UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

INFN MILANO

A simple NQS model in a discrete lattice
AND
Diagrammatic Monte Carlo for paired fermions

Carlo Barbieri

Outline:

- ***Nuclear physics*** *(motivations)*
- ***Electrons in a box***
- ***Richardson pairing model***

Thesis work by:

L. Lazzarino, G. Paravizzini, BSc

S. Brolli, MPhys

All preliminary work!

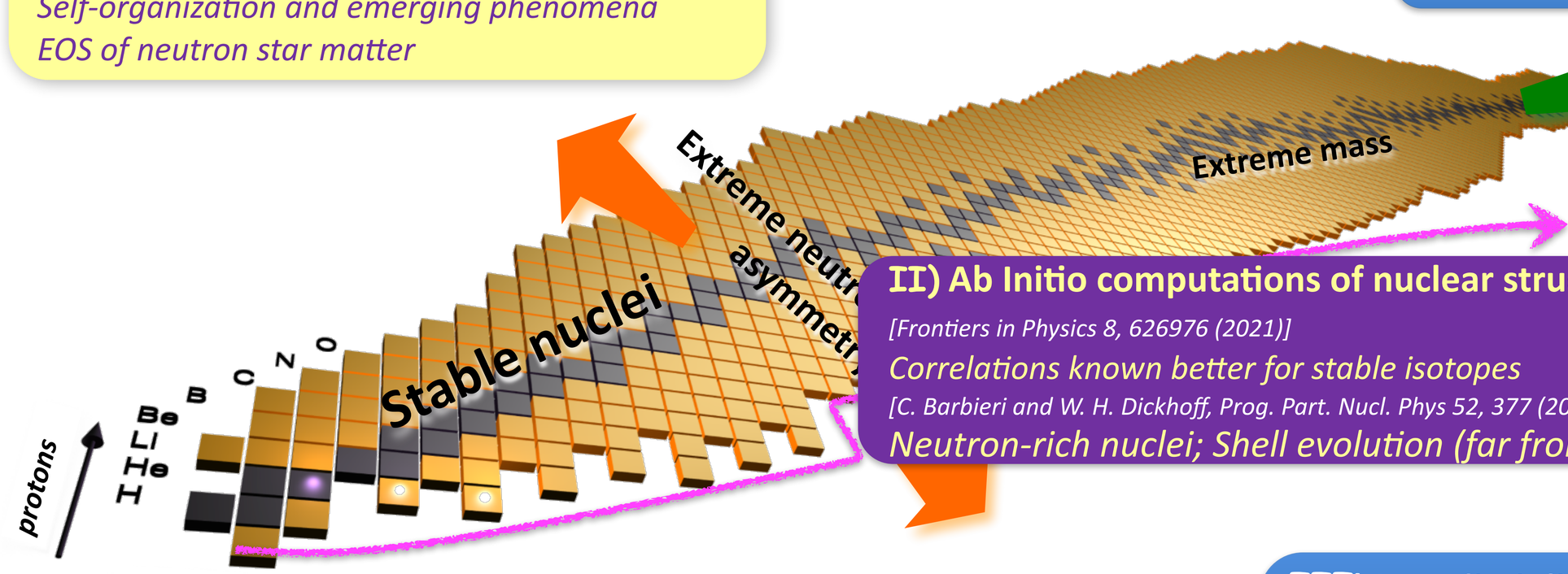
Overview of low-energy nuclear physics

Composite system of interacting fermions

Binding and limits of stability
Coexistence of individual and collective behaviors
Self-organization and emerging phenomena
EOS of neutron star matter

Experimental programs

RIKEN, FAIR, FRIB, ISAC…



II) Ab Initio computations of nuclear structure

[Frontiers in Physics 8, 626976 (2021)]
Correlations known better for stable isotopes
[C. Barbieri and W. H. Dickhoff, Prog. Part. Nucl. Phys 52, 377 (2004)]
Neutron-rich nuclei; Shell evolution (far from stability)

I) Understanding the nuclear force

QCD-derived; 3-nucleon forces (3NFs)
First principle (ab-initio) predictions

- 283 st
- ≈3,00
- ≈7,00

Nature **473**,

III) Interdisciplinary character

Astrophysics
Tests of the standard model
Other fermionic systems:
ultracold gasses; molecules;

Editors: L. Coraggio, S. Pastore, CB

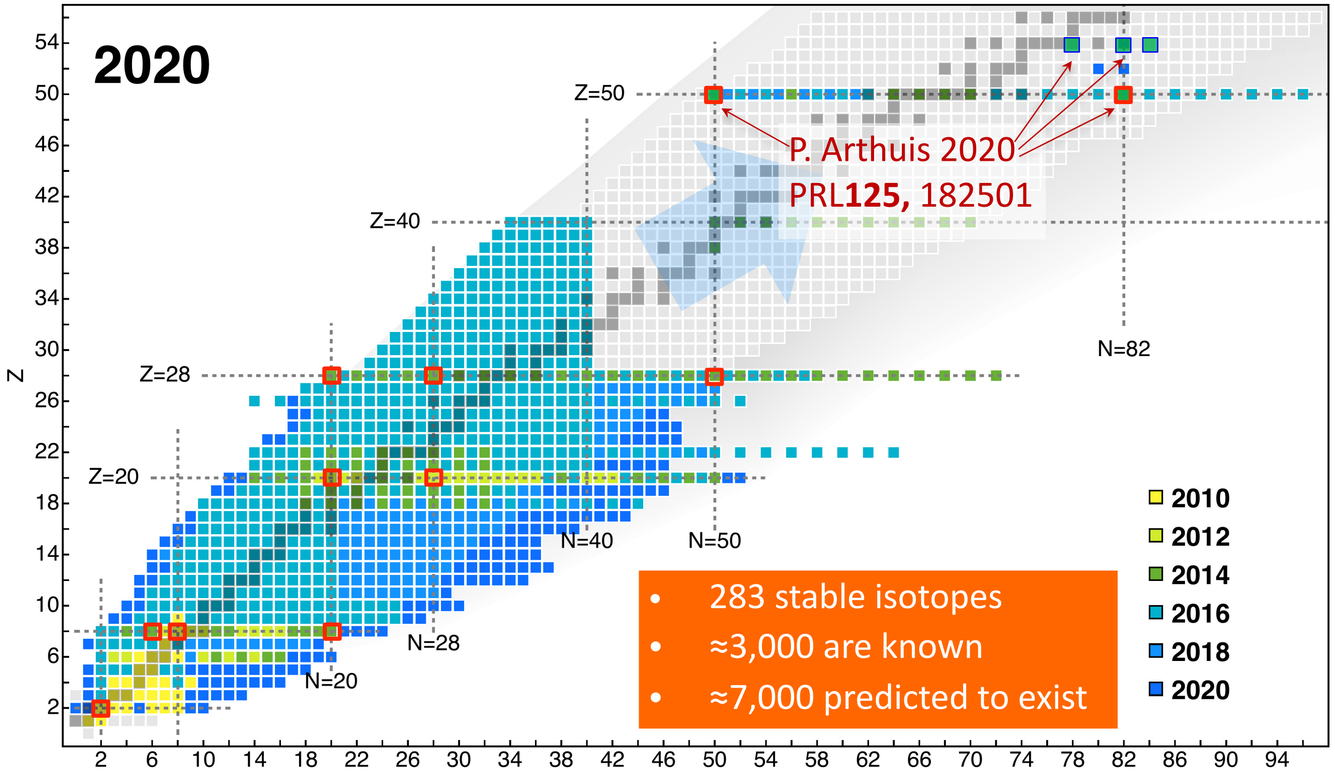
FRONTIERS topical review (doi: 10.3389/fphy.2020.626976) :

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

Reach of ab initio methods across the nuclear chart

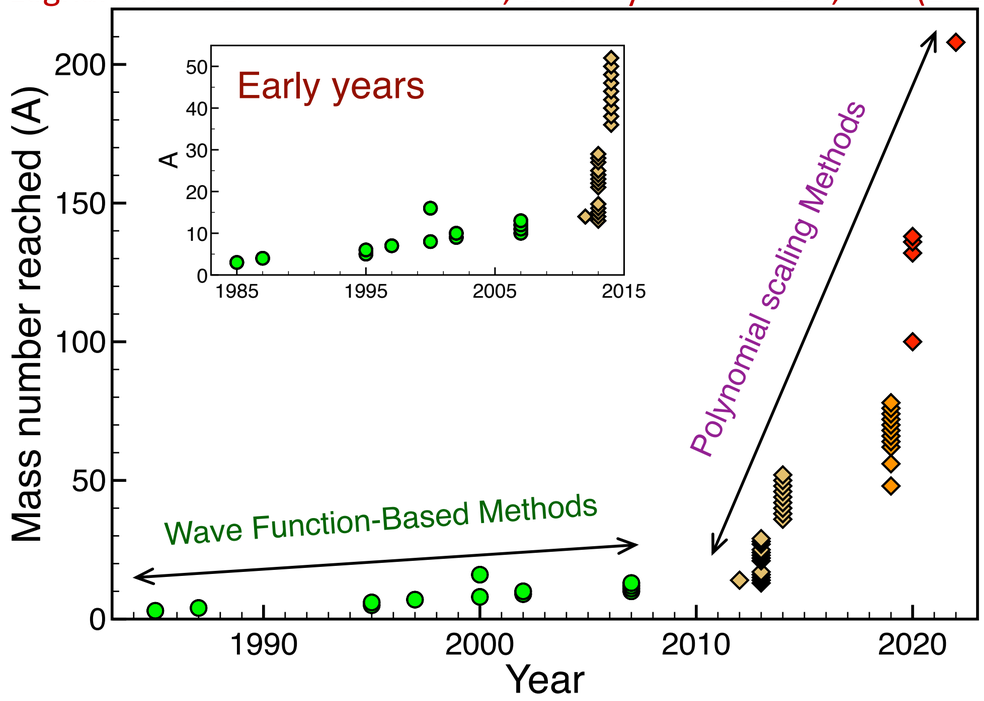
Extension beyond few-nucleons thanks to:

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



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

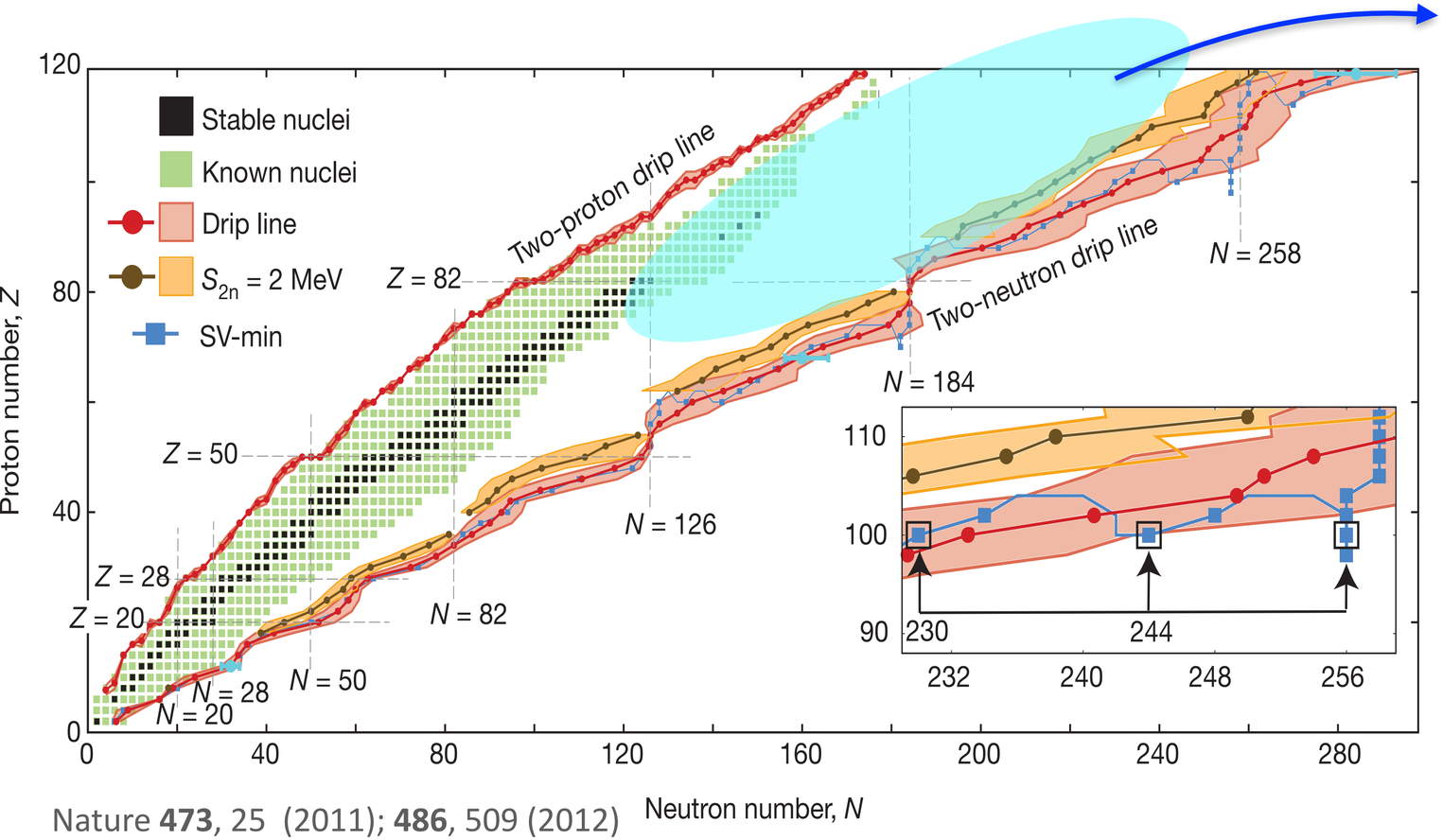
Legnaro Natl' Lab Mid Term Plan; Eur. Phys. J. Plus **138**, 709 (2023)



Open challenges:

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

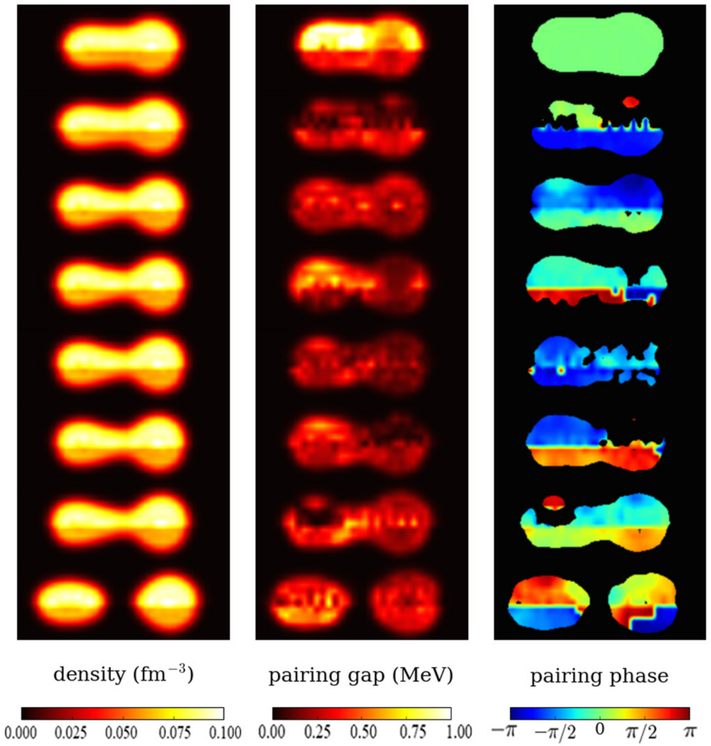
Quest to predict exotic (unstable) isotopes



Nature **473**, 25 (2011); **486**, 509 (2012)

- 283 stable isotopes
- ≈3,000 are known
- ≈7,000 predicted to exist

Most isotopes **are deformed** (even tri-axially) and change shape under external action



Bulgac et al., Phys Rev C **100**, 034615 (2019)

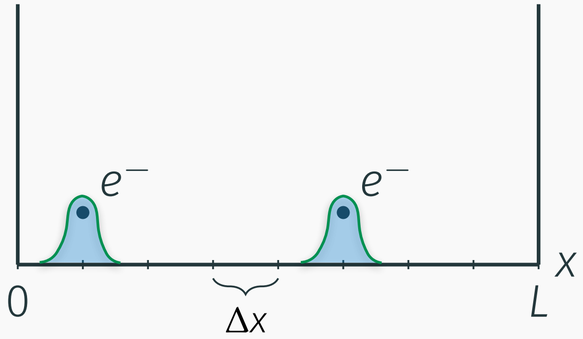
Fission of ^{240}Pu:

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

NQS for
fermions confined in a box

Confined fermions w/ a discrete coordinate space mesh

- Discretise coordinate space
- Use occupation number to locate particles



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

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***):

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

Can be solved as in Carleo and Troyer, Science **355**, 602 (2017)

NQS representation

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

$$\mathcal{P}(\mathsf{v}\cap\mathsf{h}) = \frac{1}{\mathcal{Z}}\exp\left(\mathsf{a}^{\mathsf{T}}\mathsf{v} + \mathsf{b}^{\mathsf{T}}\mathsf{h} + \mathsf{h}^{\mathsf{T}}\underline{\underline{W}}\mathsf{v}\right) \qquad \text{with:} \quad \begin{cases} \mathsf{v}\in\{-1,1\}^{N_v} \\ \mathsf{h}\in\{-1,1\}^{N_h} \end{cases} \qquad \begin{cases} \mathsf{a}\in\mathbb{C}^{N_v} \\ \mathsf{b}\in\mathbb{C}^{N_h} \\ W\in \mathrm{Mat}_{N_h\times N_v}(\mathbb{C}) \end{cases}$$

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

$$\langle x|\psi\rangle \rightarrow \quad \mathcal{P}(\mathsf{v}) = \sum_{\{\mathsf{h}\}} \mathcal{P}(\mathsf{v}\cap\mathsf{h})$$

$$\begin{cases} \mathsf{a} = \mathsf{a}^{(0)} + \Delta\mathsf{a} = \mathsf{a}^{(0)} + \sum_{i=1}^{N_h} \mathsf{a}^{(i)} \\ 1/\mathcal{Z} = \exp\left(\sum_{i=1}^{N_h} K^{(i)}\right) \\ \mathsf{W}^{(i)} = \begin{pmatrix} W_{1,i} \\ W_{2,i} \\ \vdots \\ W_{N_v,i} \end{pmatrix} \in \mathbb{C}^{N_v}, \\ \omega_i(\mathsf{v}) = \mathsf{W}^{(i)\mathsf{T}}\mathsf{v} + b_i = \sum_j W_{ji}v_j + b_i, \end{cases}$$

Restricted Boltzmann Machine

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

<— Note that $\mathbf{a}^{(i)}$ are site dependent and no hidden nodes are necessary for a single particle (N_h=0).

Energy minimization

- The Hamiltonian for N_v fermions fermions will be:

$$\mathcal{H} = T + V = \sum_i \frac{-\hbar^2}{2m_i(\Delta x)^2} \sum_j \left[\psi^\dagger_{j+1}\psi_j - 2\psi^\dagger_j\psi_j + \psi^\dagger_{j-1}\psi_j\right] + V$$

+ appropriate conditions at the walls.

- Sample E_{loc} from $|\psi(x)|^2 \sim \mathrm{RBM}^2$ using MCMC:

$$E_{\mathrm{loc}}(\mathsf{x}) = \int d\mathsf{x}'\, \mathcal{H}_{\mathsf{x}\mathsf{x}'} \frac{\psi(\mathsf{x}')}{\psi(\mathsf{x})}$$

$$\frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \langle E_{\mathrm{loc}}\rangle_{|\psi(\mathsf{x})|^2}$$

Use gradient descent w/ SR:

$$D_k(\mathsf{x};\theta) = \frac{\partial_{\theta_k}\psi^\theta(\mathsf{x})}{\psi^\theta(\mathsf{x})}$$

$$\partial_{\theta_k}\langle\mathcal{H}\rangle_\psi = \langle G_k\rangle_{|\psi(\mathsf{x})|^2}$$

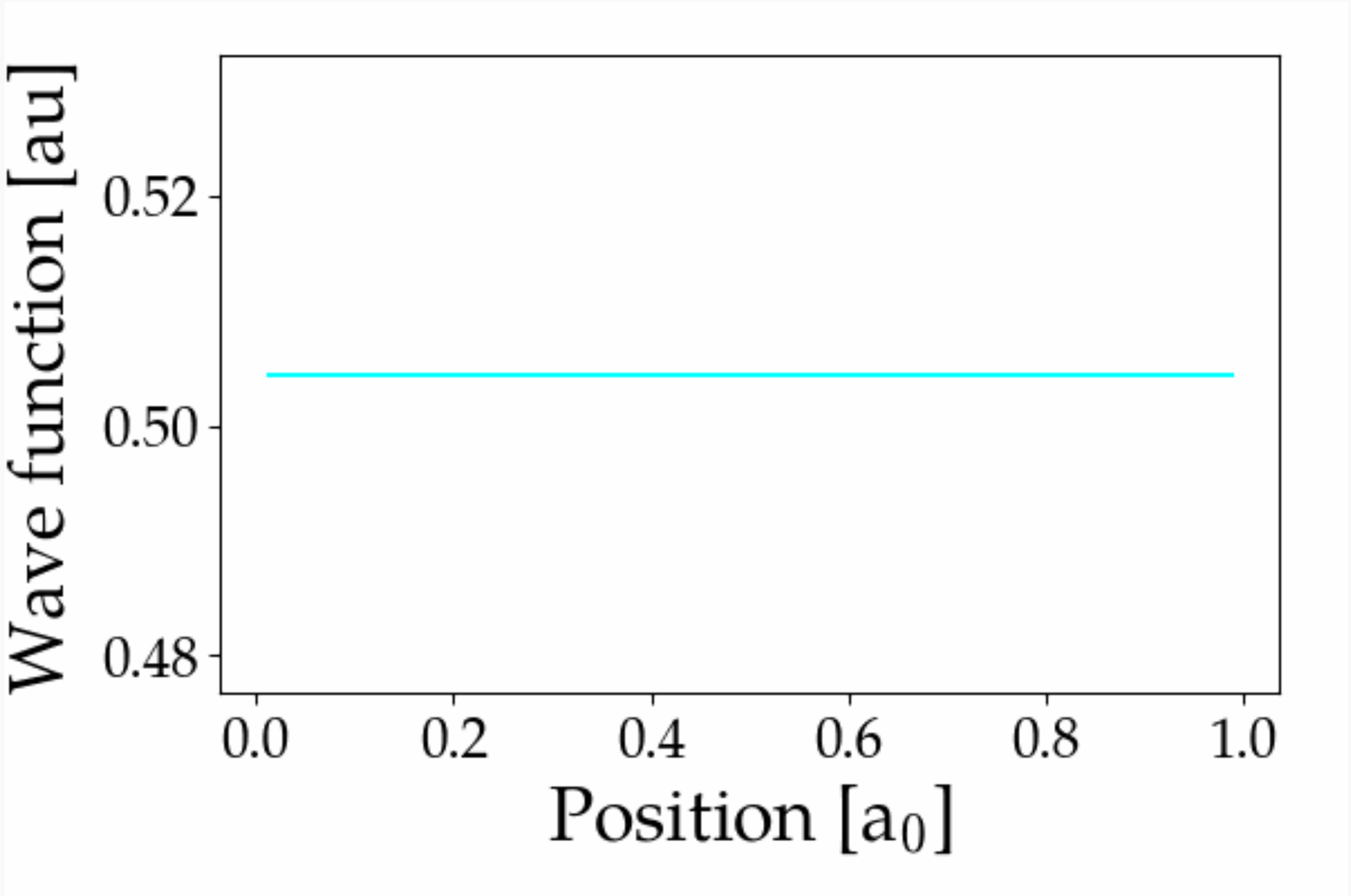
$$G_k(\mathsf{x};\theta) = 2\mathrm{Re}\left[D^*_k(\mathsf{x};\theta)\left(E_{\mathrm{loc}}(\mathsf{x}) - \langle E_{\mathrm{loc}}\rangle_{|\psi(\mathsf{x})|^2}\right)\right]$$

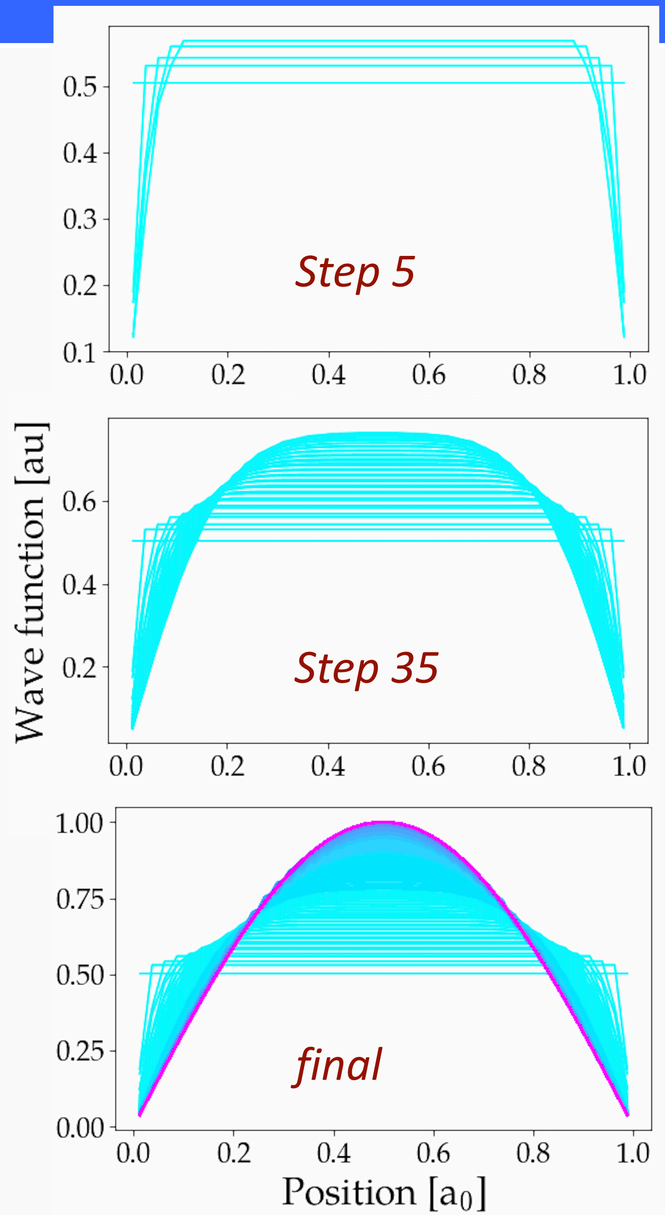
Stochastic Reconfiguration

$$\theta^{(t+1)} = \theta^{(t)} - \eta^{(t)}\, S^{-1}\, \nabla_\theta \langle\mathcal{H}\rangle_\psi,$$

$$S_{ij} = \langle D^*_i\rangle\langle D_j\rangle - \langle D^*_i D_j\rangle,$$

One fermion — optimization





Two fermions — optimization

Convergence with N_v=10

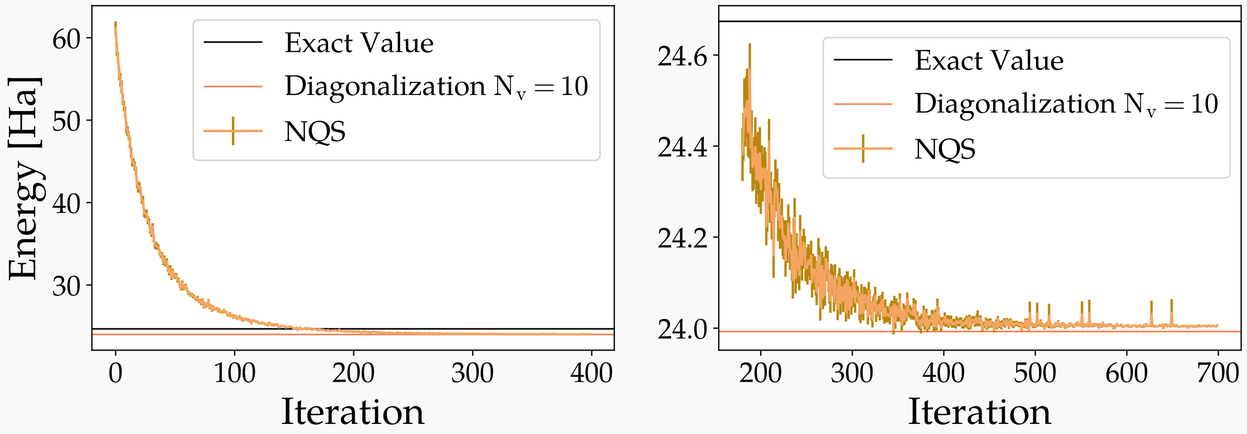


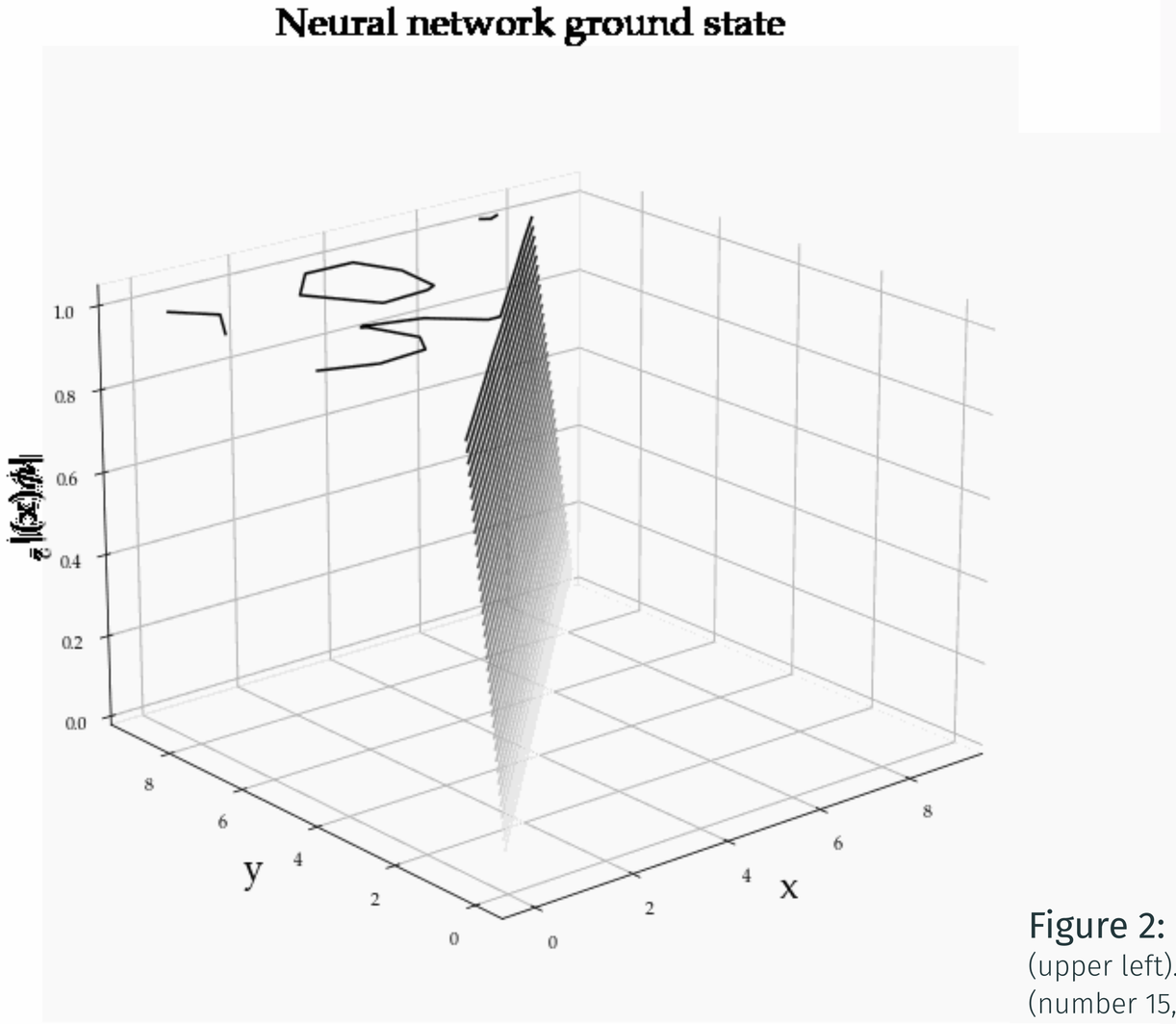
Figure 1: Solution for the two particles non-interacting problem with an RBM built with only 10 hidden nodes. This simulation proves that it is possible to have a satisfying approximation also with relatively few hyper parameters.

Hyperparameter optimization

N_h	$\langle t \rangle$ / iteration	$\Delta E / E$
40	2.75 min	2%
30	1.8 min	2.6%
20	1 min	0.03%
10	16.2 s	0.05%
5	4 s	60%

Table 1: Efficiency and quality of convergence of RBMs with various N_h to model the two non-interacting fermions in a box. N_v is set to 10 for every simulation.

Two fermions — NQS wave function



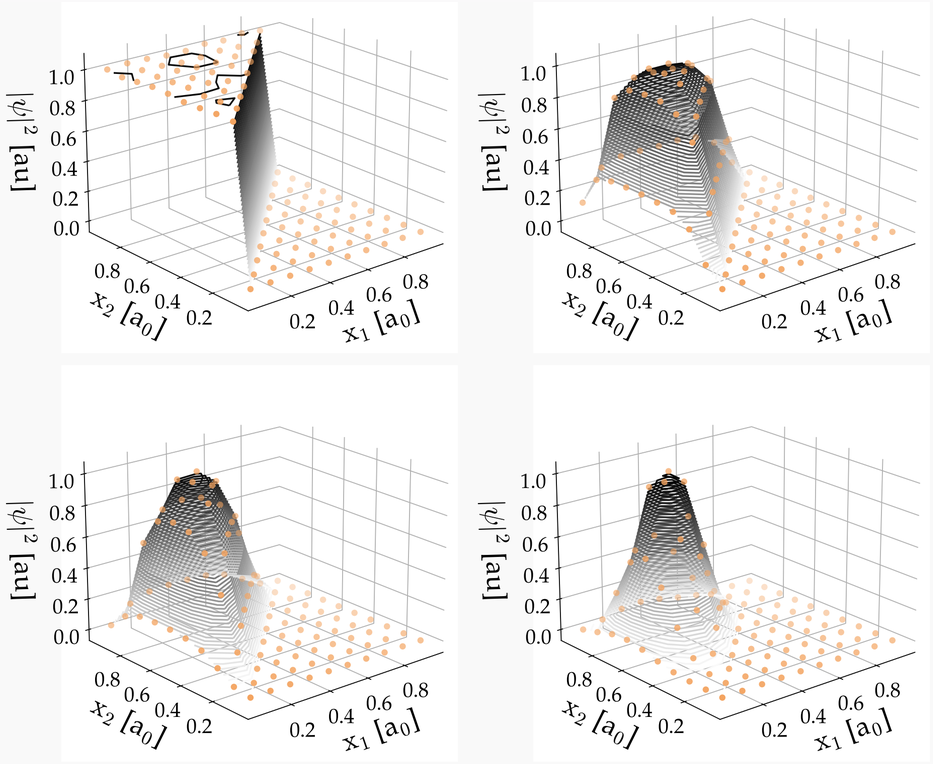


Figure 2: *Physical* learning process of an RBM with $N_h = 20$ from the starting wave function (upper left). The NN seems to be learning boundaries and antisimmetry in the following iterations (number 15, 30 and 300 are reported).

Hydrogen atom on the 3D lattice

Convergence

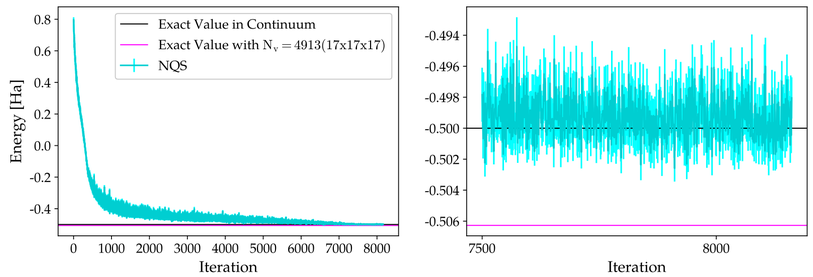


Figure 3.4: The optimization of the network for the hydrogen atom confined in a box Nv=4913(17x17x17) and a zoom of the last iterations on the right. The network seems to converge to the exact value in the continuum limit but it misses the correct result for the discretized problem.'

The cusp at the proton site is recovered

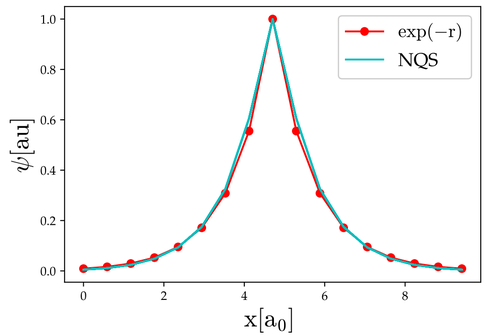
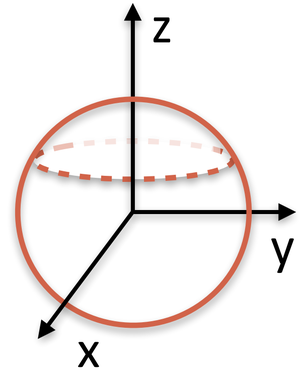
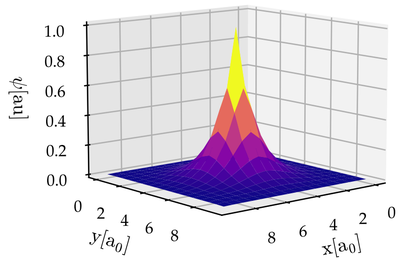


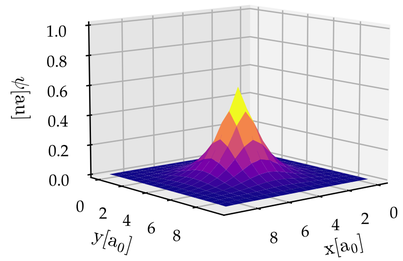
Figure 3.7: One-dimensional section of the hydrogen wave function in correspondence of the nucleus compared with theoretical behavior $\propto exp(-r)$.

RBM wave function (x-y plane at z=cons)

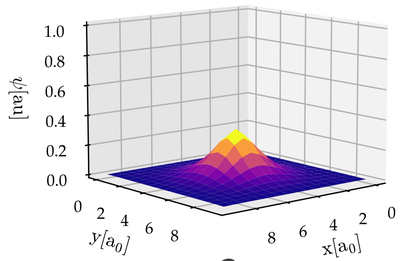




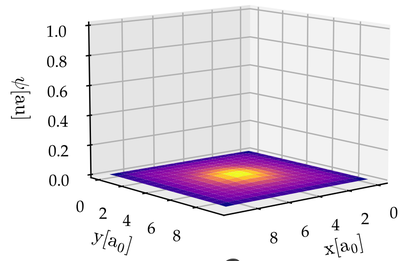
z=0



z=a_0



z=2a_0



z=3a_0

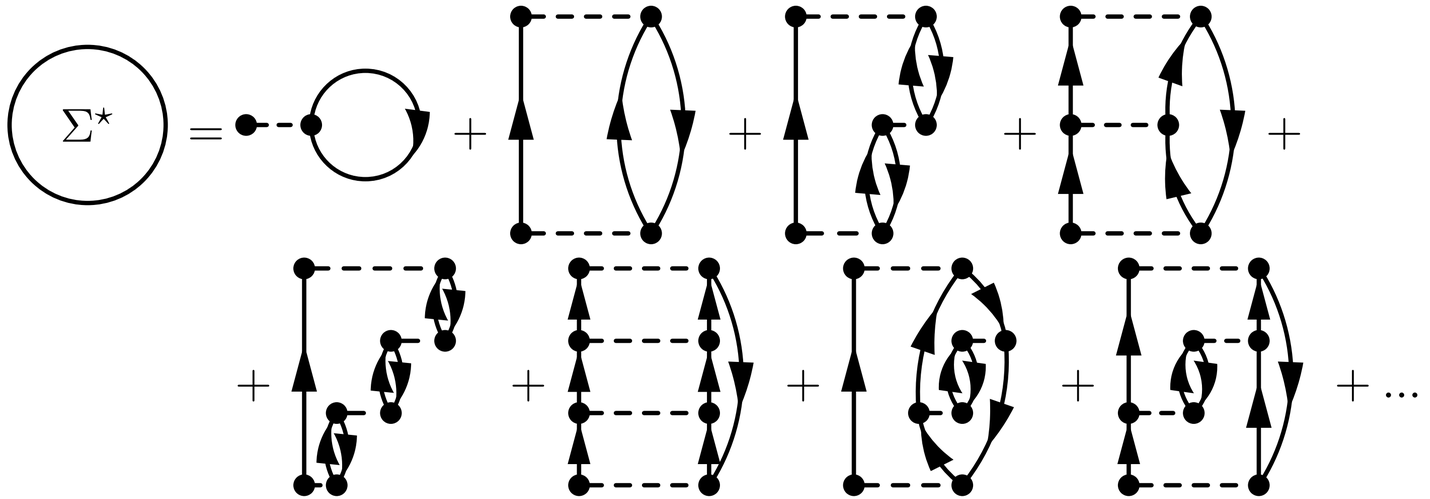
Self-consistent Green's function (SCGF)
and
Diagrammatic Monte Carlo (DiagMC)

Green's function theory for nuclei

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

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

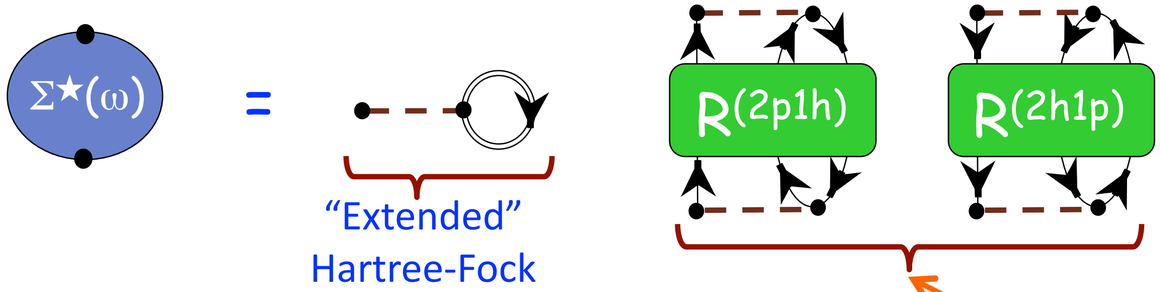
It requires knowing the self-energy which is the sum of an *infinite series* of Feynman diagrams:



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

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

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

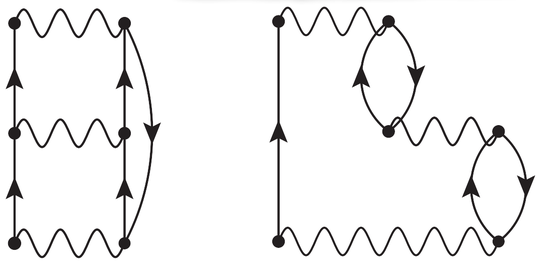


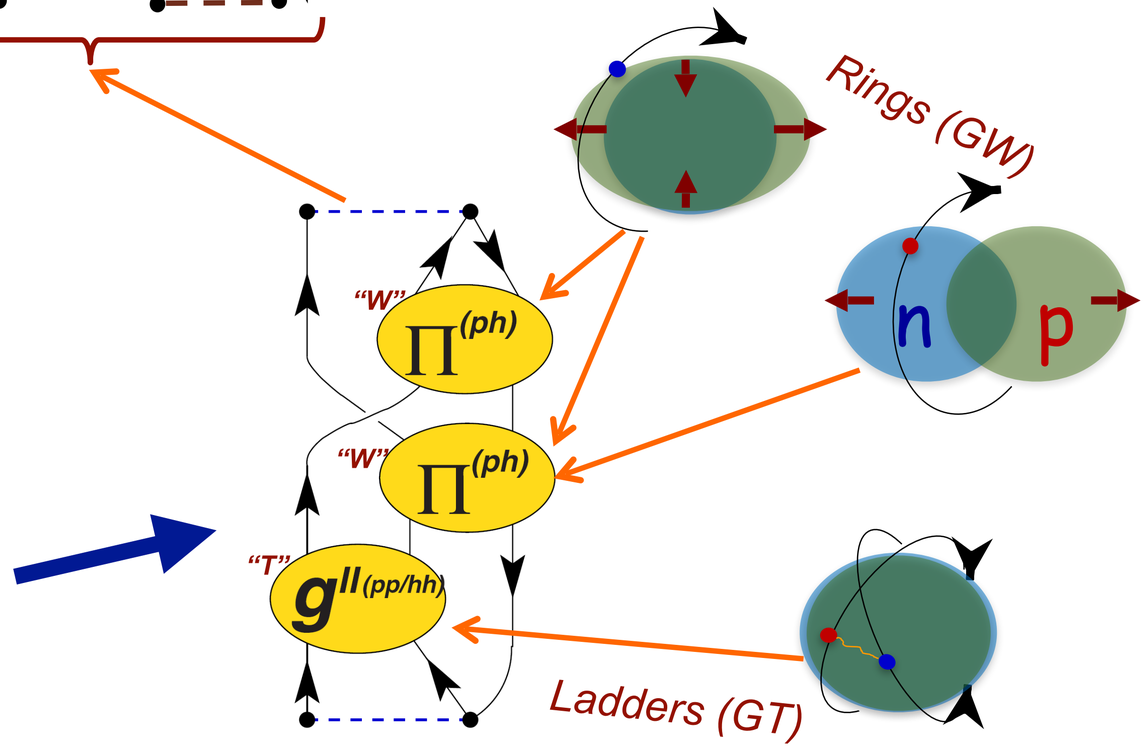
F-RPA:
*Phys. Rev. C**63**, 034313 (2001)*
*Phys. Rev. A**76**, 052503 (2007)*
*Phys. Rev. A**83**, 042517 (2011)*

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

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

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

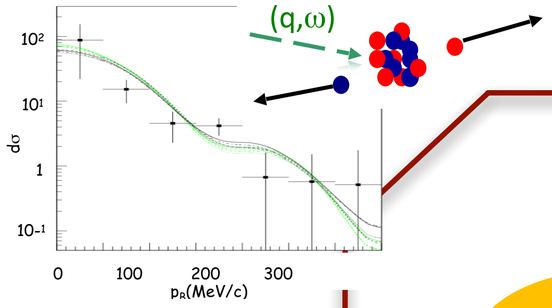




The Self-Consistent Green's Function with Faddev-RPA

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

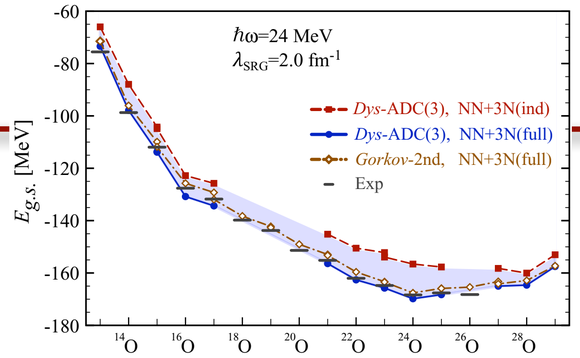
[Eur. Phys. J. A**43**, 137 (2010)]



Binding energies

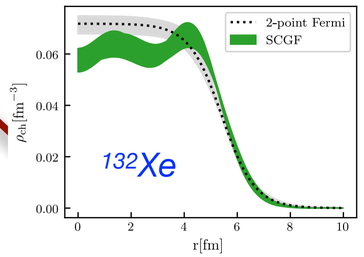
Oxygen drip line

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



Charge & matter distribution

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



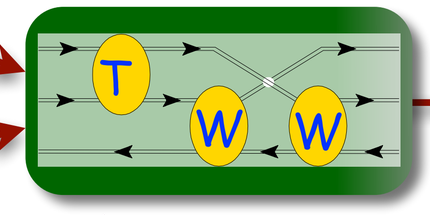
	SCGF	Exp.
^{100}Sn	4.525 – 4.707	
^{132}Sn	4.725 – 4.956	4.7093
^{132}Xe	4.700 – 4.948	4.7859
^{136}Xe	4.715 – 4.928	4.7964
^{138}Xe	4.724 – 4.941	4.8279

Spectroscopy

Ionisation energies and affinities for simple atoms and molecules

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

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



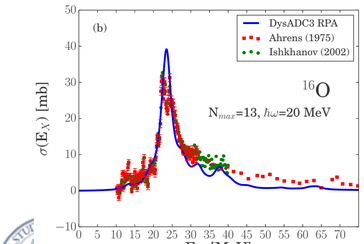
T ladders

W rings

Dyson Eq.

Nuclear ELM response and dipole polarisability, α_D

[Phys Rev C77, 024304 (2008)]

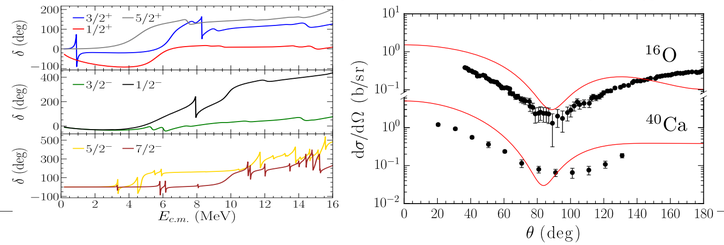


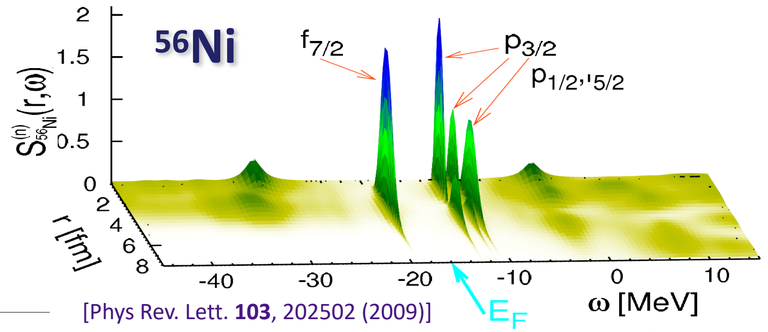
^{68}Ni:

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

Optical potential

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





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

Ab-initio Nuclear Computation & BcDor code

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

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

Code history:

2006 — core functions and FRPA

shell model charges&interactions (lowest order)

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

2012 — Coupled clusters equations

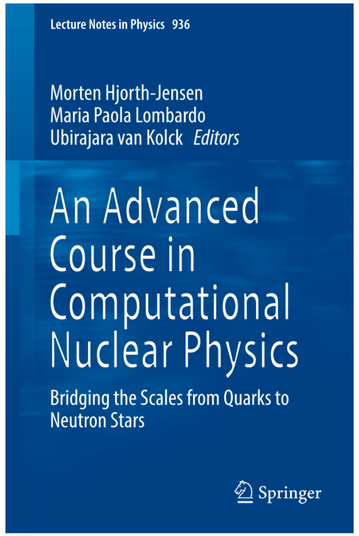
Three-nucleon forces (A. Cipollone, 2011–2015)

2013

2014 — Gorkov at 3rd order (will become massively parallel…)

2022

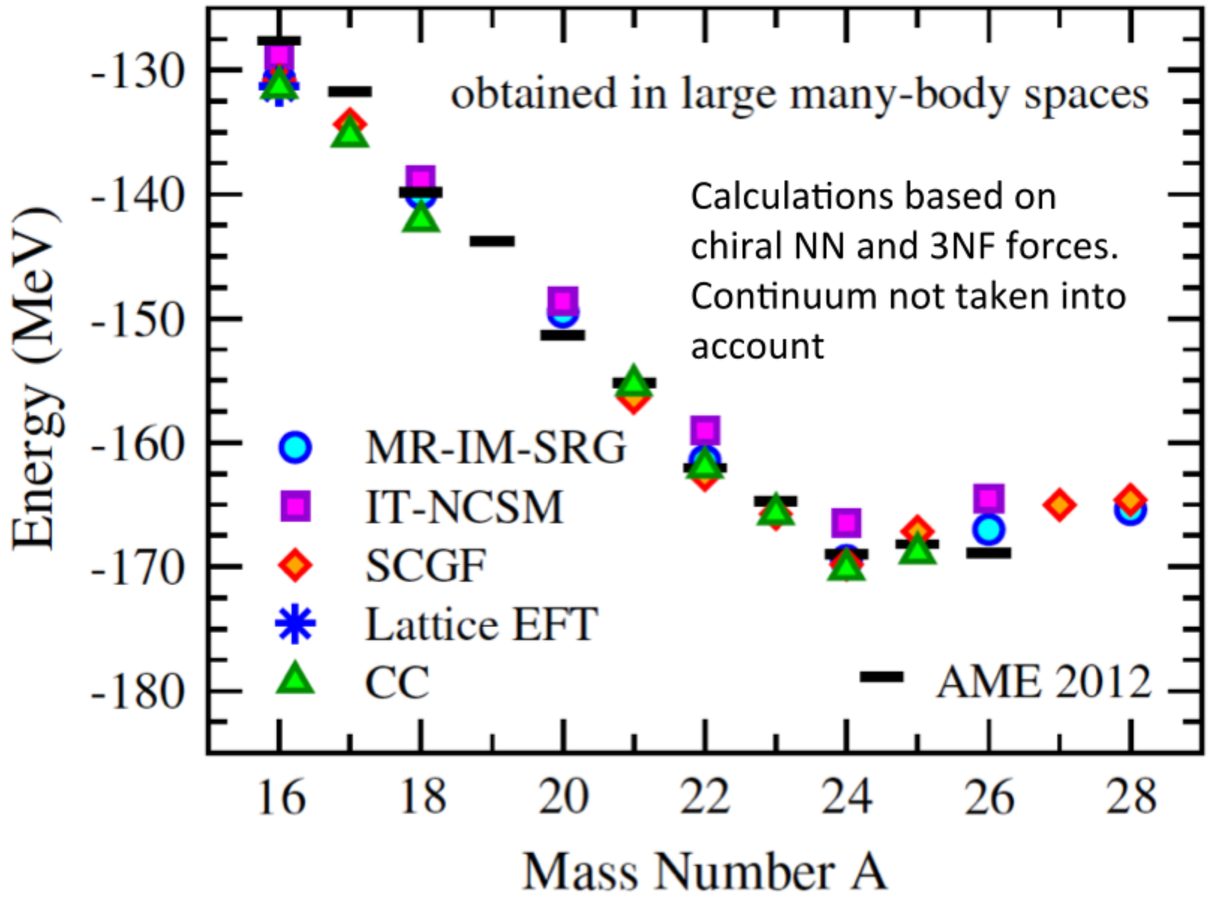
applications →



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

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

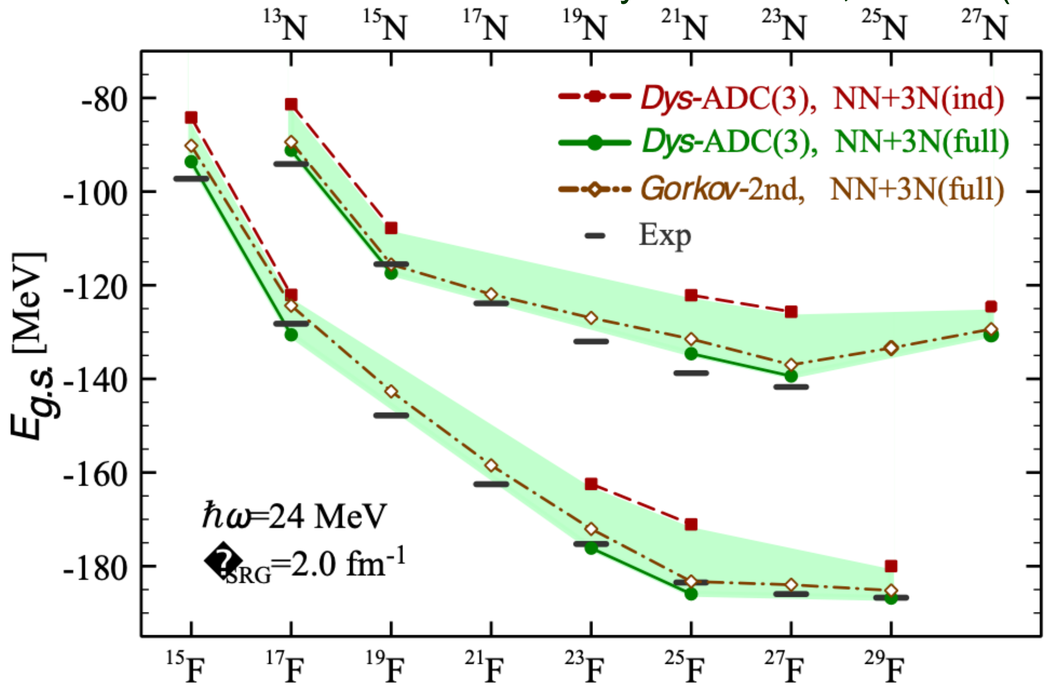
Benchmark of ab-initio methods for oxygen isotopic chain



K. Hebeler et al., Annu. Rev. Nucl. Part. Sci. **65**, 457 (2015)

A. Cipollone, CB, P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013)

and Phys. Rev. C **92**, 014306 (2015)

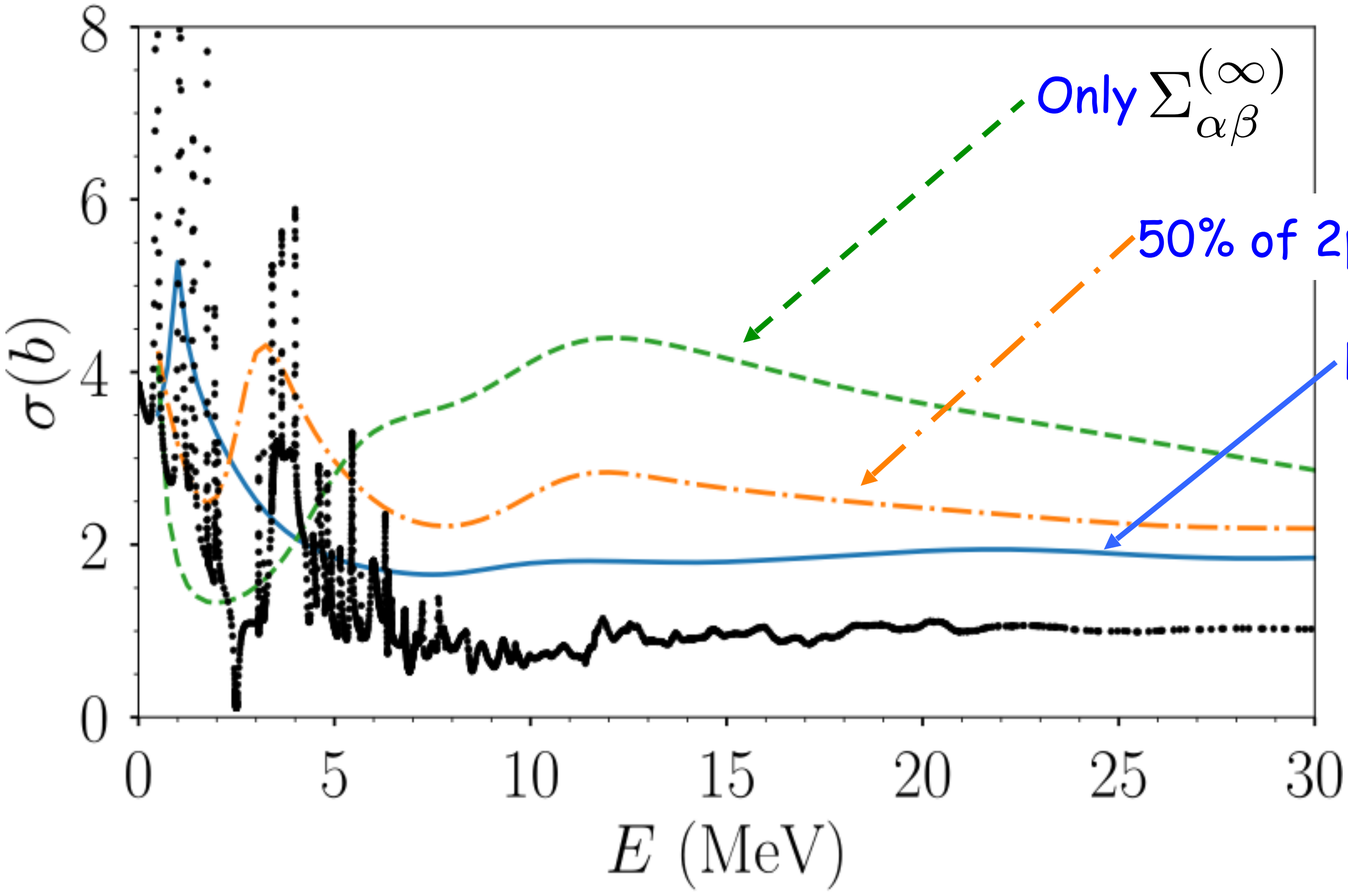


→ 3NF tensor and 3NF near flourine's dripline

Role of intermediate state configurations (ISCs)

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

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

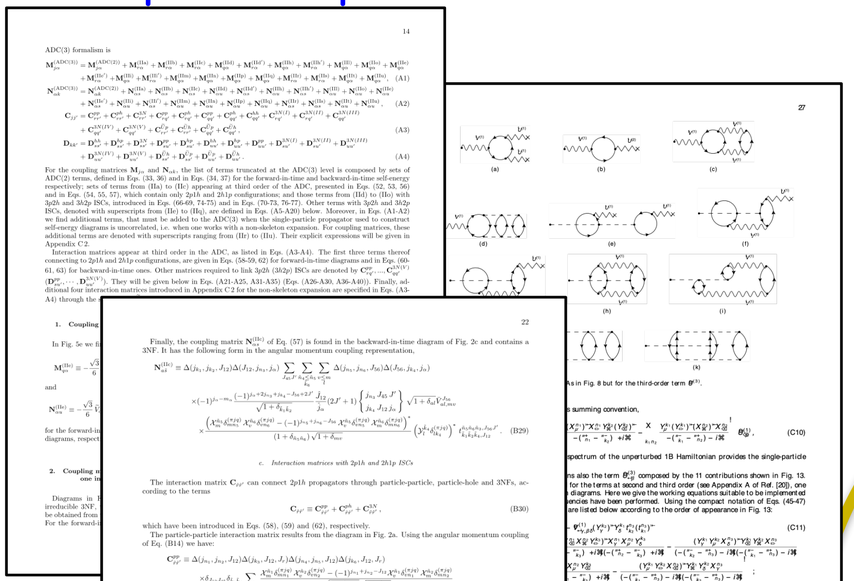


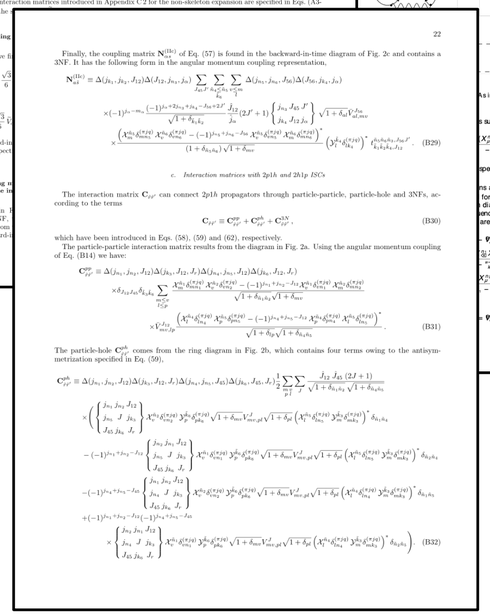
High order configurations, or ADC(n>>3), to be critical for fully ab initio optical potentials

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

Inclusion of NNN forces

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





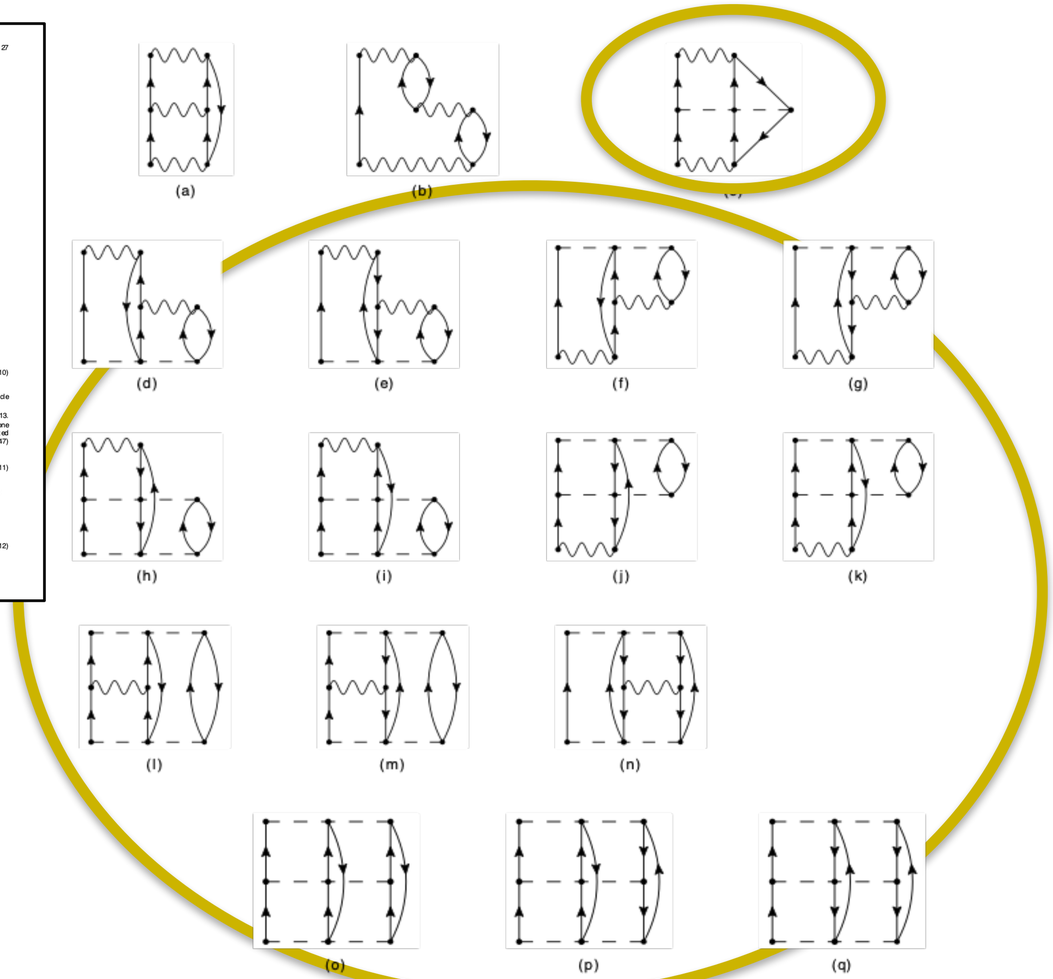


FIG. 5. 1PI, *skeleton* and *interaction irreducible* self-energy diagrams appearing at 3rd-order in perturbative expansion (7), making use of the effective hamiltonian of Eq. (9).

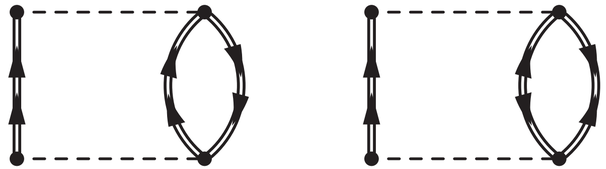
Formalism already laid out:

F. Raimondi, CB, Phys. Rev. C**97**, 054308 (2018).

Nambu-Covariant approach to build (Gorkov) propagators

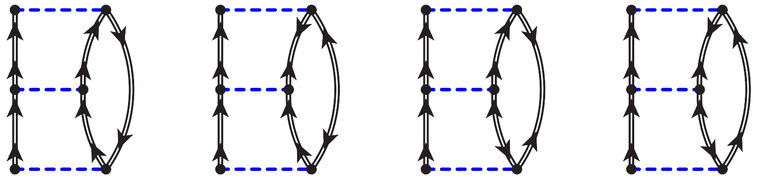
Gorkov at 2nd order:

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

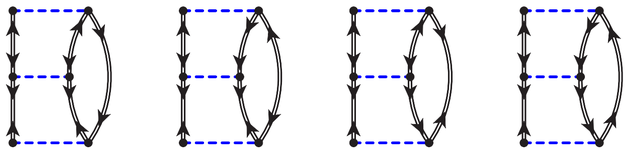


Gorkov at 3rd order:
(ONLY NN forces)

pp-ladders:

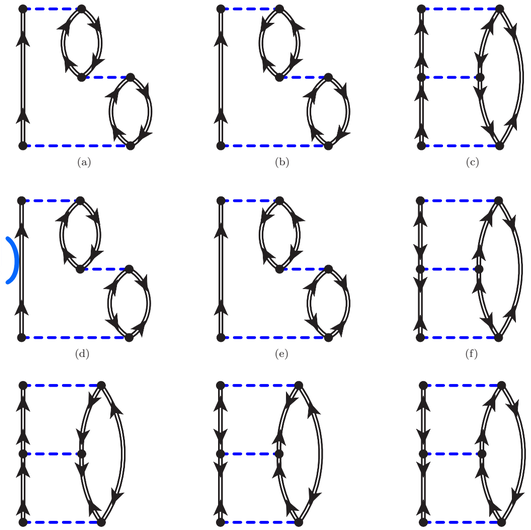


hh-interactions (hh int. among pp ladders!!!)



(NN ONLY forces)

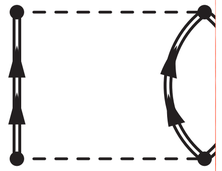
ph-rings:



Nambu-Covariant approach to build (Gorkov) propagators

Gorkov at 2nd order:

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



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

Gorkov algebraic diagrammatic construction formalism at third order

Carlo Barbieri
Department of Physics, Via Celoria 16, 20133, Milano, Italy
and INFN, Via Celoria 16, 20133, Milano, Italy

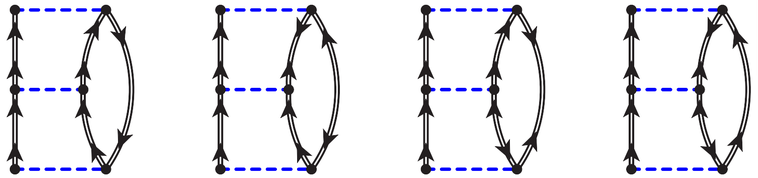
Thomas Duguet
IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France
and KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium

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

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

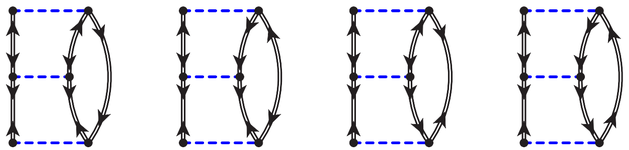
$$\widetilde{\Sigma}^{12}_{\alpha\beta}(\omega) = \sum_{rr'} \left\{ \mathcal{C}_{\alpha,r} \left[\frac{1}{\omega\mathbb{I} - \mathcal{E} + i\eta} \right]_{r,r'} \mathcal{D}^{*}_{r',\beta} + \bar{\mathcal{D}}^{\dagger}_{\alpha,r} \left[\frac{1}{\omega\mathbb{I} + \mathcal{E}^{T} - i\eta} \right]_{r,r'}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

pp-ladders:



Gorkov at 3rd order:
(ONLY NN forces)

hh-interactions (hh int. among pp ladders



(NN ONLY forces)

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

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

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

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

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

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

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

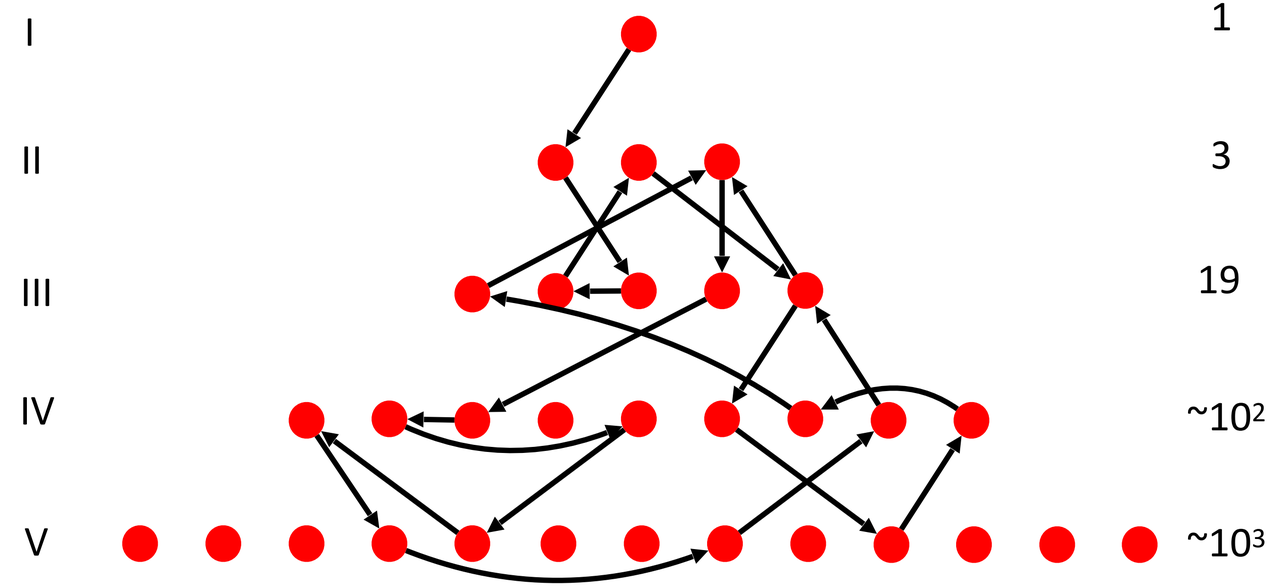
$$\mathcal{C}^{(\mathrm{IIf})}_{\alpha,r} = \frac{1}{\sqrt{6}} \mathcal{A}_{123} \sum_{\substack{\mu\nu\lambda \\ k_7k_8}} v_{\alpha\lambda,\mu\nu} \left(\mathcal{U}^{k_7}_{\lambda} \bar{\mathcal{V}}^{k_8}_{\mu} \right)^{*} \mathcal{U}^{k_1}_{\nu} t^{k_8k_2}_{k_7k_3}, \tag{50b}$$

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

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

Diagrams grow factorially (more than exponentially) with the order

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



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

Overview of the math

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

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

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

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

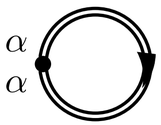
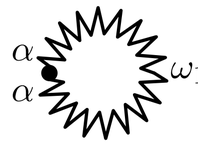
- $W_o(N)$ is an order dependent reweighting factor
- $\mathcal{Z}^{\omega}_{\alpha\beta} = \int d\mathcal{C} \; |\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})| W_o(N)$ is a normalization factor
- $w^{\omega}_{\alpha\beta}(\mathcal{C}) := \frac{|\mathcal{D}^{\omega}_{\alpha\beta}(\mathcal{C})| W_o(N)}{\mathcal{Z}^{\omega}_{\alpha\beta}}$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

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

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

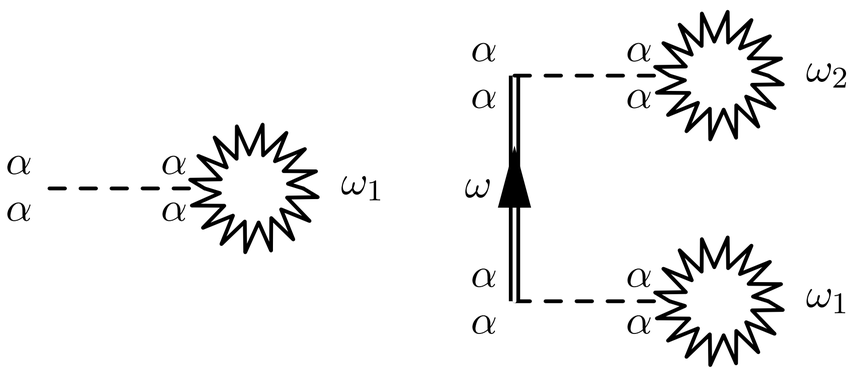
where the normalization $\mathcal{Z}^{\omega}_{\alpha\beta}$ is unknown but it can be estimated.

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

$e^{i\omega_1\eta}G_{\alpha}(\omega_1) =$  $\omega_1 \longrightarrow$  $\omega_1 := -ie^{-k\omega_1^2}$

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

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



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

$\mathcal{S}_N$ has weight:

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

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

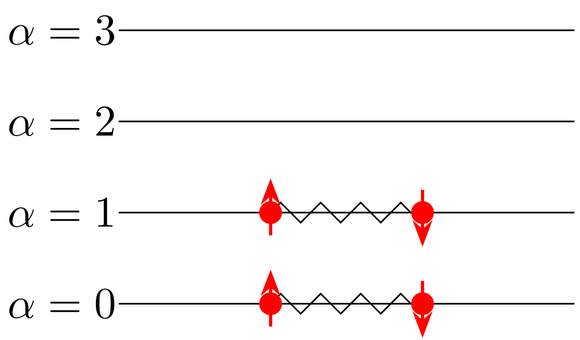
$$\frac{\mathcal{Z}_{N\alpha}^{\omega}}{\mathcal{Z}_\alpha^\omega} = \lim_{n\to\infty}\frac{\mathcal{N}}{n}$$

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

Pairing Hamiltonian

Application to the Richardson-Gaudin pairing model with D levels (of spin 1/2) and M=4 fermions:

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



The updates

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

} Standard Monte Carlo

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

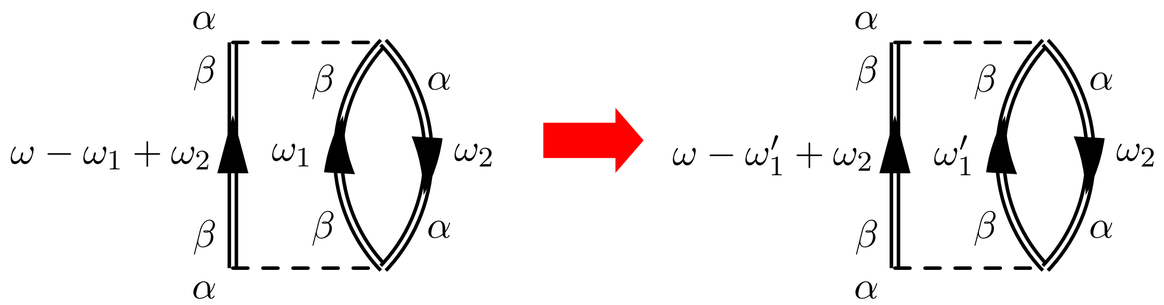
} Monte Carlo on the topology

The updates

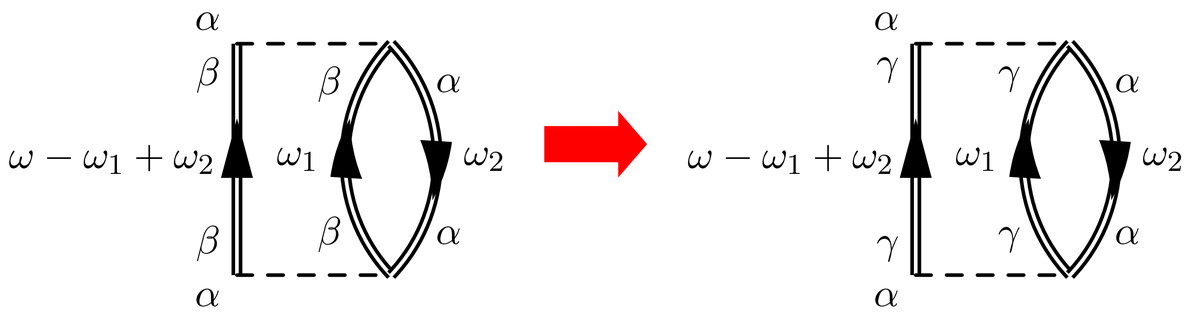
1. *Change Frequency*
2. *Change Single-Particle Quantum Numbers*

} Standard Monte Carlo

Change Frequency:



Change Single-Particle Quantum Numbers:

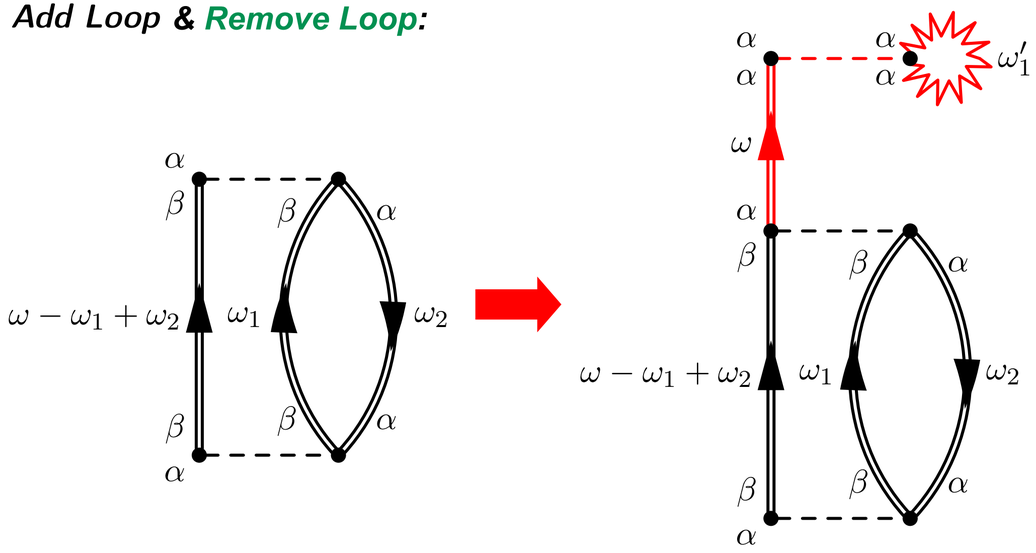


The updates

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

} Monte Carlo on the topology

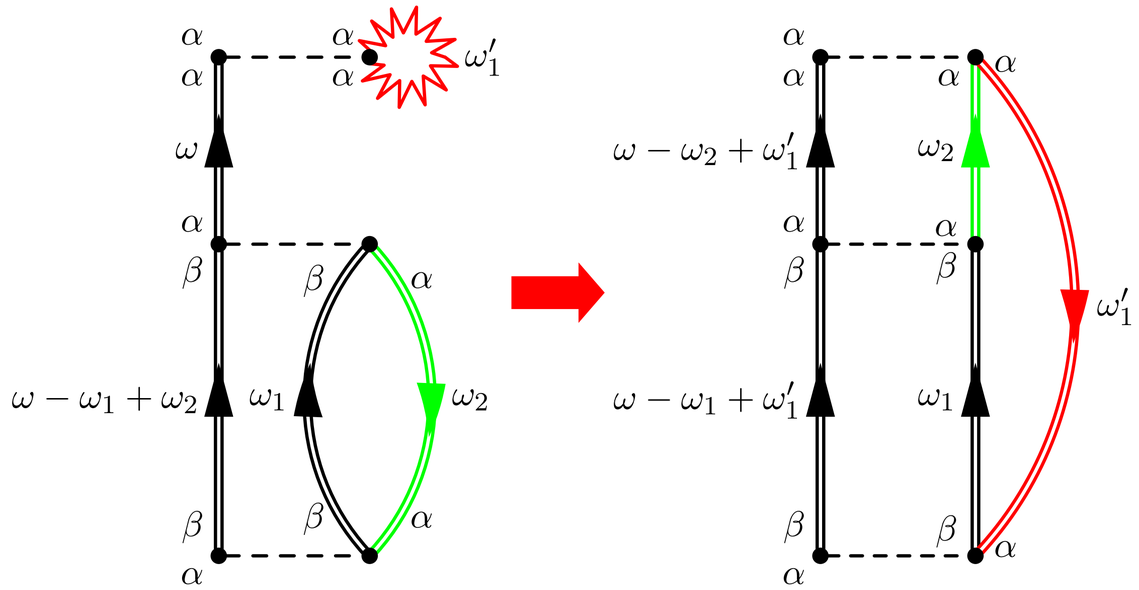
***Add Loop* & *Remove Loop*:**



ω_1' is drawn from the probability distribution $W_f\left(\omega_1'\right)$.

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

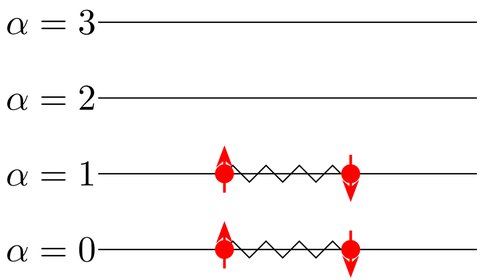
***Reconnect*:**



The unphysical propagators are turned into physical ones when reconnected.

Results of the simulation for D=4

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



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

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

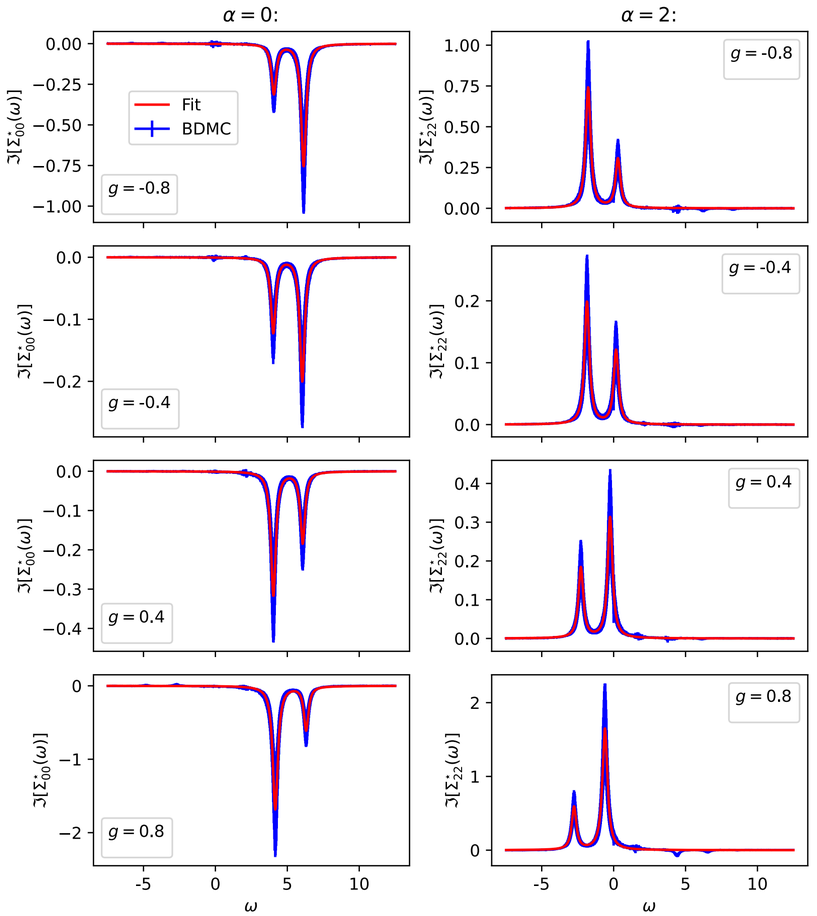
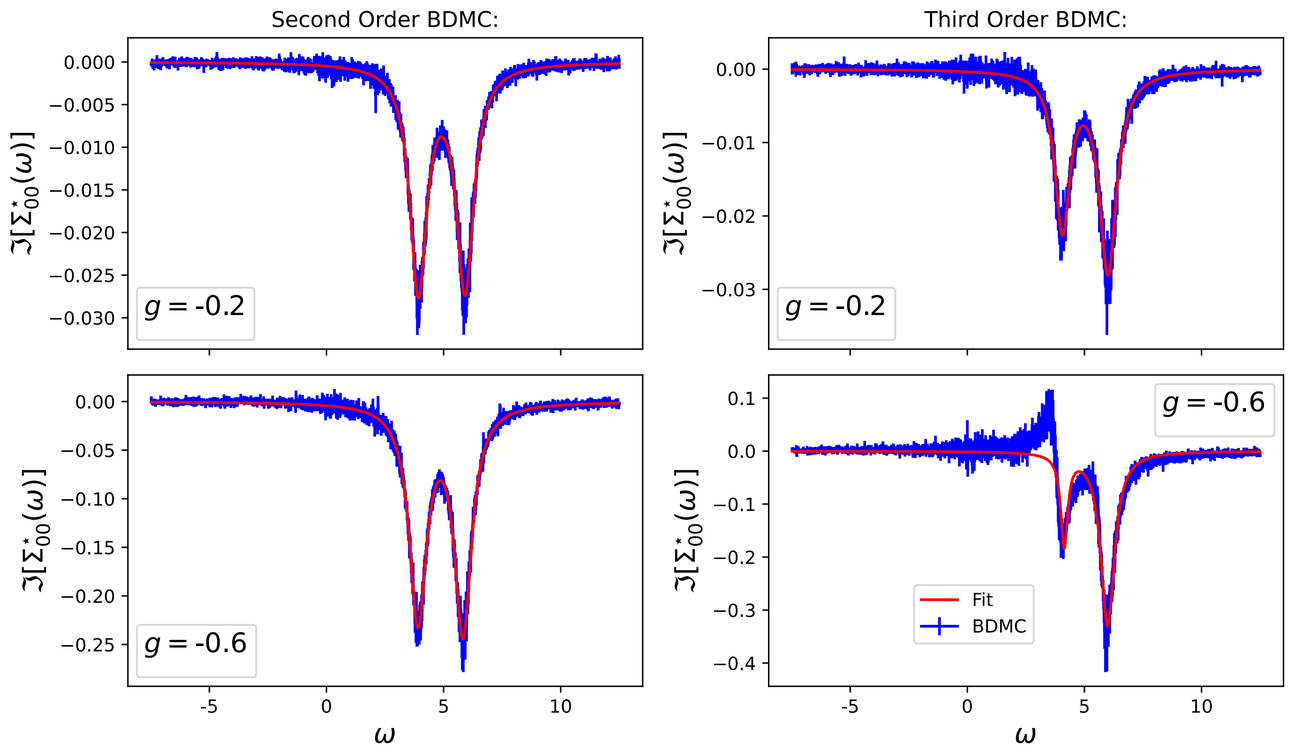


Figure 4.1: Components $\alpha = 0$ and $\alpha = 2$ of the imaginary part of the self-energy for different values of the coupling g. The blue line is the results obtained with the BDMC simulation, while the red line is the best fit as a sum of two Lorentzians. The results for the two values of $\alpha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

Results of the simulation for D=4

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

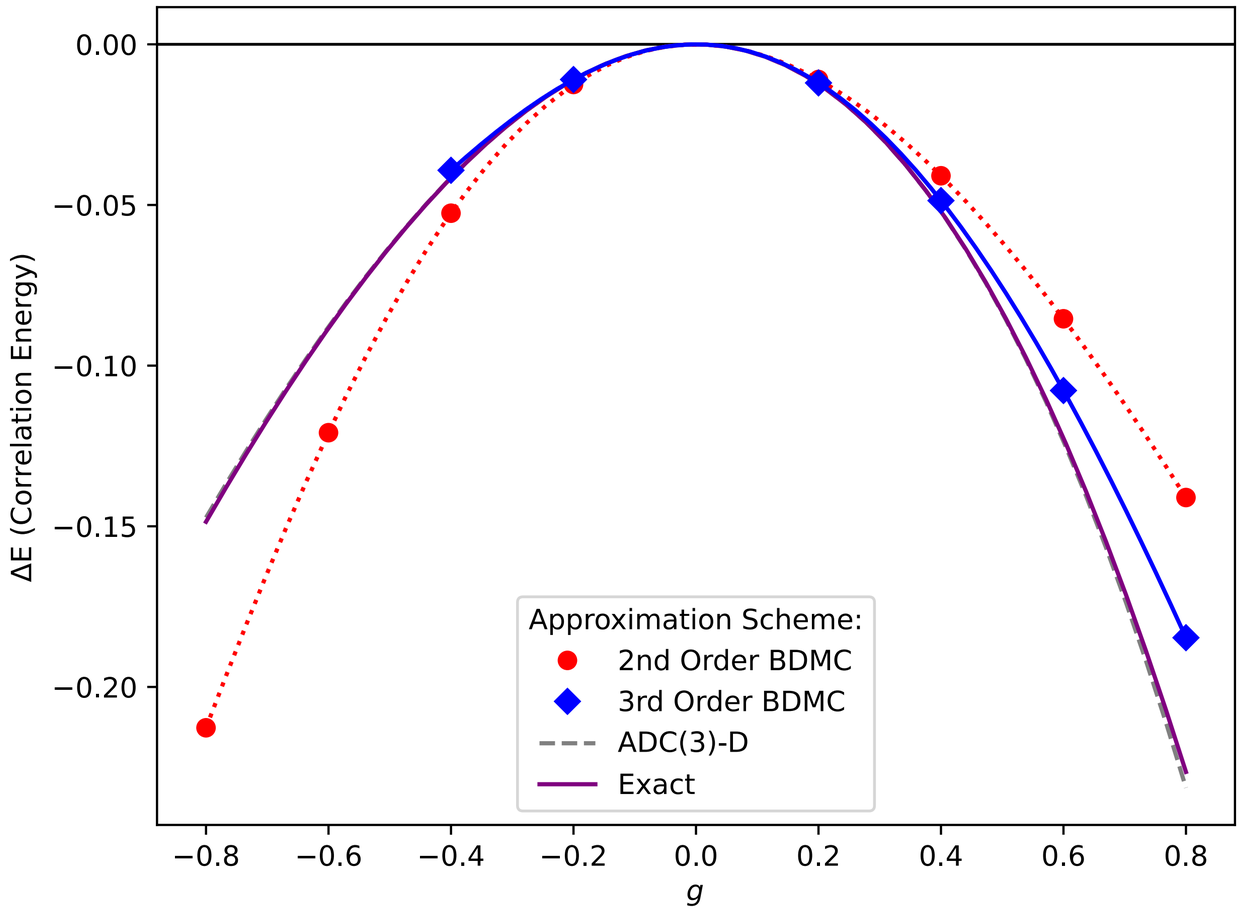


$$H = \xi \sum_{\alpha=0}^{D-1} \sum_{\sigma=+,-} \alpha c^\dagger_{\alpha\sigma} c_{\alpha\sigma} - \frac{g}{2} \sum_{\alpha,\beta=0}^{D-1} c^\dagger_{\alpha+} c^\dagger_{\alpha-} c_{\beta-} c_{\beta+}$$

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

Results of the simulation for D=4

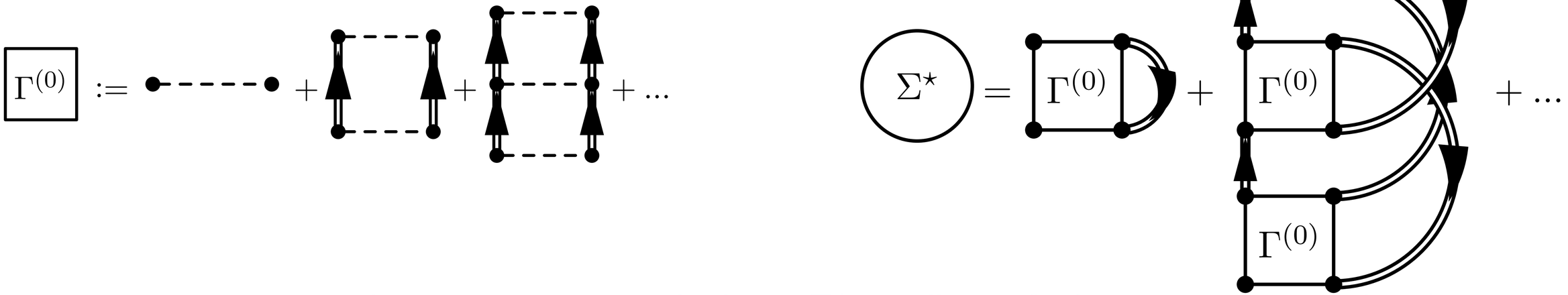
Correlation energy $\Delta E = E - E_{HF}$ as a function of interaction strength (g):



Reorganization in terms of ladders (Γ)

Breaking of the spectral representation is mostly due to truncation in partial all order resummations

—> Can reformulate DiagMC/BDMC in terms of complete lattes (now 3rd oder in Γ)



—> New resummations scheme, now up to 3rd oder in Γ (actually, we find convergence at order 1)

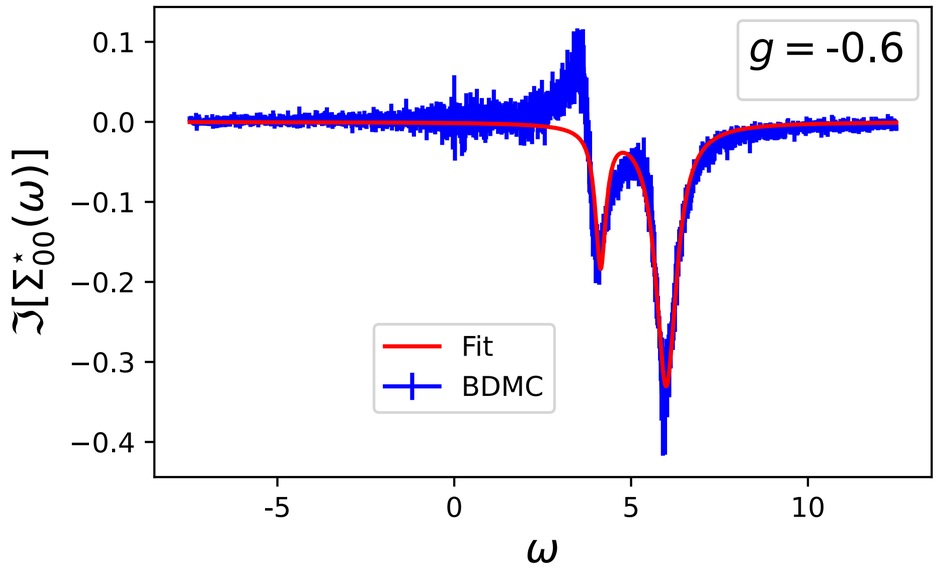
—> New set of diagrammatic update rules

—> New normalisation sectors.

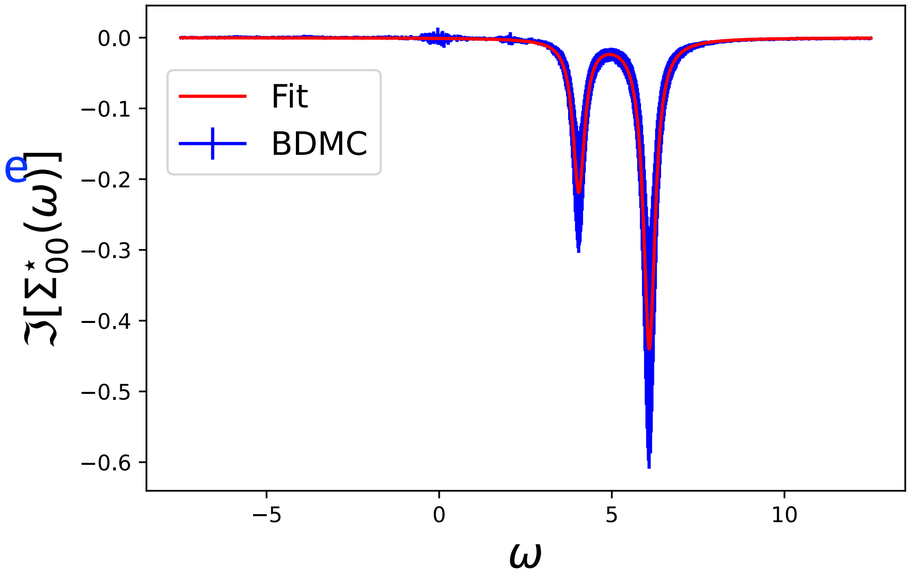
Reorganization in terms of ladders (Γ)

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

Old updating scheme:



New updating scheme:

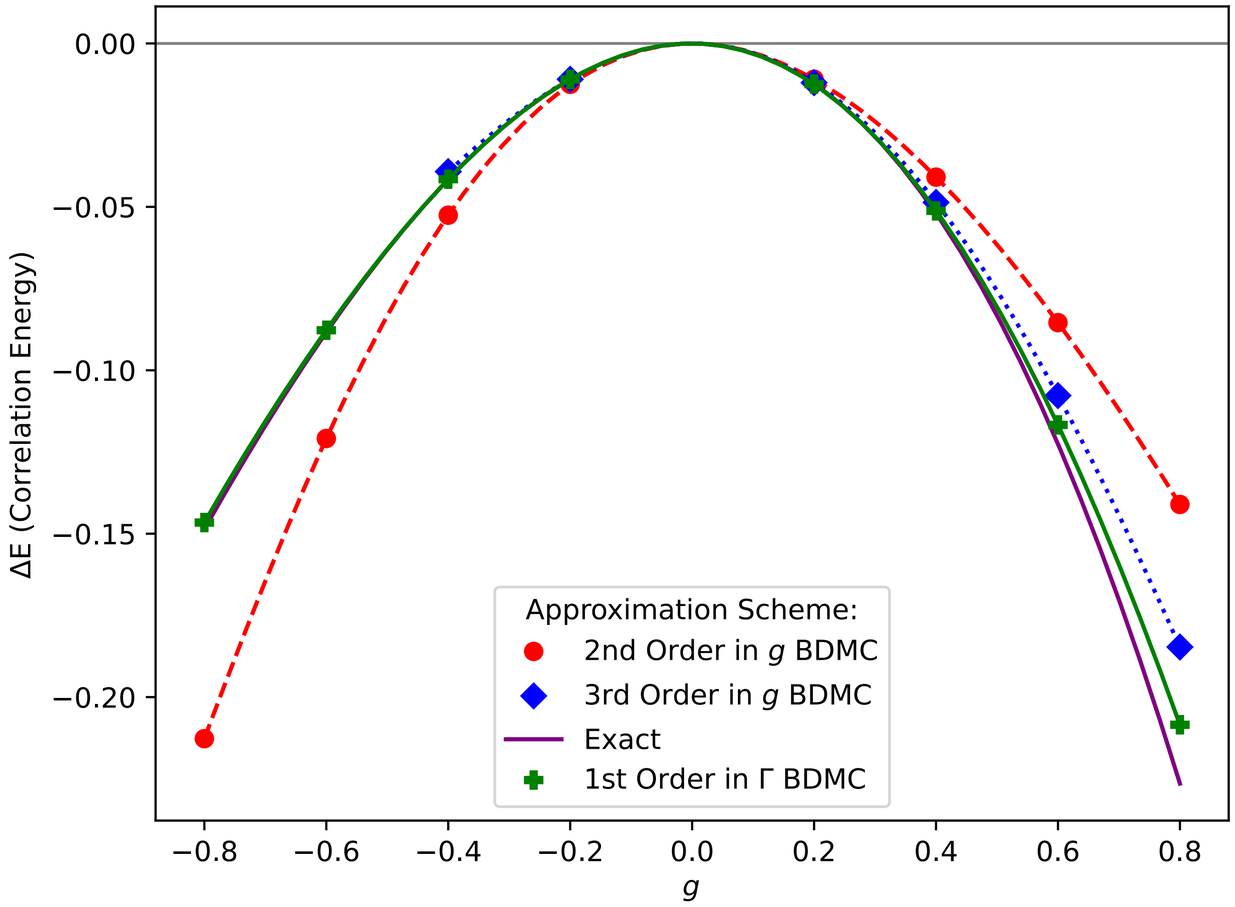


the

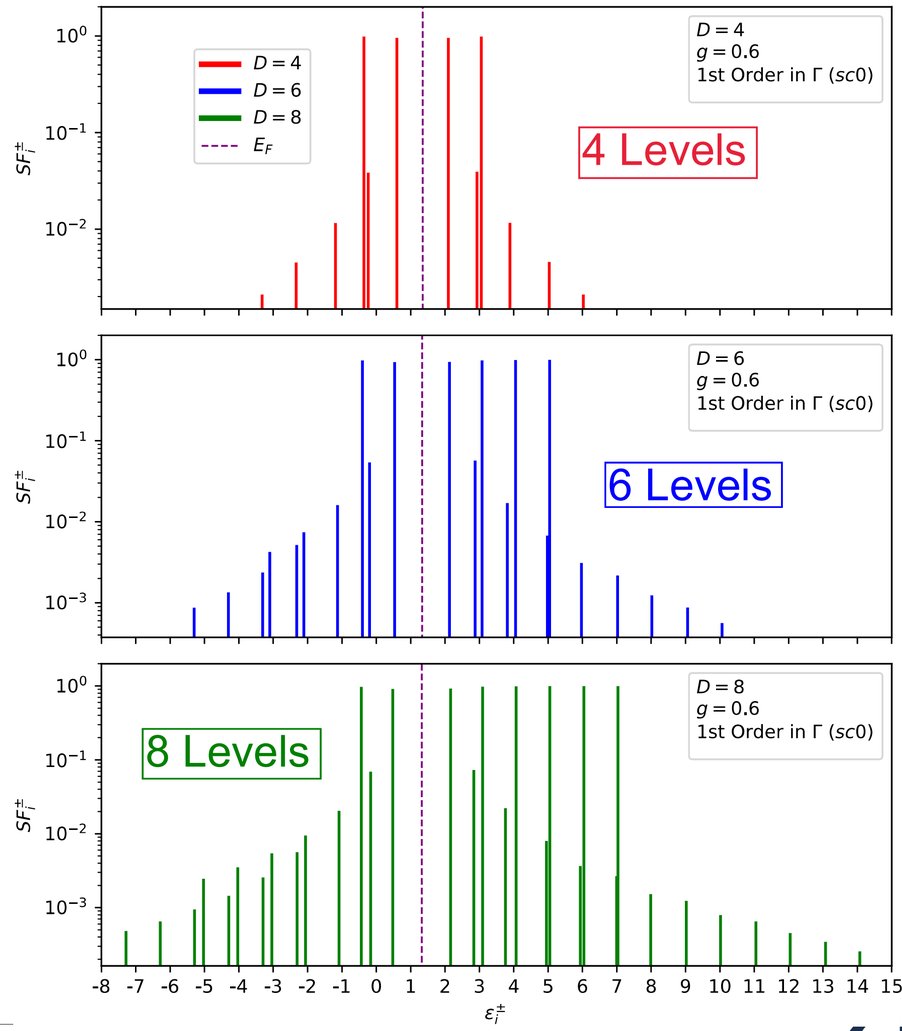
It restores the correct spectral representation also for g < −0.4!

Reorganization in terms of ladders (Γ)

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



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



Take home messages on DiagMC

- We were able to obtain results in good agreement with the exact ones and the ones predicted by other state-of-the-art techniques.
- In future developments we need to extend the algorithm to higher order diagrams.
- A different updating scheme or a different method to sample higher order contributions can be considered.
- The application to realistic interactions is something that has to be studied in the next years

All merits goes to:

L. Lazzarino, G. Paravizzini (NQS)

S. Brolli (DiagMC)

Thank you for your attention!!!