A hybrid Gorkov-Dyson SCGF for infinite matter and Neural Network based methods in nuclei

PAINT26

Vancouver, Feb. 24-27, 2026

Carlo Barbieri

Università degli Studi di Milano & INFN

UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

INFN MILANO

Rooting Nuclear Density Functional into 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*

F. Marino (EPS PhD thesis prize, 2025)

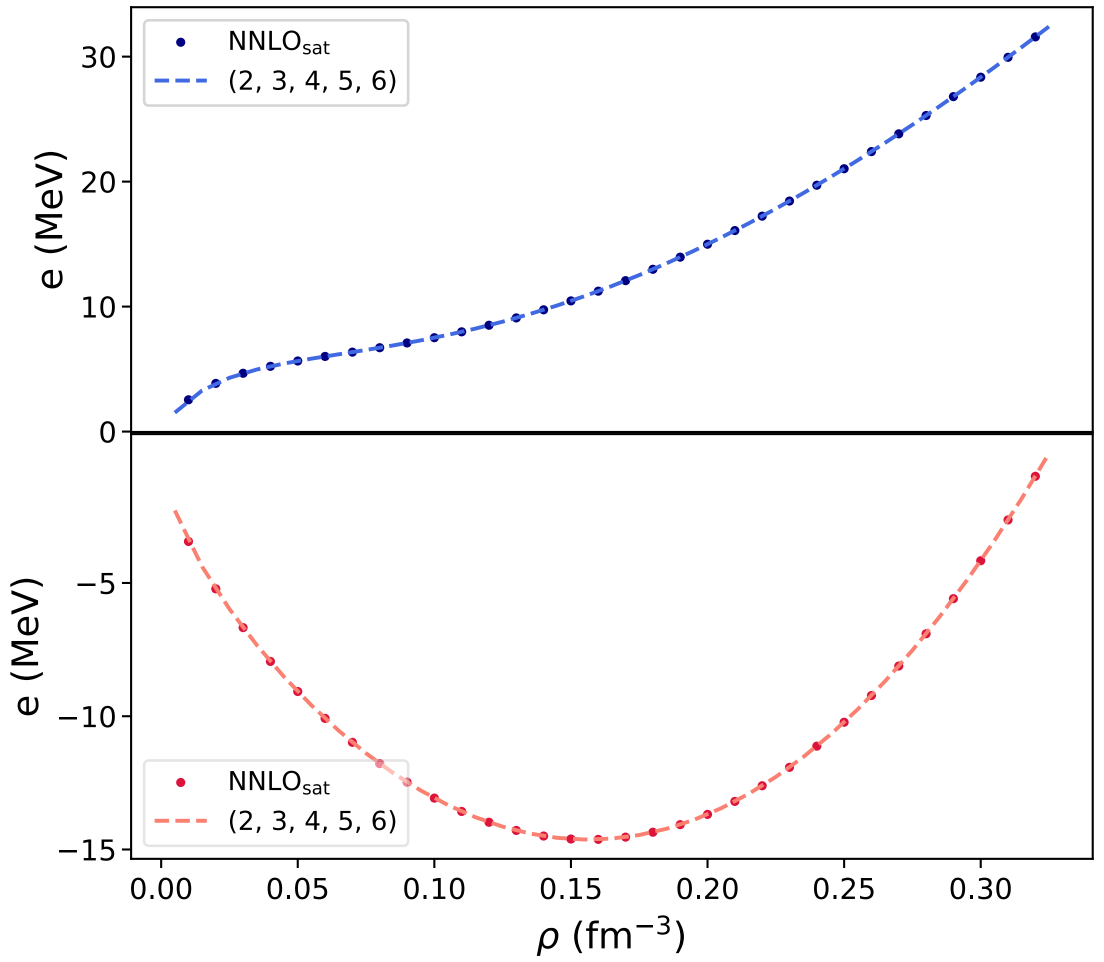
DFT is in principle exact – but the energy density functional (EDF) is not known

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

Machine-learn DFT functional on the nuclear equation of state

Jacob's ladder

+ approximate GA



Benchmark in finite systems

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

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

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

Benchmark on finite systems

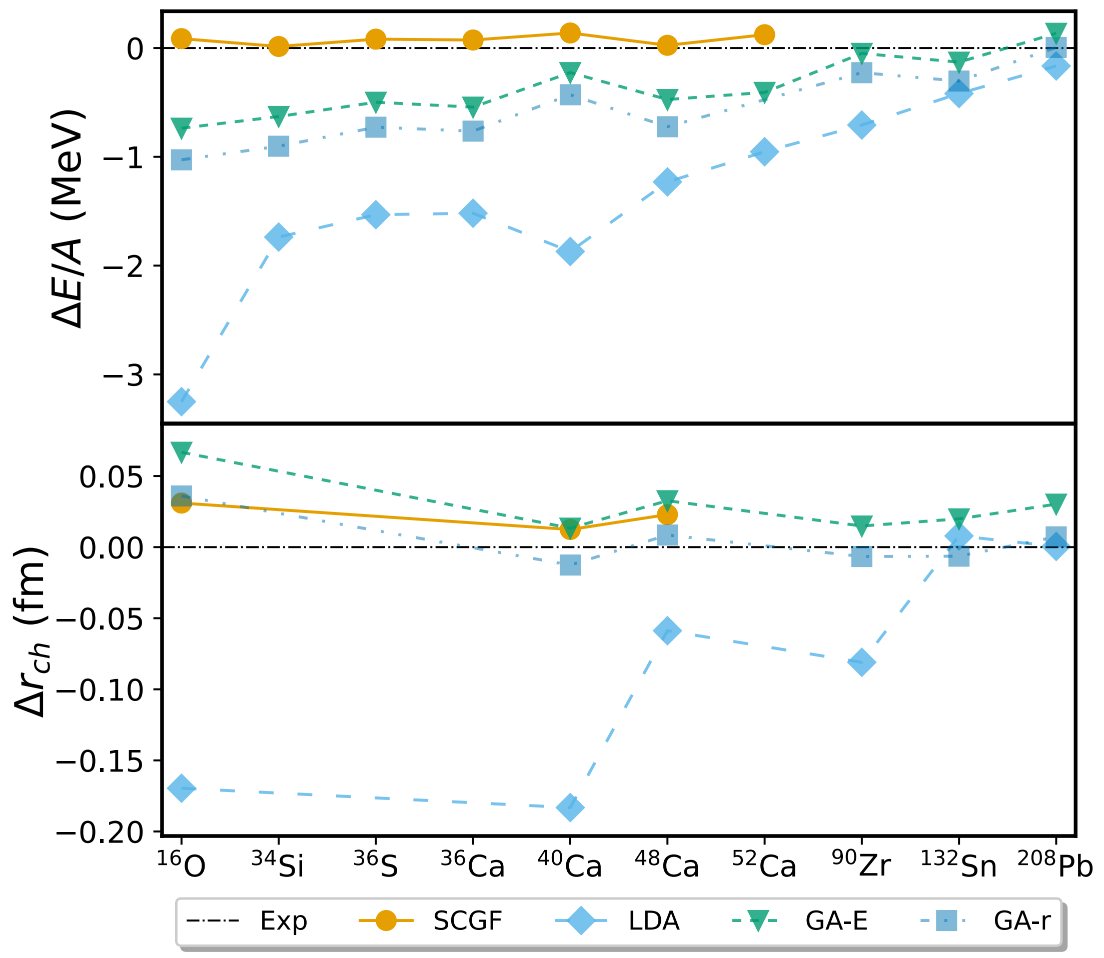
Machine-learn DFT functional on the nuclear equation of state

Jacob's ladder

+ approximate GA

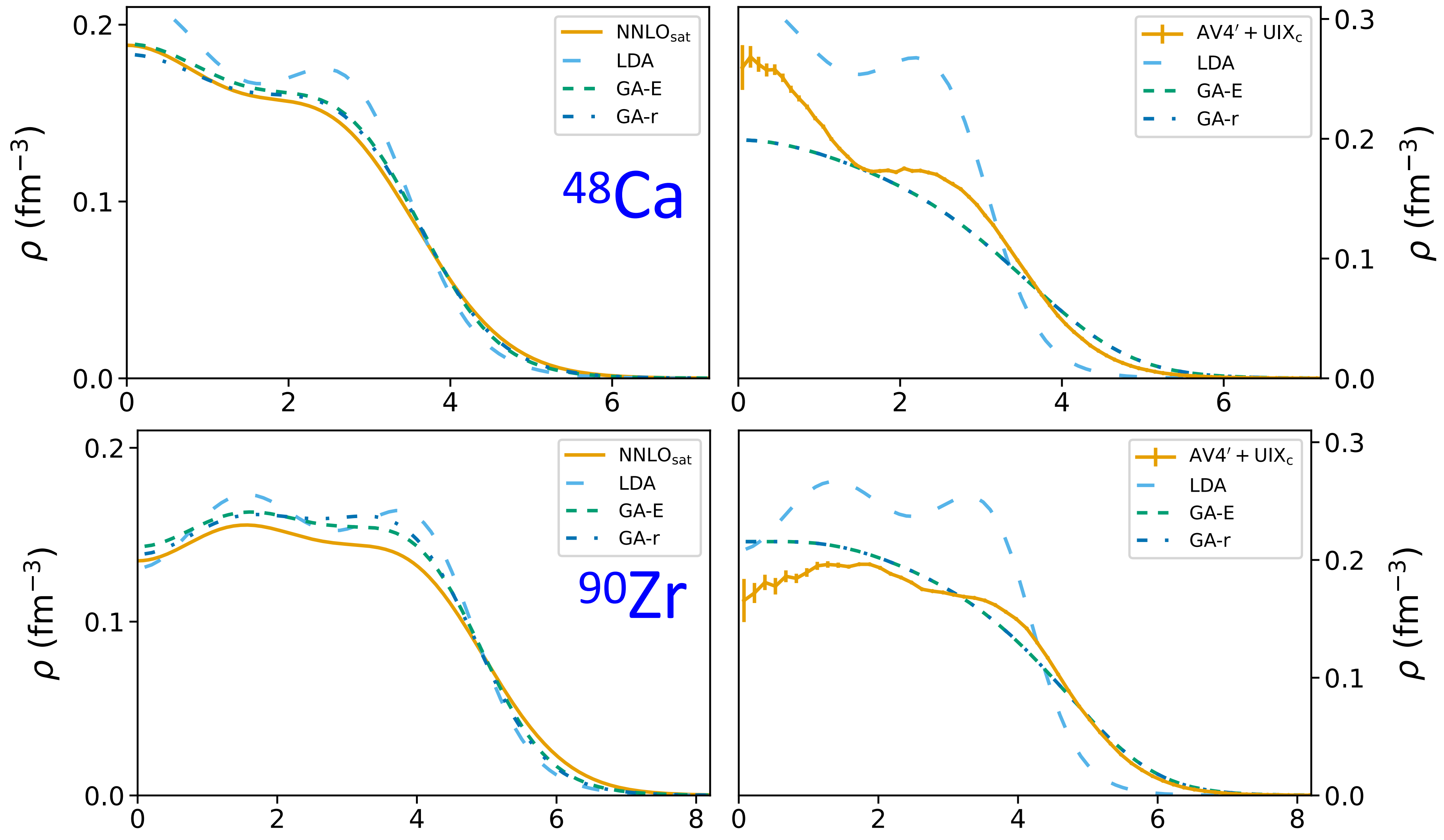
Benchmark in finite systems

Gradient terms are important!



SCGF/NNLO-sat :

AFDMC/AV4' :



Problem: gradients here were added *ad hoc* to the EDF, so far.

—>

Need to extract gradient information from non-uniform matter. E.g., external (monocromatic) perturbations:

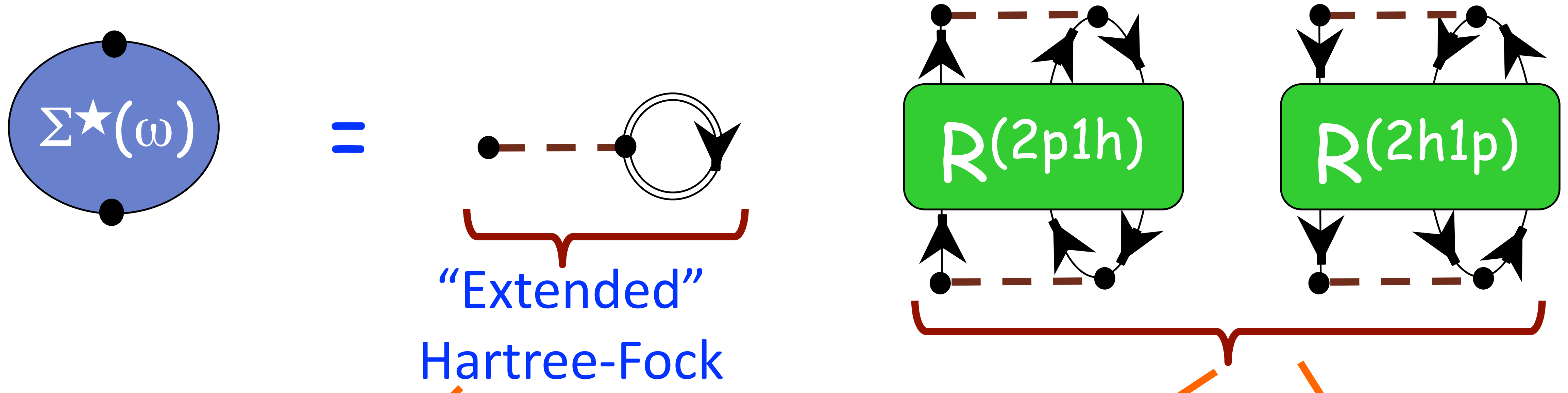
$$v(\mathbf{x}) = v_q e^{i\mathbf{q}\cdot\mathbf{x}} + c.c. = 2v_q \cos(\mathbf{q}\cdot\mathbf{x})$$
$$\delta\rho(\mathbf{x}) = 2\rho_q \cos(\mathbf{q}\cdot\mathbf{x})$$

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

Algebraic Diagramatic Construction at 3rd order [ADC(3)] in a few words

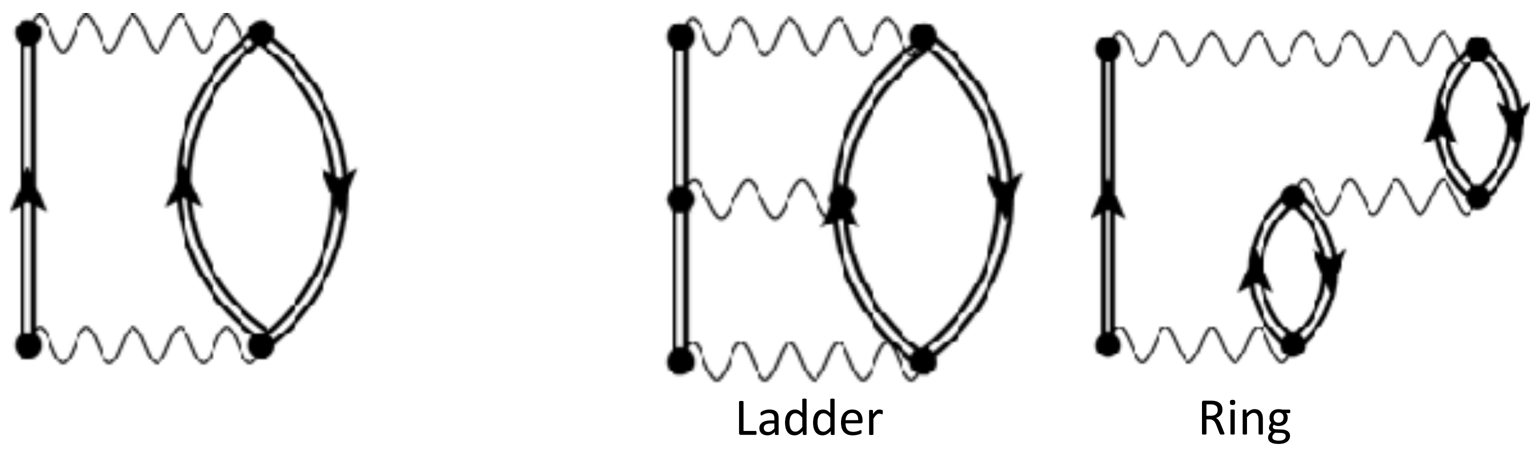
The nuclear self-energy includes both *mean field* and *dynamical correlations* (leading to optical potentials and spectroscopy)

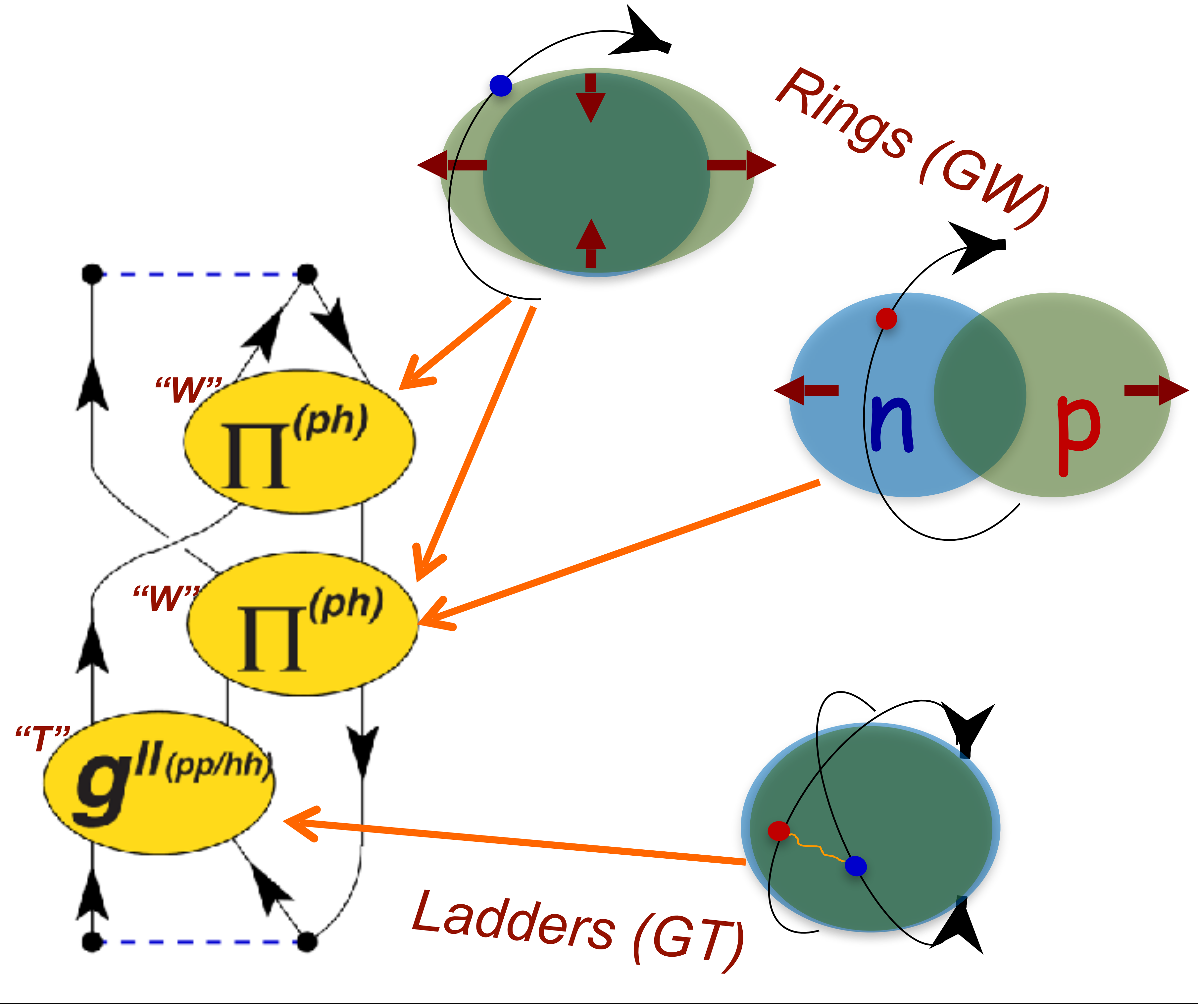
ADC(3): Lect. Notes in Phys ***936*** *(2017) — Chapter 11.*



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

The ADC(3) truncation level uses diagrams up to 3rd order as 'seeds' for all-orders summations:





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

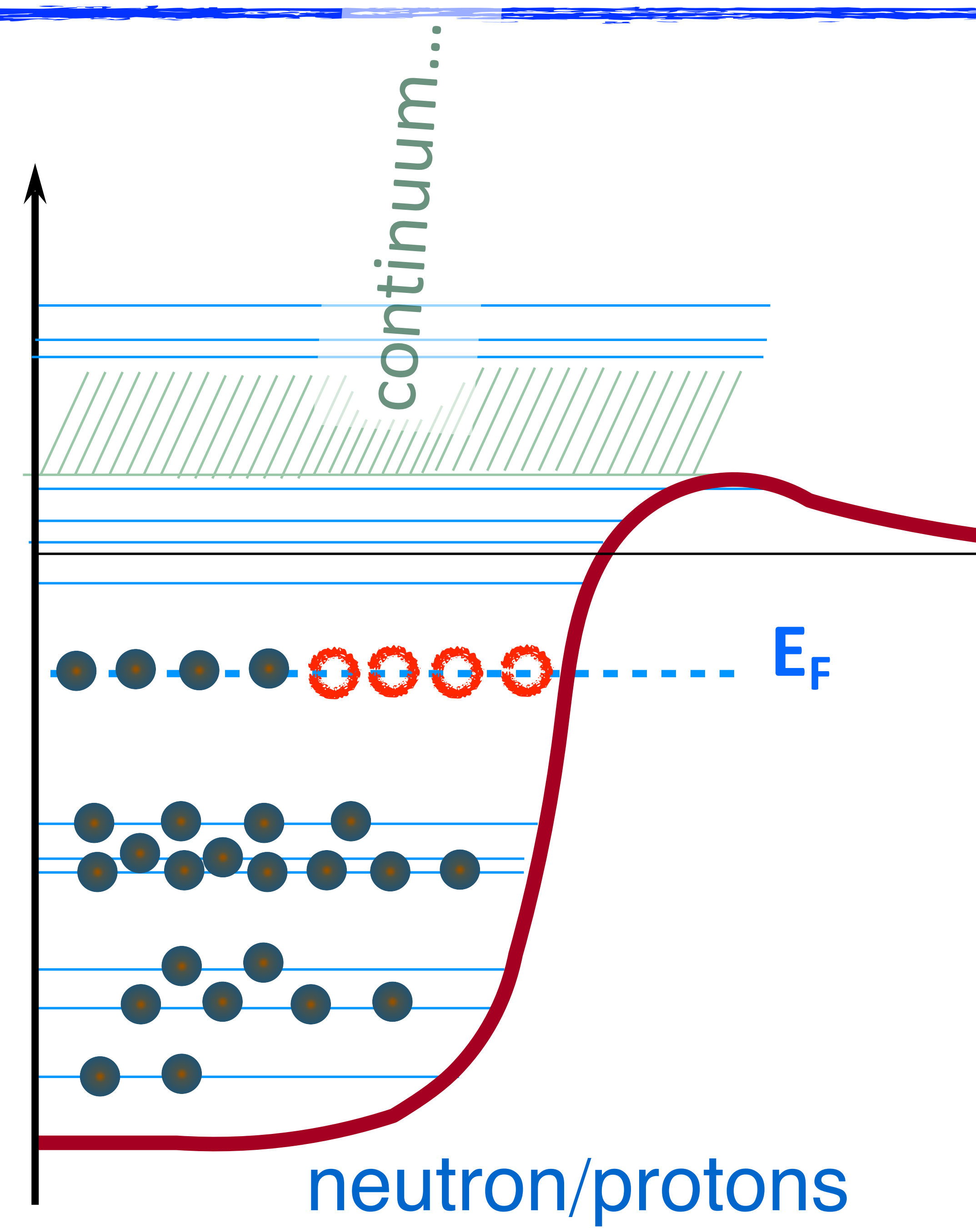
Gorkov ansatz… for atomic nuclei

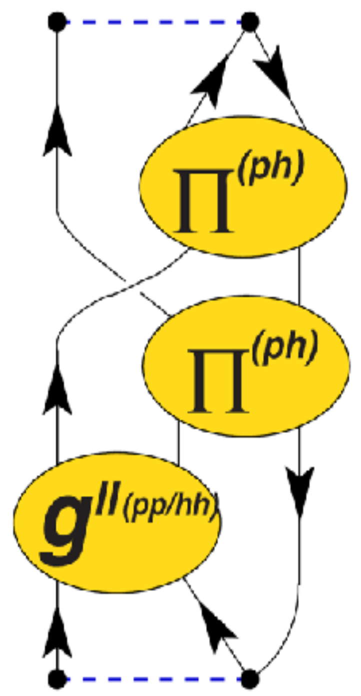
➢ In the presence of degenracies (vanishing ph- gaps), enforce (two nucleon) pairing to mitigate unstabilities:

➢ 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 $\Omega_0 = \min\limits_{|\Psi_0\rangle} \{\langle \Psi_0 | \Omega | \Psi_0 \rangle\}$ under the constraint $\mathrm{N} = \langle \Psi_0 | N | \Psi_0 \rangle$





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

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

[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:

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

Gorkov superfluid formulation

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

Normal self-energy Pairing field

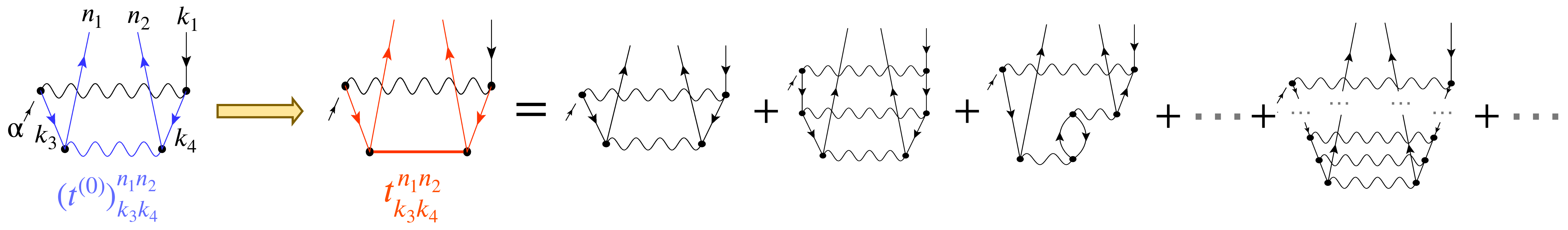
$$\Sigma^\star(\omega) = \begin{pmatrix} \Sigma^{11}(\omega) & \Delta \\ -\Delta^* & \Sigma^{22}(\omega) \end{pmatrix}$$

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

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

Extension of ADC(3) ⟹ **ADC(3)-D**

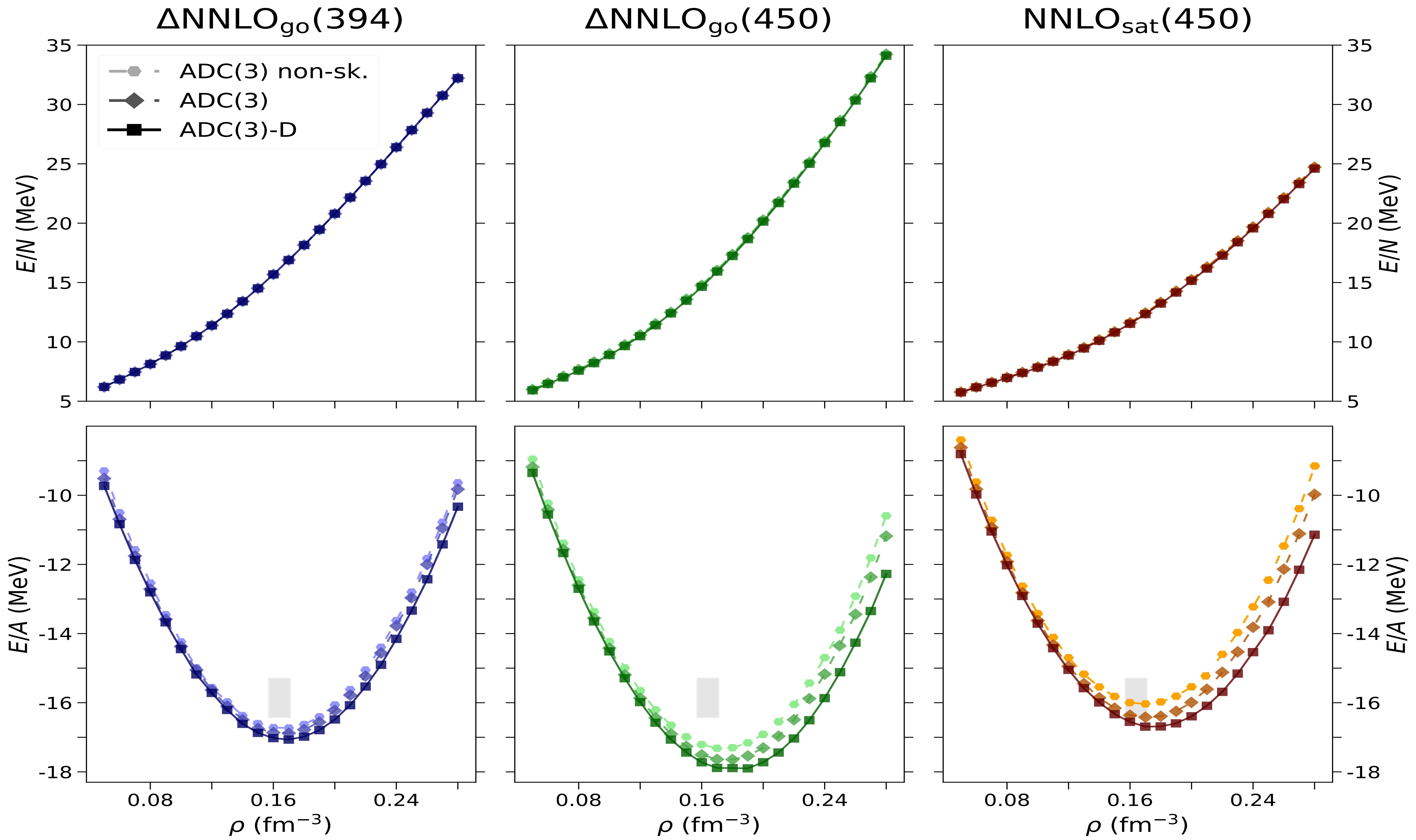
In $\tilde{\Sigma}(\omega)$, replace $t^{(0)}$ with converged $\boldsymbol{T_2}$ **amplitudes**



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

F. Marino, CB, and G. Colò, arXiv:2601.03763 [nucl-th]

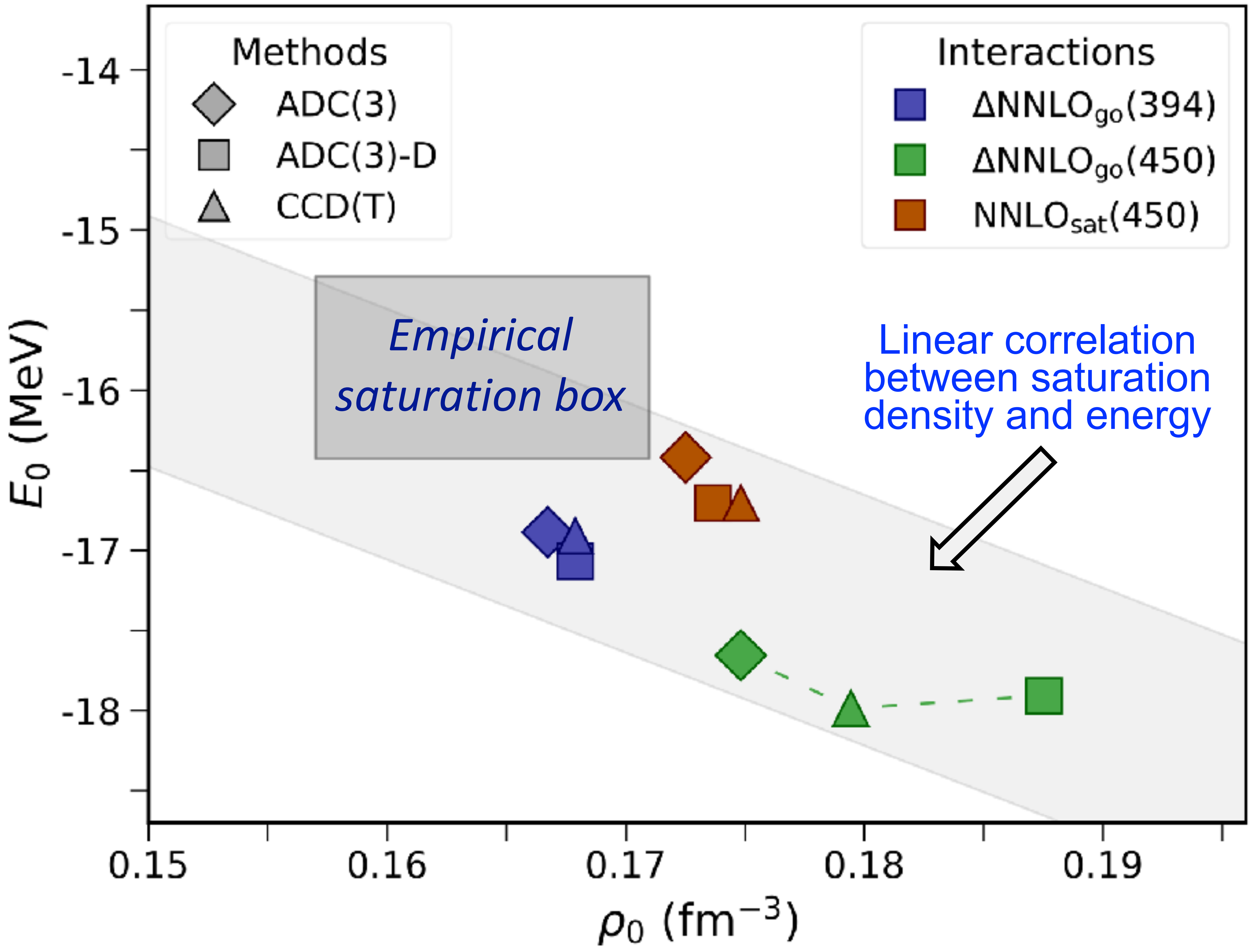
Equations of state (T=0)



EOS available at:

F. Marino, CB, and G. Colò, arXiv:2601.03763 [nucl-th]

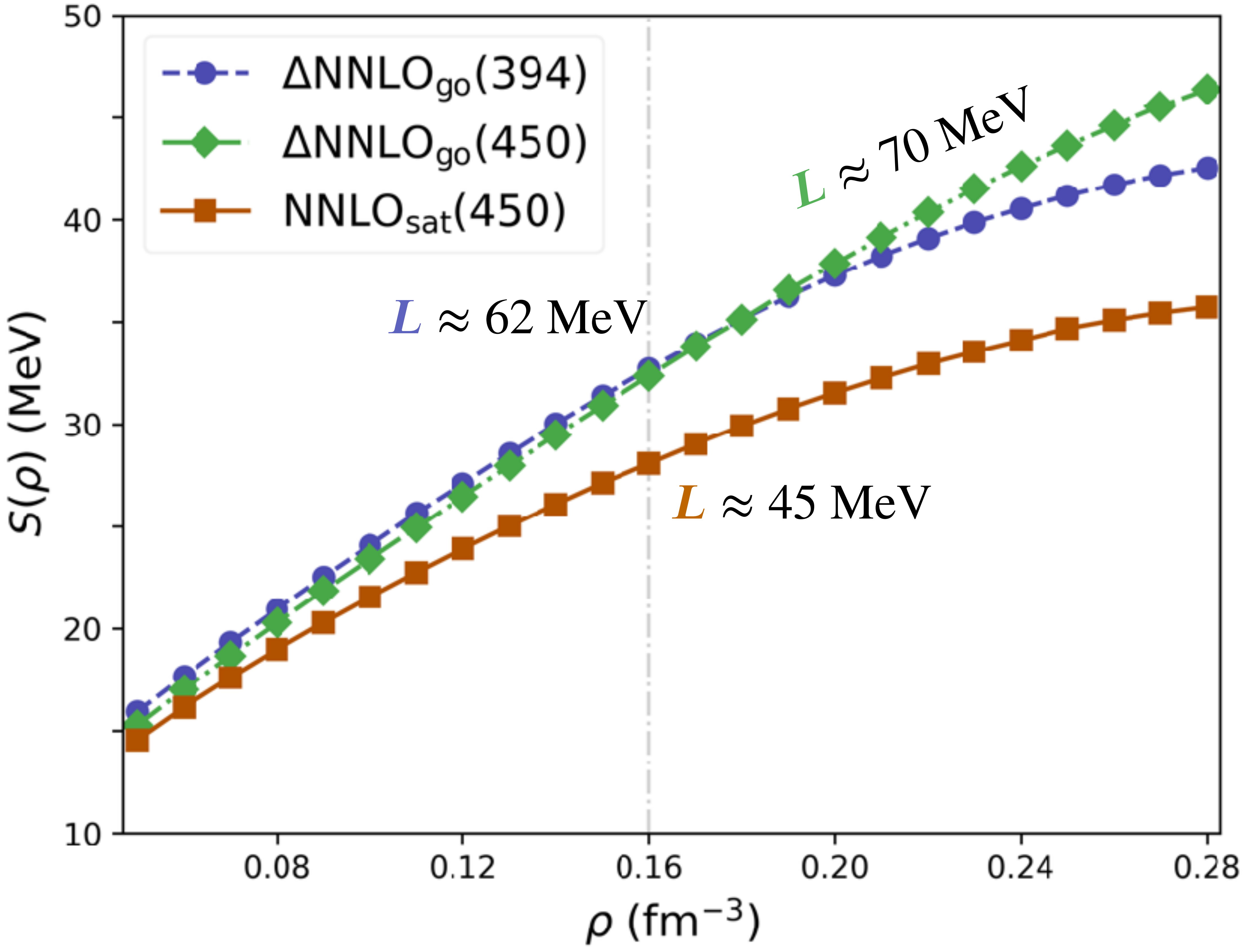
Saturation point of symmetric nuclear matter

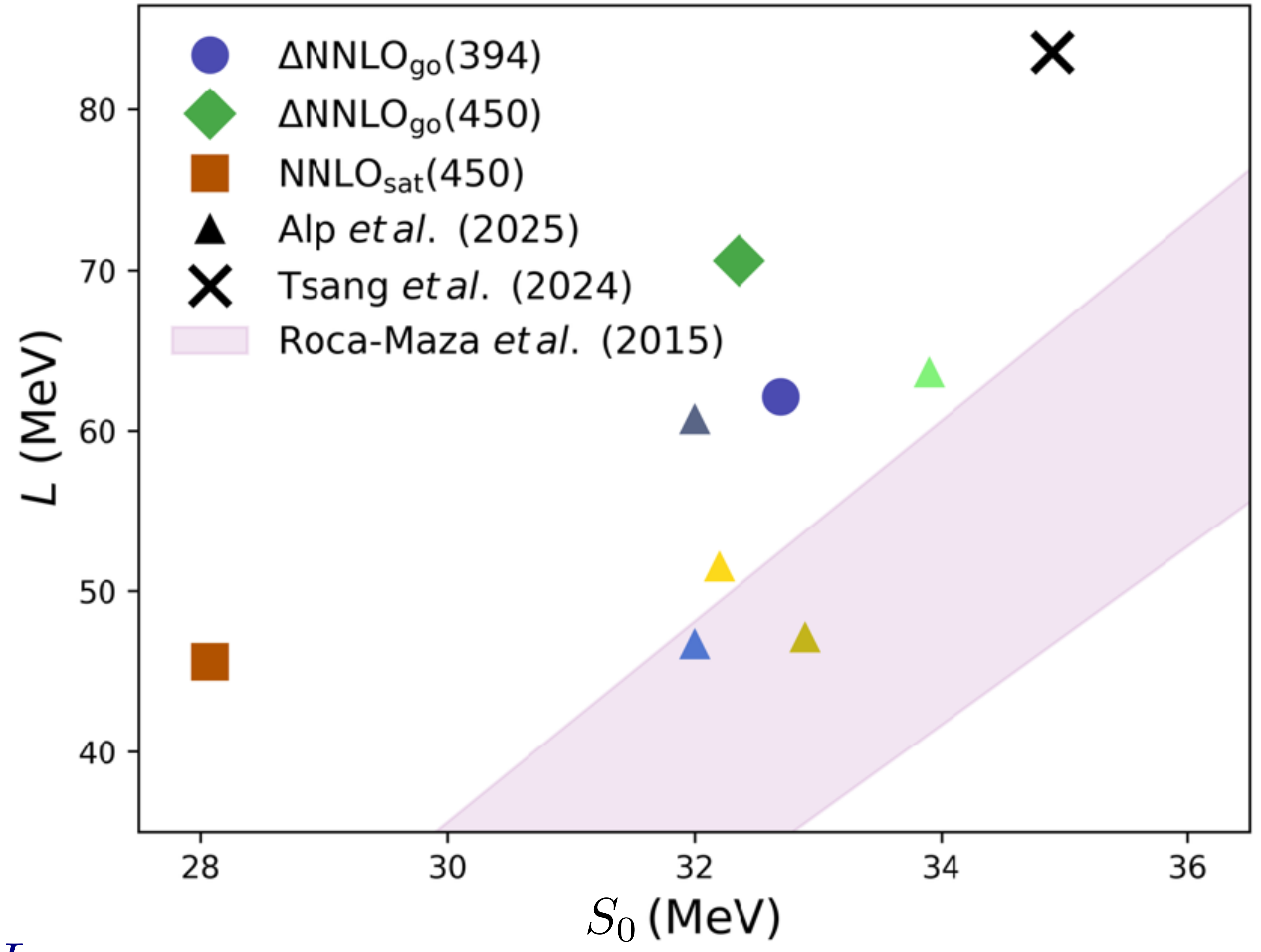


- Generally good agreement across many-body methods
- **Interaction-dependence** is the dominant uncertainty

F. Marino et al., Phys. Rev. C **110**, 054322 (2024)

Symmetry energy





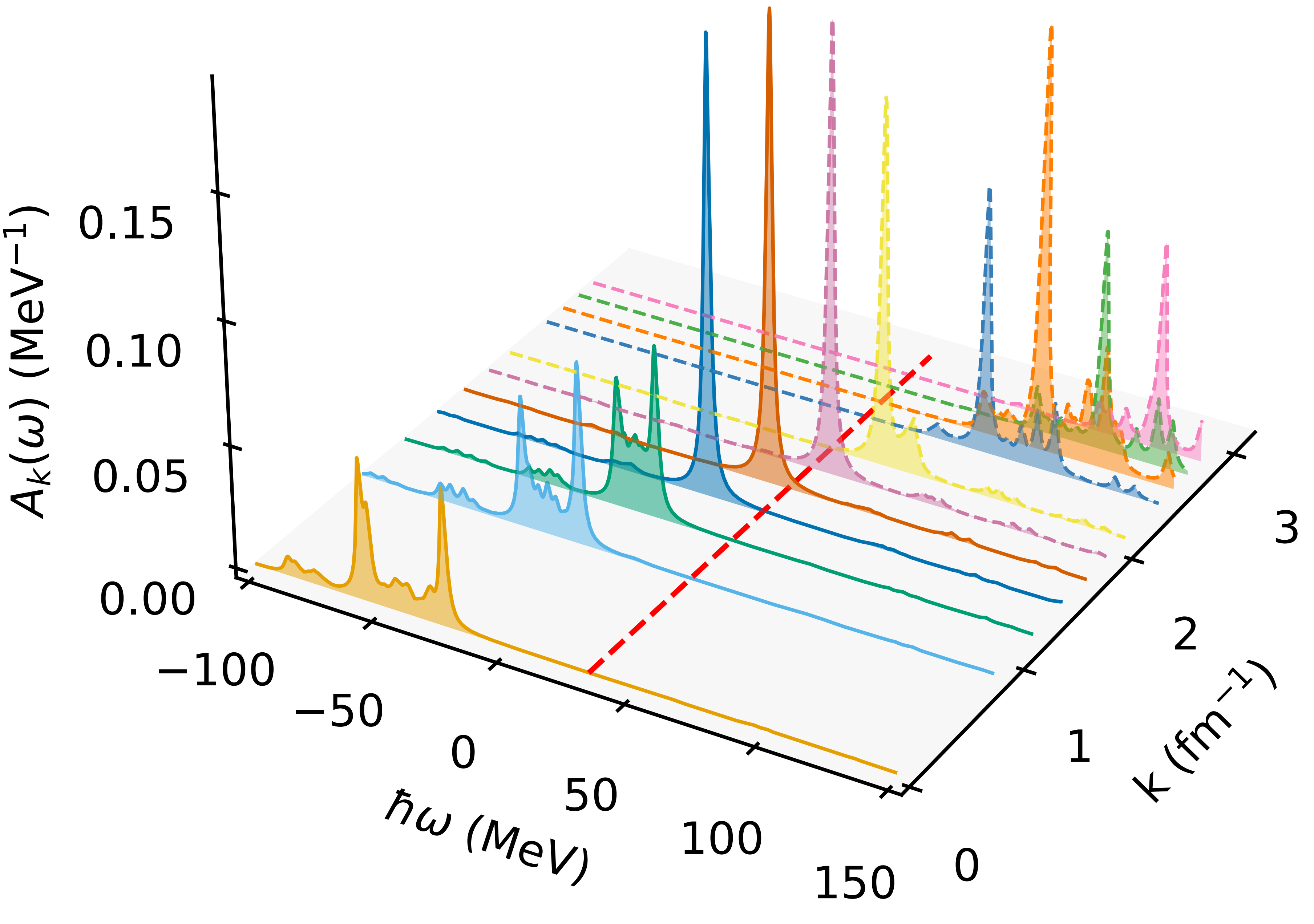
$$S(\rho) = S(\rho_0) + \frac{L}{3\rho_0}(\rho - \rho_0) + \cdots$$

F. Marino, CB, and G. Colò, arXiv:2601.03763 [nucl-th]

Alp et al., arXiv:2504.18259
Burgio et al., Front. Astron. Space Sci. **11**, 1505560 (2024)
Lynch and Tsang, Phys. Lett. B **830**, 137098 (2022)
Roca-Maza et al., Phys. Rev. C **92**, 064304 (2015)

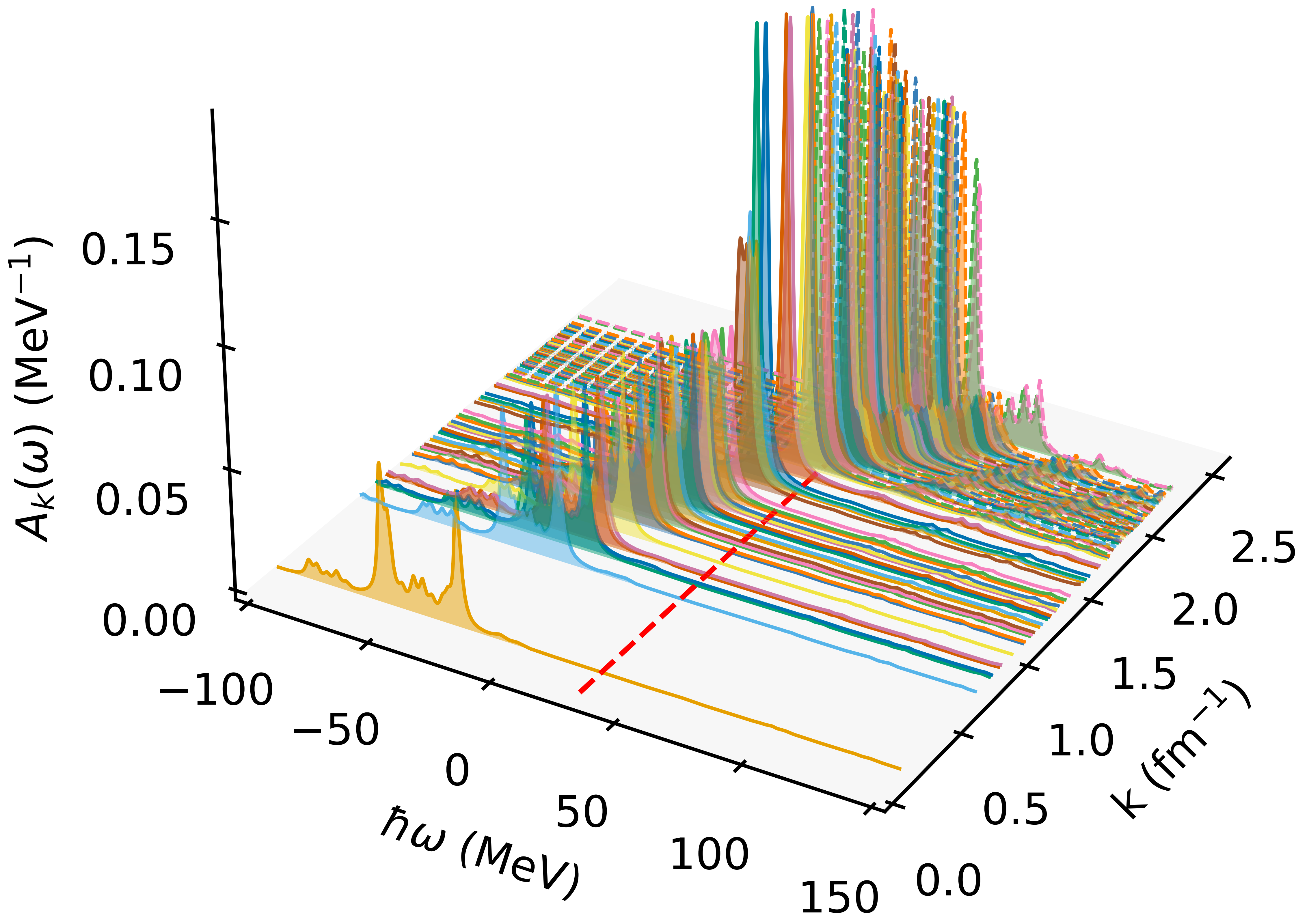
Removing finite size effects - Twisted Angle BC

Ordinary PBC



sp-TABC: chose just one set of twisted angles

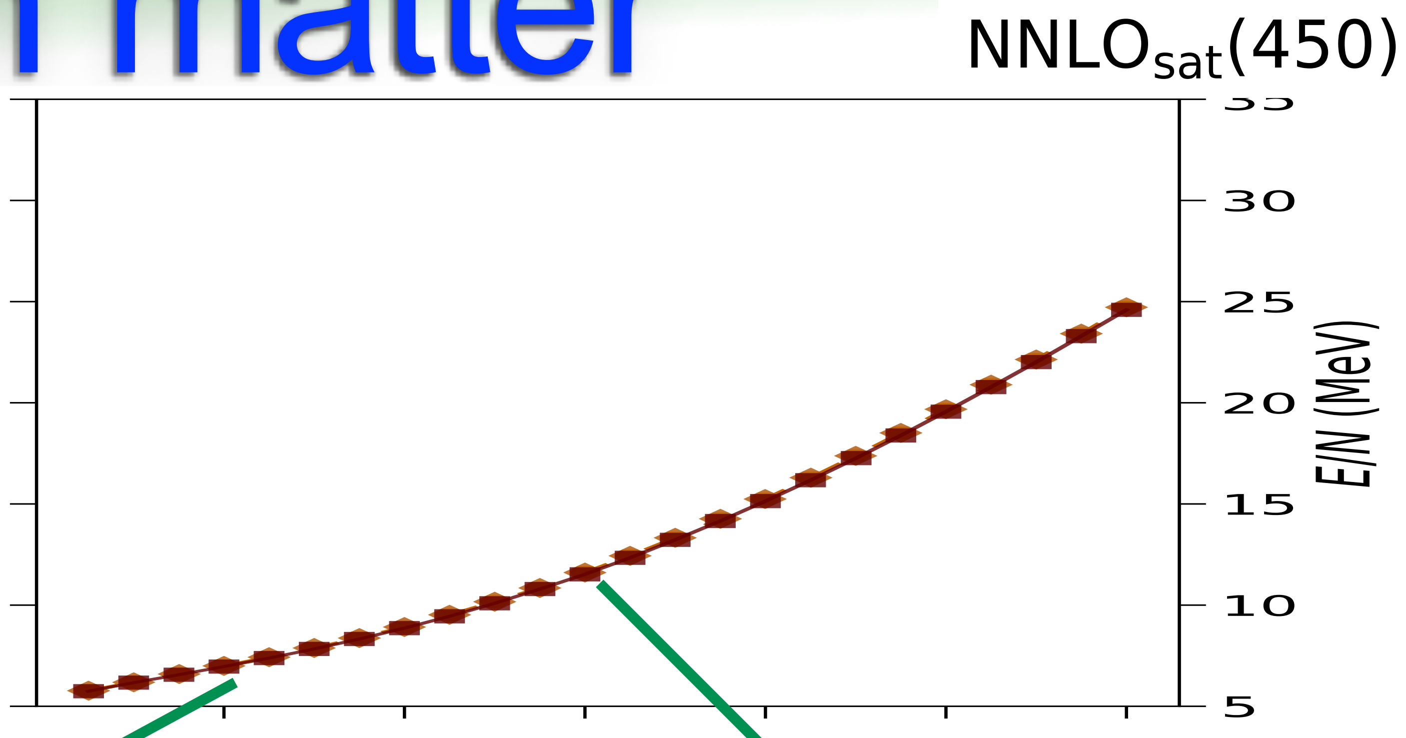
- Finer resolution in momenta
- Better description of the thermodynamic Limit

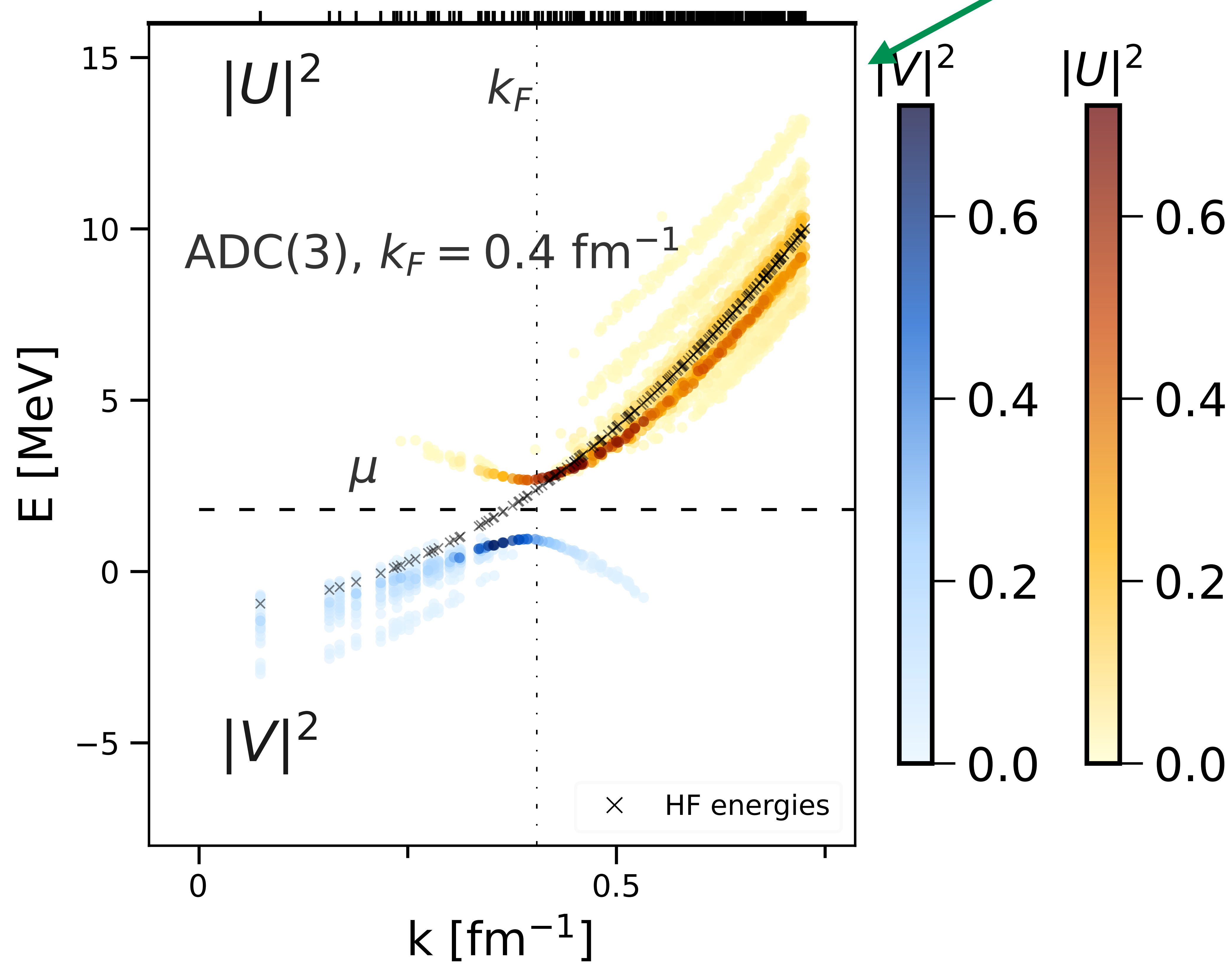


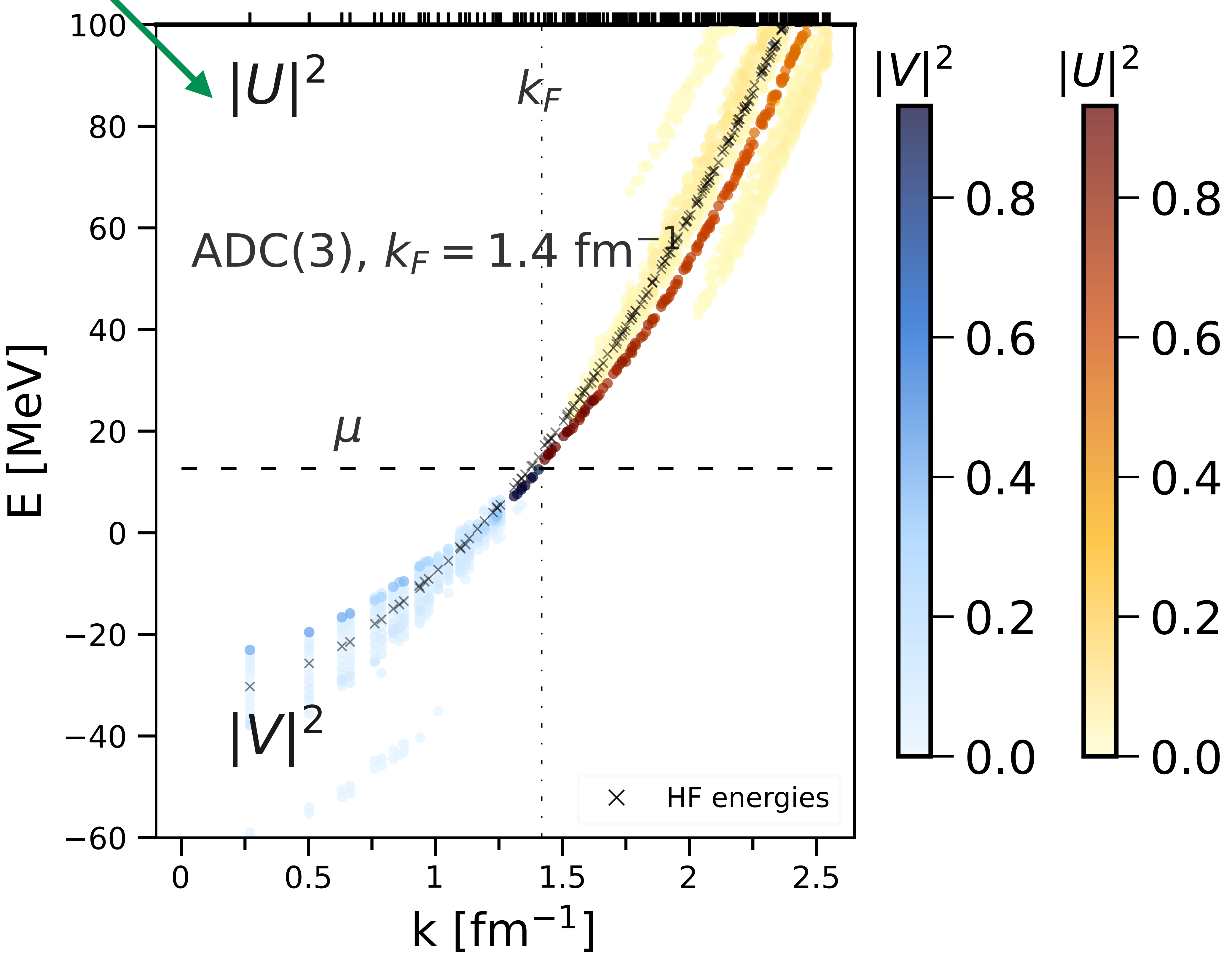
$$S^p(\mathbf{p},\omega) = \sum_n \left|\langle \Psi_n^{A+1} | \psi_{\mathbf{p}}^\dagger | \Psi_0^A \rangle\right|^2 \delta\left(\hbar\omega - (E_n^{A+1} - E_0^A)\right)$$

$$S^h(\mathbf{p},\omega) = \sum_k \left|\langle \Psi_k^{A-1} | \psi_{\mathbf{p}} | \Psi_0^A \rangle\right|^2 \delta\left(\hbar\omega - (E_0^A - E_k^{A-1})\right)$$

Pairing regime, neutron matter

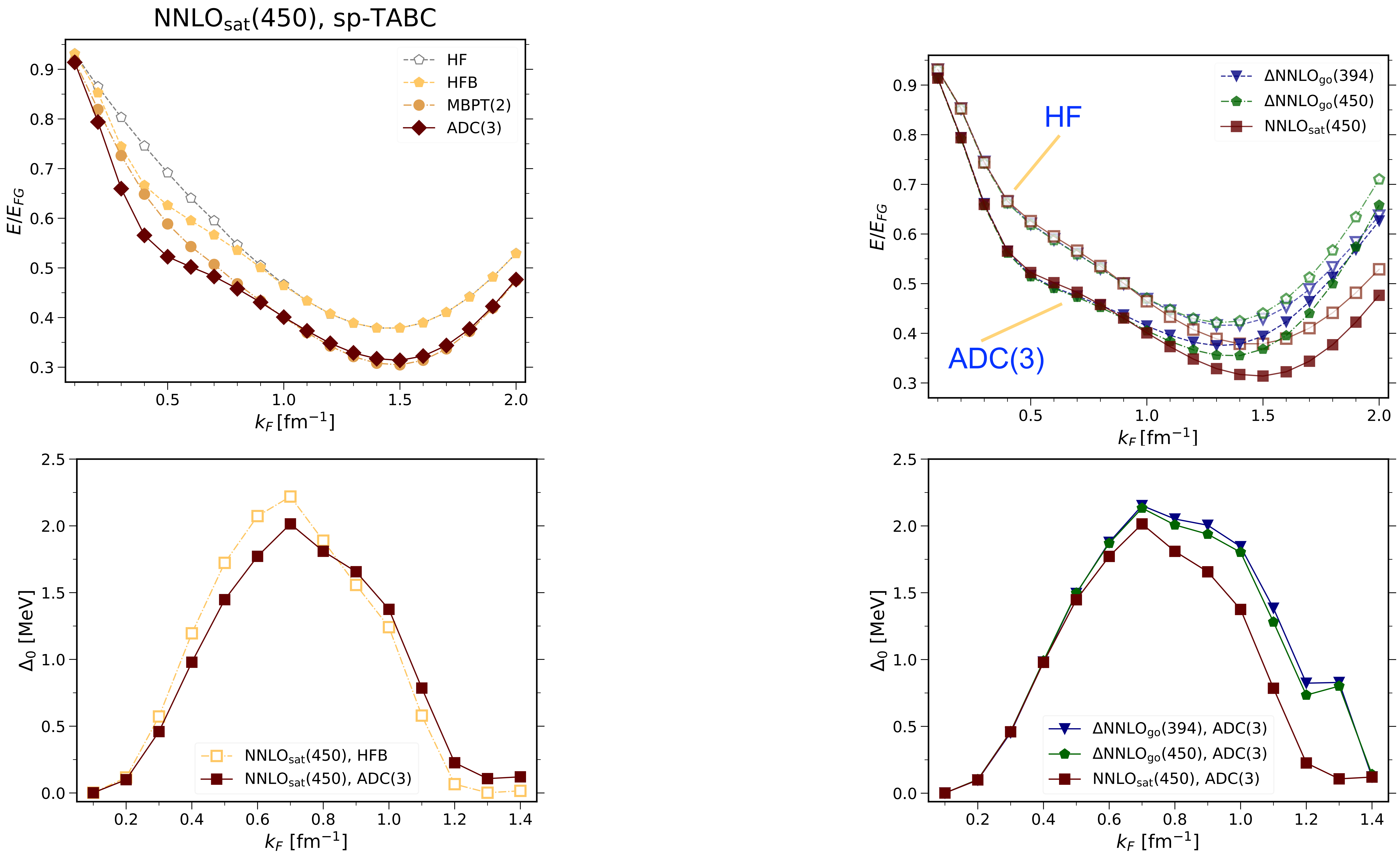






F. Marino, CB, and G. Colò, in preparation

Pairing in neutron matter



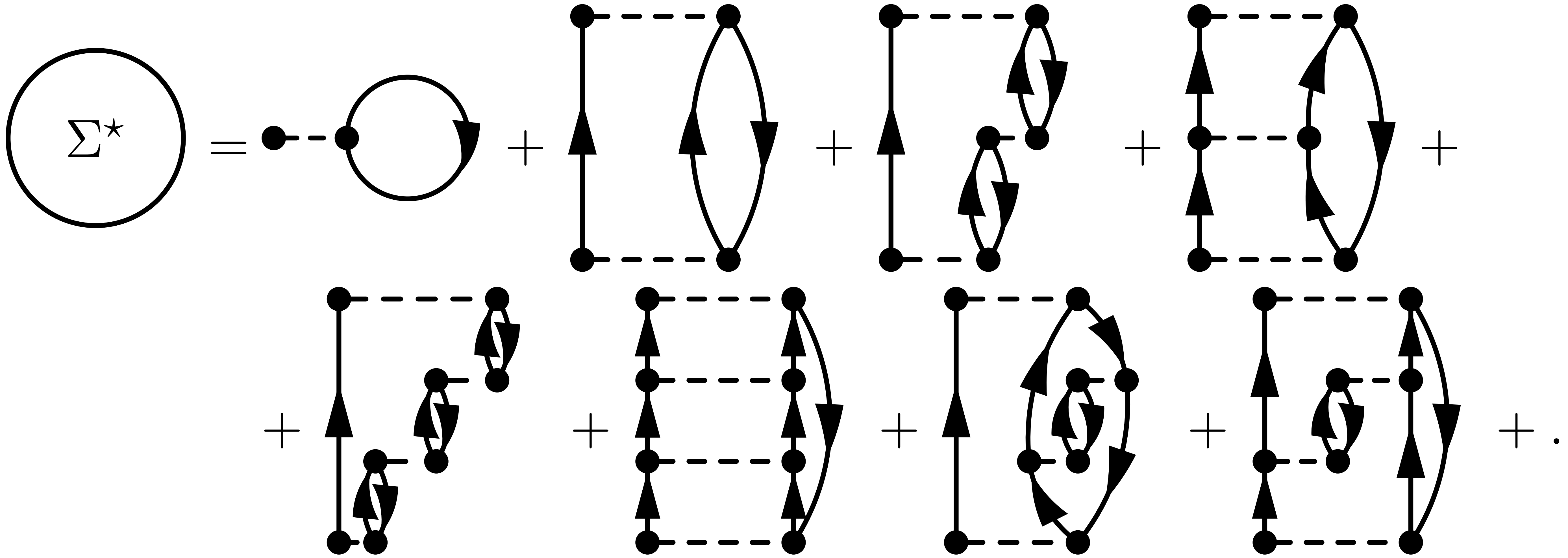
Green's function theory beyond ADC(3)? DiagMC !!

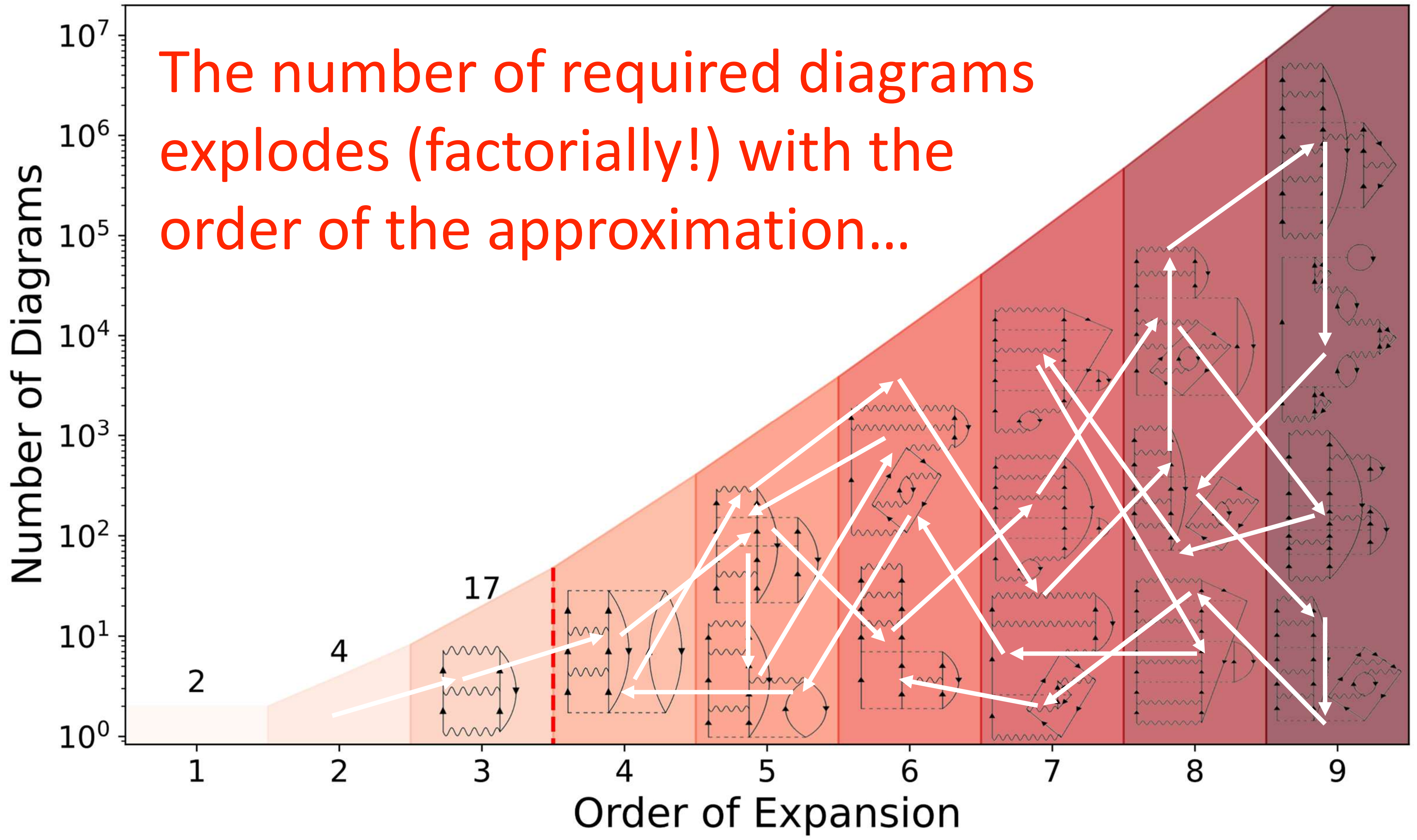
S. Brolli (PhD candidate, Milan)

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:

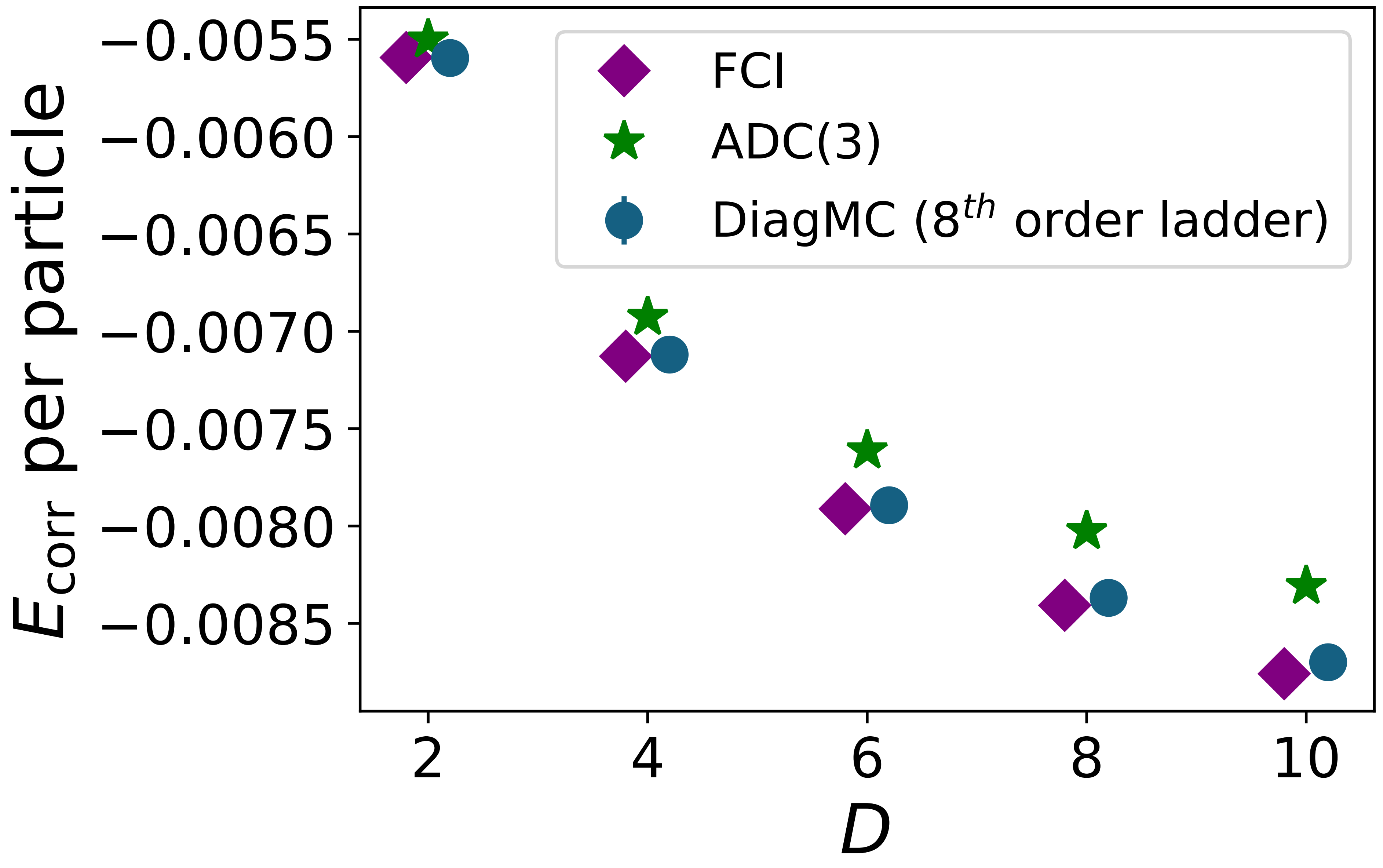


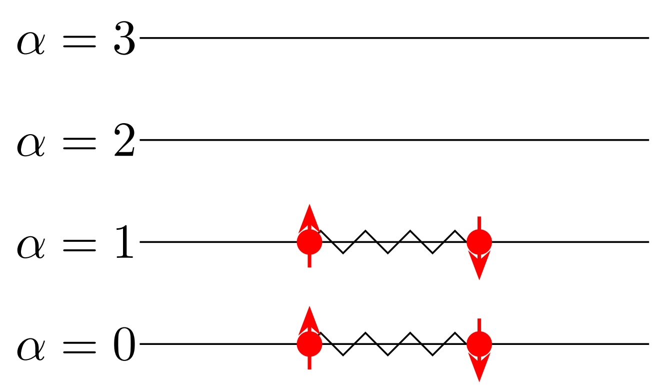


Diagrammatic Monte Carlo (DiagMC) ***samples diagrams in their topological space*** using a Markov chain.

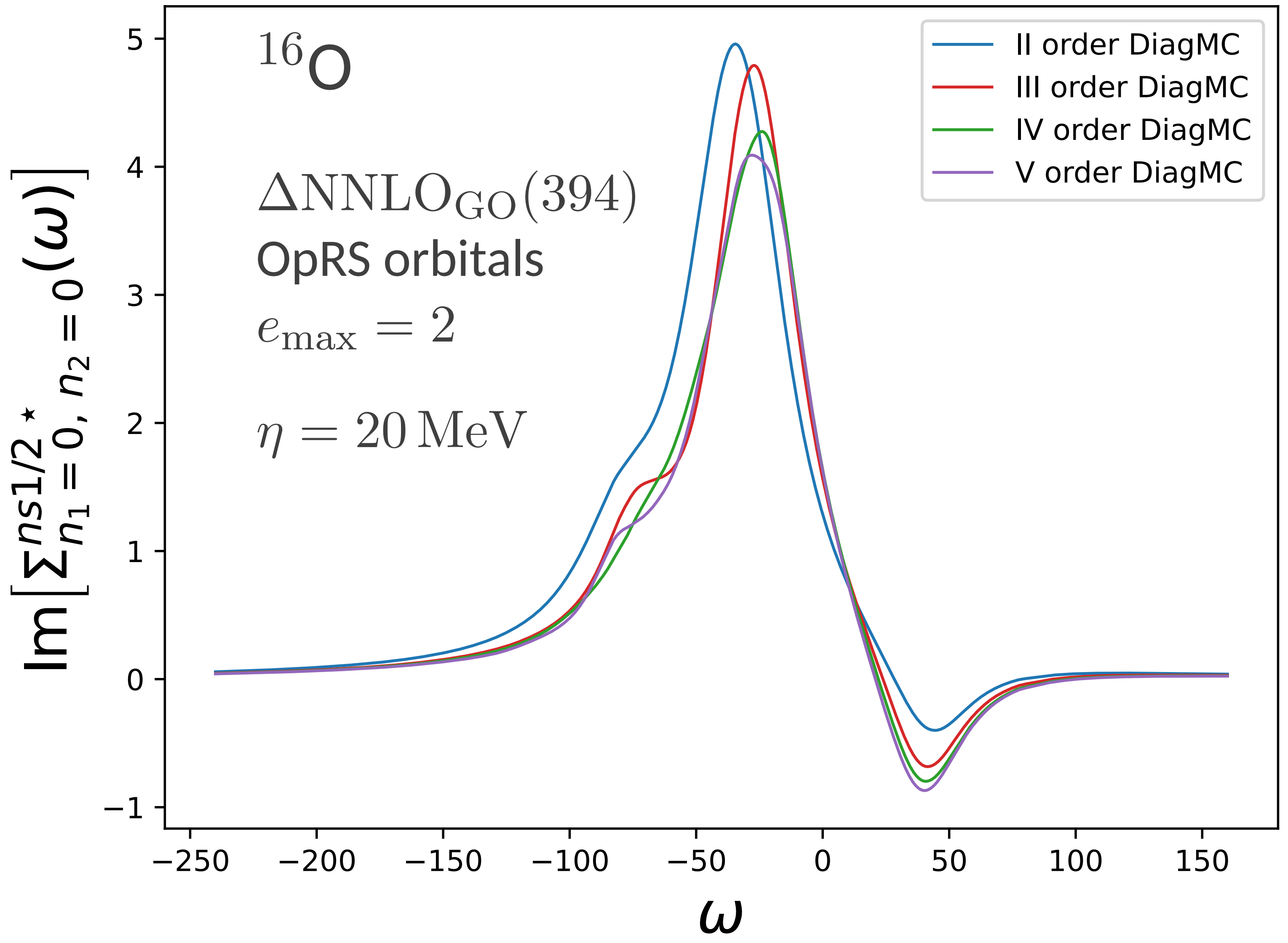
[Brolli, CB, Vigezzi, Phys. Rev. Lett. **134**, 182502 (2025)]

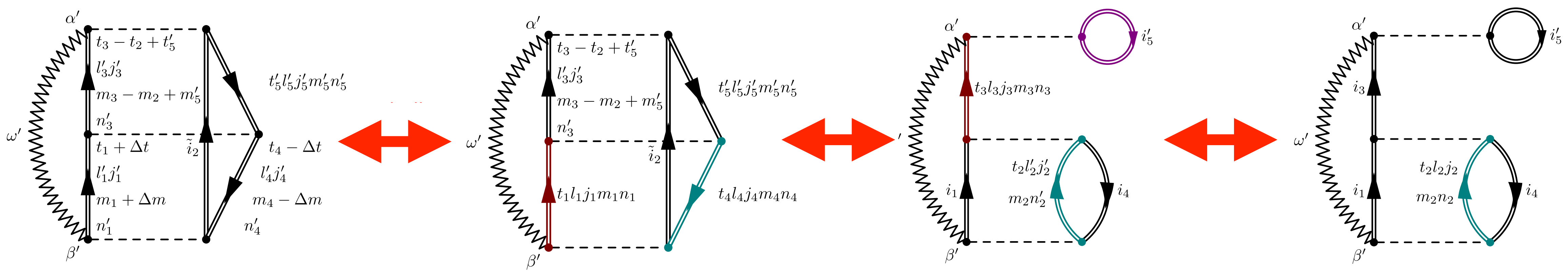
Richardson pairing model model up to *D=10* levels:





Up to 5th order calculations are now possible in nuclei:





S. Brolli, CB, Vigezzi, Phys. Rev. Lett. **134**, 182502 (2025)
S. Brolli, CB, in preparation.

Neural Network Quantum States (NQS):

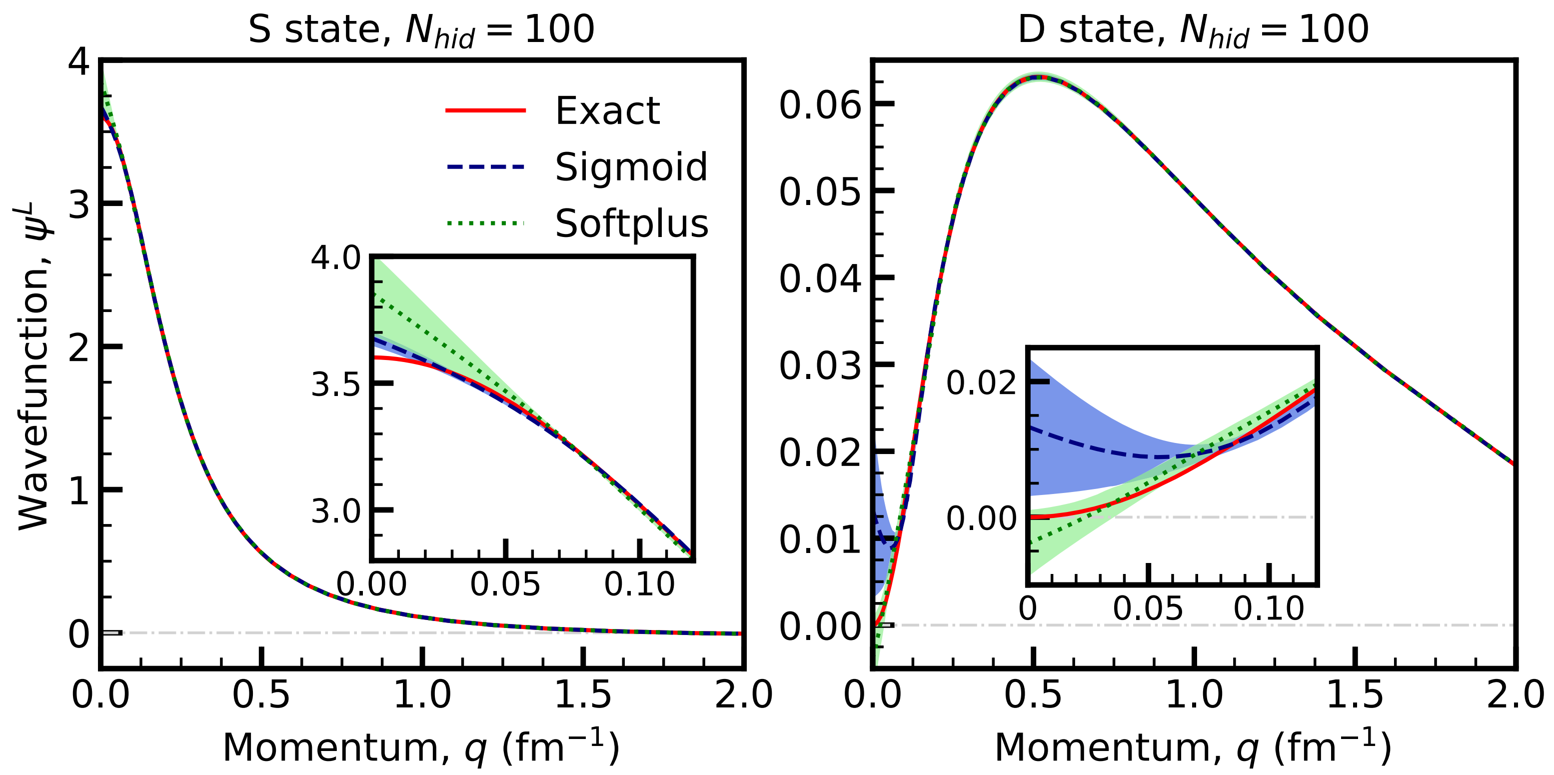
$$\frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = E_V \geq E_0$$

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

neural networks

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

The deuteron:



Keeble, Rios, Phys. Lett. B **809**, 135743 (2020)
Rozalén Sarmiento, Keeble, EPJ Plus **139**, 189 (2024)

Light nuclei:

	Λ	VMC-ANN	VMC-JS	GFMC	GFMC$_c$
^{2}H	4 fm^{-1}	−2.224(1)	−2.223(1)	−2.224(1)	-
	6 fm^{-1}	−2.224(4)	−2.220(1)	−2.225(1)	-
^{3}H	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)
^{4}He	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)

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

Neural Network Quantum States (NQS):

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

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

neural networks

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

- **NQS often surpass traditional VMC**, with accuracy similar to GFMC/DMC but a a fraction of the cost
- Sometimes referred 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 $f(\mathbf{x}),\ \partial f(\mathbf{x})/\partial x_i, \ldots$

- 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 $\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots)$
- Many-body PINN cost function:

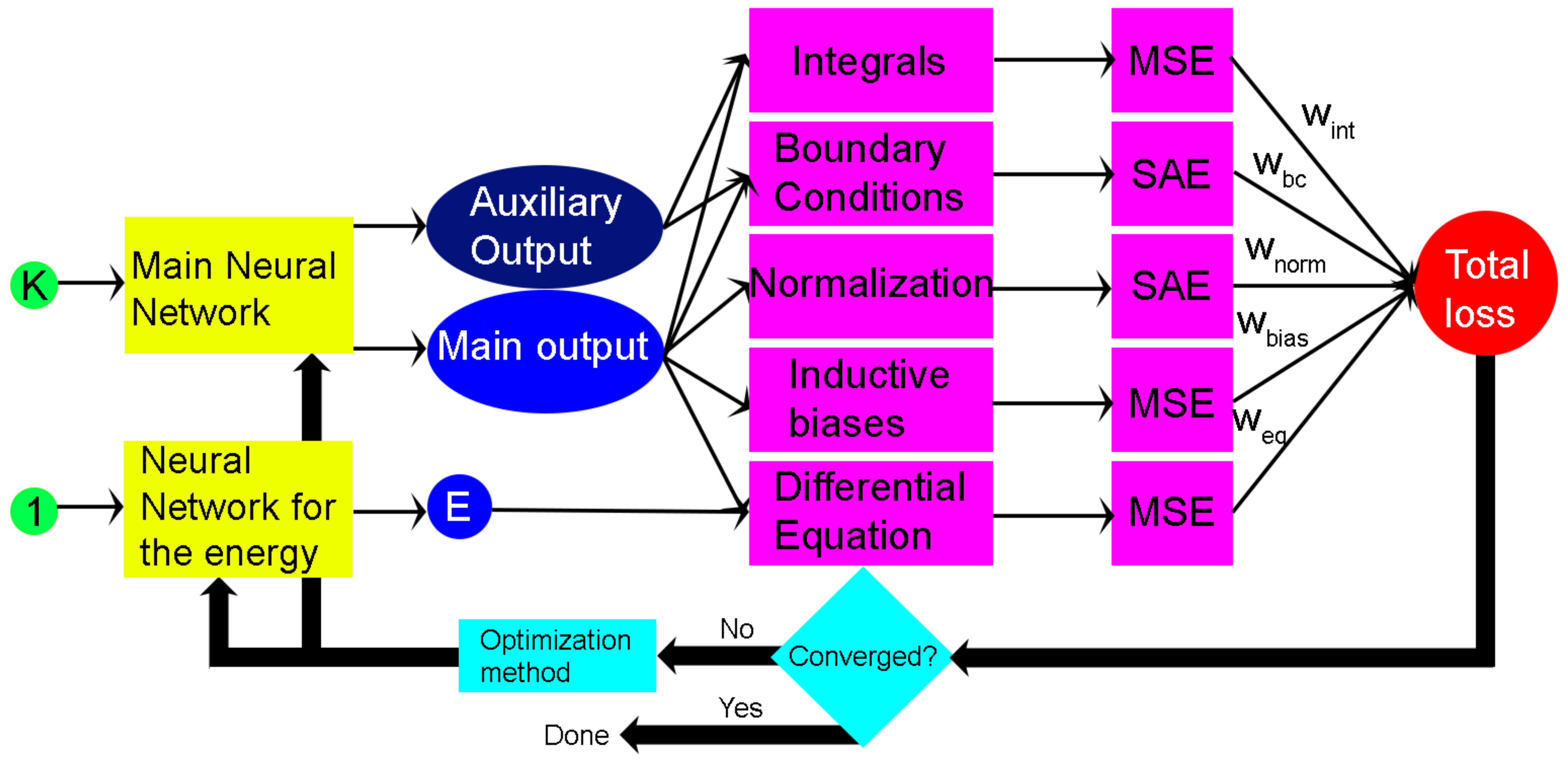
$$\mathcal{L}_{PINN} = \mathcal{L}_{PDE} + \mathcal{L}_{phys} + \cancel{\mathcal{L}_{data}}$$

Schrod. eq.

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

Physics constraints

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



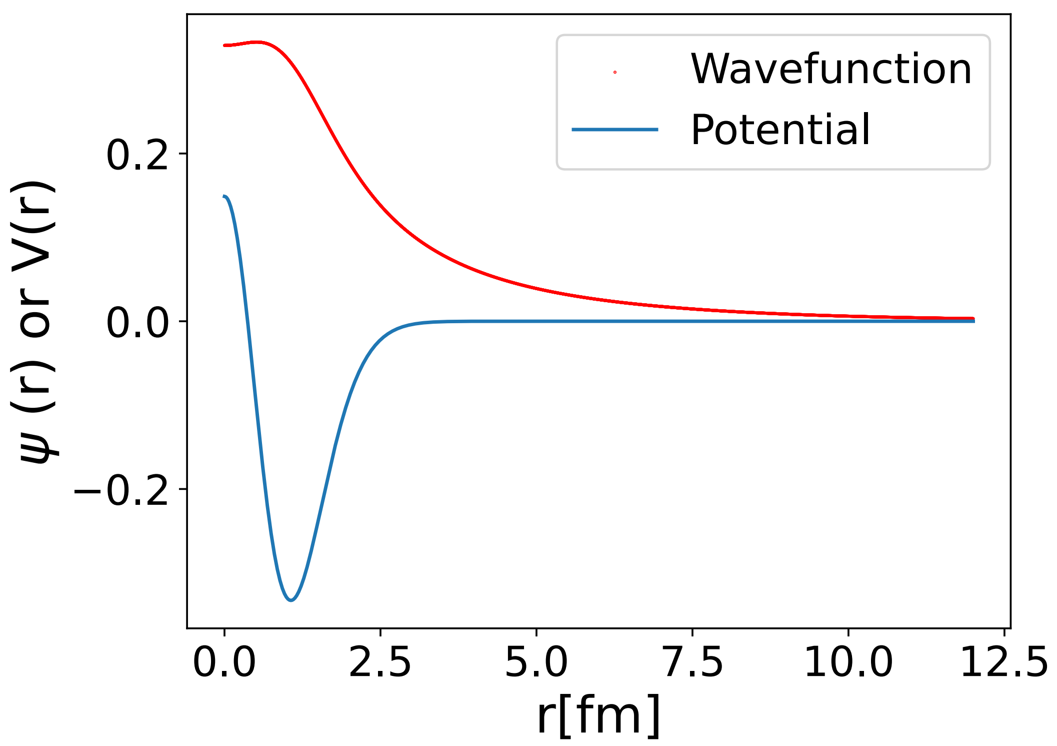
- Through boundary conditions, one may target excited (and scattering) states.

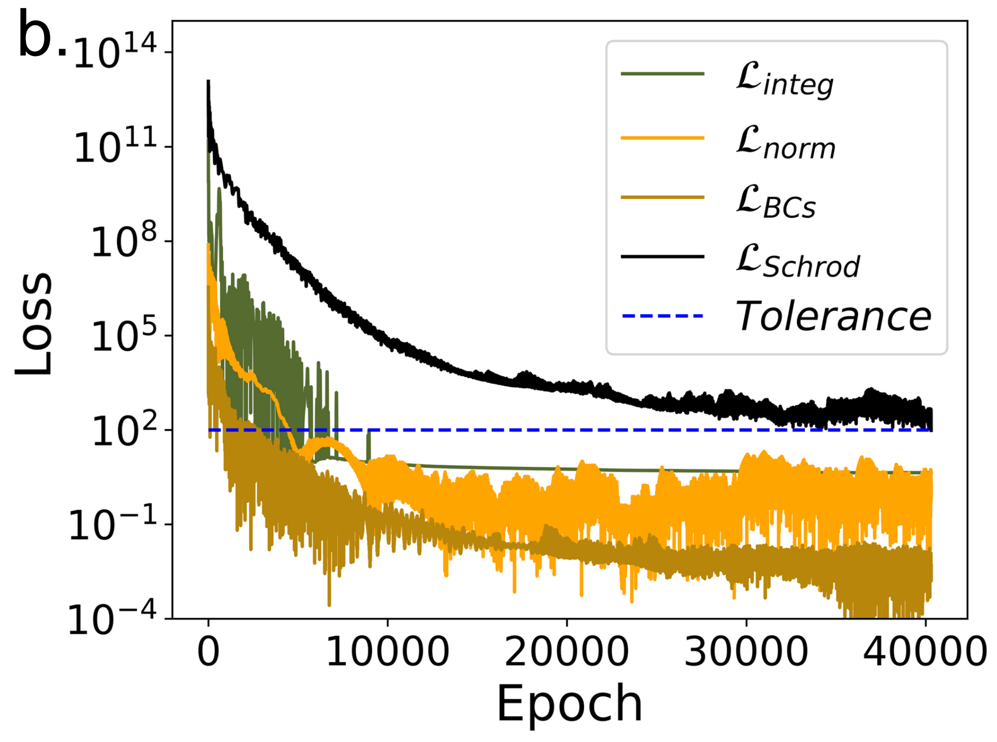
L. Brevi, A. Mandarino, E. Prati,
Technologies 12, 174 (2024); New J. Phys. **26**, 103015 (2024).

Physics Informed Neural Networks for the deuteron

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

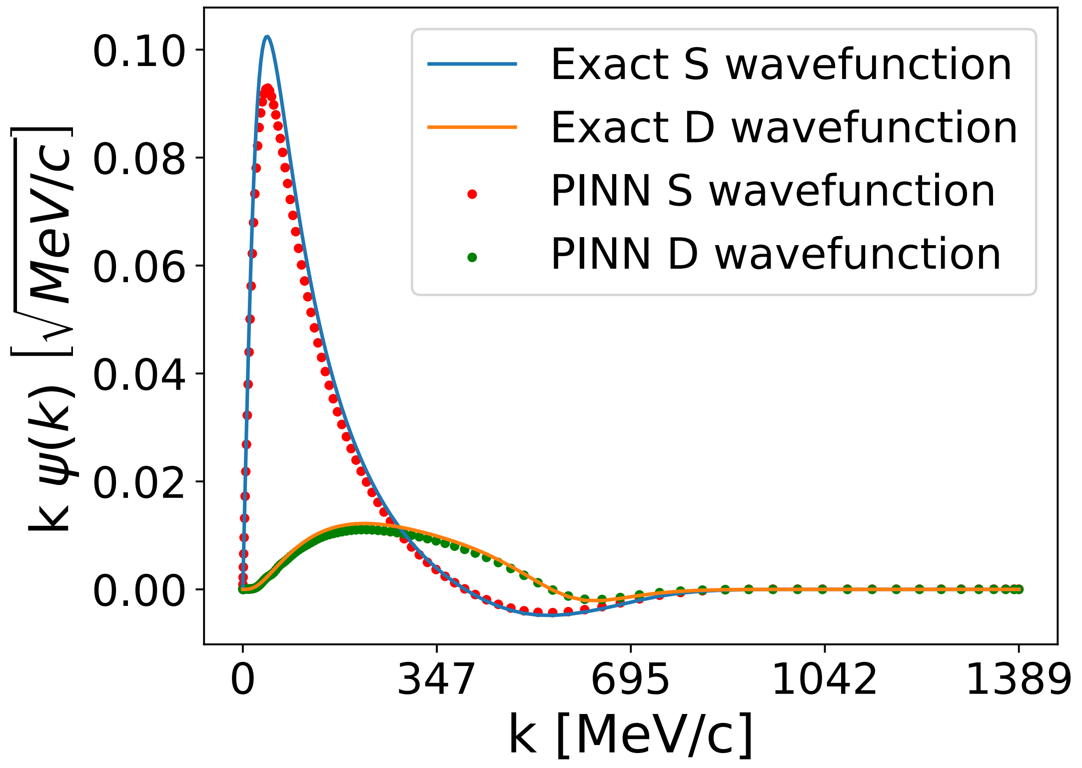
✦ Coordinate space, Minnesota potential:

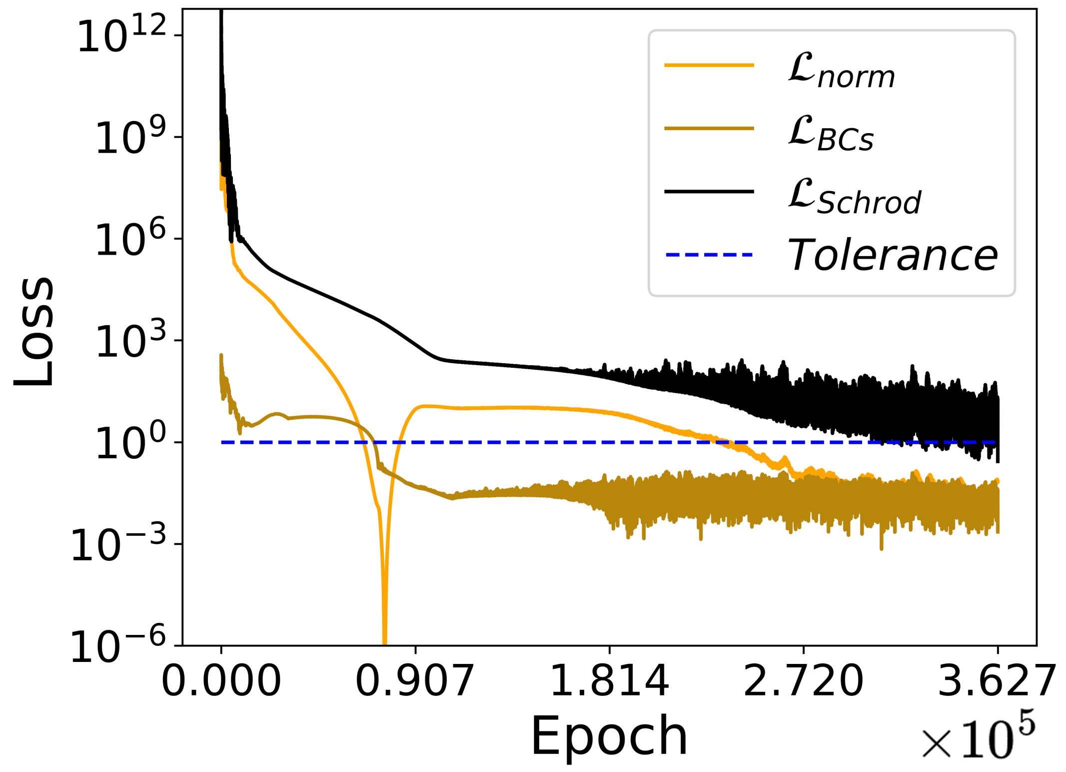


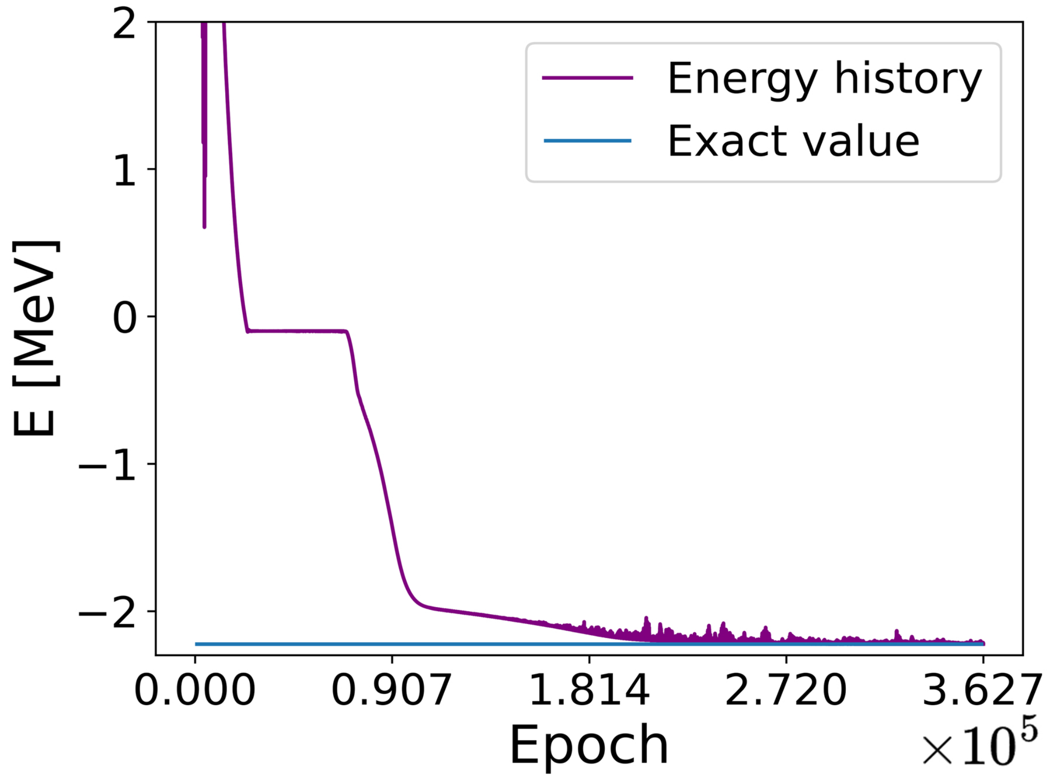


	$Err_{E,exp}$	$Err_{E,Num}$	$1-\mathcal{F}_\psi$
Minnesota	0.01	1×10^{-8}	
N4LO(550)	-5.96×10^{-6}	-5.21×10^{-5}	1×10^{-5}
CD-Bonn	-6.01×10^{-4}	-2.76×10^{-7}	1×10^{-9}

✦ Momentum space with N4LO(550) from EMN:







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

Toward Lattice Simulations with Neural Networks

Work in progress...

L. Lazzarino, G. Borroni, E. Redaelli - BSc theses U. Of Milan

Why NQS on the Lattice?

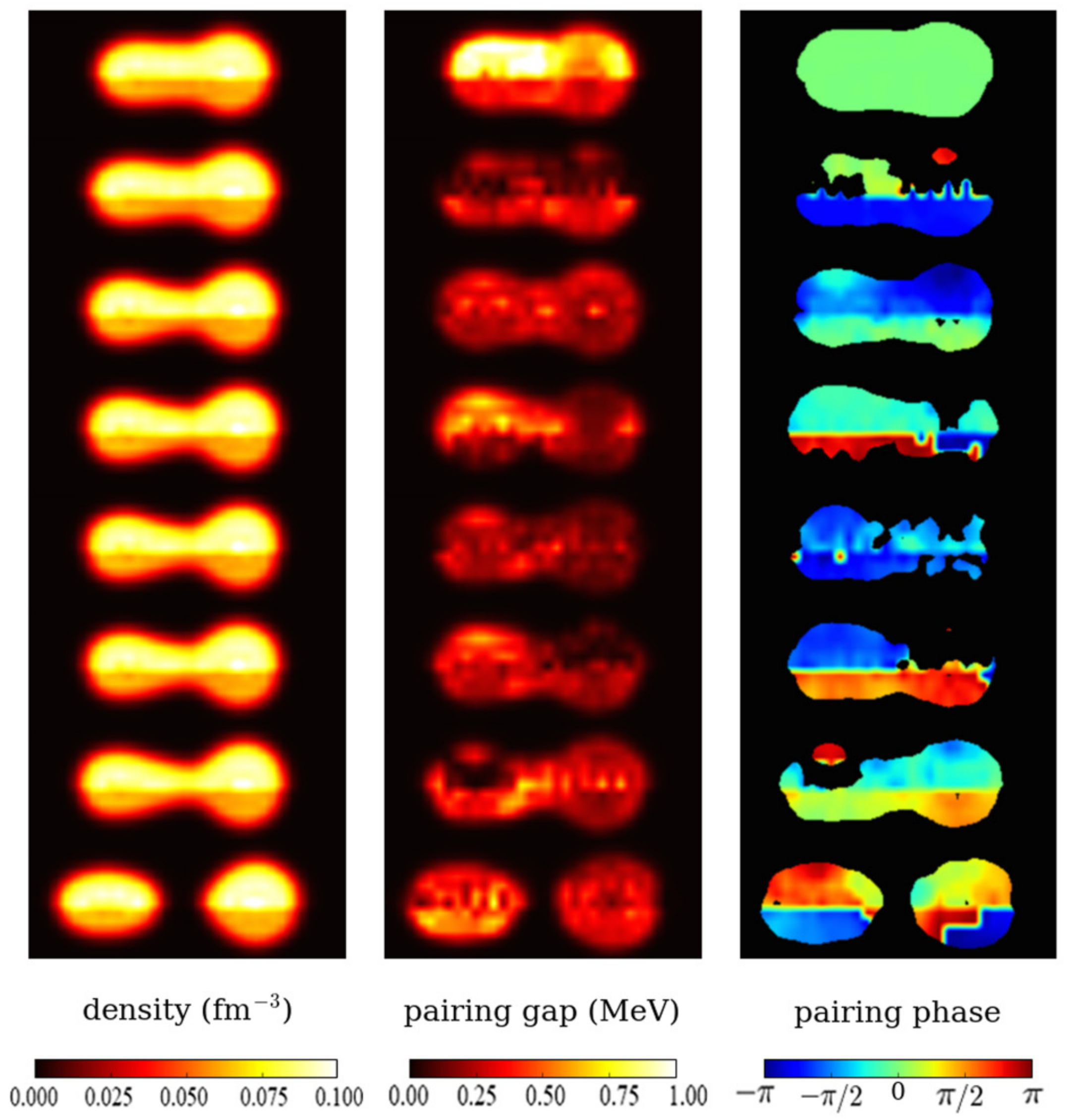
Advantages of a lattice-NQS for nuclei:

- Fermi-Pauli statistics comes for free (Fock space).

- Not tied to spherical or partially deformed ansätze (full deformation, etc…).

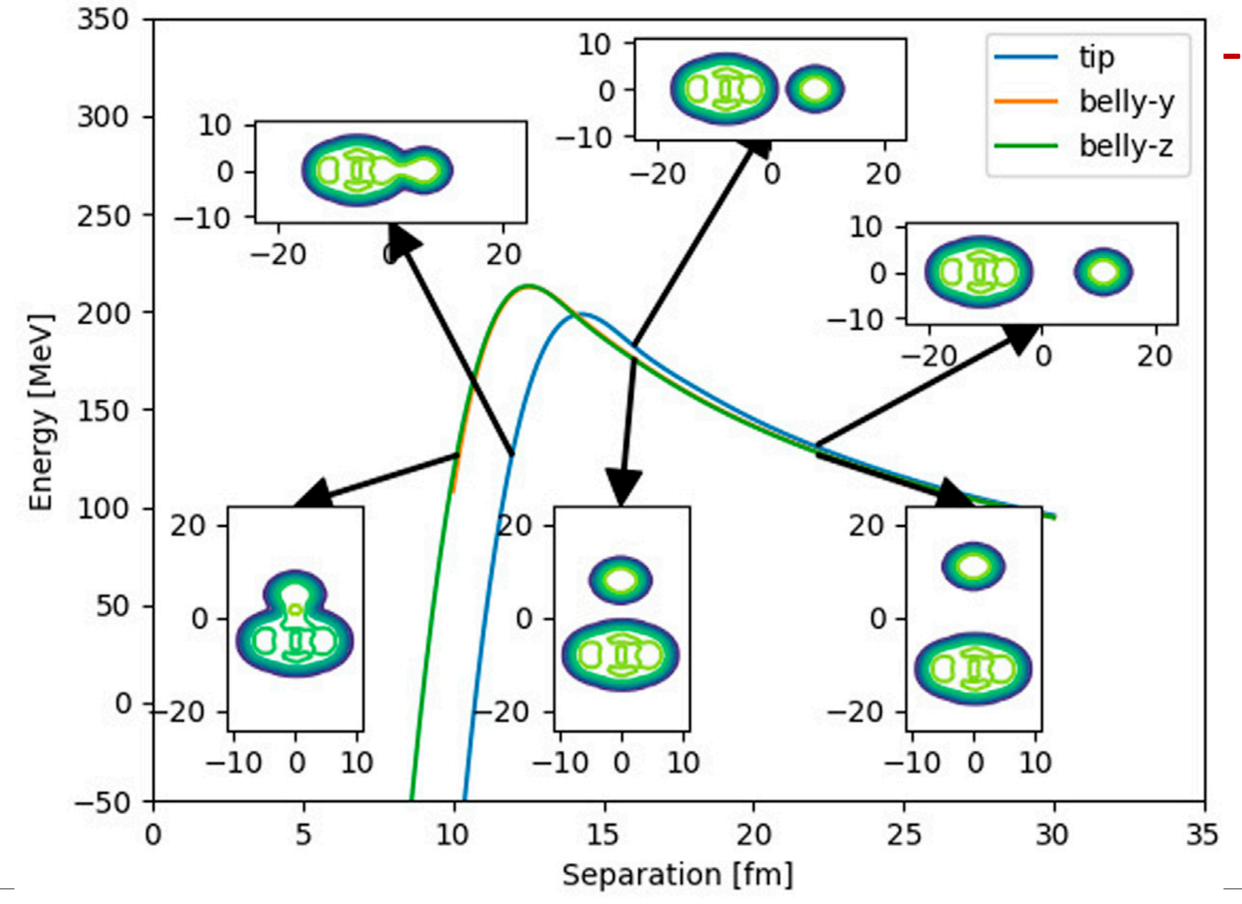
- Transfer learning (train few-nucleon first).

- Many-body dynamics.



Fission of ^{240}Pu:

- time dependent DFT inspired, in 3D
- 30 x 30 x 60 fm^3 box
- 24 x 24 x 48 = 27,000 pts mesh



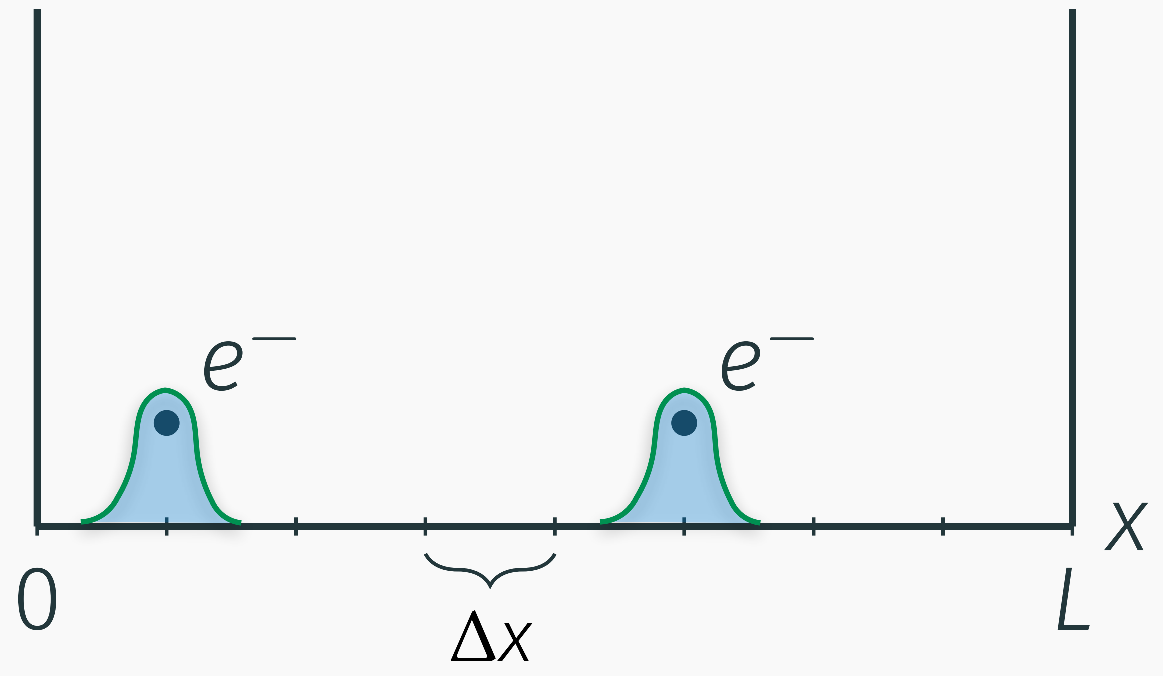
Mean-field simulations of Es-254 + Ca-48 heavy-ion reactions

P. Stevenson et al., Frontiers **10**, 1019285 (2022)

Confined fermions w/ a discrete coordinate space mesh

- Discretise coordinate space

- Use occupation number to locate particles



$\Longleftrightarrow$ $(0, 1, 0, 0, 0, 1, 0, 0, 0)$

no need to worry about antisymmetrization!

- Use a Fock space basis to represent particle configurations:

$$|\psi\rangle = \prod_i \psi^\dagger(x_i)\,|0\rangle \;= |n_0\!=\!0,\, n_1\!=\!1,\, n_2\!=\!0,\, n_3\!=\!0,\, n_4\!=\!0,\, n_5\!=\!1,\, \ldots n_L\!=\!0\rangle$$

- Can be mapped into a system of spins (*with **fixed magnetisation***):

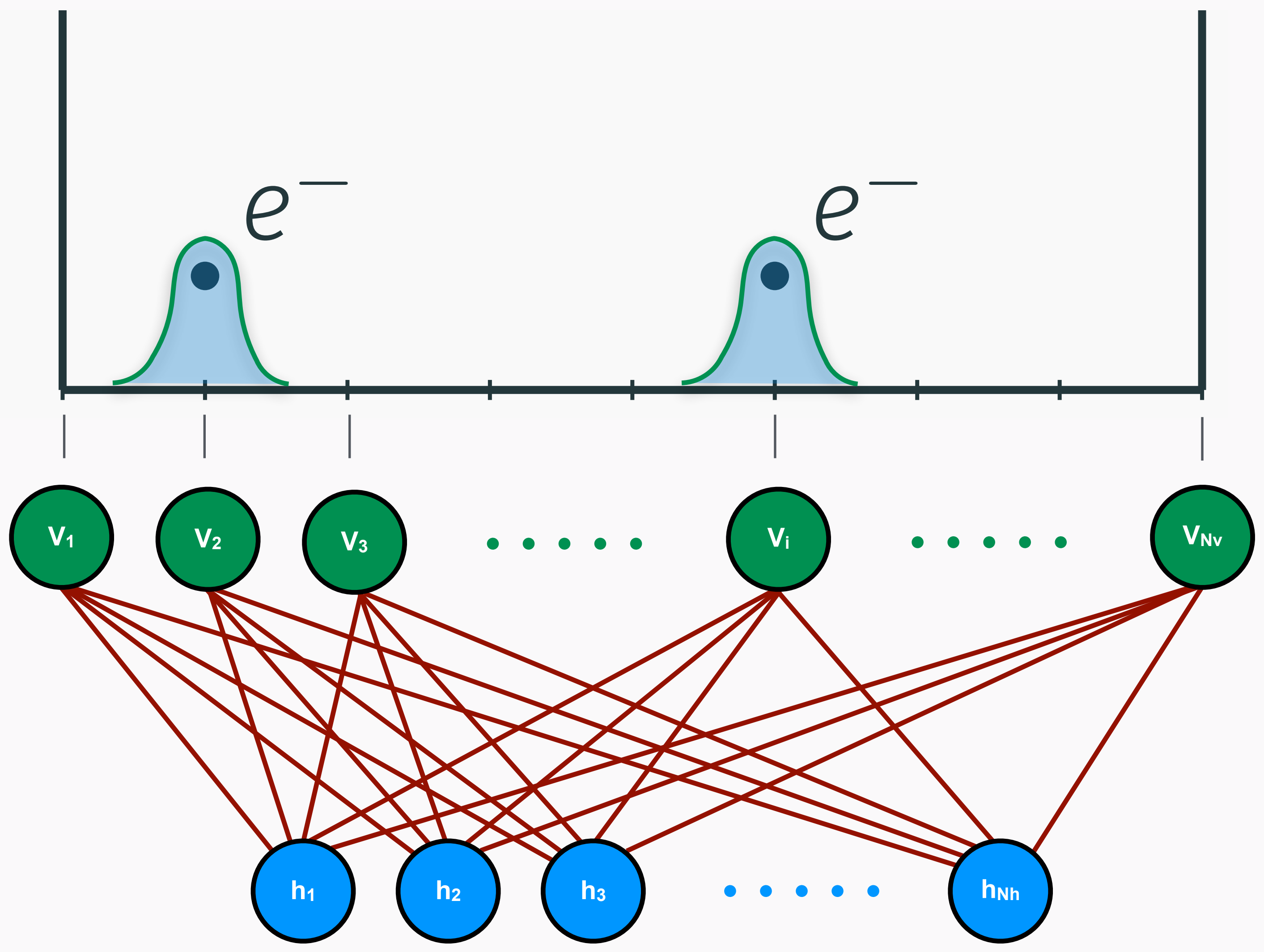
$$\langle x|\psi\rangle \to \langle S|\psi\rangle \Leftrightarrow \begin{cases} c_{\uparrow\uparrow\uparrow\ldots} \doteq \langle\uparrow\uparrow\uparrow\ldots|\psi\rangle = \psi(\uparrow\uparrow\uparrow\ldots) \\ c_{\downarrow\uparrow\uparrow\ldots} \doteq \langle\downarrow\uparrow\uparrow\ldots|\psi\rangle = \psi(\downarrow\uparrow\uparrow\ldots) \\ \quad\vdots \\ c_{\downarrow\downarrow\downarrow\ldots} \doteq \langle\downarrow\downarrow\downarrow\ldots|\psi\rangle = \psi(\downarrow\downarrow\downarrow\ldots) \end{cases}$$

NQS representation

- Use a Restricted Boltzmann Machine with complex parameter to represent the w.f.:

$$\mathcal{P}(\mathrm{v} \cap \mathrm{h}) = \frac{1}{\mathcal{Z}} \exp\left(\mathrm{a}^\intercal \mathrm{v} + \mathrm{b}^\intercal \mathrm{h} + \mathrm{h}^\intercal \underline{\underline{W}}\, \mathrm{v}\right)$$

with:
$$\begin{cases} \mathrm{v} \in \{-1,1\}^{N_v} \\ \mathrm{h} \in \{-1,1\}^{N_h} \end{cases} \qquad \begin{cases} \mathrm{a} \in \mathbb{C}^{N_v} \\ \mathrm{b} \in \mathbb{C}^{N_h} \\ W \in \mathrm{Mat}_{N_h \times N_v}(\mathbb{C}) \end{cases}$$



NOTE: The RBM architecture will be independent from the particle number.

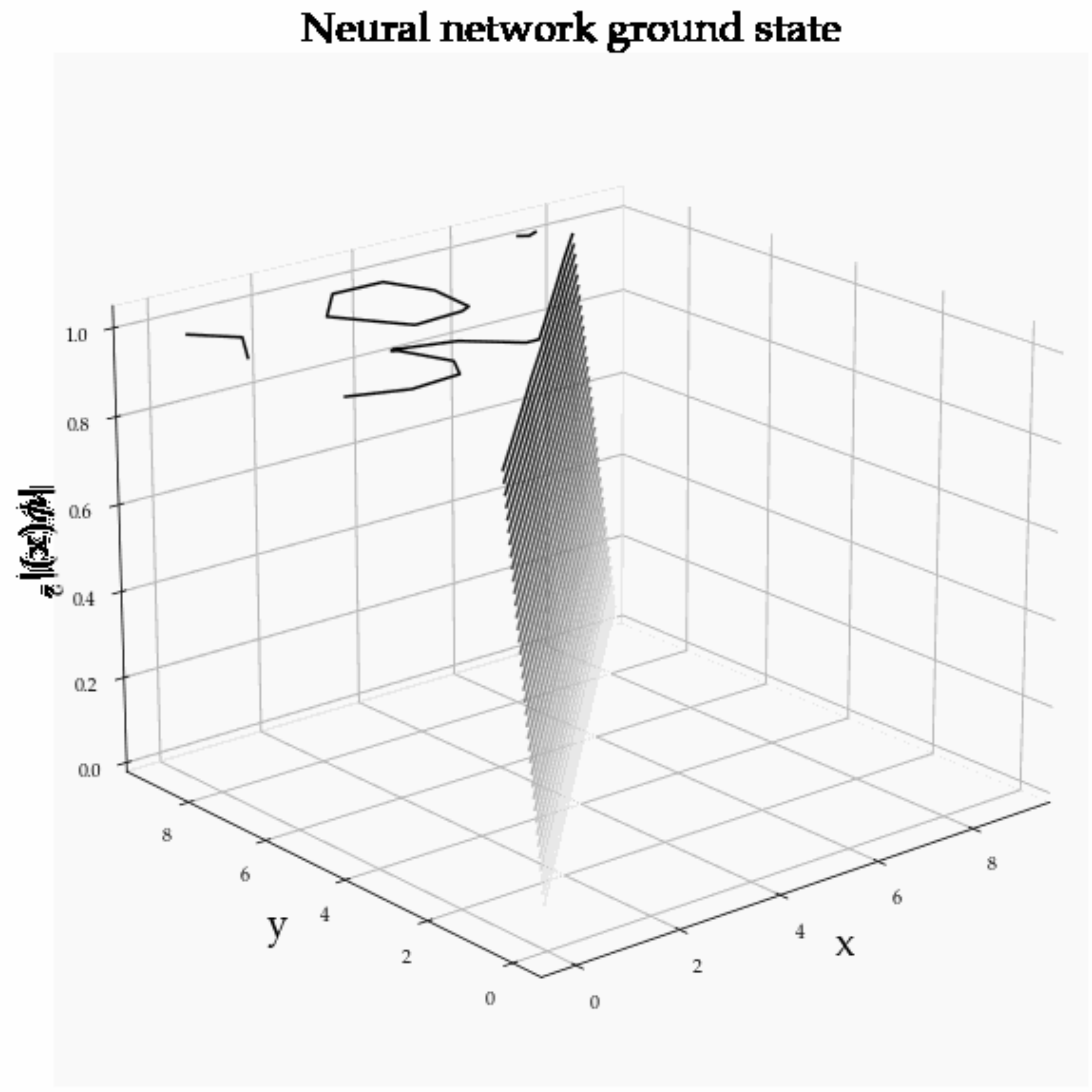
- Marginalize w.r.t. the hidden nodes:

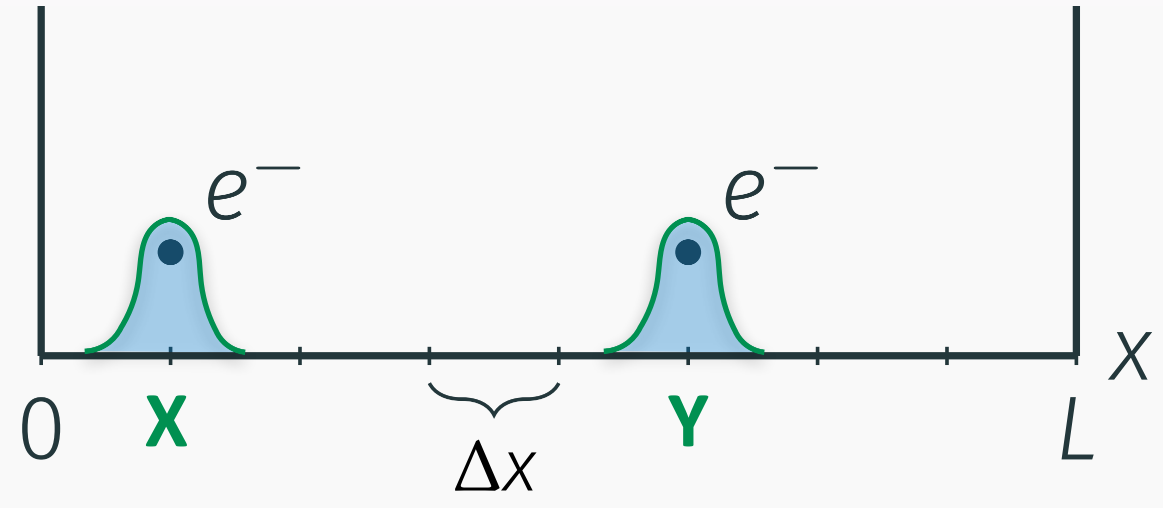
$$\langle x|\psi\rangle \to \mathcal{P}(\mathrm{v}) = \sum_{\{\mathrm{h}\}} \mathcal{P}(\mathrm{v} \cap \mathrm{h})$$

Restricted Boltzmann Machine

$$\psi(\mathbf{v}) = 2^{N_h} \exp\left(\mathrm{a}^{(0)\intercal} \mathrm{v}\right) \prod_{i=1}^{N_h} \left[\exp\left(K^{(i)} + \mathrm{a}^{(i)\intercal} \mathrm{v}\right) \cosh(\omega_i(\mathrm{v}))\right]$$

Two fermions — NQS wave function





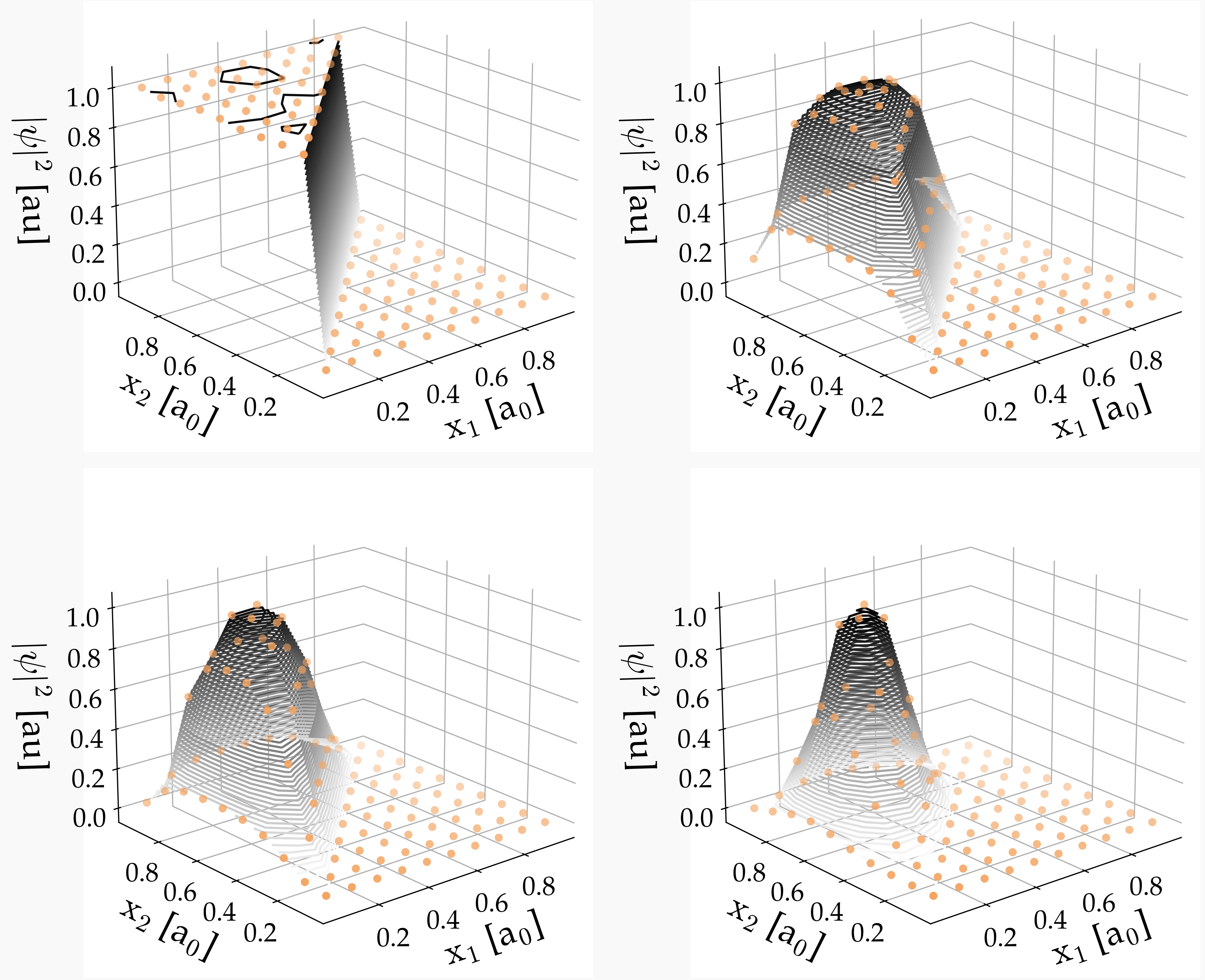
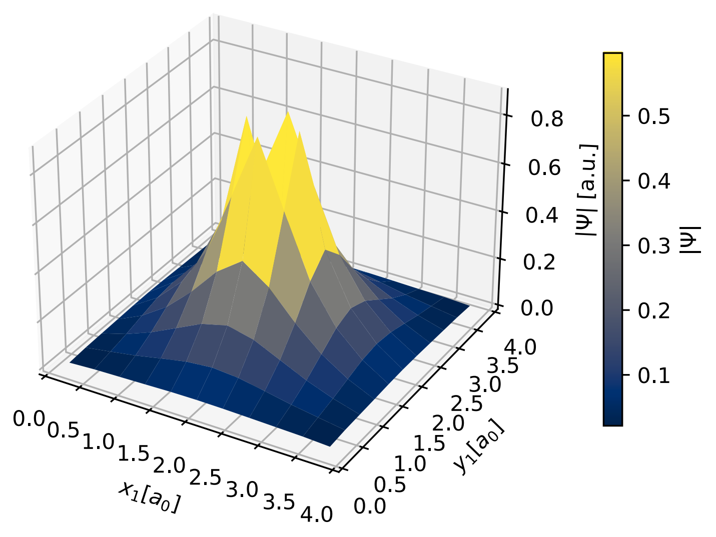


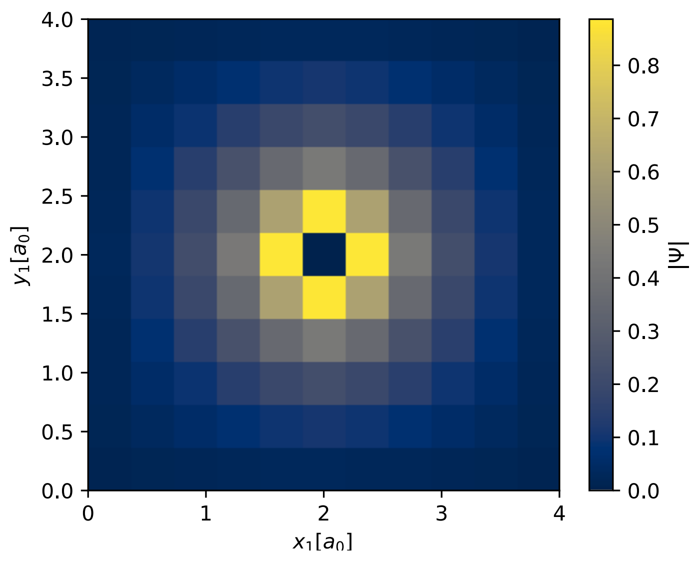
Figure 2: *Physical* learning process of an RBM with $N_h = 20$ from the starting wave function (upper left). The NN seems to be learning boundaries and antisimmetry in the following iterations (number 15, 30 and 300 are reported).

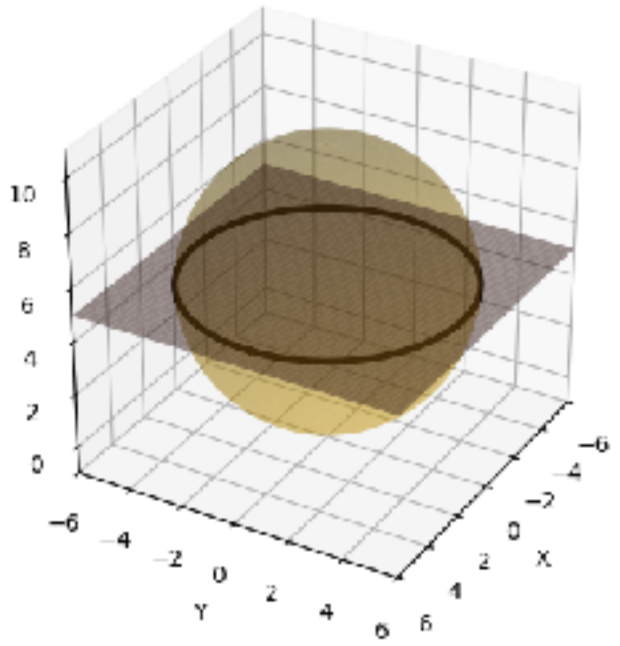
Examples for 2- and 3-fermion systems

Lithium atom
(3 electrons)

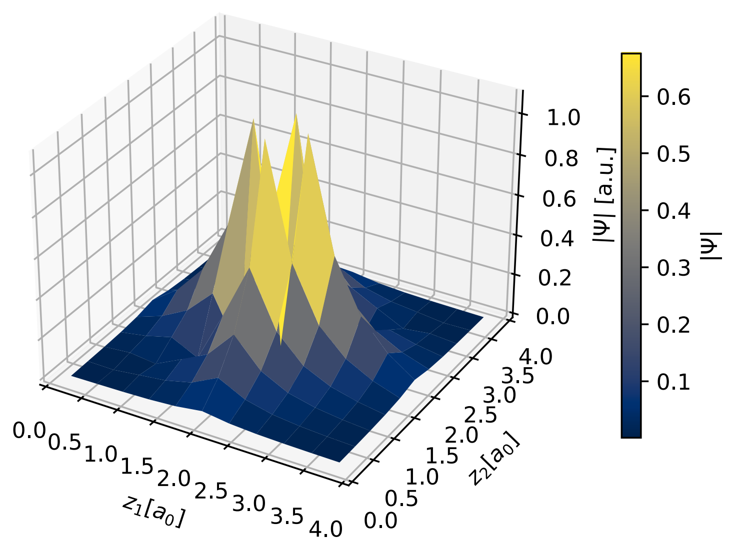
Motion of one electron on the equatorial plan, with the other two (spin up and down) near the atom's center.

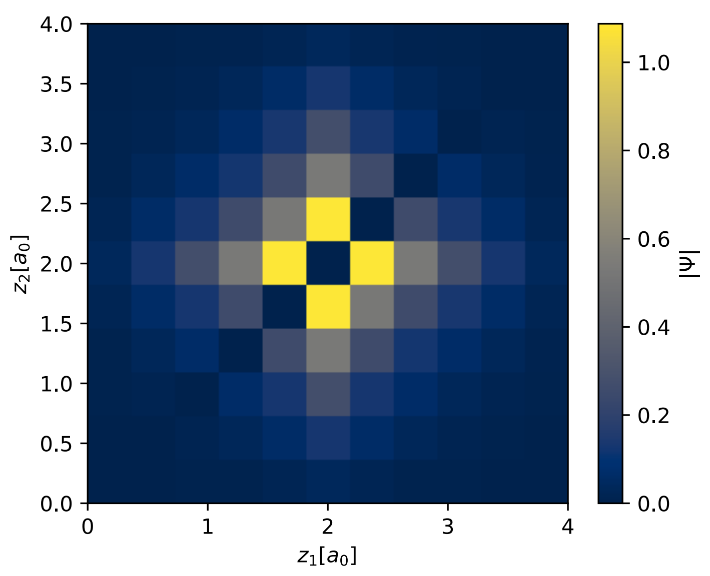






Two spin-up electrons on a vertical line passing through the nucleus; and with the third (spin-down) near the atom's center.





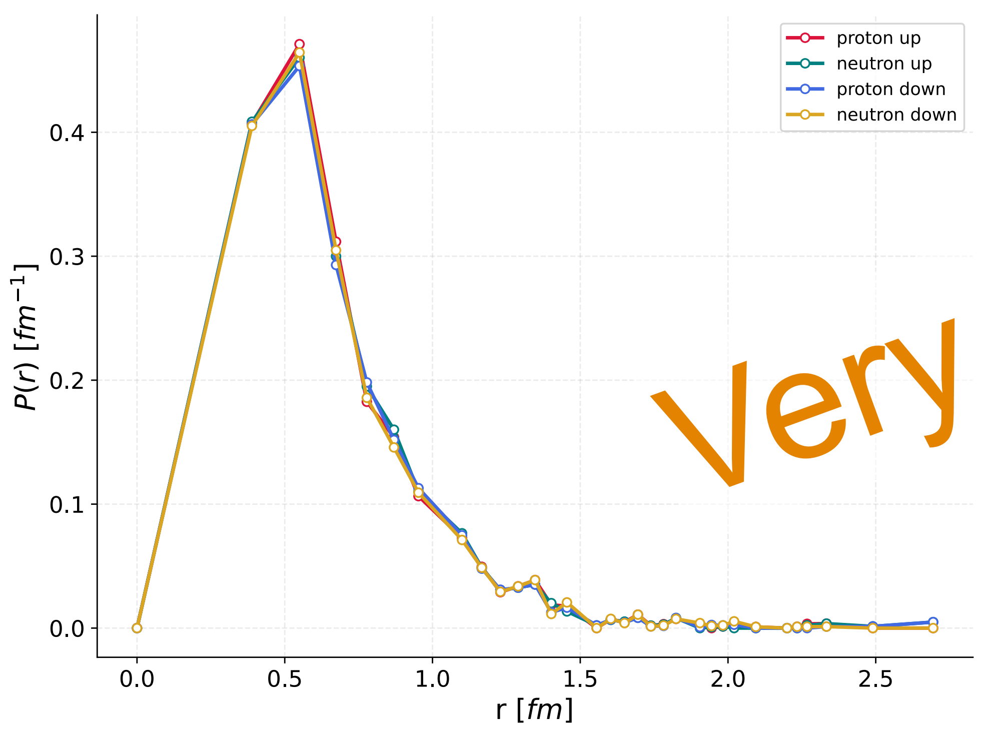
The deuteron
(proton-neutron)

Extension to a **4-fold** *RBM lattice* to account for spin and isospin.

Semi-realistic Argonne V6 potential

$$V = \sum_{i=1}^{6} V_i(r)\hat{O}_i$$

$$O_1 = \mathbb{I}, \quad O_2 = \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, \quad O_3 = \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2, \quad O_4 = (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2),$$
$$O_5 = S_{12}, \quad O_6 = S_{12}(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)$$



Very preliminary!

Recent Progress in Many-Body Theories (RPMBT-23)

https://rpmbt23.mi.infn.it/

RPMBT-23 conference in Milan, Sept 14-18, 2026

School on Quantum Simulation, Sept. 9-11, 2026

Abstract submission opens in a few days!

(...and Thank You for your Attention!!!!!).