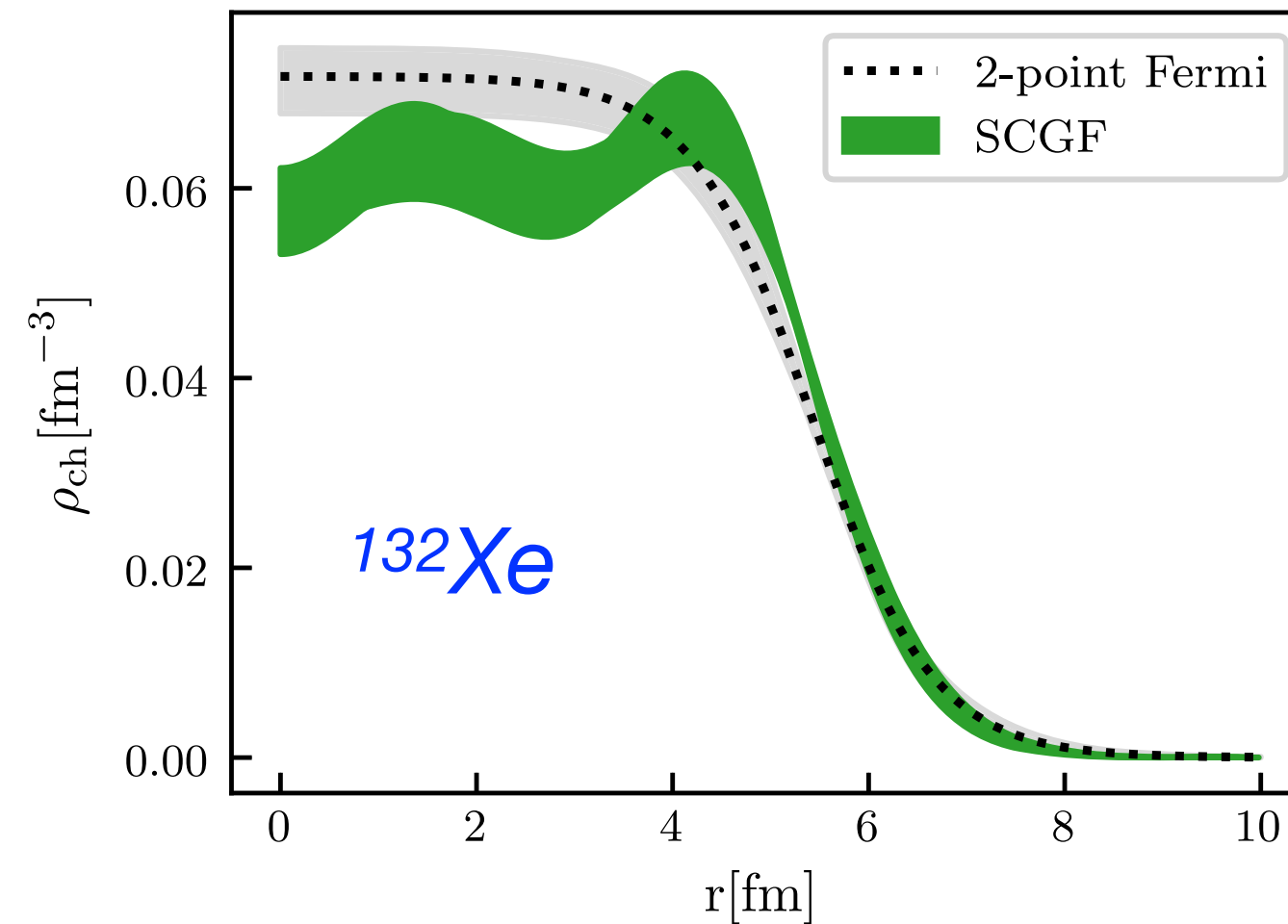
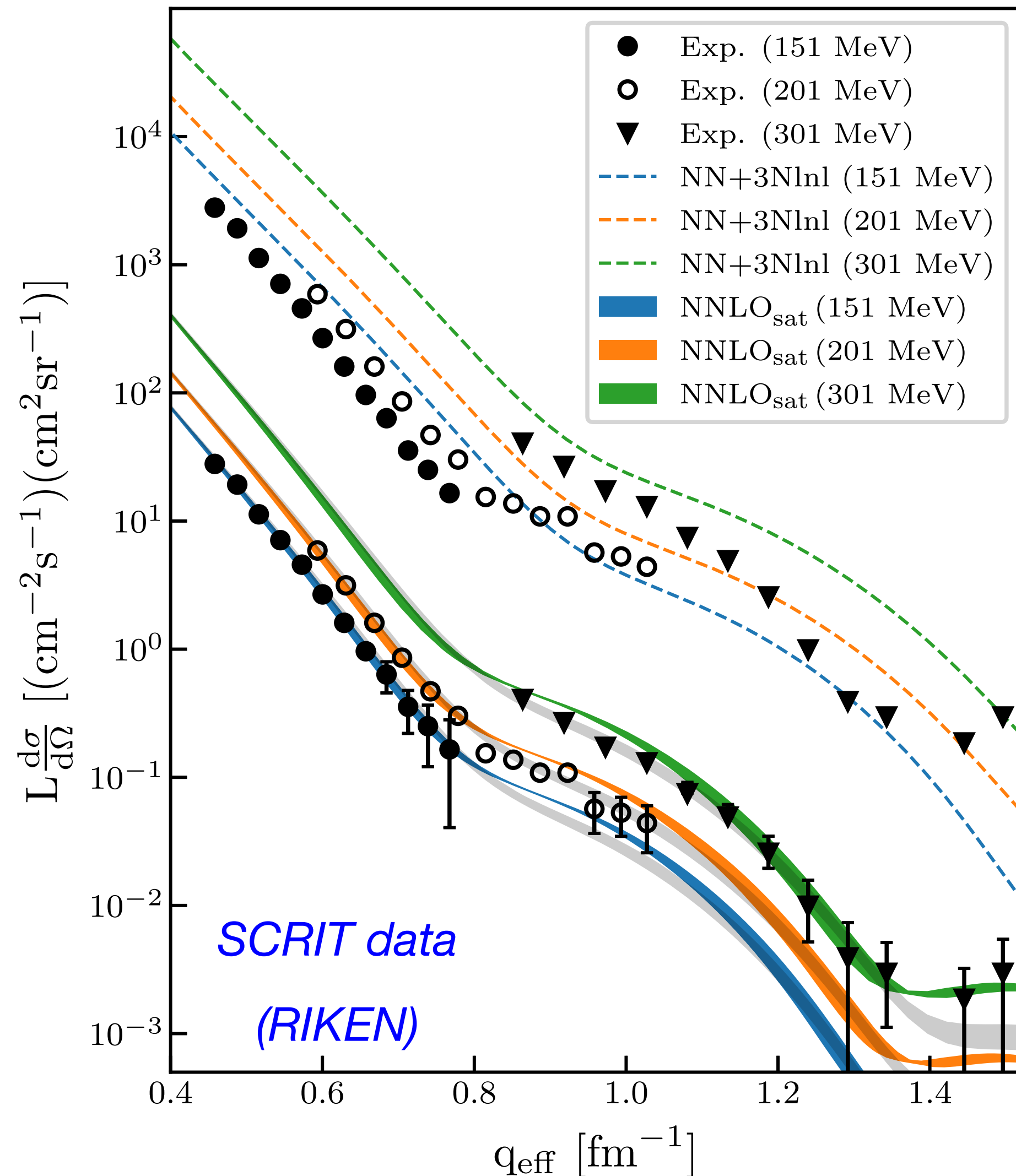


First ever measurement of charge radii through electron scattering with and ion trap setting that can be used on radioactive isotopes !!

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



Charge radii (NNLO_{sat}):

	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

...and accompanying predictions
for neutron skins (see paper).



Inclusion of NNN forces

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

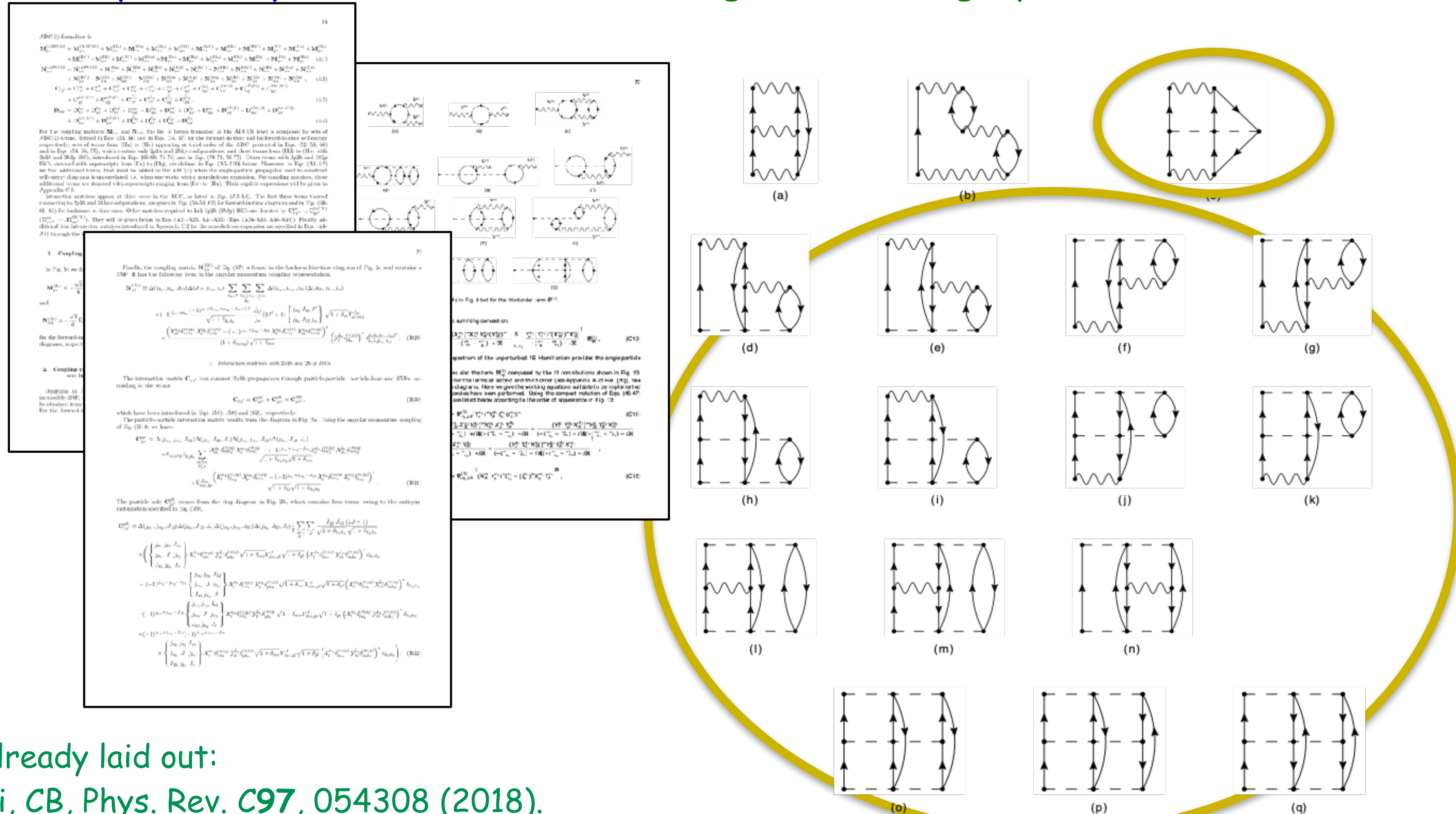


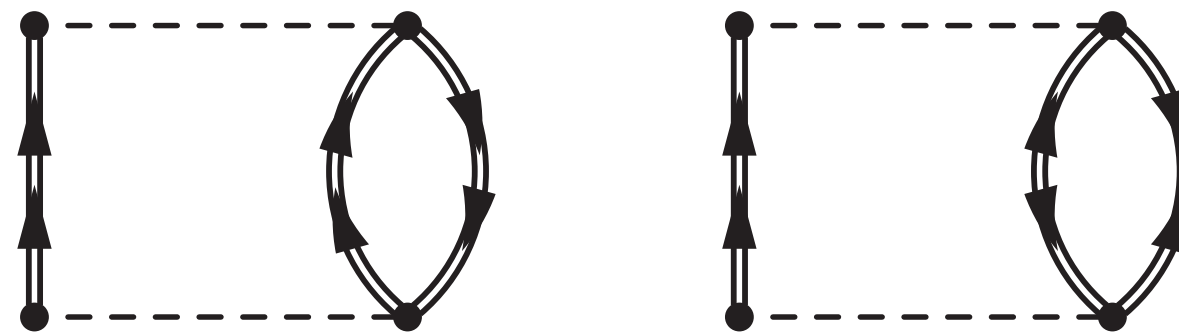
FIG. 5. 1PI, skeleton and interaction irreducible self-energy diagrams appearing at 3^{rd} -order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

Formalism already laid out:

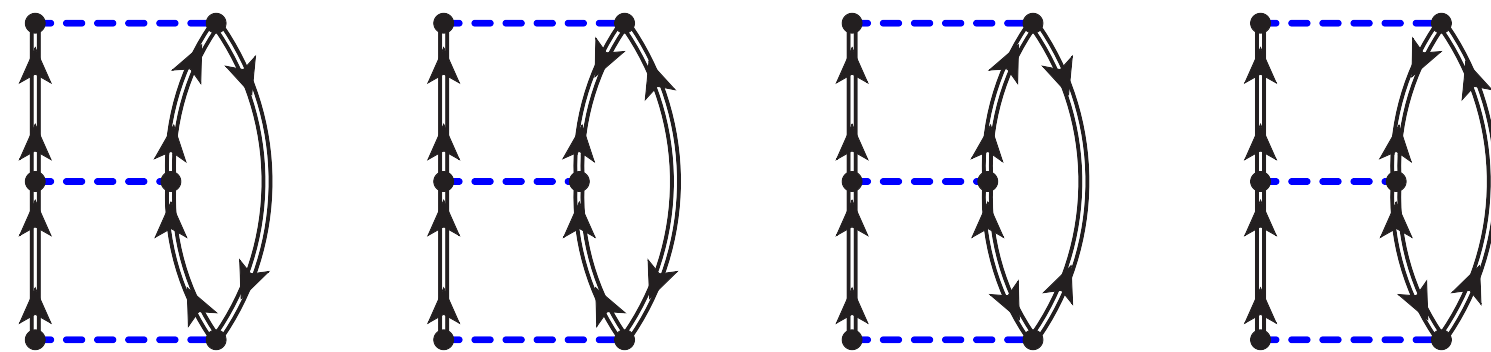
F. Raimondi, CB, Phys. Rev. C97, 054308 (2018).

Extending Gorkov to ADC(3) level...

Gorkov at
2nd order:

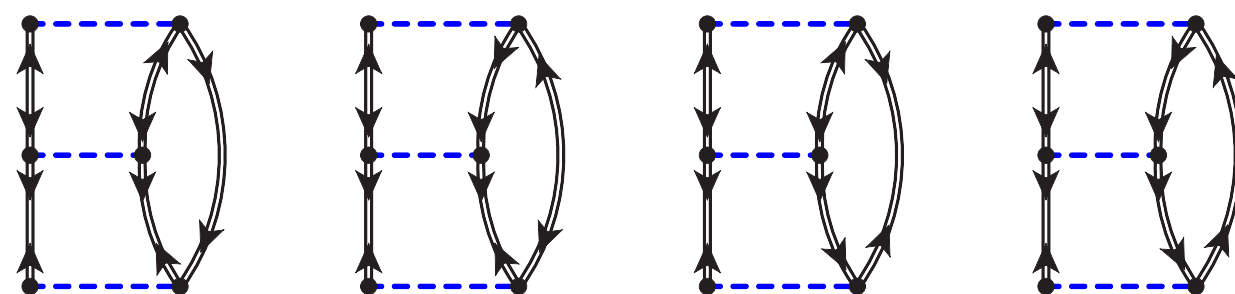
$$\Sigma_{\alpha\beta}^{11}(\omega) =$$


pp-ladders:



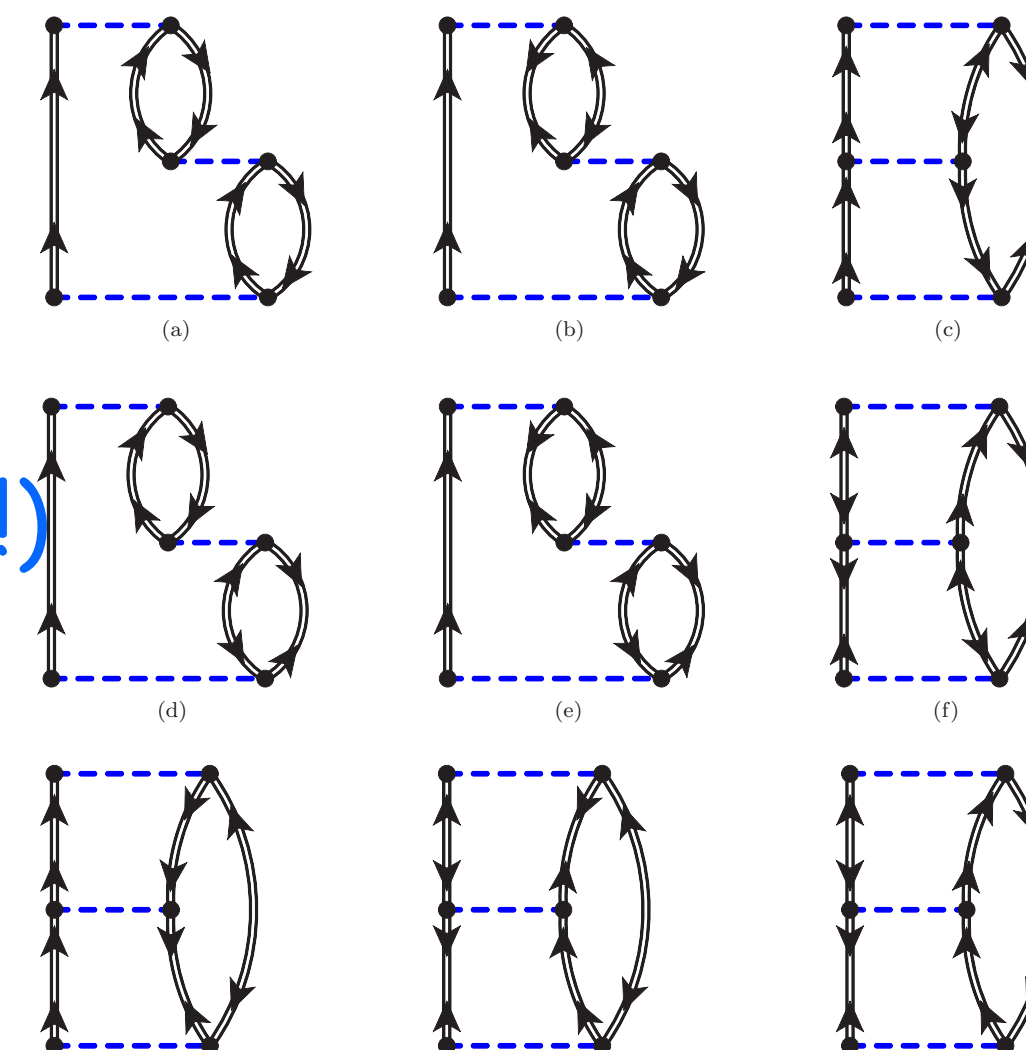
Gorkov at
3rd order:
(ONLY NN forces)

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



(NN ONLY forces) LI STUDI DI MILANO

ph-rings:

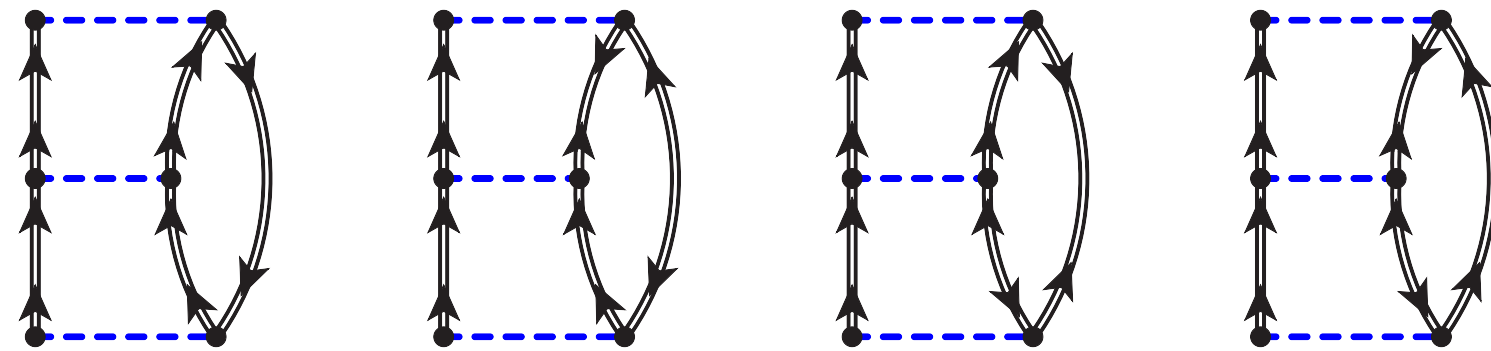


Extending Gorkov to ADC(3) level...

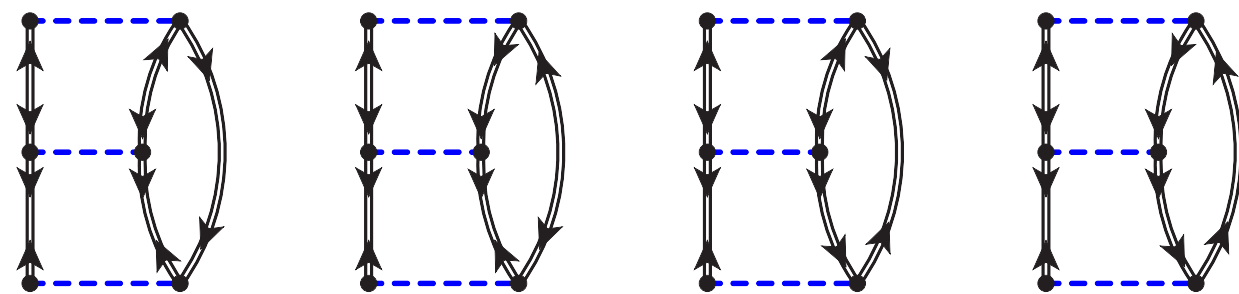
Gorkov at
2nd order:

$$\Sigma_{\alpha\beta}^{11}(\omega) = \text{diagram}$$

pp-ladders:



hh-interactions (hh int. among pp ladders)



Gorkov at
3rd order:
(ONLY NN forces)

(NN ONLY forces) LI STUDI DI MILANO

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

Gorkov algebraic diagrammatic construction formalism at third order

Carlo Barbieri

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Thomas Duguet

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

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

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

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

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

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

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

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

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

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

$$\mathcal{C}_{\alpha,r}^{(\text{IIe})} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\mu\nu\lambda} v_{\alpha\lambda,\mu\nu} (\bar{\mathcal{V}}_\nu^{k_7} \mathcal{U}_\lambda^{k_8})^* \mathcal{U}_\mu^{k_1} t_{k_7k_8}^{k_3k_2}, \quad (50a)$$

$$\mathcal{C}_{\alpha,r}^{(\text{IIIf})} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\mu\nu\lambda} v_{\alpha\lambda,\mu\nu} (\mathcal{U}_\lambda^{k_7} \bar{\mathcal{V}}_\mu^{k_8})^* \mathcal{U}_\nu^{k_1} t_{k_7k_8}^{k_3k_2}, \quad (50b)$$

$$\mathcal{C}_{\alpha,r}^{(\text{IIg})} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\mu\nu\lambda} v_{\alpha\lambda,\mu\nu} (\bar{\mathcal{V}}_\mu^{k_7} \bar{\mathcal{V}}_\nu^{k_8})^* \bar{\mathcal{V}}_\lambda^{k_1} t_{k_7k_8}^{k_3k_2}, \quad (50c)$$

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

Gorkov Green's functions and equations

Set of 4 Gorkov Green's functions:

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

[Gorkov 1958]

In terms of Nambu fields:

$$\mathbf{G}_{\alpha\beta}(t, t') = -i\langle\Psi_0|T \left[\underbrace{\mathbf{A}_{\alpha}(t)\mathbf{A}_{\beta}^{\dagger}(t')}_{\text{Don't (anti)commute}} \right] |\Psi_0\rangle \quad \mathbf{A}_{\alpha}(t) \equiv \begin{bmatrix} c_{\alpha}(t) \\ c_{\alpha}^{\dagger}(t) \end{bmatrix}$$

[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:

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

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

(contravariant)

$$\mathcal{B} \equiv \{ |b\rangle \}$$

(covariant)

$$\bar{\mathcal{B}} \equiv \{ \langle \bar{b} | \}$$

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

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 @ TD Darmstadt)

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:

$$A^{(b,1)} \equiv a_b$$

$$A^{(b,2)} \equiv \bar{a}_b$$

$$\bar{A}_{(b,1)} \equiv \bar{a}_b$$

$$\bar{A}_{(b,2)} \equiv a_b$$



$$\bar{A}_\mu = \sum_\nu g_{\mu\nu} A^\nu$$

$$\bar{A}_\mu = \sum_\nu g_\mu{}^\nu \bar{A}_\nu$$

$$A^\mu = \sum_\nu g^{\mu\nu} \bar{A}_\nu$$

$$A^\mu = \sum_\nu g^\mu{}_\nu A^\nu$$



$$\{ A^\mu, A^\nu \} = g^{\mu\nu}$$

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

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

$$\{ \bar{A}_\mu, \bar{A}_\nu \} = g_{\mu\nu}$$

Drissi, Rios & Barbieri, Ann. Phys. 469 169729 (2024)
Drissi, Rios & Barbieri, Ann. Phys. 469 169730 (2024)



Nambu-Covariant approach to build (Gorkov) propagators

Combine w/ dual-basis:

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

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

(contravariant) $\swarrow$ $\searrow$ (covariant)

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

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

Generalised states:

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M. Drissi (Surrey, now @ TD Darmstadt)

Covariant (contravariant) of operators:

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

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

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

$$O_{\mu_1 \dots \mu_{2k}} = \sum_{\alpha_1 \dots \alpha_k} g_{\mu_1 \alpha_1} \dots g_{\mu_k \alpha_k} O^{\alpha_1 \dots \alpha_k}_{\mu_{k+1} \dots \mu_{2k}}$$

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

Drissi, Rios & Barbieri, Ann. Phys. 469 169729 (2024)
Drissi, Rios & Barbieri, Ann. Phys. 469 169730 (2024)

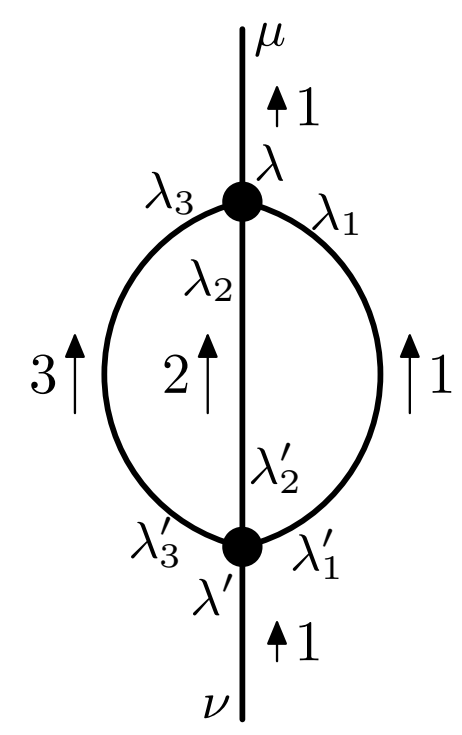


Nambu-Covariant approach to build (Gorkov) propagators

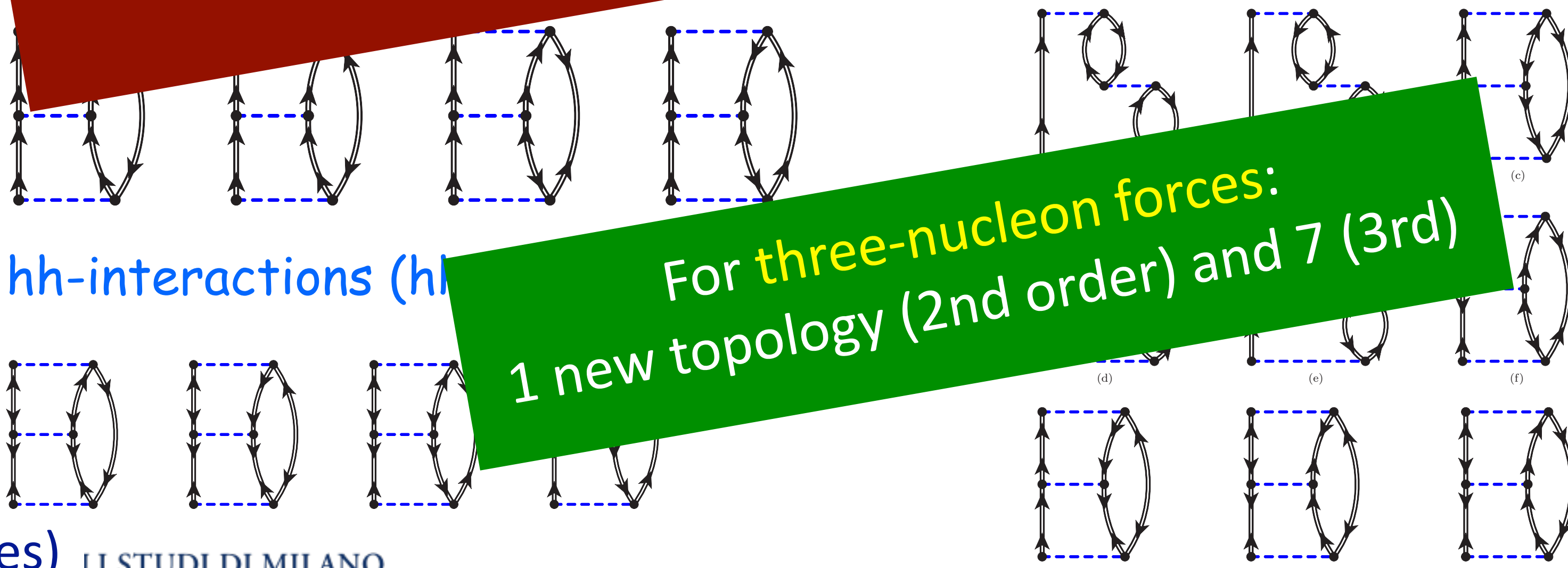
Gorkov at
2nd order:



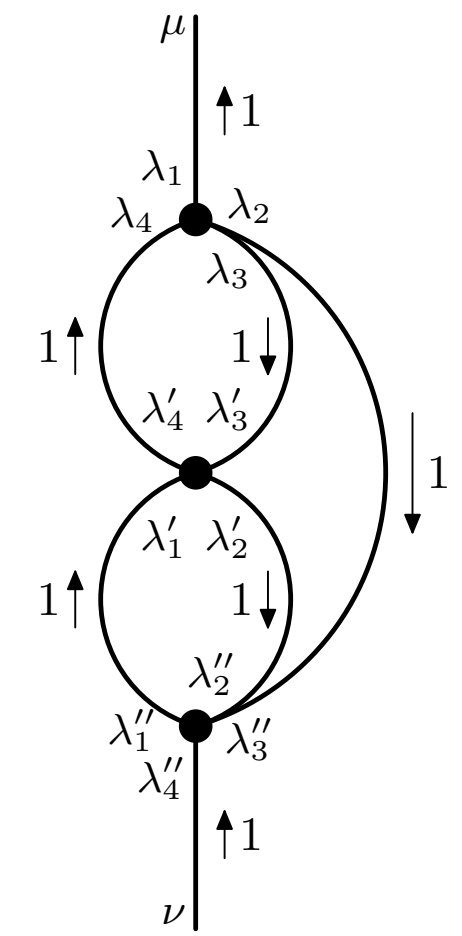
Just ONE topology at 2nd and 3rd order!
(2-body forces only)



Gorkov at
3rd order:
(ONLY NN forces)



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



(NN ONLY forces) LI STUDI DI MILANO

Ab initio optical potentials from propagator theory

Relation to Feshbach 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)

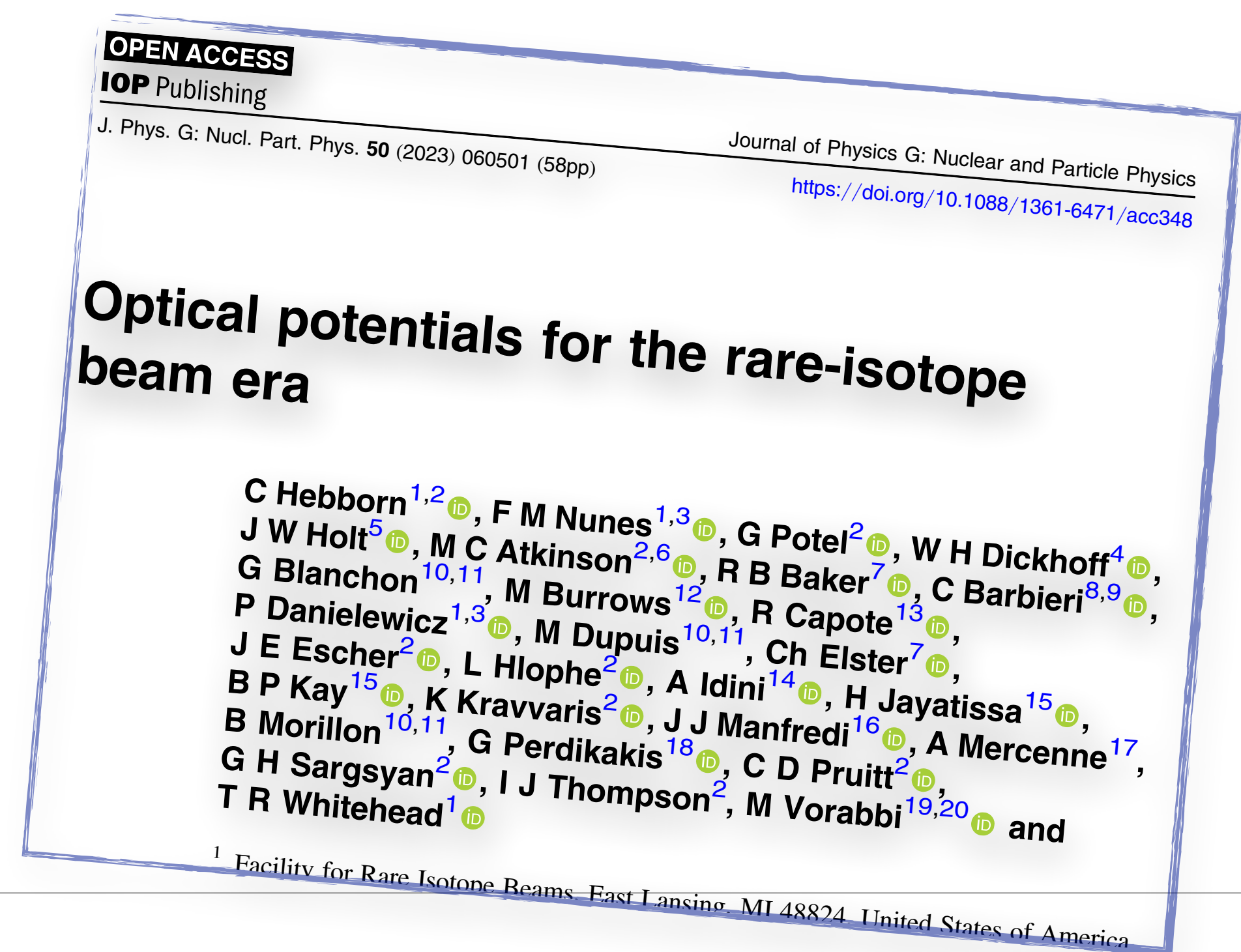
S. Waldecker, CB, W. Dickhoff, Phys. Rev. C **84**, 034616 (2011)

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

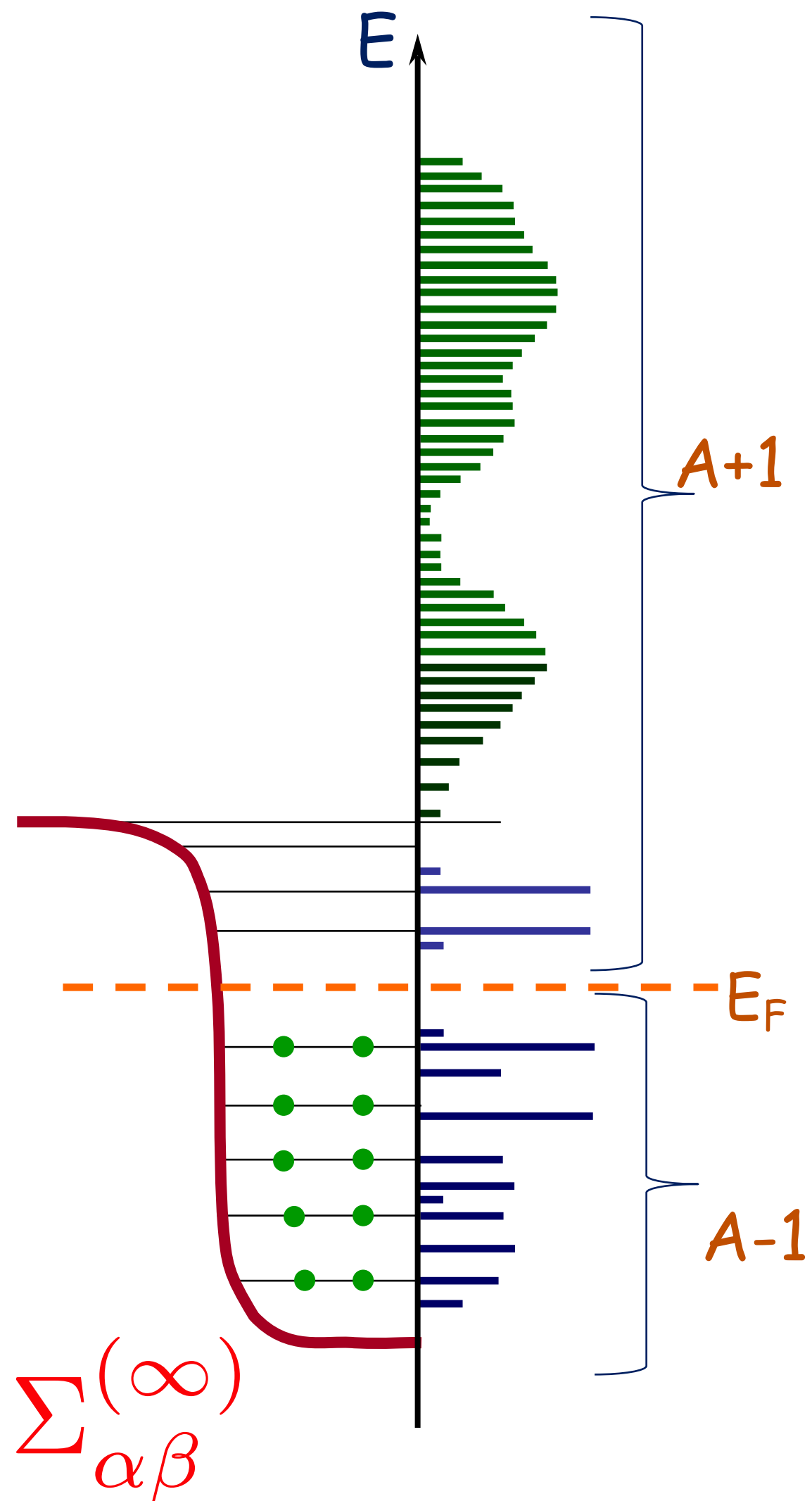
M. Vorabbi, CB, et al., Phys Rev C **109**, 034613 (2024)

State-of-the-art of the field:

C. Hebborn, et al., CB, “*Optical potentials for the rare-isotope beam era*”, Jour. Phys. G **50**, 060501 (2023)



Microscopic optical potential

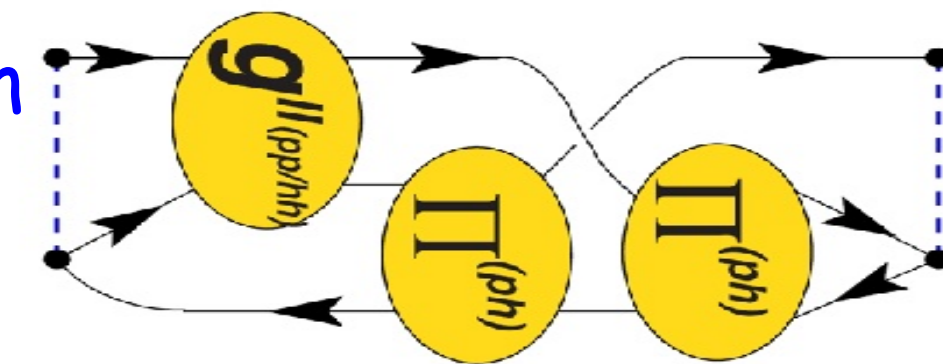


Nuclear self-energy $\Sigma^*(\mathbf{r}, \mathbf{r}'; \varepsilon)$:

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

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

Particle-vibration couplings:



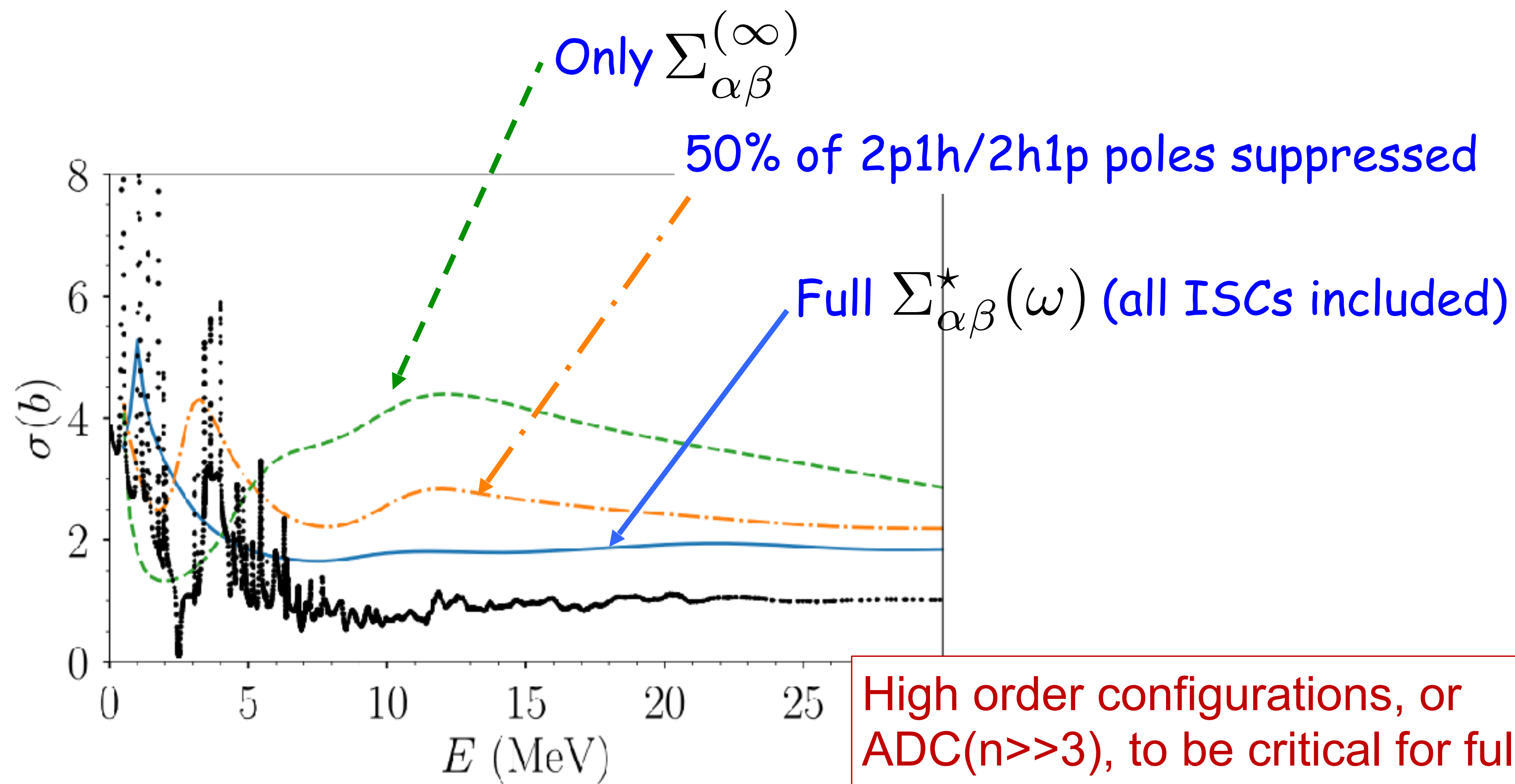
Solve scattering and overlap functions directly in momentum space:

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

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

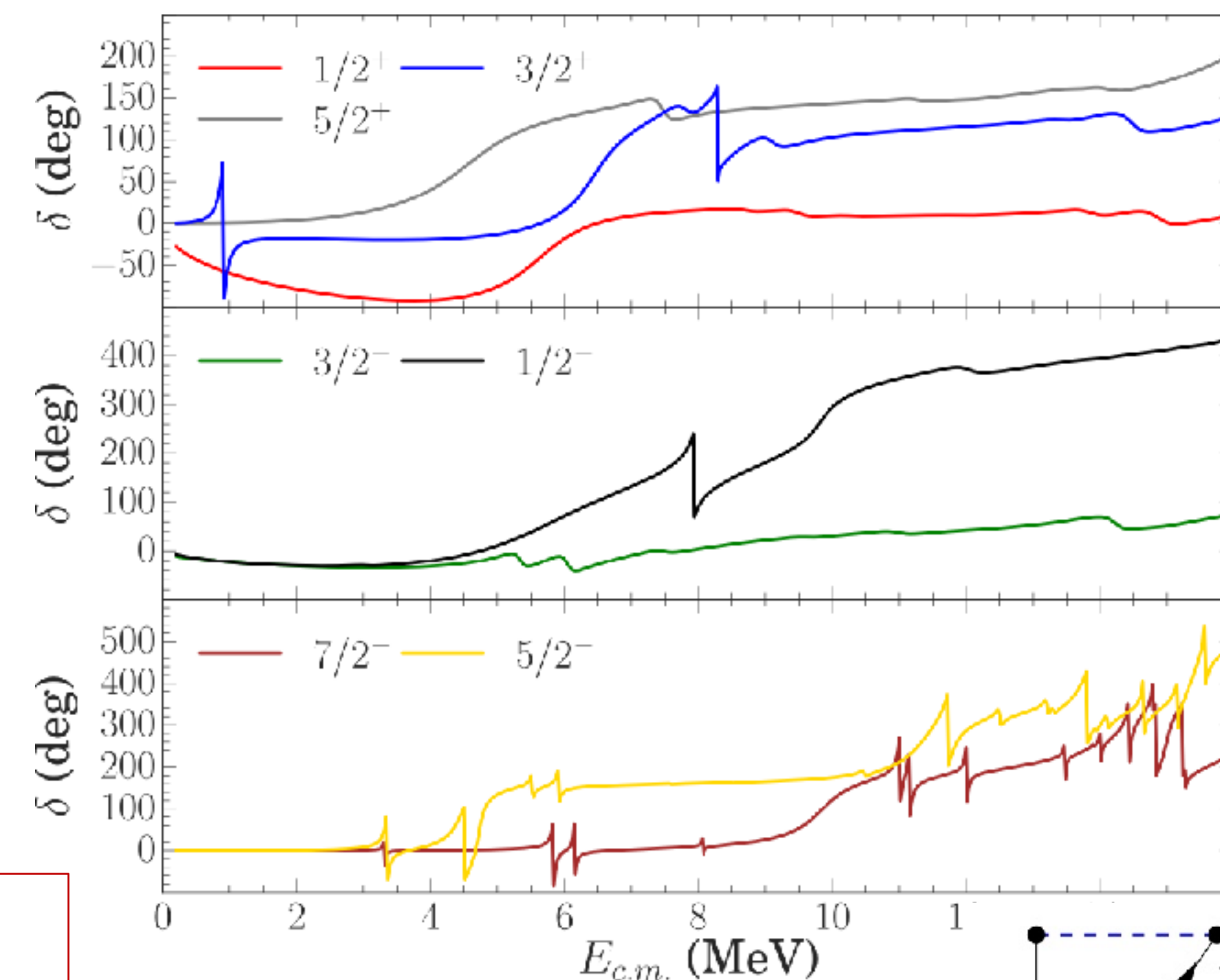
Role of intermediate state configurations (ISCs)

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

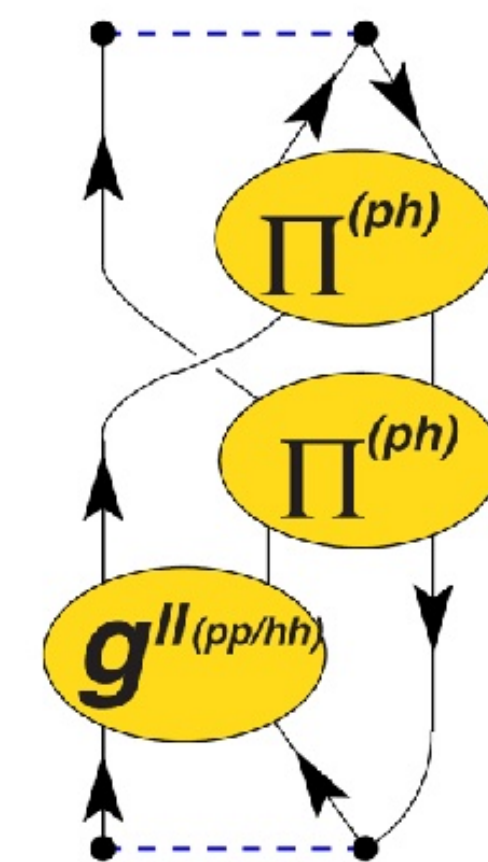


High order configurations, or ADC($n \gg 3$), to be critical for fully ab initio optical potentials

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

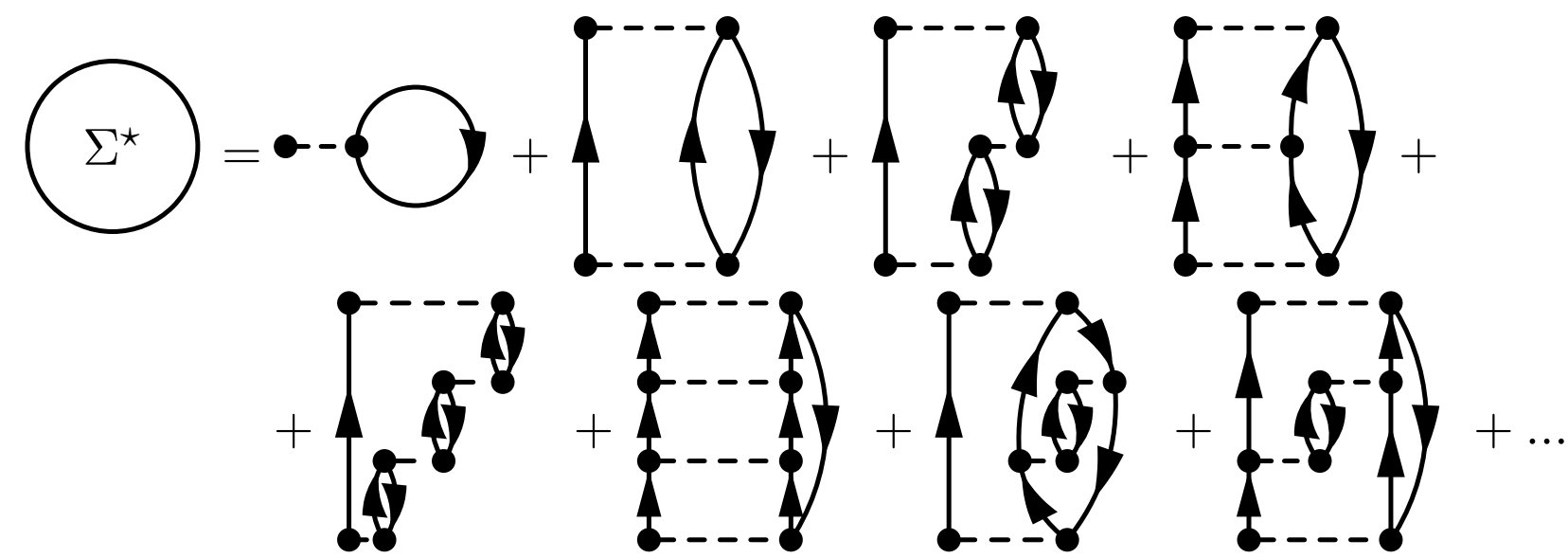


$$\Sigma_{\alpha\beta}^*(\omega) = \Sigma_{\alpha\beta}^{(\infty)} + \underbrace{\sum_{i,j} \mathbf{M}_{\alpha,i}^\dagger \left(\frac{1}{E - (\mathbf{K}^> + \mathbf{C}) + i\Gamma} \right)_{i,j} \mathbf{M}_{j,\beta}}_{2p1h} + \underbrace{\sum_{r,s} \mathbf{N}_{\alpha,r} \left(\frac{1}{E - (\mathbf{K}^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



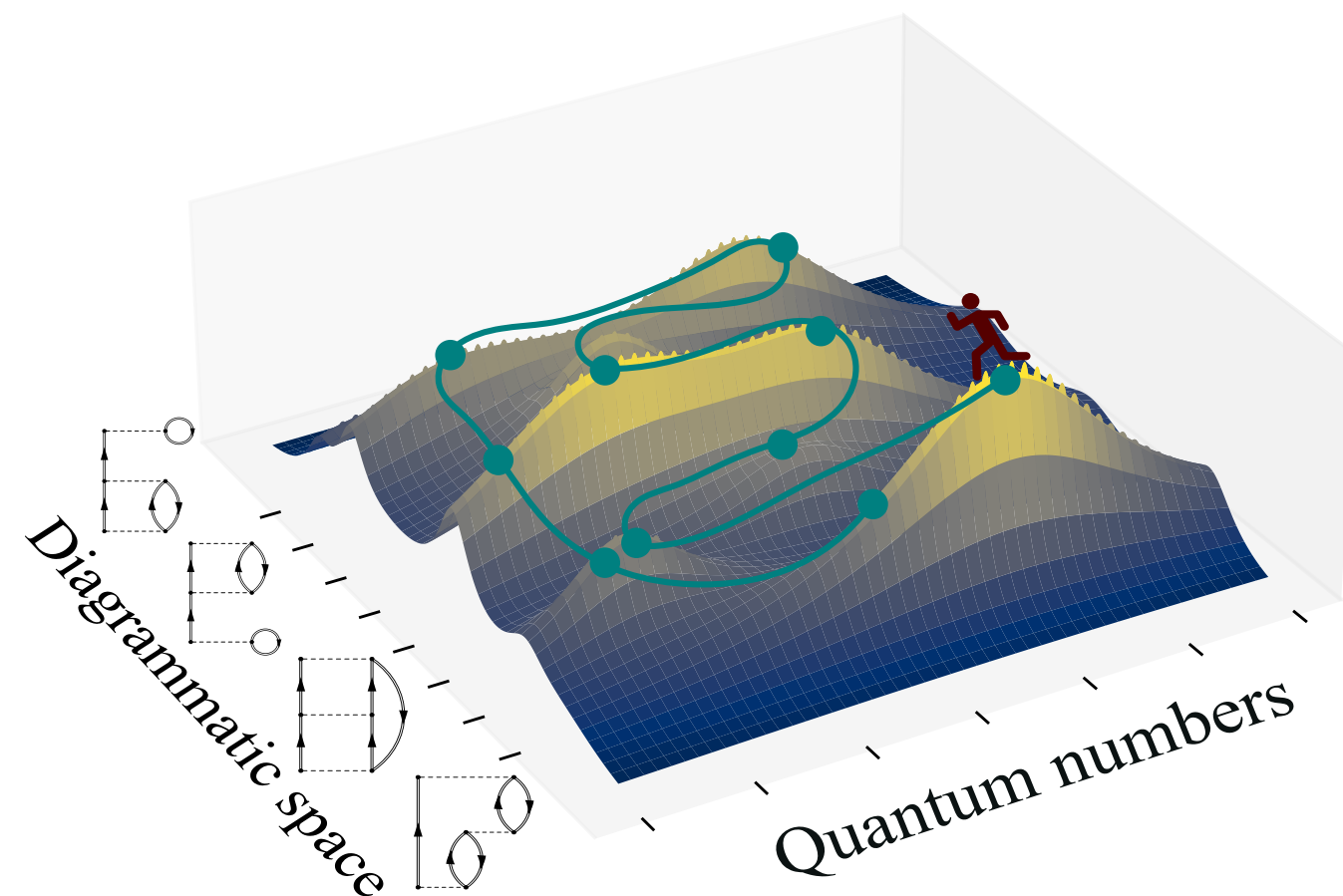
Green's function theory beyond ADC(3)? **DiagMC !!**

Infinte Feynman
series of diagrams



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

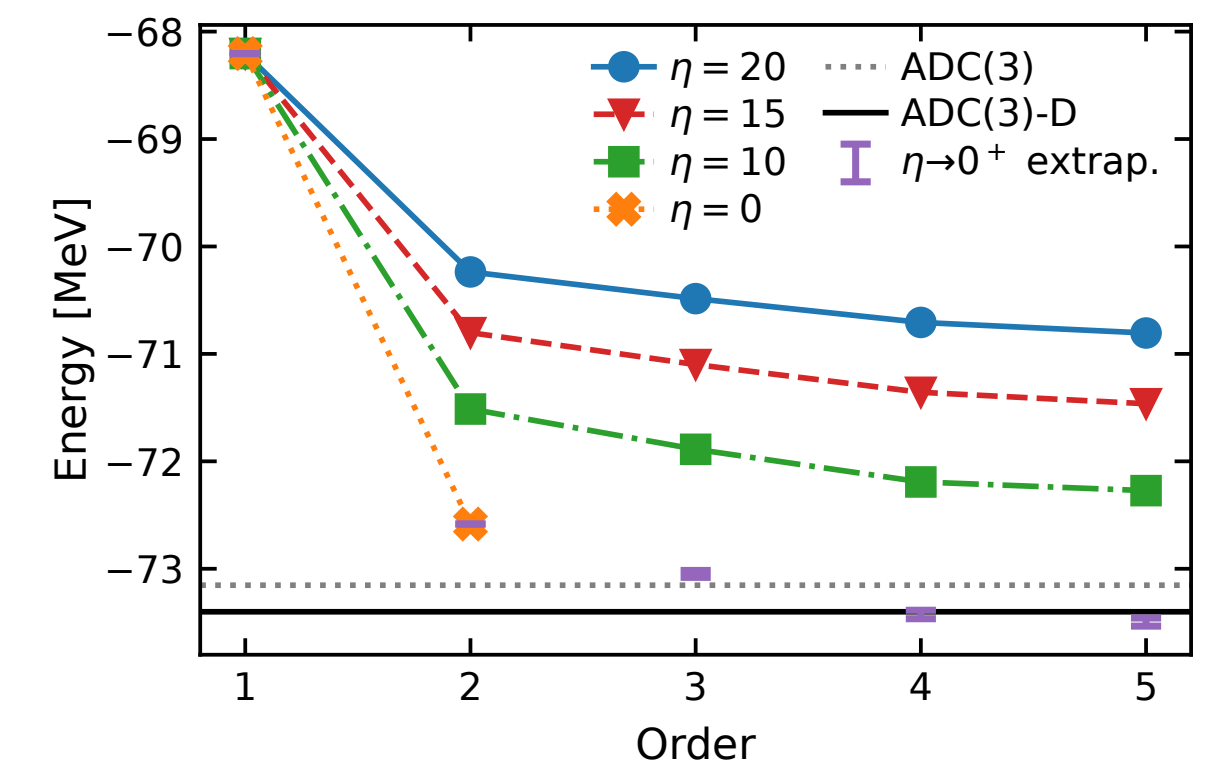
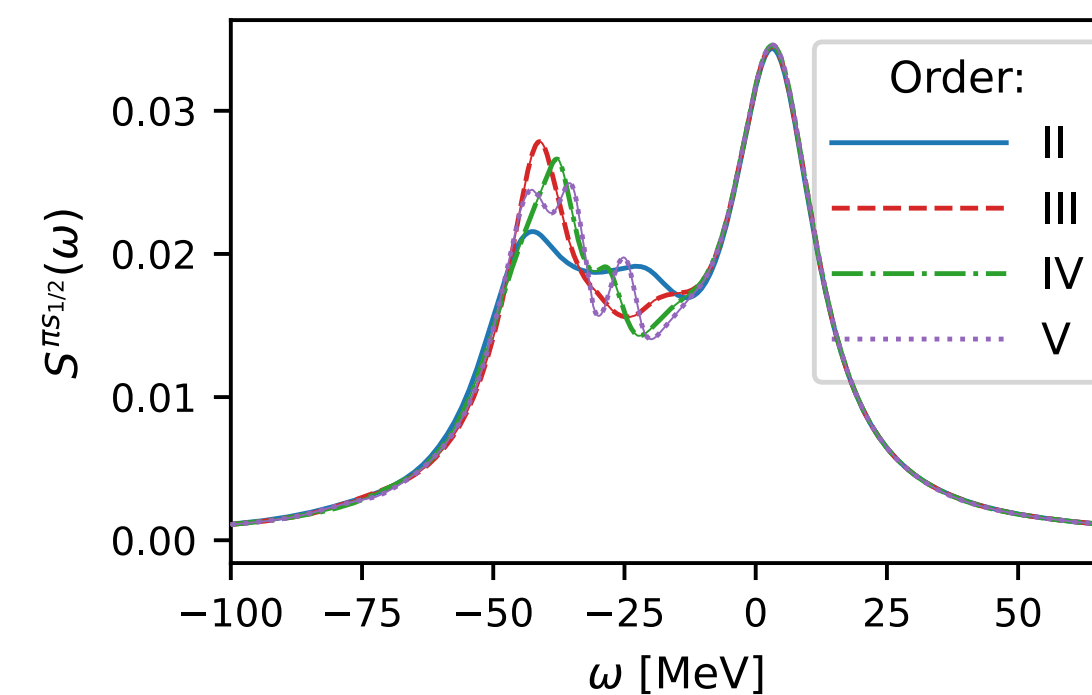
Monte Carlo integration
in the topological space
of Feynman diagrams:



Time-ordered Diagrammatic Monte Carlo for ^{16}O

Stefano Brolli^{1,2,*} and Carlo Barbieri^{1,2,†}

¹Dipartimento di Fisica "Aldo Pontremoli," Università degli Studi di Milano, via Celoria 16, I-20133 Milano, Italy
²INFN, Sezione di Milano, via Celoria 16, I-20133 Milano, Italy
(Dated: May 8, 2026)



See talk by S. Brolli later this
morning !!!



Emulating the Green's Function

Consider a Hamiltonian with an affine dependence on a parameter g . We compute a set of snapshots $\{|\Psi(g_j)\rangle\}_j$.

- Ground state (from eigenvector continuation):

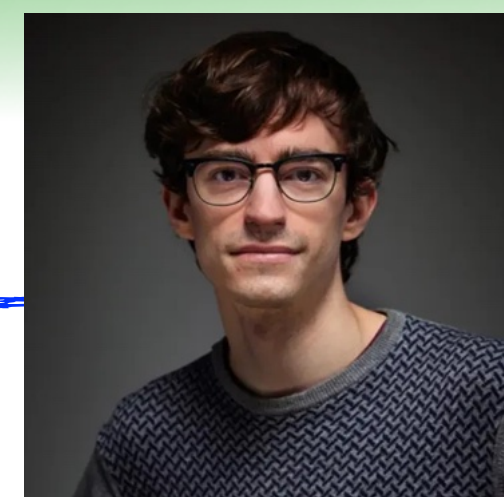
$$|\Psi_0^A(g)\rangle \approx \sum_{k=1}^N v_k |\Psi_0^A(g_k)\rangle.$$

- Excited states:

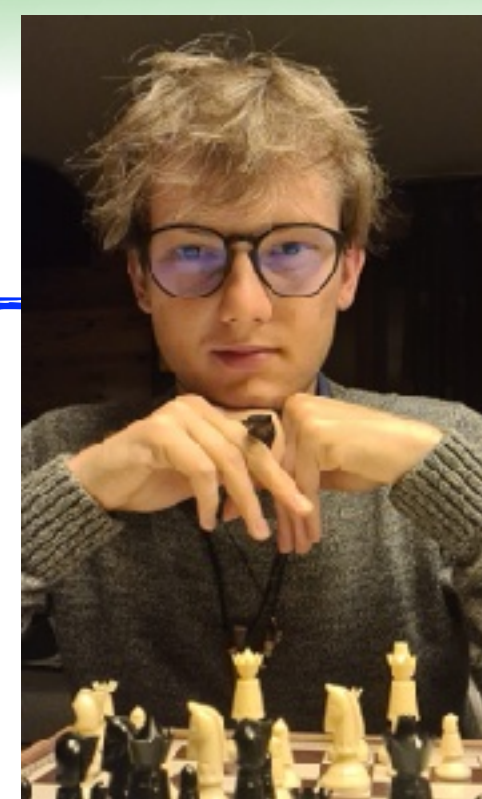
$$|\Psi_n^{A+1}(g)\rangle \approx \sum_{k\alpha} A_{k\alpha}^n c_\alpha^\dagger |\Psi_0^A(g_k)\rangle$$

$\mathcal{M}$ and $\mathcal{N}$ can be computed exactly or extracted from SCGF calculations and used as the primary matrices of a Parametric Matrix Model (PMM). Cook et al., Nat. Commun. 16, 5929 (2025)

$$H \equiv H(g)$$



A. Scalesi
@ Chalmers
(and in the audience...)



S. Brolli
(PhD candidate,
Milan)

—> *Linear equations alike to a parametric Matrix Model:*

$$\sum_{k\alpha} \langle \Psi_0^A(g_j) | c_\beta H(g) c_\alpha^\dagger | \Psi_0^A(g_k) \rangle A_{k\alpha}^n = E_n^{A+1} \sum_{k\alpha} \langle \Psi_0^A(g_j) | c_\beta c_\alpha^\dagger | \Psi_0^A(g_k) \rangle A_{k\alpha}^n$$

Linear in g . $\sum_{k\alpha} \boxed{\mathcal{M}_{j\beta,k\alpha}(g)} A_{k\alpha}^n = E_n^{A+1} \sum_{k\alpha} \boxed{\mathcal{N}_{j\beta,k\alpha}} A_{k\alpha}^n$ Does not depend on g .

$$\langle \Psi_n^{A+1}(g) | c_\beta^\dagger | \Psi_0^A(g) \rangle = \sum_{jk\alpha} v_j \mathcal{N}_{j\beta,k\alpha} A_{k\alpha}^n \quad \epsilon_n^+ = E_n^{A+1} - E_0^A$$

Emulating the Green's Function

Richardson Model:

$$\sum_{k\alpha} \mathcal{M}_{j\beta,k\alpha}(g) A_{k\alpha}^n = E_n^{A+1} \sum_{k\alpha} \mathcal{N}_{j\beta,k\alpha} A_{k\alpha}^n$$

$$\langle \Psi_n^{A+1}(g) | c_\beta^\dagger | \Psi_0^A(g) \rangle = \sum_{jk\alpha} v_j \mathcal{N}_{j\beta,k\alpha} A_{k\alpha}^n \quad \epsilon_n^+ = E_n^{A+1} - E_0^A$$

$$p = D \quad \text{---}$$

$$\vdots$$

$$p = \frac{D}{2} + 1 \quad \text{---}$$

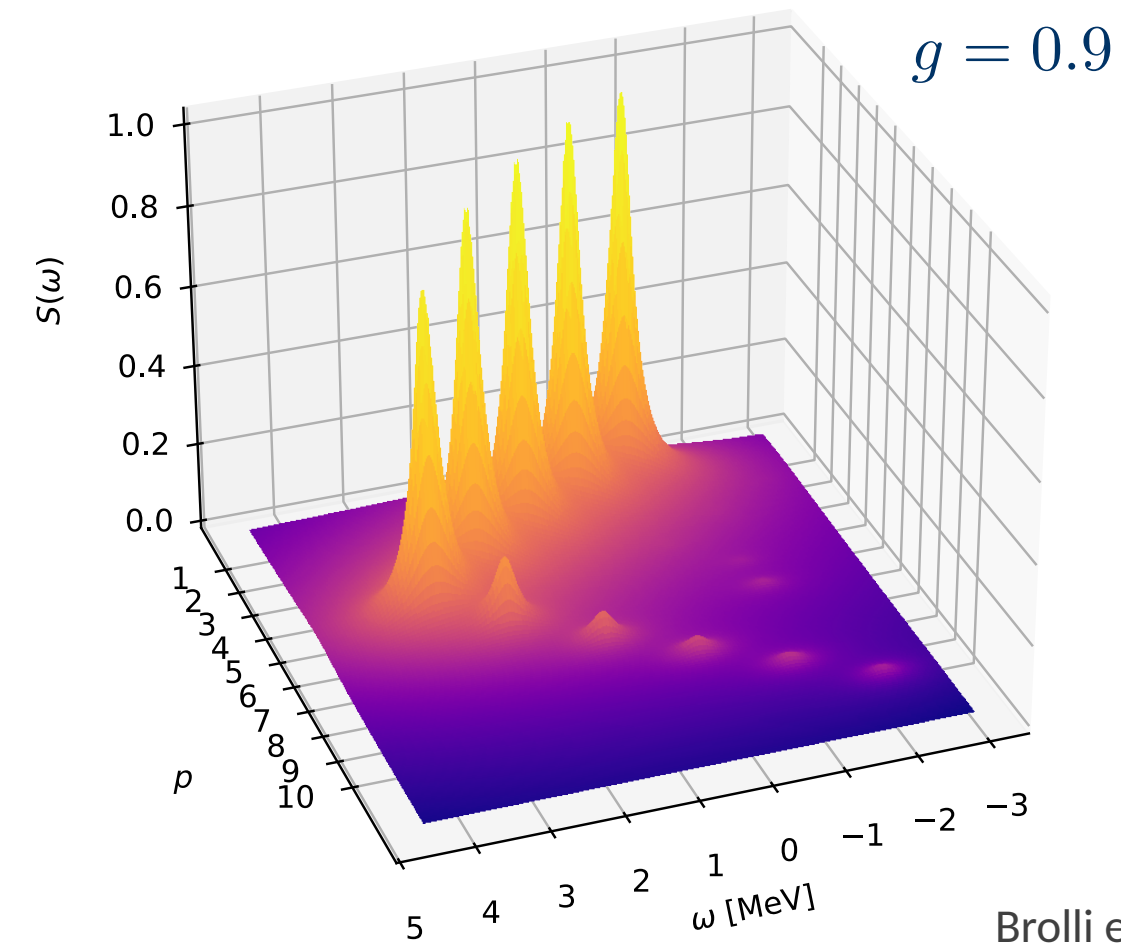
$$p = \frac{D}{2} \quad \text{---} \quad \propto -\frac{g}{2}$$

$$\vdots$$

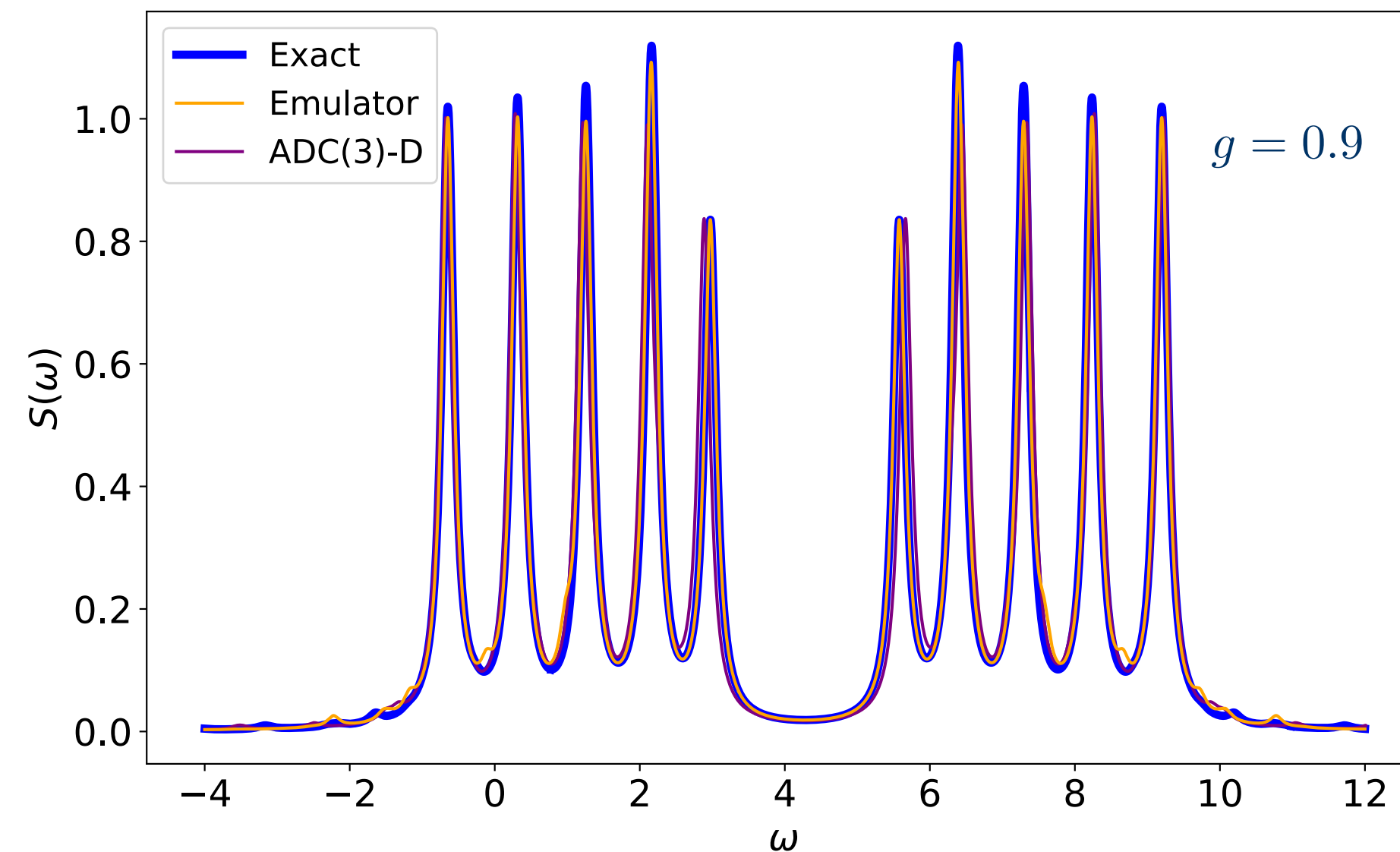
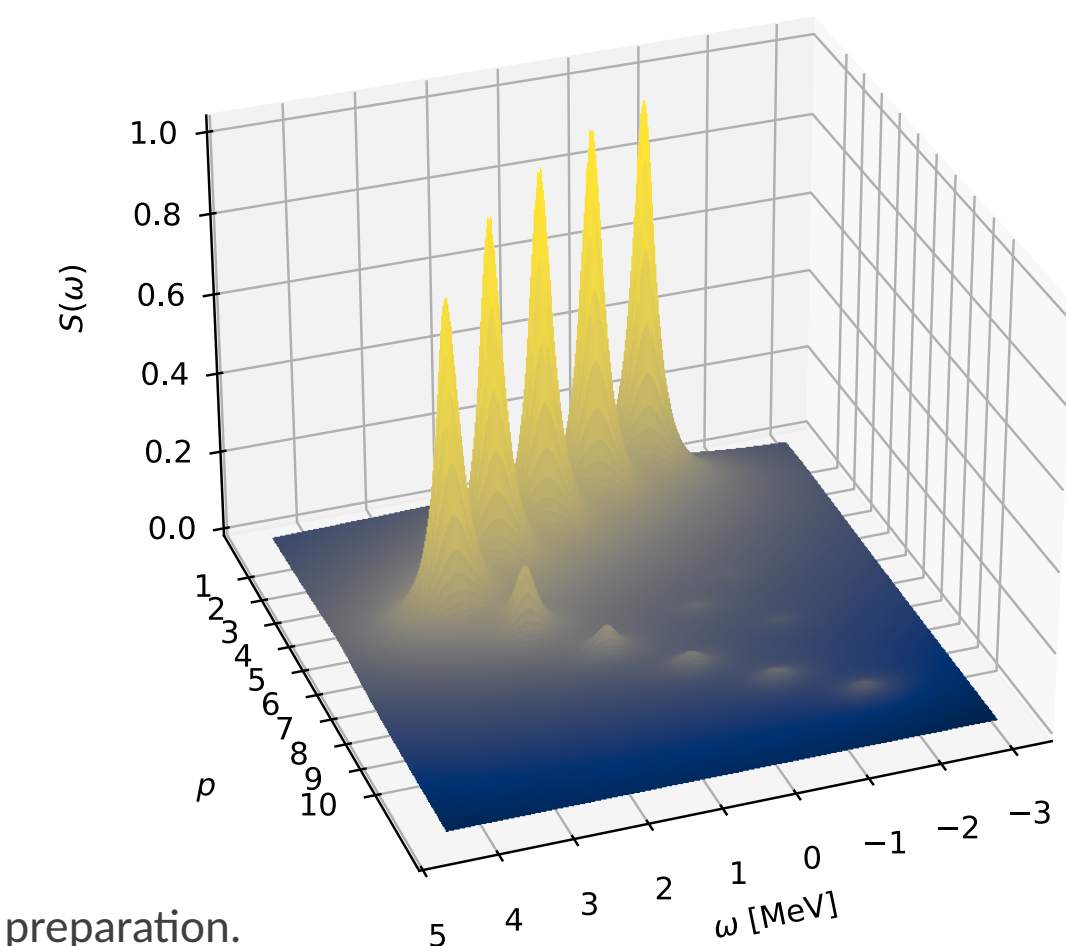
$$p = 2 \quad \text{---} \quad \propto -\frac{g}{2}$$

$$p = 1 \quad \text{---} \quad \propto -\frac{g}{2}$$

Emulator:



Exact:



$$\mathcal{L}_{\text{emul}} = 0.007$$

$$\mathcal{L}_{\text{exact}} = 0.04$$

Brolli et al., In preparation.



SCGF for infinite Matter



Gorkov ansatz... for atomic nuclei

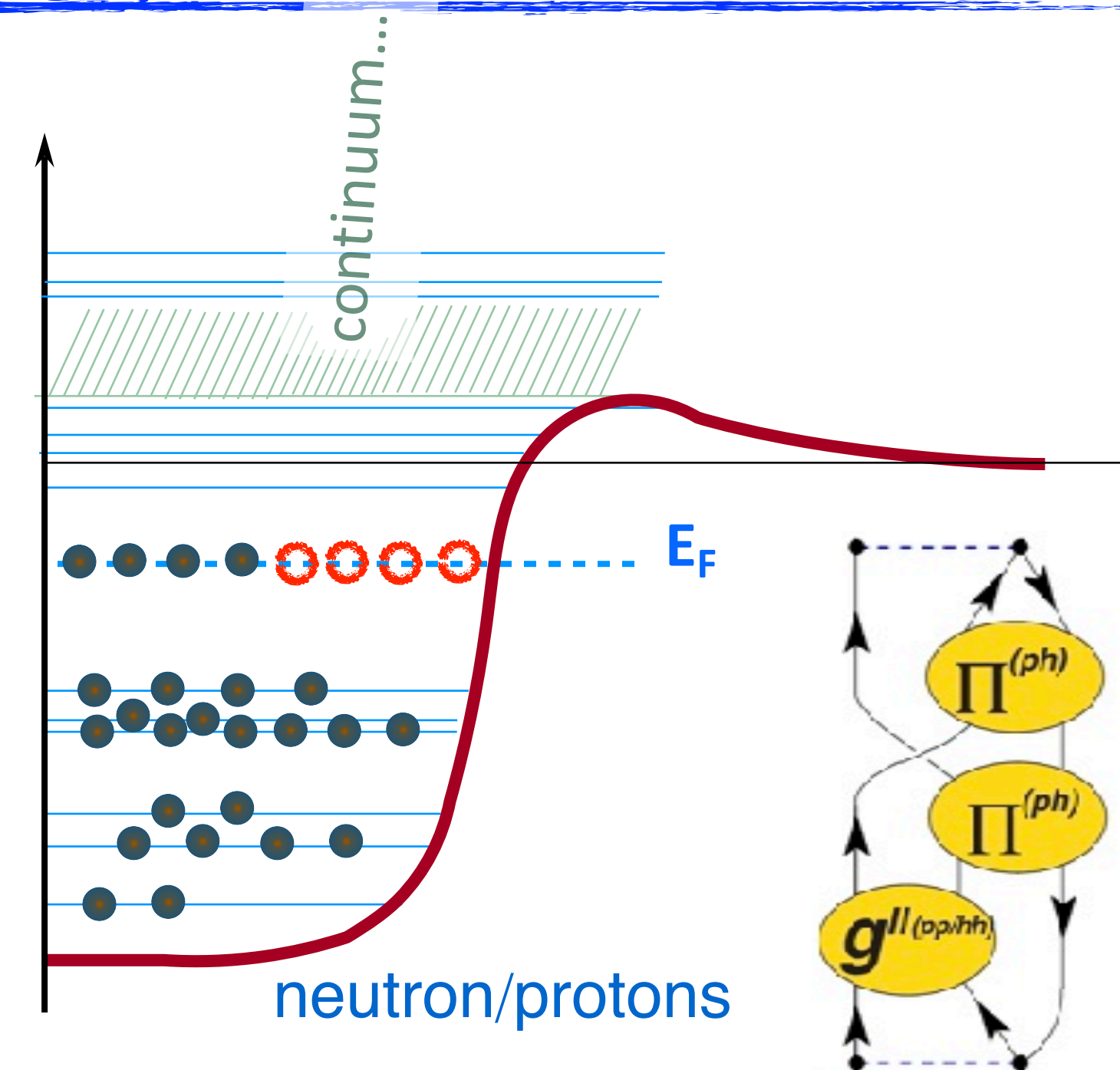
- In the presence of degeneracies (vanishing ph- gaps), enforce (two nucleon) pairing to mitigate unstabilities:

- 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 $N = \langle \Psi_0 | N | \Psi_0 \rangle$

- Generates a set of two normal and two anomalous self-energies:



$$\Sigma_{\alpha\beta}^*(\omega) = \Sigma_{\alpha\beta}^{\infty} + \tilde{\Sigma}_{\alpha\beta}(\omega) = \begin{pmatrix} \Sigma_{\alpha\beta}^{11,\infty} & \Sigma_{\alpha\beta}^{12,\infty} \\ \left(\Sigma_{\beta\alpha}^{12,\infty}\right)^* & -\Sigma_{\beta\alpha}^{11,\infty} \end{pmatrix} + \begin{pmatrix} \tilde{\Sigma}_{\alpha\beta}^{11}(\omega) & \cancel{\tilde{\Sigma}_{\alpha\beta}^{12}(\omega)} \\ -\left(\cancel{\tilde{\Sigma}_{\beta\alpha}^{12}(-\omega)}\right)^* & -\tilde{\Sigma}_{\beta\alpha}^{11}(-\omega) \end{pmatrix}$$

[Gorkov 1958]

In the limit of particle number restoration:

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)



Algebraic diagrammatic construction [ADC(3)] for infinite matter

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

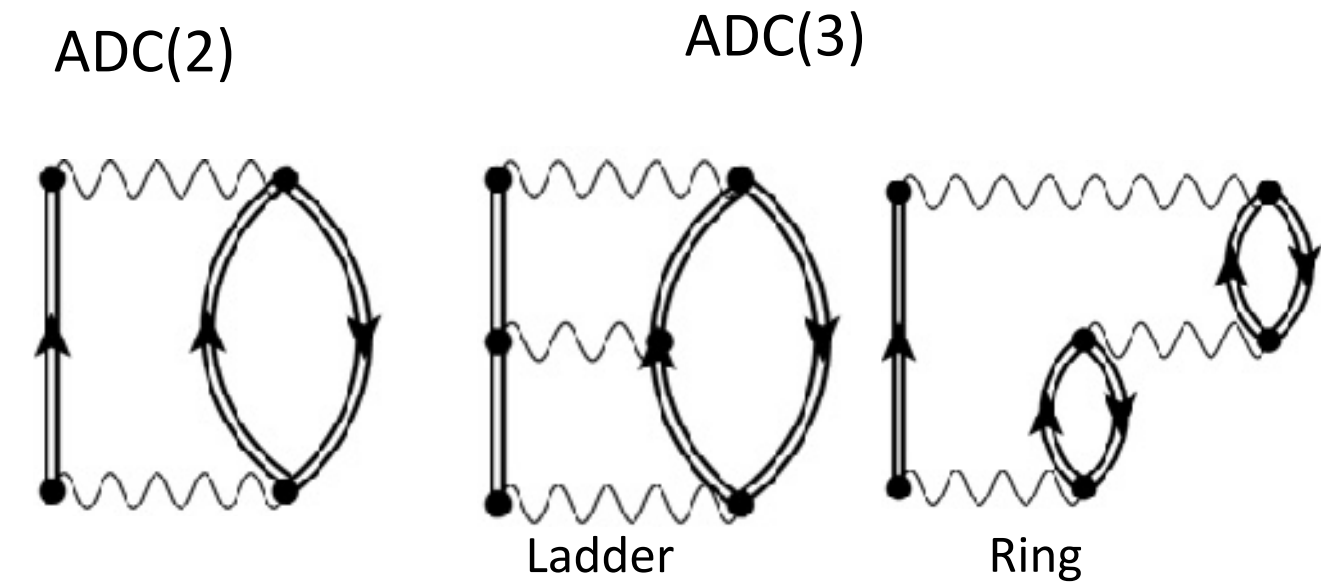
$$\rho = \frac{A}{L} \quad p_F = \sqrt[3]{\frac{6\pi^2\rho}{v_d}} \quad \mathbf{k} = \frac{1}{L} \left(2\pi\mathbf{n} + \boldsymbol{\theta} \right), \quad |\mathbf{k}|^2 = k_x^2 + k_y^2 + k_z^2 \leq \frac{4\pi^2}{L^2} N_{max}$$

$$\hat{H} = \sum_{\alpha} \varepsilon_{\alpha}^0 a_{\alpha}^{\dagger} a_{\alpha} - \sum_{\alpha\beta} U_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{4} \sum_{\substack{\alpha\gamma \\ \beta\delta}} V_{\alpha\gamma,\beta\delta} a_{\alpha}^{\dagger} a_{\gamma}^{\dagger} a_{\delta} a_{\beta} + \frac{1}{36} \sum_{\substack{\alpha\gamma\epsilon \\ \beta\delta\eta}} W_{\alpha\gamma\epsilon,\beta\delta\eta} a_{\alpha}^{\dagger} a_{\gamma}^{\dagger} a_{\epsilon}^{\dagger} a_{\eta} a_{\delta} a_{\beta}.$$

$$\Sigma^{11}(\omega) = \boxed{\Sigma^{11}(\infty)} + \tilde{\Sigma}(\omega)$$

Static self-energy Dynamical self-energy

Self-consistent GF $\Sigma^{\star} = \Sigma^{\star}[g(\omega)]$



↓
Algebraic diagrammatic construction (ADC)

ADC(3) self energy:

ADC(3) includes third-order perturbation theory, ladders, rings...

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

Raimondi et al., Phys Rev C **97**, 054308 (2018)

Barbieri et al., Phys. Rev. C **105**, 044330 (2022)



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DIPARTIMENTO DI FISICA

F. Marino, CB, and G. Colò, Phys. Rev. C **113**, 064301 (2026).



Algebraic diagrammatic construction [ADC(3)] for infinite matter

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

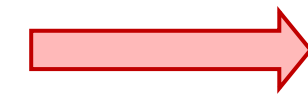
$$\rho = \frac{A}{L} \quad p_F = \sqrt[3]{\frac{6\pi^2\rho}{v_d}} \quad \mathbf{k} = \frac{1}{L} \left(2\pi\mathbf{n} + \boldsymbol{\theta} \right), \quad |\mathbf{k}|^2 = k_x^2 + k_y^2 + k_z^2 \leq \frac{4\pi^2}{L^2} N_{max}$$

Gorkov superfluid formulation

$$\mathbf{g}(\omega) = \mathbf{g}^{(0)}(\omega) + \mathbf{g}^{(0)}(\omega) \mathbf{\Sigma}^*(\omega) \mathbf{g}(\omega)$$

Normal self-energy Pairing field

$$\mathbf{\Sigma}^*(\omega) = \begin{pmatrix} \Sigma^{11}(\omega) & \Delta \\ -\Delta^* & \Sigma^{22}(\omega) \end{pmatrix}$$



$$\begin{pmatrix} T+\Lambda-1\mu_q & M^\dagger & N \\ M & E^>+C-1\mu_q & \\ N^\dagger & & E^<+D-1\mu_q \end{pmatrix} \bigg| \begin{pmatrix} \Delta \\ \\ \end{pmatrix} \bigg/ \begin{pmatrix} \Delta^\dagger & & \\ & -(T+\Lambda)^*+1\mu_q & -M^T \\ & -M^* & -(E^>+C)^*+1\mu_q \\ & -N^T & & -(E^<+D)^*+1\mu_q \end{pmatrix} \begin{pmatrix} \mathcal{U}^q \\ \mathcal{W}^q \\ \mathcal{Z}^q \\ \mathcal{V}^q \\ \mathcal{R}^q \\ \mathcal{S}^q \end{pmatrix} = \hbar\omega_q \begin{pmatrix} \mathcal{U}^q \\ \mathcal{W}^q \\ \mathcal{Z}^q \\ \mathcal{V}^q \\ \mathcal{R}^q \\ \mathcal{S}^q \end{pmatrix}$$

Normal self-energy in full ADC(3) but use pairing only at 1st order

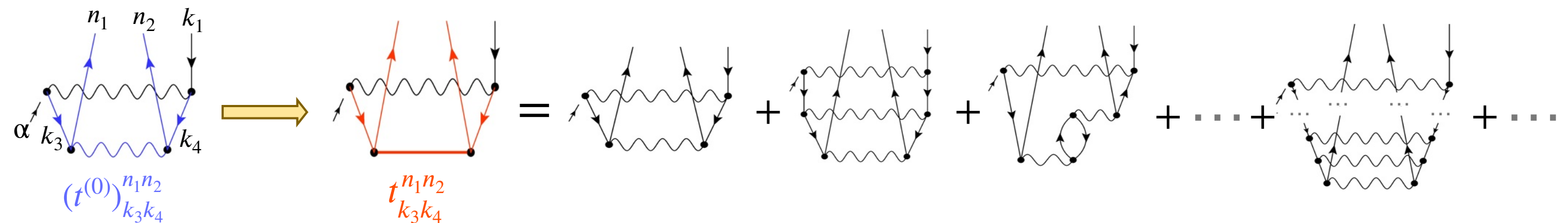
Extension of ADC(3)



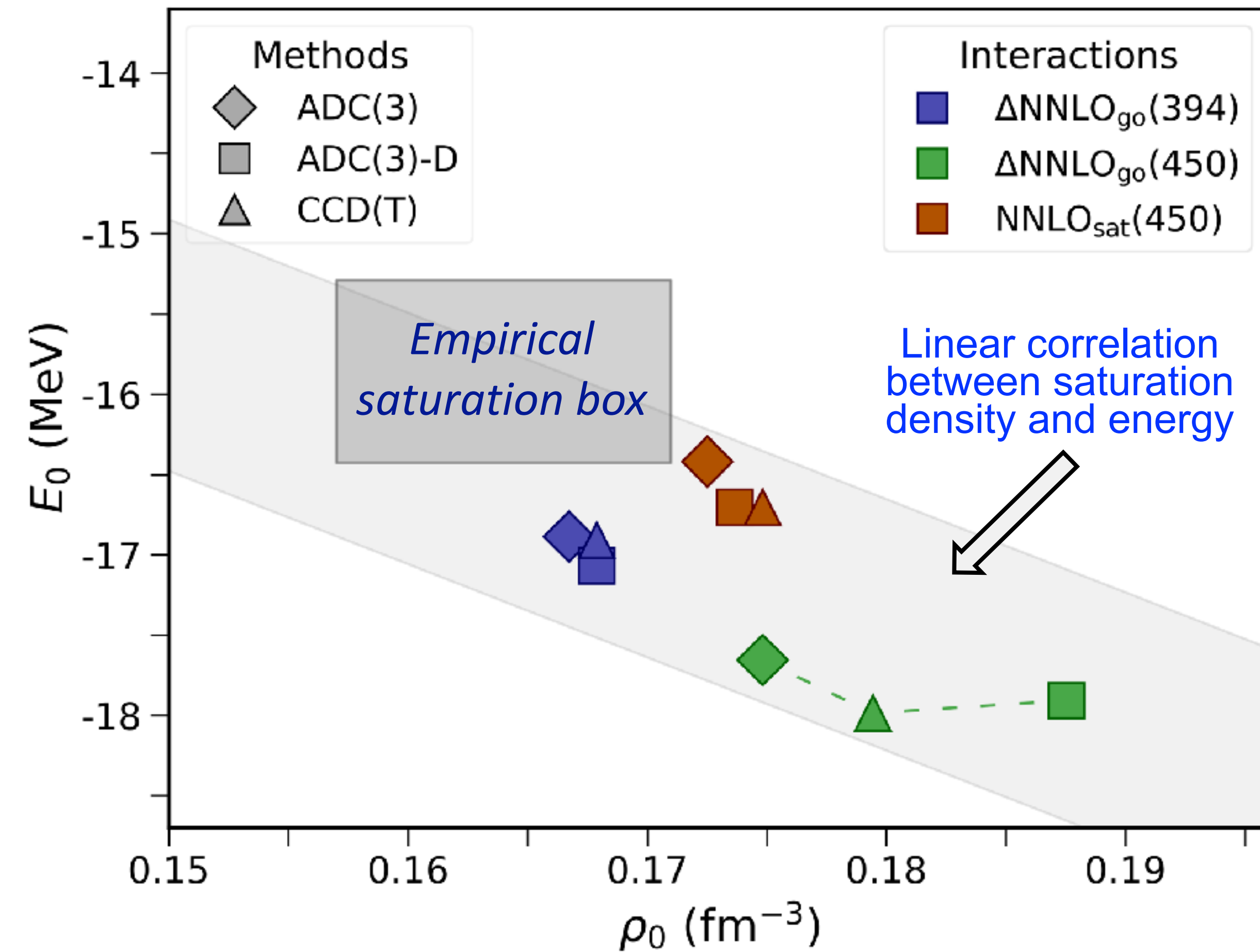
ADC(3)-D

In $\tilde{\Sigma}(\omega)$, replace $t^{(0)}$ with converged T_2 amplitudes

$$(t^{(0)})_{ij}^{ab} = \frac{\langle ab | v | ij \rangle_A}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

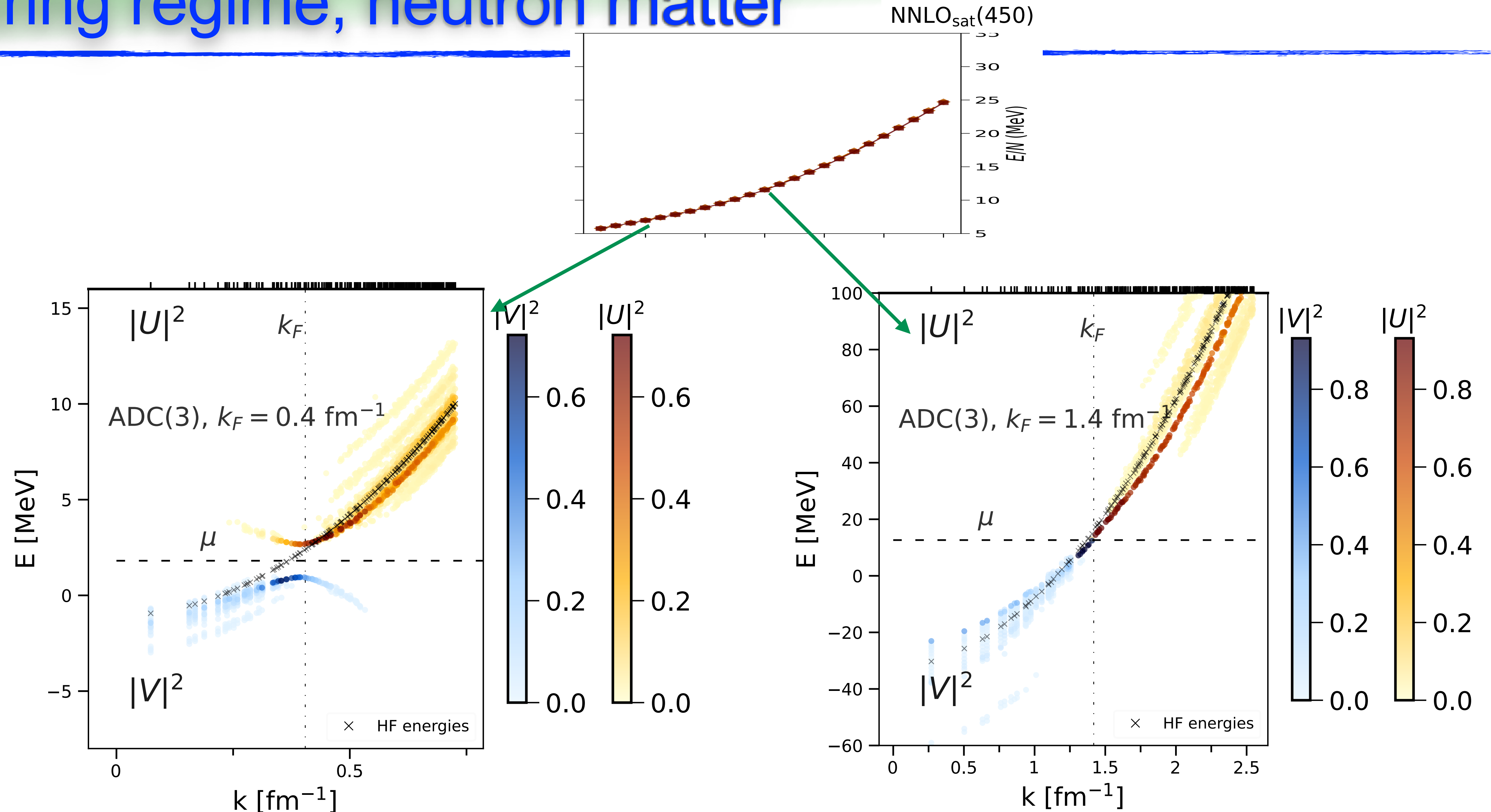


Saturation point of symmetric nuclear matter



- ◆ Generally good agreement across many-body methods
- ◆ **Interaction-dependence** is the dominant uncertainty

Pairing regime, neutron matter



Neural Network Quantum States



Neural Network Quantum States (NQS):

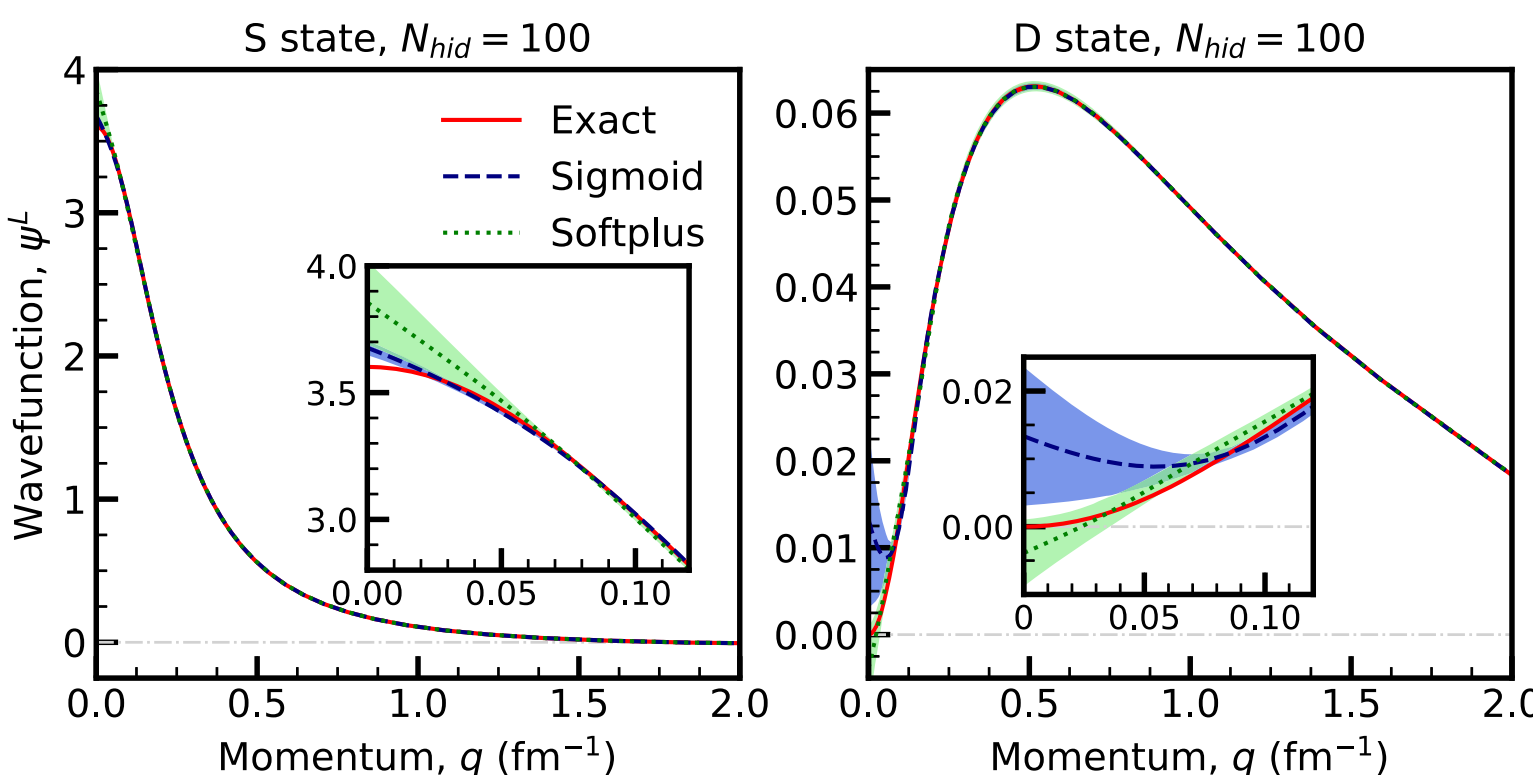
$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = E_V \geq E_0$$

$$|\Psi_V^J\rangle = \prod_{i<j<k} \left(1 - \sum_{\text{cyc}} u(r_{ij}) u(r_{jk}) \right) \prod_{i<j} f(r_{ij}) |\Phi\rangle$$

In short: a VMC with a NN trial wave function!

neural networks

The
deuteron:



Light nuclei:

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC _c
^2H	4 fm^{-1}	$-2.224(1)$	$-2.223(1)$	$-2.224(1)$	-
	6 fm^{-1}	$-2.224(4)$	$-2.220(1)$	$-2.225(1)$	-
^3H	4 fm^{-1}	$-8.26(1)$	$-7.80(1)$	$-8.38(2)$	$-7.82(1)$
	6 fm^{-1}	$-8.27(1)$	$-7.74(1)$	$-8.38(2)$	$-7.81(1)$
^4He	4 fm^{-1}	$-23.30(2)$	$-22.54(1)$	$-23.62(3)$	$-22.77(2)$
	6 fm^{-1}	$-24.47(3)$	$-23.44(2)$	$-25.06(3)$	$-24.10(2)$

Keeble, Rios, Phys. Lett. B **809**, 135743 (2020)

Rozalén Sarmiento, Keeble, EPJ Plus **139**, 189 (2024)

C. Adams, G. Carleo, A. Lovato, N. Rocco,
Phys. Rev. Lett. **127**, 022502 (2021)



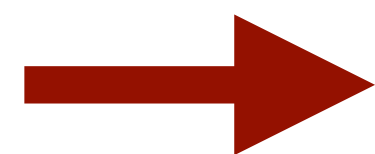
Neural Network Quantum States (NQS):

$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = E_V \geq E_0 \quad |\Psi_V^J\rangle = \prod_{i < j < k} \left(1 - \sum_{\text{cyc}} u(r_{ij}) u(r_{jk}) \right) \prod_{i < j} f(r_{ij}) |\Phi\rangle$$

In short: a VMC with a NN trial wave function!

neural networks

- **NQS often surpass traditional VMC**, with accuracy similar to GFMC/DMC but at a fraction of the cost
- Sometimes referred to as “**science driven learning**”: it is not supervised and the cost function is the variational principle.
- However: the **variational principle is the only guiding principle** exploited, what about the rest??



Use Physics Informed Neural Networks (PINN) !

Physics Informed Neural Networks

- ◆ Generally used for solving ODE and PDE: NN represent the solution $f(\mathbf{x})$, $\partial f(\mathbf{x})/\partial x_i, \dots$
- ◆ General PINN cost function:

$$\mathcal{L}_{PINN} = \mathcal{L}_{PDE} + \mathcal{L}_{phys} + \mathcal{L}_{data}$$

constraint from
diff. equations

Physics constraints
(e.g. boundary conditions)

Any known (measured) data

Physics Informed Neural Networks for nuclei

- ♦ The Schrödinger problem is an integro-differential eq.: use NN to represent $\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots)$
- ♦ Many-body PINN cost function:

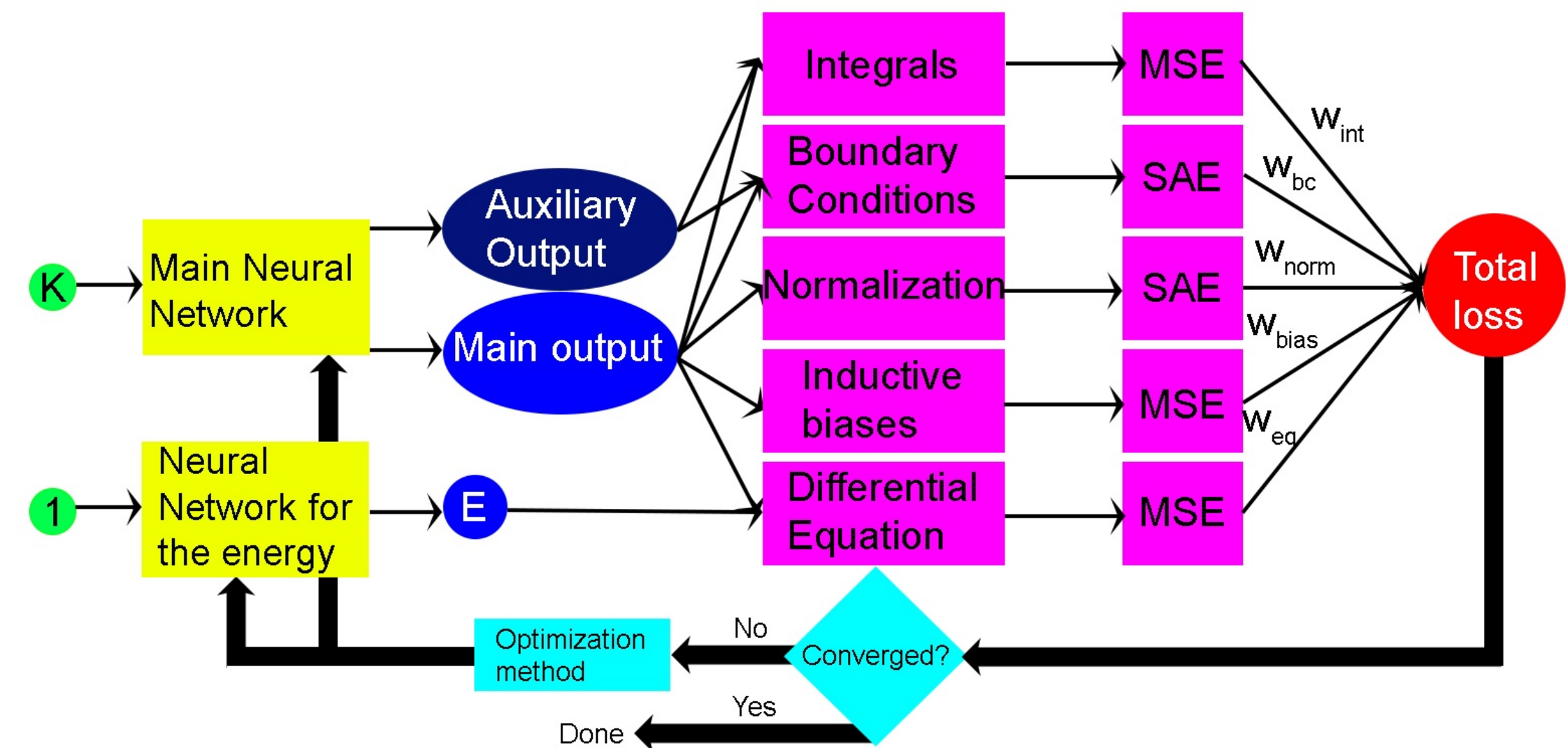
$$\mathcal{L}_{PINN} = \mathcal{L}_{PDE} + \mathcal{L}_{phys} + \cancel{\mathcal{L}_{data}}$$

Schrod. eq.

$$\mathcal{L}_{PDE} = \sum_{i=0}^{N_c} |[H\psi](x_i) - E\psi(x_i)|^2 \quad \text{with} \quad E = \frac{\langle \psi | H | \psi \rangle}{\mathcal{I}[\psi]}$$

Physics constraints

$$\mathcal{L}_{phys} = w_{int} \mathcal{L}_{int} + w_{BCs} \mathcal{L}_{BCs} + w_{norm} \mathcal{L}_{norm} + w_{var} \mathcal{L}_{var} + \dots$$



- ♦ Through boundary conditions, one may target excited (and scattering) states.

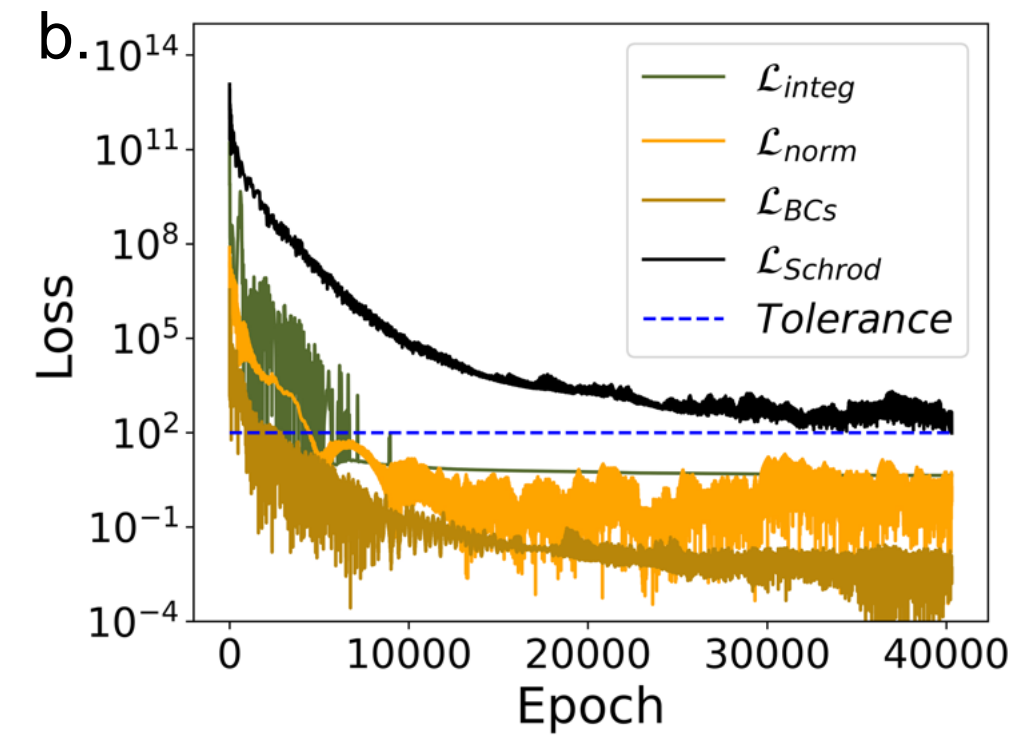
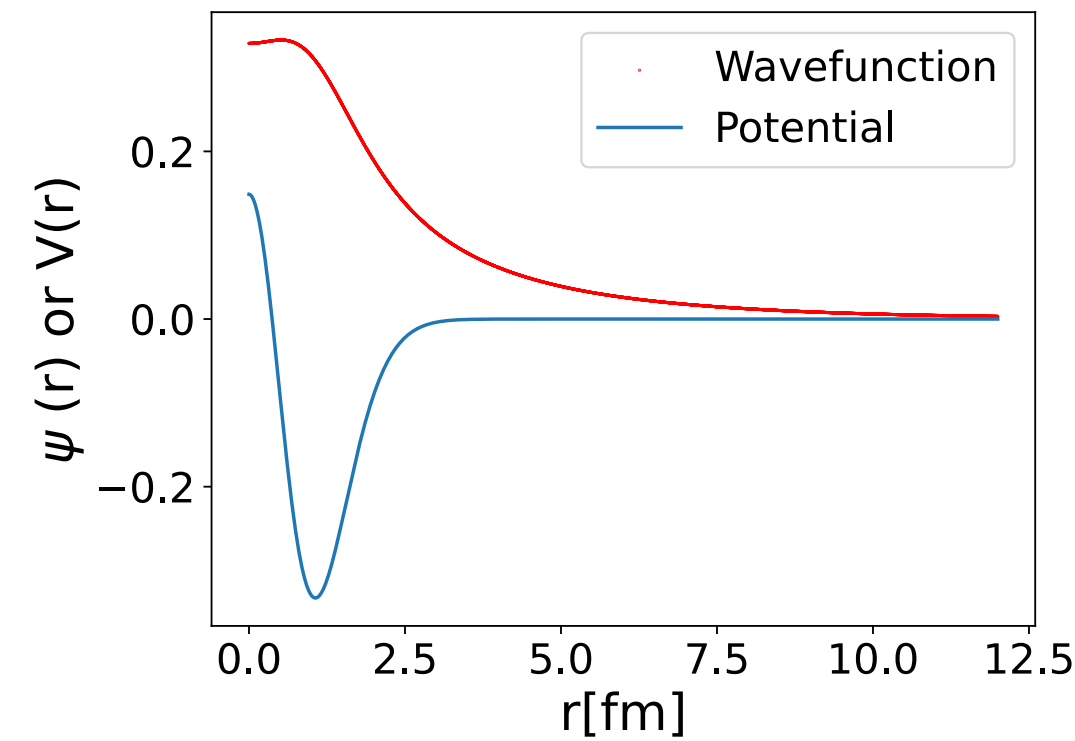
L. Brevi, A. Mandarino, E. Prati,
Technologies 12, 174 (2024); New J. Phys. **26**, 103015 (2024).

L. Brevi, A. Mandarino, CB, E. Prati, arXiv:2602.11193

Physics Informed Neural Networks for the deuteron

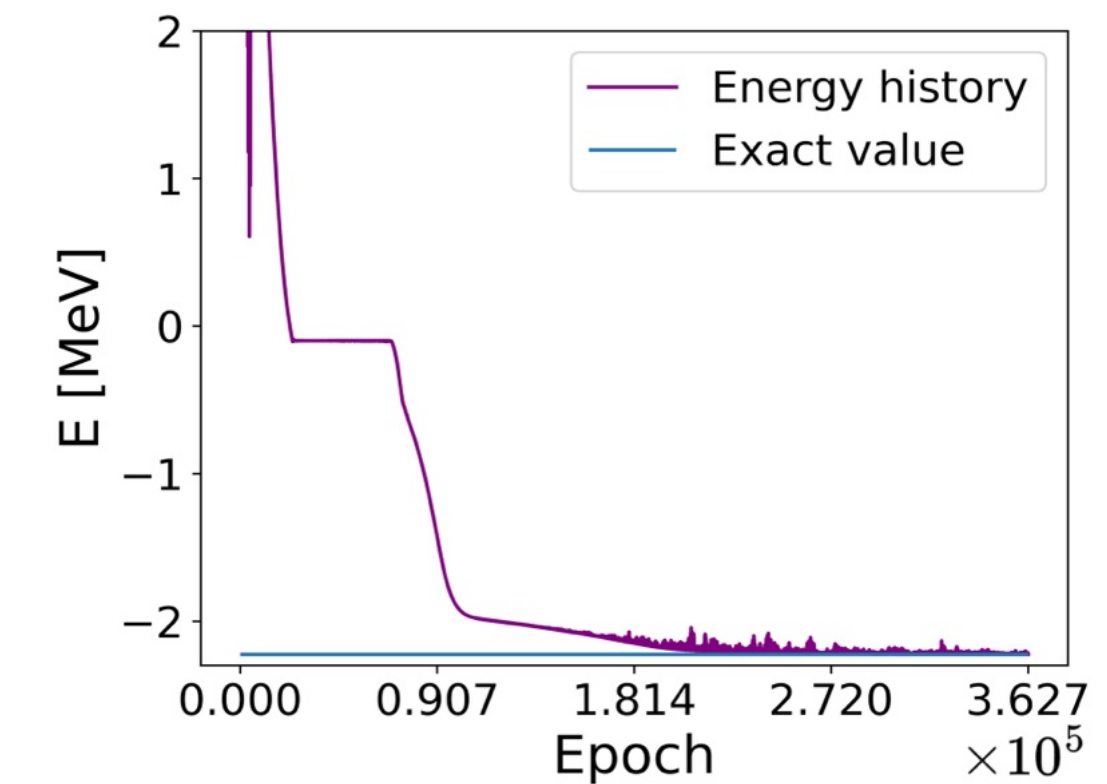
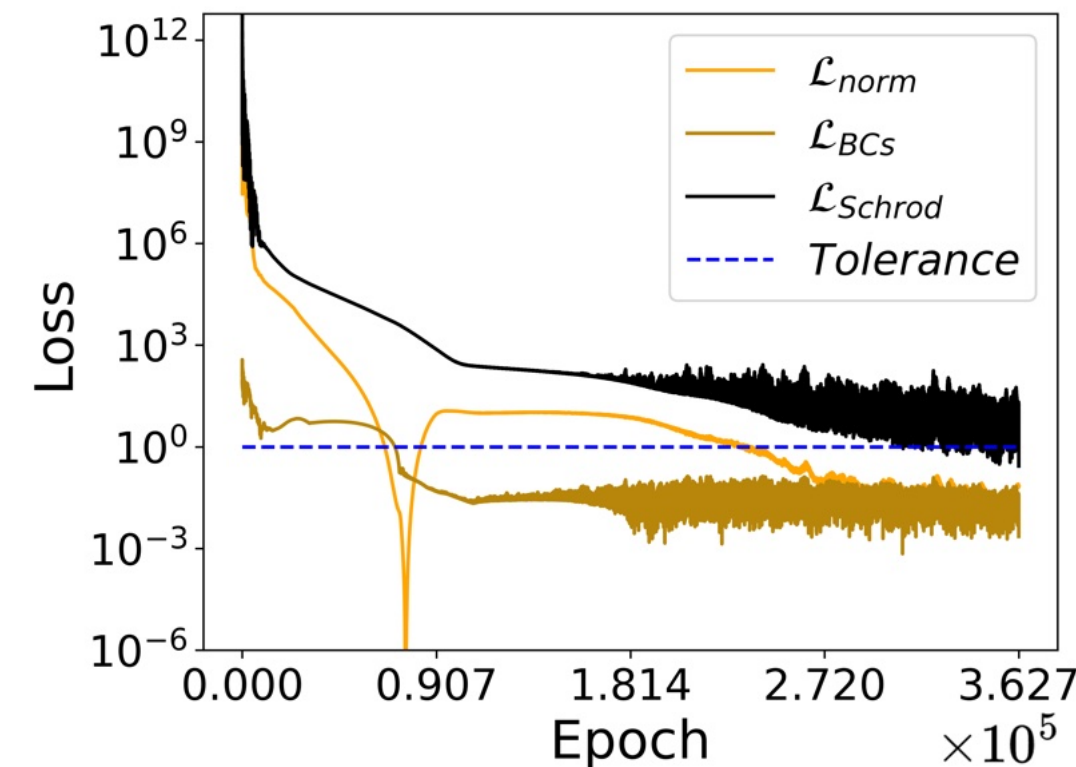
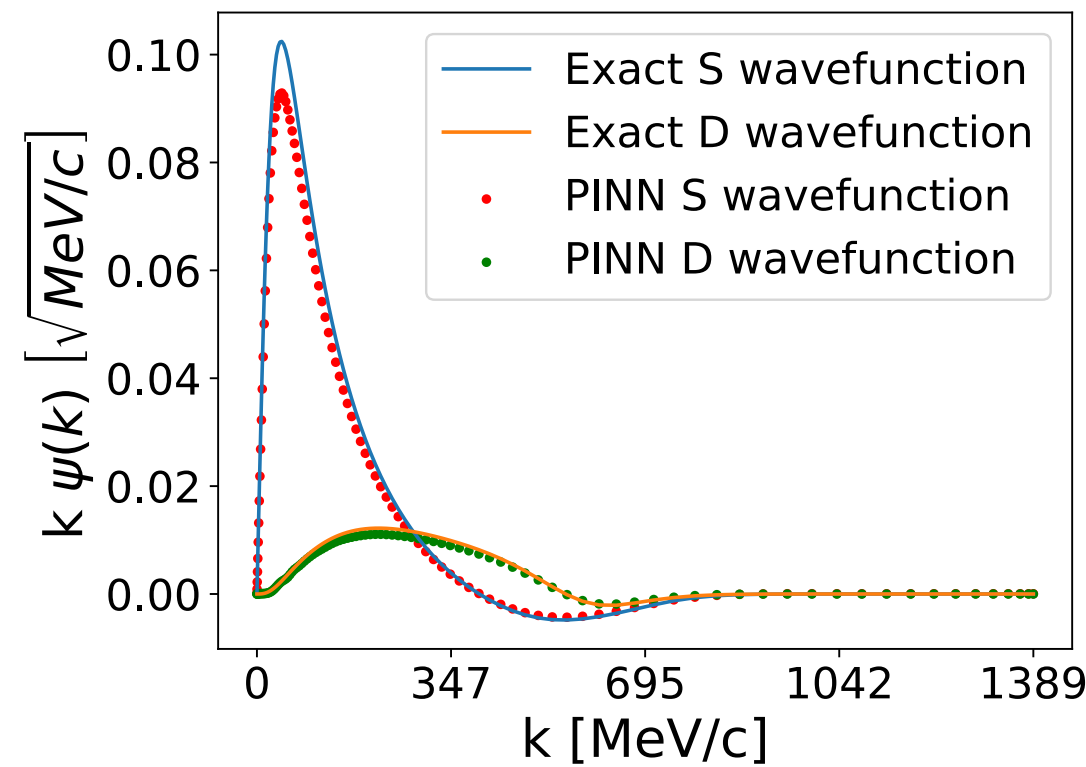
L. Brevi, A. Mandarino, CB, E. Prati, arXiv:2602.11193

◆ Coordinate space, Minnesota potential:



	$Err_{E,exp}$	$Err_{E,Num}$	$1 - \mathcal{F}_\psi$
Minnesota	0.01	1×10^{-8}	
N4LO(550)	-5.96×10^{-6}	-5.21×10^{-5}	1×10^{-5}
CD-Bonn	-6.01×10^{-4}	-2.76×10^{-7}	1×10^{-9}

◆ Momentum space with N4LO(550) from EMN:



$$\mathcal{L}_{phys} = w_{ODE} \mathcal{L}_{ODE} + (w_{int} \mathcal{L}_{int} + w_{norm} \mathcal{L}_{norm}) + w_{BCs} \mathcal{L}_{BCs} + w_{var} \mathcal{L}_{var}$$

Conclusions

- ◆ Faddeev Random Phase Approximation (FRPA) and Algebraic diagrammatic construction (ADC) — provide a systematic way
- ◆ Currently, NP advances in precision beyond ADC(3)/FRPA are needed to address scattering process
- ◆ Gorkov formulation (for open shells) and three-nucleon forces
- ◆ Partial Gorkov-ADC(3) simulations are within reach. For infinite matter and...
- ◆ Novel developments: breakthrough in DiagrammaticMC for nuclei and Emulators for SCGF (PMM based)
- ◆ Novel developments: Physics Informed Neural Network (PINN) as an alternative to NQS.

**Thank you for
your attention !!!**

