FROM RESEARCH TO INDUSTRY

MPMH TO TAILOR NUCLEAR EFFECTIVE INTERACTIONS

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Caroline Robin	University of Washington, USA
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FROM RESEARCH TO INDUSTRY

ARCHEOLOGY OF THE SCIENTIFIC WORK OF D. GOGNY, THEN MPMH TO TAILOR NUCLEAR EFFECTIVE INTERACTIONS

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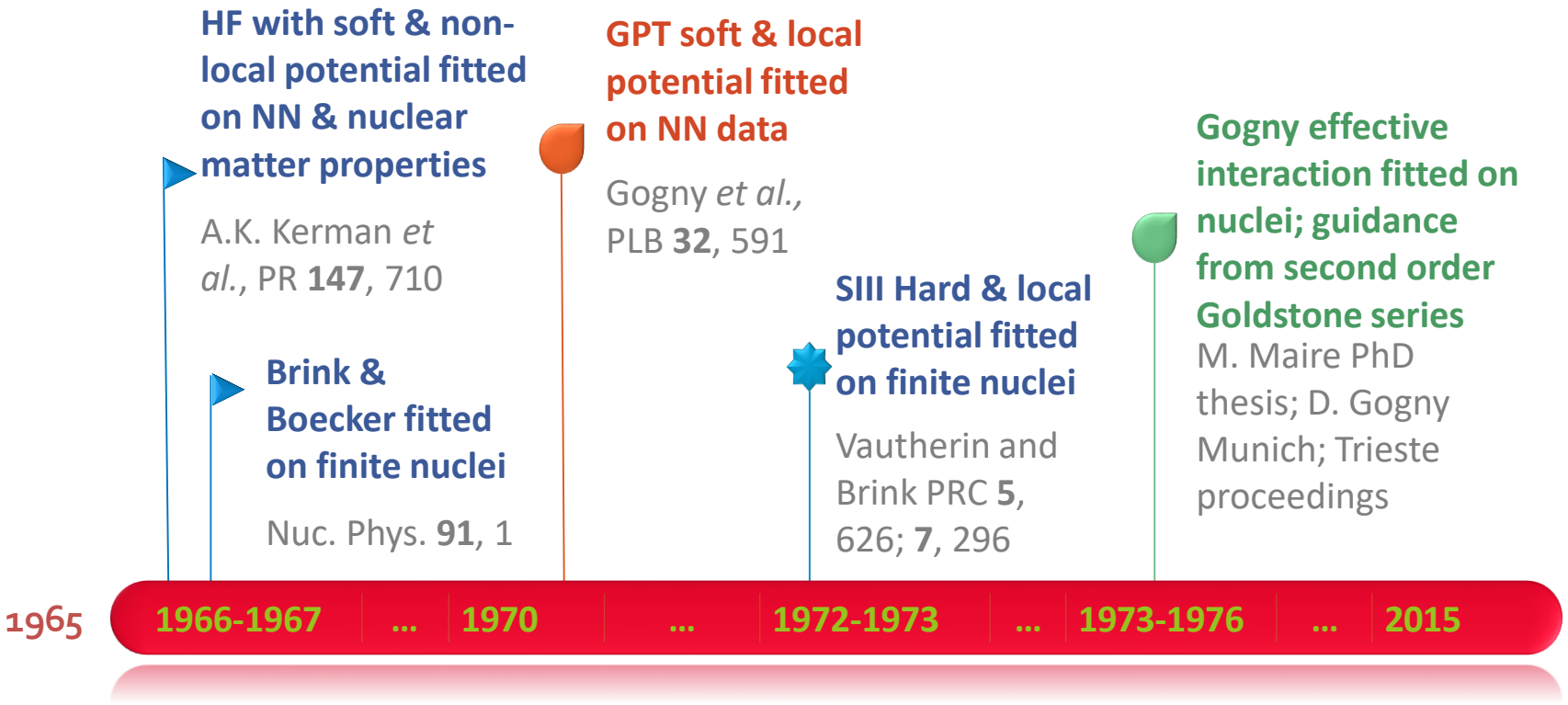
(PARTIAL) TIMELINE



Realistic potential for HF

SIII

Skyrme effective interaction

Gogny effective interaction

GOGNY, PIRES AND DE TOURREIL REALISTIC INTERACTION

1. All the key components of a realistic NN interaction.
2. Soft such that convergence can be achieved with HF+Goldstone series (~150MeV)
3. Three Gaussians for short repulsive, intermediate and long-range (3 fm)
4. But does not fit OPEP
5. Local

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

$$V_i(r) = \sum_\alpha V_\alpha e^{-r^2/\mu_\alpha}$$

Spatial dependence are expressed with a sum of Gaussian (fit done per channel χ^2 =8.4)

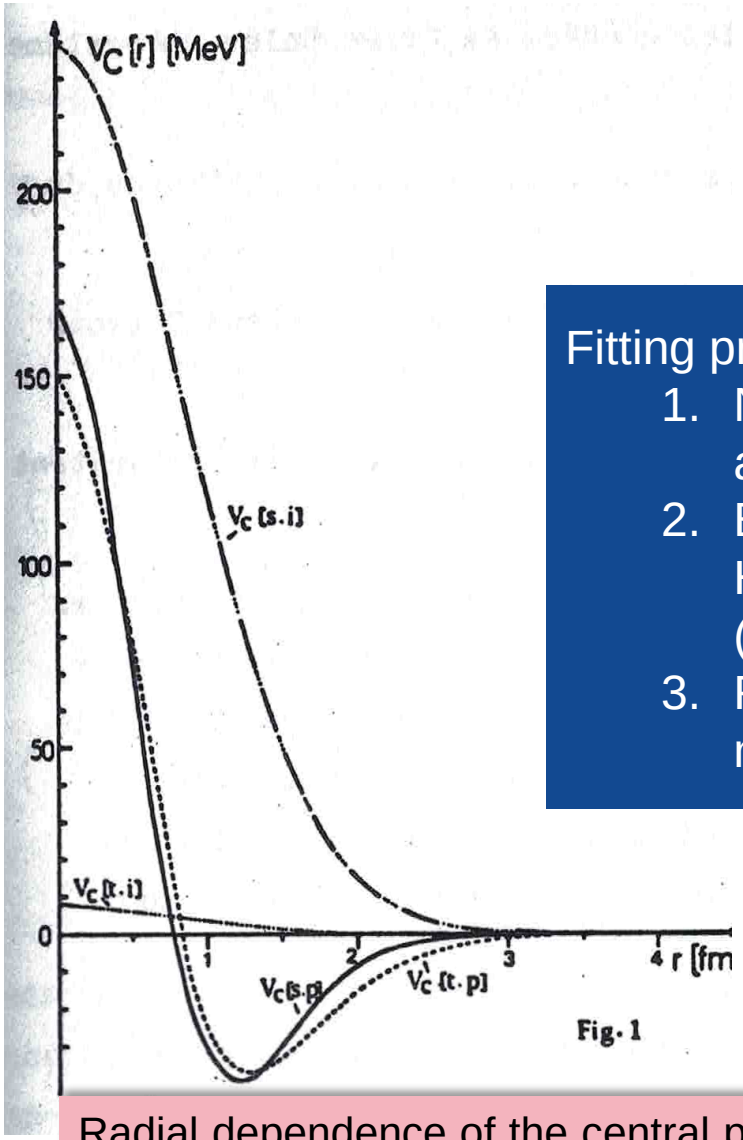
Table 1

Parameters of the potential. The strengths V_α are in MeV and the ranges α are in fm

forces / subspaces		V_C						V_{LL}	
S	T	V_μ	μ	V_ν	ν	V_ρ	ρ	V_μ	μ
0	1	560.0	0.8109	- 390.7	1.031	- 1.501	3.205	- 6.279	1.069
1	0	265.7	0.7482	- 113.9	1.418	- 1.000	2.412	50.82	0.8877
0	0	240.0	1.200	- 0.9000	2.000	0.1000	3.000	- 175.0	0.7000
1	1	9.335	1.184	- 1.37	2.099	0.1663	3.193	13.23	0.8097

forces / subspaces		V_T						V_{LS}	
S	T	V_μ	μ	V_ν	ν	V_ρ	ρ	V_μ	μ
1	0	82.49	0.5162	- 24.51	1.687	- 2.656	3.225	86.97	0.6718
1	1	12.24	1.539	- 31.64	0.4039	0.8111	3.015	- 114.5	0.9296

GOGNY, PIRES AND DE TOURREIL REALISTIC INTERACTION



Radial dependence of the central part of the GPT NN potential.

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

Fitting prescriptions:

1. NN phase shifts to be reproduced up to 300 MeV and correct deuteron properties.
2. Basic properties of spherical nuclei reproduced at HF, particularly radii while E/A expected ~3 MeV (higher order bring important corrections).
3. Reasonable saturation properties of nuclear matters (not achieved in practice).

Note that the choice of Gaussian is guided by:

1. Will behave like separable interaction at HF/HFB level.
2. Soft interaction with UV cutoff.

GOGNY, PIRES AND DE TOURREIL REALISTIC INTERACTION

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

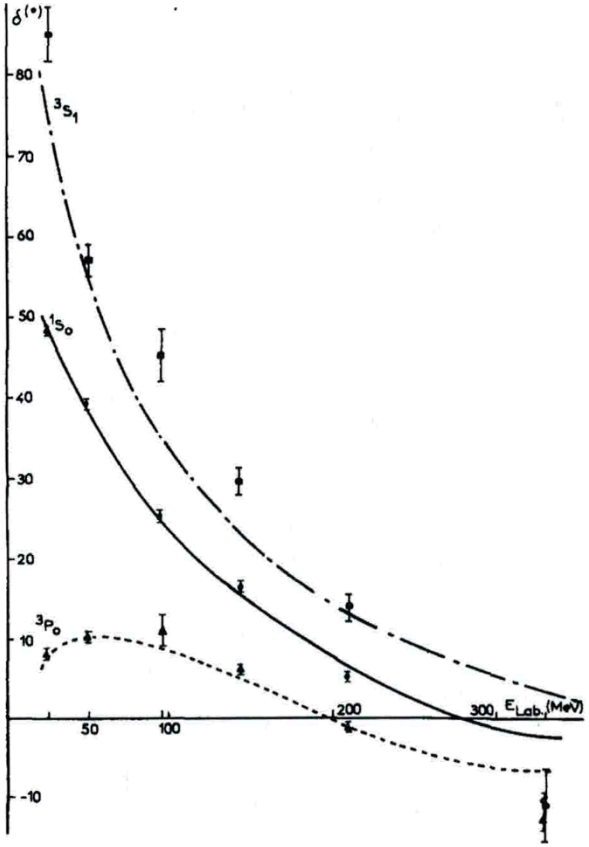


Fig. 1. $^1S_0$, $^3S_1$ and $^3P_0$ phase shift.
● $^1S_0$ experimental phase shift;

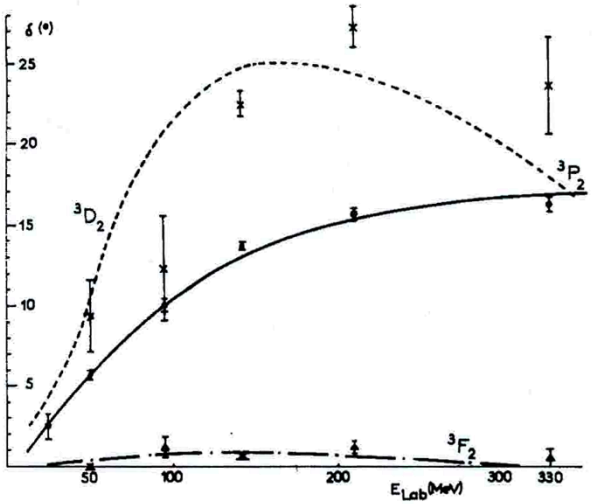


Fig. 2. $^3P_2$, $^3D_2$ and $^3F_2$ phase shifts.
● $^3P_2$ experimental phase shift;
——— $^3P_2$ theoretical phase shift;
× $^3D_2$ experimental phase shift;
----- $^3D_2$ theoretical phase shift;
▲ $^3F_2$ experimental phase shift;
-·-·- $^3F_2$ theoretical phase shift.

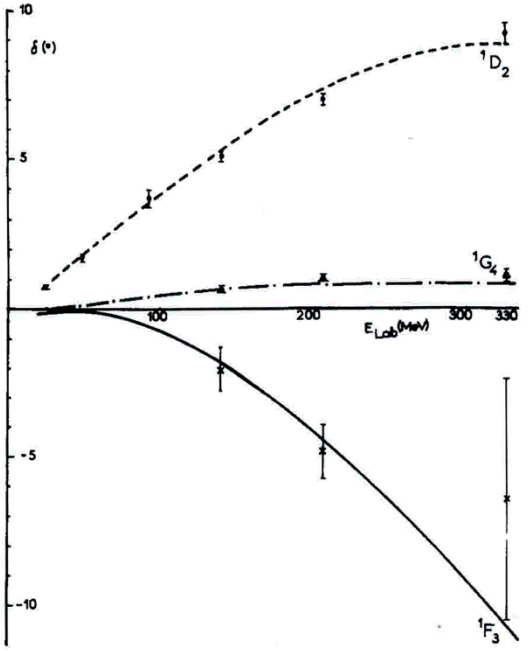


Fig. 4. $^1D_2$, $^1G_4$ and $^1F_3$ phase shifts.
● $^1D_2$ experimental phase shift;
----- $^1D_2$ theoretical phase shift;
▲ $^1G_4$ experimental phase shift;
-·-·-: $^1G_4$ theoretical phase shift;
× $^1F_3$ experimental phase shift;
——— $^1F_3$ theoretical phase shift.

NN scattering phase-shifts analysis.

GOGNY, PIRES AND DE TOURREIL REALISTIC INTERACTION

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

Table 2

The low energy and deuteron properties

	theoretical	experimental	
even singlet scattering length a_s	- 22.12 fm	- 23.7 ± 0.1 fm	[20, 21]
even singlet effective range r_{os}	2.83 fm	2.70 ± 0.08 fm	[21]
even triplet scattering length a_t	5.24 fm	5.40 ± 0.01 fm	[20, 21]
even triplet effective range r_{ot}	1.93 fm	1.73 ± 0.02 fm	[20, 21]
deuteron binding energy E_D	- 2.6 MeV	- 2.2246 ± 0.0005 MeV	[22]
deuteron quadrupole moment Q	0.271 fm^2	0.2796 ± 0.0005 fm^2	[23]
deuteron magnetic moment μ	0.861 n.m.	0.85741±0.00008 n. m.	[21]
deuteron D-state probability P_D	3.8 %	4 to 6%	[21]

Deuteron properties with GPT interaction.

1. No information about 3N and 4N systems from which behavior in light systems can be inferred.
2. Deuteron is overbound.
3. Tensor force is not that good.

SECOND ORDER CORRECTION TO GPT; INFINITE NUCLEAR MATTER

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

First order (HF)

k_F = 1.75 F_m^{-1}	T = + 38.1 MeV	$V^{(1)}$ = - 52.63 MeV	$E^{(1)}$ = - 14.548 MeV	m^*/m = 0.400

Second order correction

S T	Central		L12		C-L12	Tenseur	LS	Tenseur-L12	Total
	1er ordre	2ème ordre	1er ordre	2ème ordre	2ème ordre	2ème ordre	2ème ordre	2ème ordre	2ème ordre
0 0	+ 16.45	- 1.33	+ 5.27	- 0.900	- 1.88				- 4.11
0 1	- 37.40	- 1.17	+ 2.20	- 0.035	+ 0.16				- 1.04
1 0	- 46.69	- 1.33	+ 1.95	- 0.06	+ 0.019	- 2.64	- 0.005	- 0.21	- 4.
1 1	+ 3.24	- 0.01	+ 2.33	- 0.012	- 0.02	- 0.69	- 1.12	- 0.41	- 1.59
Total	- 64.40	- 3.81	+ 11.75	- 1.	- 1.55	- 3.33	- 1.125	- 0.72	- 10.74

E/A at saturation is way to high (25.2 instead of 16 MeV) !

SECOND ORDER CORRECTION TO GPT; INFINITE NUCLEAR MATTER

Replacing long-range behavior with a Yukawa

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

First order (HF)

$k_F = 1.5\ F^{-1}$	T = + 28 MeV	$V^{(1)}$ = -36 MeV	E^1 = - 8 MeV	m^*/m = .444

Second order correction

	central		L_{12}		Central-L_{12}	Tenseur	L.S	tenseur-L_{12}	Total du
S T	1° ordre	2°ordre	1° ordre	2° ordre	2° ordre	2° ordre	2° ordre	2° ordre	2° ordre
0 0	+ 12.	- 1.06	+ 2.58	- 0.53	- 1.28				- 2.87
0 1	- 25.	- 0.94	+ 0.88	- 0.02	+ 0.08				- 0.88
1 0	- 33.	- 1.11	+ 0.75	- 0.03	+ 0.11	- 2.66	- 0.00	+ 0.02	- 3.67
1 1	+ 4.5	- 0.00	+ 1.15	- 0.00	- 0.01	- 0.57	- 0.78	- 0.07	- 1.45
Total	- 41.5	- 3.12	+ 5.5	- 0.58	- 1.10	- 3.23	- 0.78	- 0.05	- 8.87

When including the proper OPEP asymptotic, E/A correct at second order…

SECOND ORDER CORRECTION TO GPT; FINITE NUCLEI

GPT NN potential

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

Yukawa at long-range

S	T	^{16}O	^{40}Ca	^{90}Zr	^{208}Pb	Matière Nucléaire	
						POT2	GPT
0	0	16%	22%	26%	30%	32%	38%
0	1	14,5%	12,5%	12%	11,5%	10%	10%
1	0	61,5%	55%	49%	43%	41%	37%
1	1	8%	11%	13%	15%	16%	15%

GPT ^{208}Pb 2nd order correction is similar to infinite matter with correct asymptotic

SECOND ORDER CORRECTION TO GPT; FINITE NUCLEI

GPT NN potential

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

Second order

Hartree-Fock

D1 effective interaction "functional"

$$v_{12}(\rho) = \sum_{j=1}^{2}\left(W_j + B_jP_\sigma - H_jP_\tau - M_jP_\sigma P_\tau\right)e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_j}$$
$$+t_3(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha\left(\vec{r}_1-\vec{r}_2/2\right)$$
$$+iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\wedge\overleftarrow{\nabla}_{12}(\vec{\sigma}_1+\vec{\sigma}_2)$$

16_O	G.P.T.	SKYRME	CAMPI SPRUNG	GOGNY	Valeurs expérimentales
Neutrons					
1S 1/2	- 38.69	- 35.20	- 36.36	- 39.65	- 47.
1P 3/2	- 19.41	- 19.84	- 21.25	- 21.82	- 21.8
1P 1/2	- 15.44	- 15.14	- 15.81	- 16.02	- 15.8
Protons					
1S 1/2	- 35.39	- 31.21	- 33.16	- 36.35	- 40±8.
1P 3/2	- 16.21	- 16.26	- 18.13	- 18.54	- 18.4
1P 1/2	- 12.33	- 11.64	- 12.78	- 12.83	- 12.1

Density dependent interaction are able to retrieve ESP spectrum at HF level…

SECOND ORDER CORRECTION TO GPT; FINITE NUCLEI

GPT NN potential

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

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$$+iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\wedge\overleftarrow{\nabla}_{12}(\vec{\sigma}_1+\vec{\sigma}_2)$$

^{40}Ca	G.P.T.	SKYRME	CAMPI SPRUNG	GOGNY	Valeurs expérimentales
Neutrons					
1S 1/2		- 49.67	- 49.48	- 52.61	- 50.
1P 3/2	- 38.91	- 34.06	- 36.03	- 37.75	- 30.
1P 1/2	- 36.83	- 29.62	- 32.58	- 34.01	- 27.
1D 5/2	- 21.21	- 20.23	- 23.39	- 23.04	- 21.9
2S 1/2	- 20.73	- 13.92	- 16.73	- 17.66	- 18.2
1D 3/2	- 16.20	- 14.14	- 17.16	- 16.54	- 15.6
Protons					
1S 1/2		- 41.38	- 42.38	- 45.28	- 50±11.

Density dependent interaction are able to retrieve ESP spectrum at HF level…

SECOND ORDER CORRECTION TO GPT; CONCLUSIONS

GPT NN potential

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

D1 effective interaction "functional"

$$v_{12}(\rho) = \sum_{j=1}^{2}\left(W_j + B_jP_\sigma - H_jP_\tau - M_jP_\sigma P_\tau\right)e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_j}$$
$$+t_3(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha\left(\vec{r}_1-\vec{r}_2/2\right)$$
$$+iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\wedge\overleftarrow{\nabla}_{12}(\vec{\sigma}_1+\vec{\sigma}_2)$$

1. Non-locally is not exploited but a soft potential is obtained.
2. Second order reproduced by density dependent interaction at HF approximation.
3. OPEP is not necessary for finite nuclei (probably only true for $A \geq 16$). D1 drops long range $V(r)$ and use infinite matter as a weak constraint.

μ_1, μ_2	W	B	H	M MeV
0.7	-402.4	-100.	-496.2	-23.56
1.2	-21.30	-11.77	37.27	-68.81
α=1/3 x_0=1 W_{LS}=-115MeV t_0=1350MeV.fm^6				

Gogny D1 parametrization

SECOND ORDER CORRECTION TO GPT; CONCLUSIONS

GPT NN potential

$$V(r) = V_C(r) + V_T(r)S_{12} + V_{LS}(r)L.S + V_{LL}(r)L_{12}$$

D1 effective interaction "functional"

$$v_{12}(\rho) = \sum_{j=1}^{2}\left(W_j + B_jP_\sigma - H_jP_\tau - M_jP_\sigma P_\tau\right)e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_j}$$
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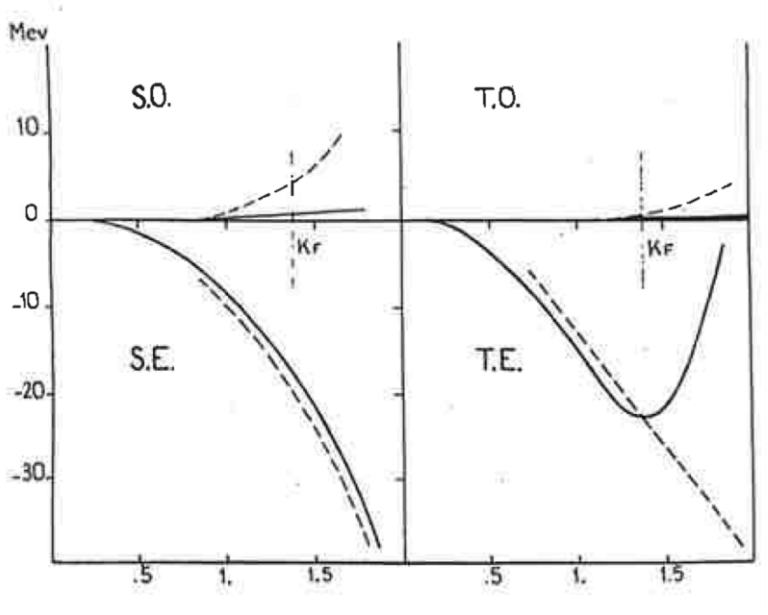
$$+iW_{LS}\overleftarrow{\nabla}_{12}\delta(\vec{r}_1-\vec{r}_2)\wedge\overleftarrow{\nabla}_{12}(\vec{\sigma}_1+\vec{\sigma}_2)$$

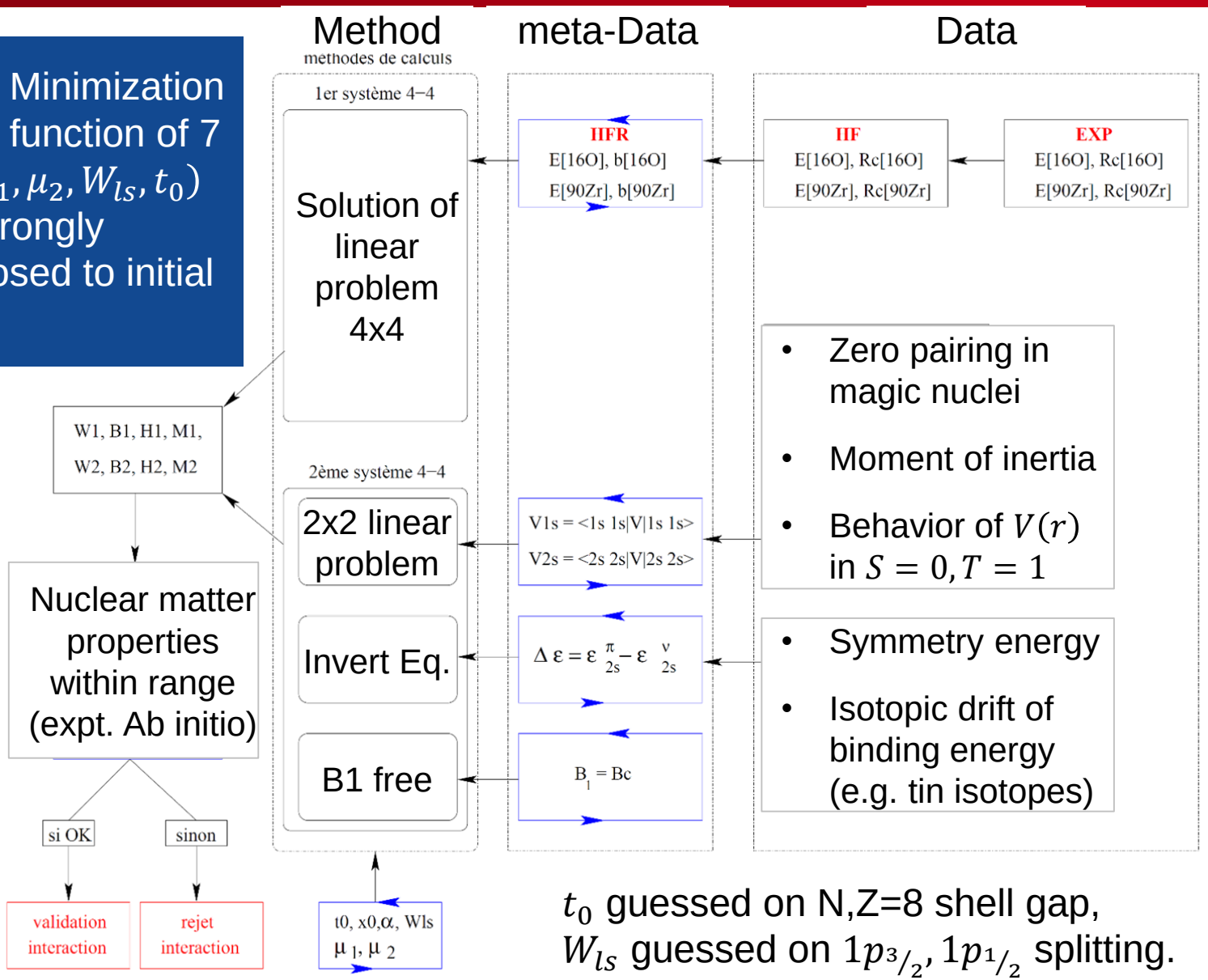
1. Non-locally is not exploited but a soft potential is obtained.
2. Second order reproduced by density dependent interaction at HF approximation.
3. OPEP is not necessary for finite nuclei (probably only true for $A \geq 16$). D1 drops long range $V(r)$ and use infinite matter as a weak constraint.
4. Infinite matter result from realistic BHF+GPT is used to give guidance on per channel trend.



GOGNY FITTING PROCEDURE

From the PhD thesis of F. Chappert (2008); F. Chappert *et al.* PRC 91 (2015); N. Pillet *et al.* EPJA 83 (2017)

14 parameters Minimization of an objective function of 7 variables, 4 $(\mu_1, \mu_2, W_{ls}, t_0)$ of which are strongly constrained closed to initial guess.



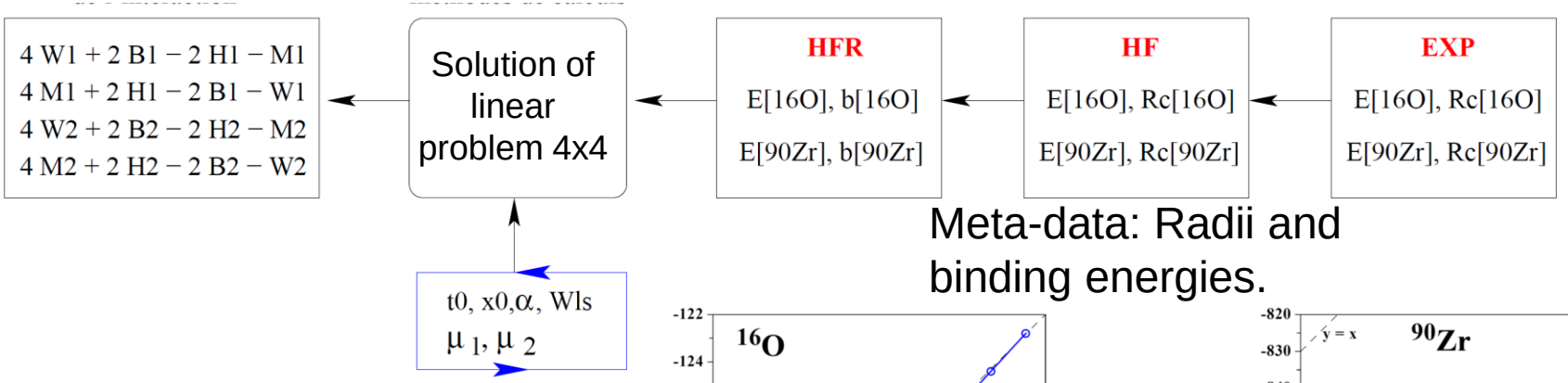
t_0 guessed on N,Z=8 shell gap,
W_{ls} guessed on $1p_{3/2}, 1p_{1/2}$ splitting.

GOGNY FITTING PROCEDURE : FIT TO SPHERICAL CLOSED SHELL ^{16}O AND ^{90}Zr

Procedure follows the need of analytical relations between the exchange coefficient of the central term.

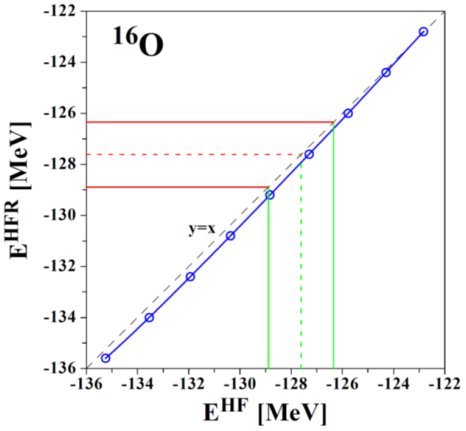
$$\rho_{\alpha\beta} = \delta_{\alpha\beta}\rho_{\alpha\alpha} \text{ avec } \rho_{\alpha\alpha} = \left\{ \begin{array}{l} 1 \text{ si } \alpha \leq A \\ 0 \text{ sinon.} \end{array} \right\}$$

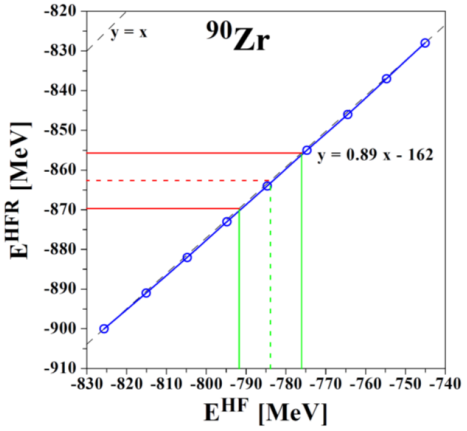
$$E^{HFR} = \sum_{\alpha} t_{\alpha\alpha}\rho_{\alpha\alpha} + \frac{1}{2}\sum_{\alpha,\beta} V^{(a)}_{\alpha\beta\alpha\beta}\rho_{\alpha\alpha}\rho_{\beta\beta}$$



Meta-data: Radii and binding energies.

Meta-data used in the fitting routine generated from correlation function between E^{HFR} and E^{HF}.



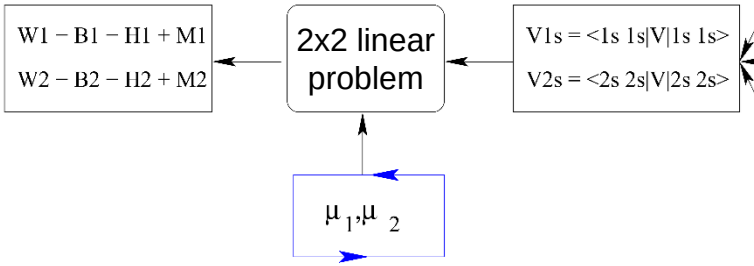


GOGNY FITTING PROCEDURE : PAIRING

Analytical solution using two pairing matrix elements as meta-data.

Meta-data used in the fitting routine generated from HFB $E^{pairing}$, $\Im_k^{IB}$ and shape of $V^{S=0,T=1}(r)$.

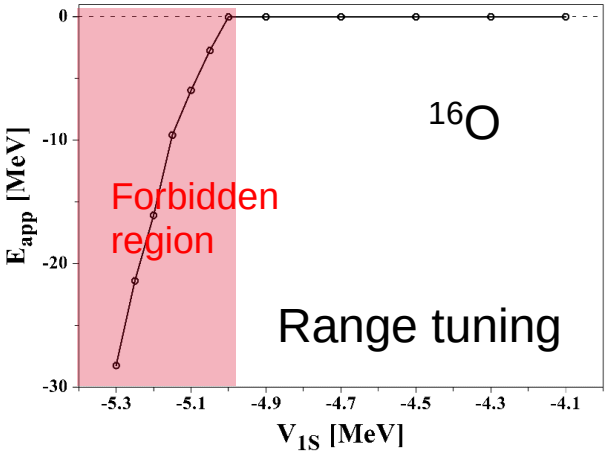
Meta-data pairing s-wave m.e. in S,T=0,1 channel.



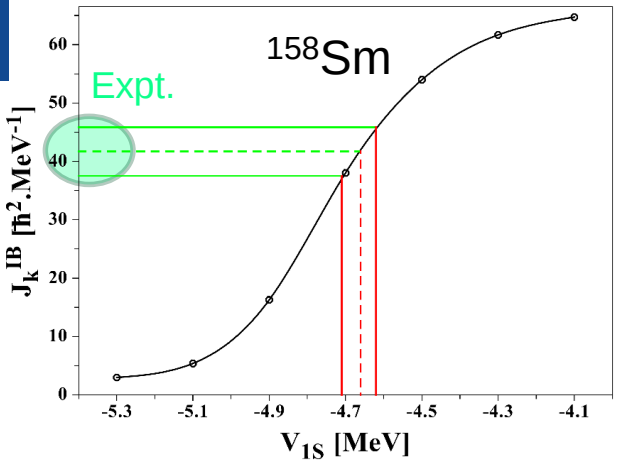
Zero pairing in magic nuclei

Moment of inertia

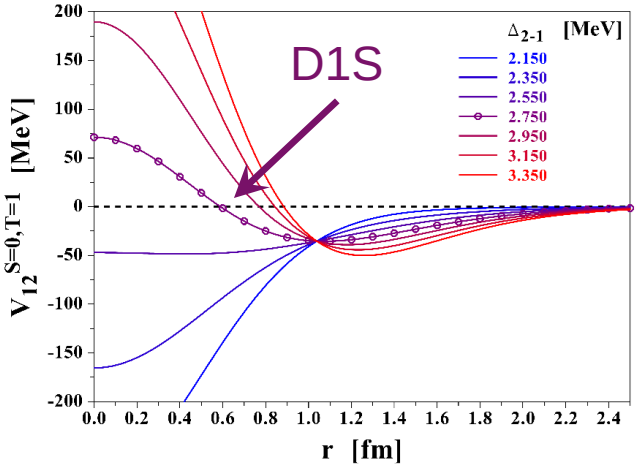
Behavior of $V(r)$ in $S = 0, T = 1$



V_{1S} extraction



V_{2S} extraction



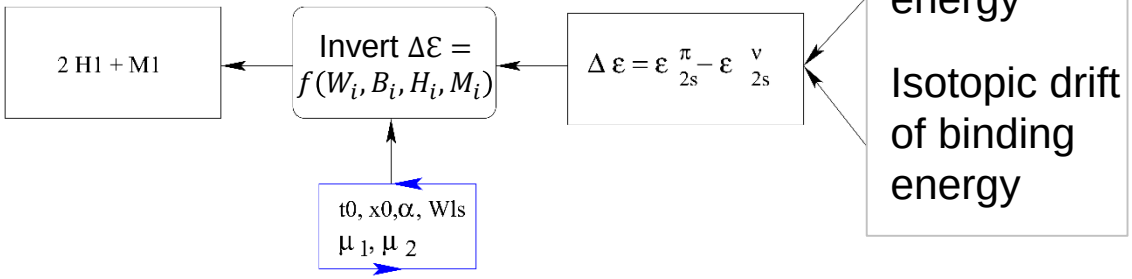
$\Im_k^{IB} = f(V_{1s})$ at HFB

Radial shape of central interaction

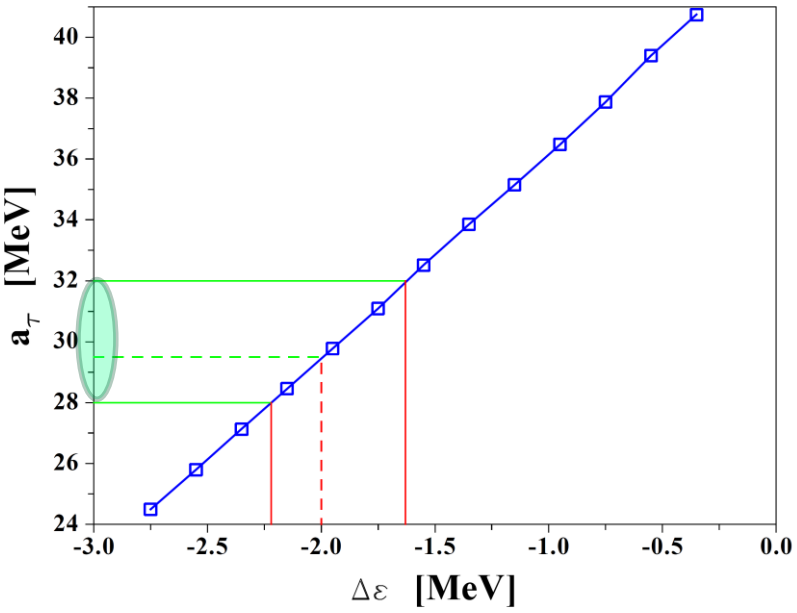
GOGNY FITTING PROCEDURE : ISOSPIN

One meta-data but fine tune to bulk and shell properties of nuclei. Restricted HF is used to express $\Delta\mathcal{E} = f(W_i, B_i, H_i, M_i)$

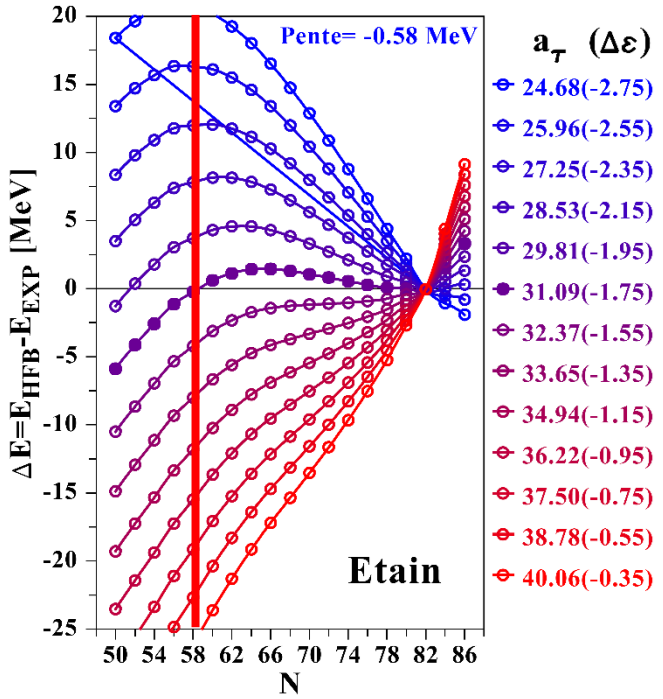
Meta-data $\Delta\mathcal{E}$ is ^{48}Ca proton and neutron $2s_{1/2}$ splitting.



Crude tuning on liquid drop model

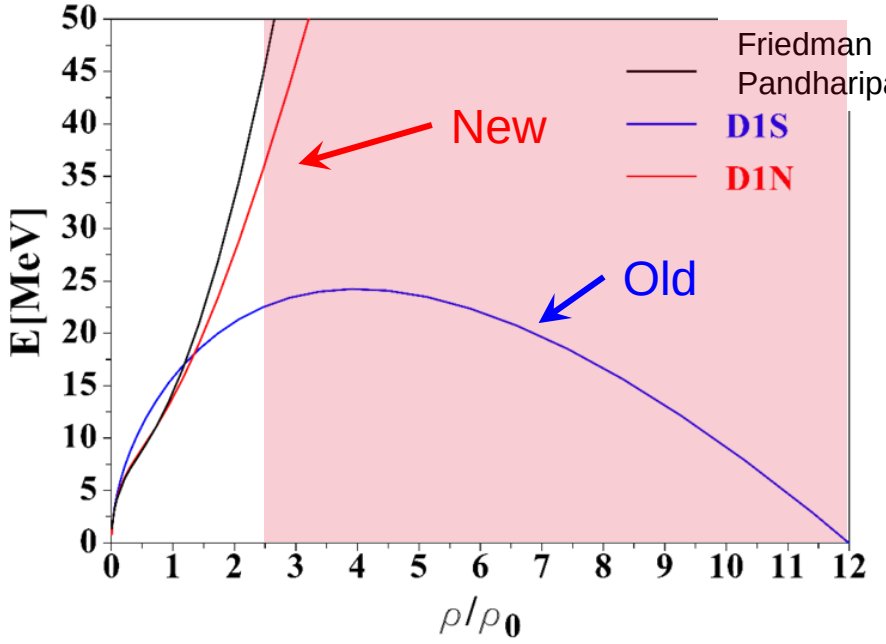


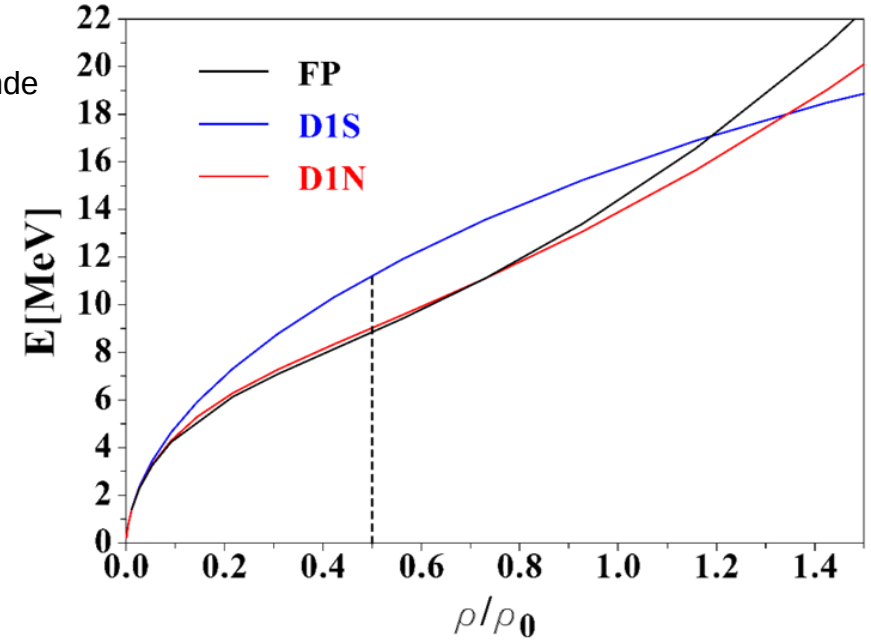
Fine tuning on shell closure



INSTRUCTIVE EXAMPLE: D1N

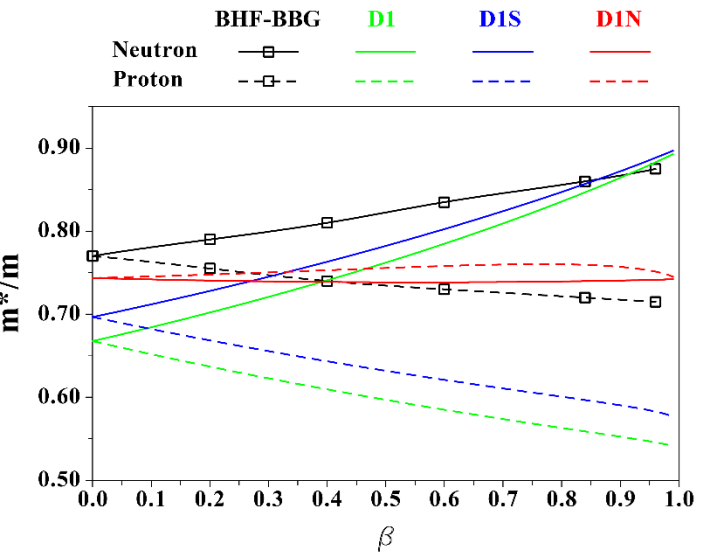
AIM: introduce a new weak constrained on neutron matter based on *ab initio* result.



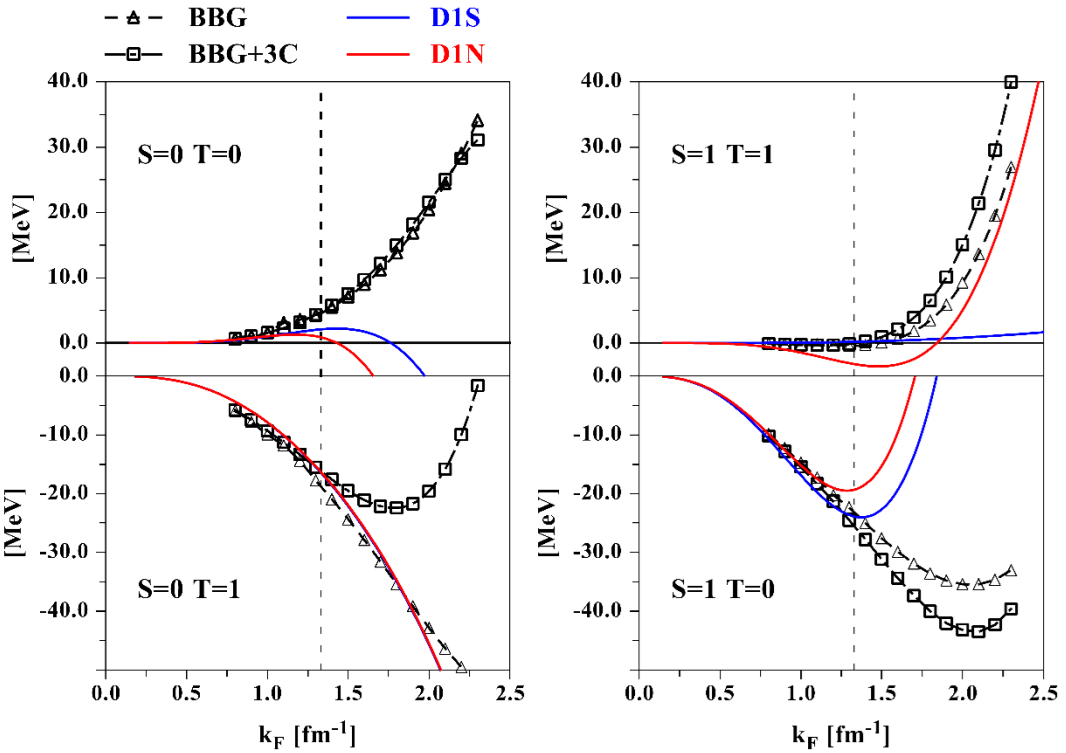


INSTRUCTIVE EXAMPLE: D1N

Results: on average properties in nuclear matter and finite nuclei are degraded.



Effective mass as function of isospin asymmetry



Potential energy by ST channel

Functional form of the Gogny interaction is too weak to sustain all the constraints.

TOWARDS GENERALIZED FINITE RANGE INTERACTION

To make room for additional constrained, the density dependent term can be generalized

$$V_{dens} = (W_3 + B_3 P_\sigma - H_3 P_\tau - M_3 P_\sigma P_\tau) \frac{e^{-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\mu_3^2}}}{(\mu_3\sqrt{\pi})^3} \frac{\rho^\alpha(\vec{r}_1) + \rho^\alpha(\vec{r}_2)}{2}$$

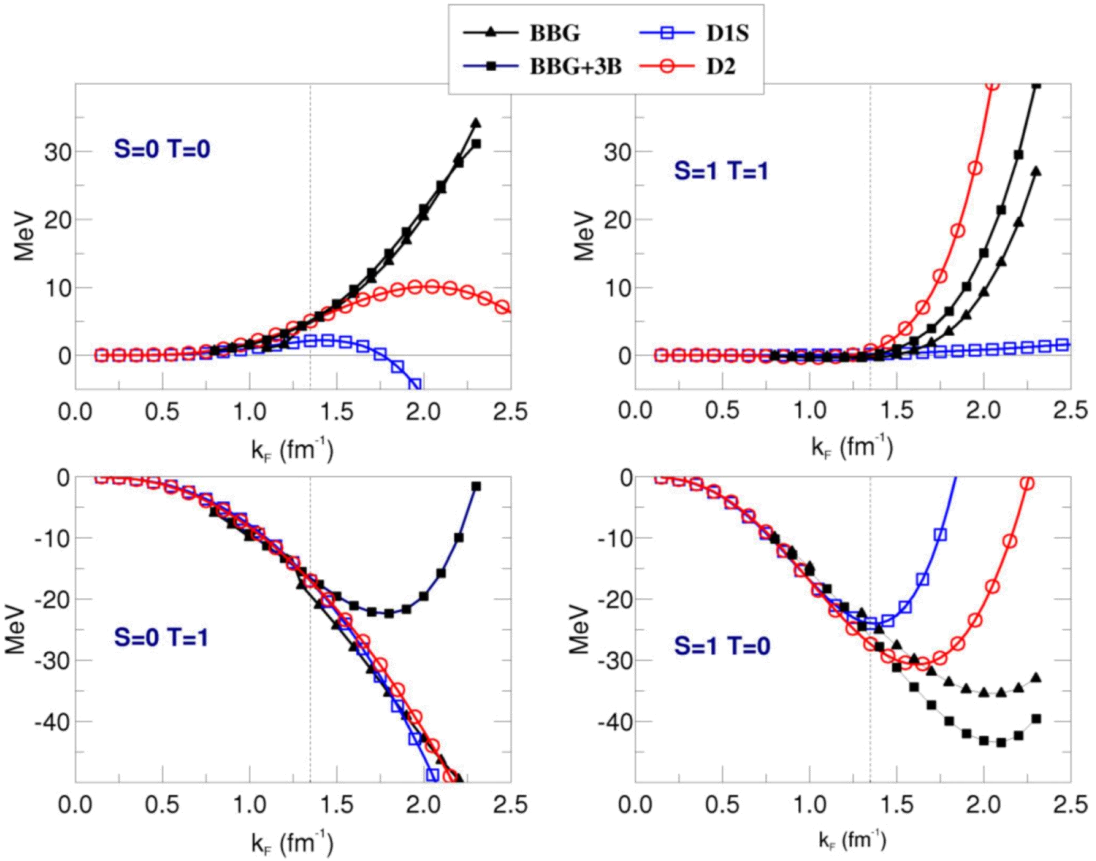
Finite range density dependent term in D2

Advantages:

- More freedom in the contribution of exchange term.
- Finite-range is suited for beyond MF calculation.

Disadvantages:

- One more system of equation for the fit (from ^{100}Sn data)



TOWARDS GENERALIZED FINITE RANGE INTERACTION

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Finite range density dependent term in D2

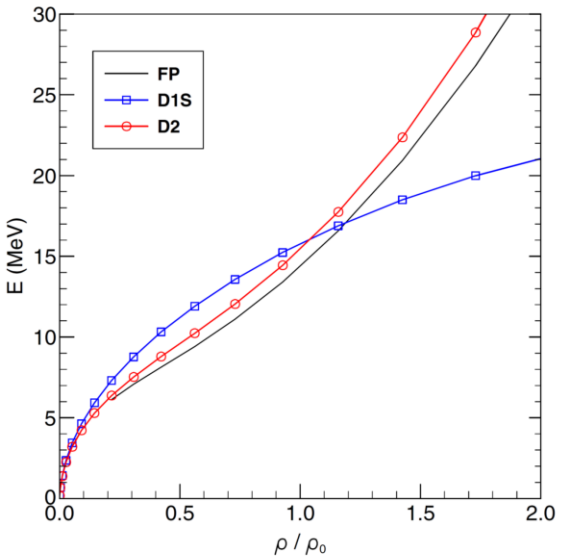
Advantages:

- More freedom in the contribution of exchange term.
- Finite-range is suited for beyond MF calculation.

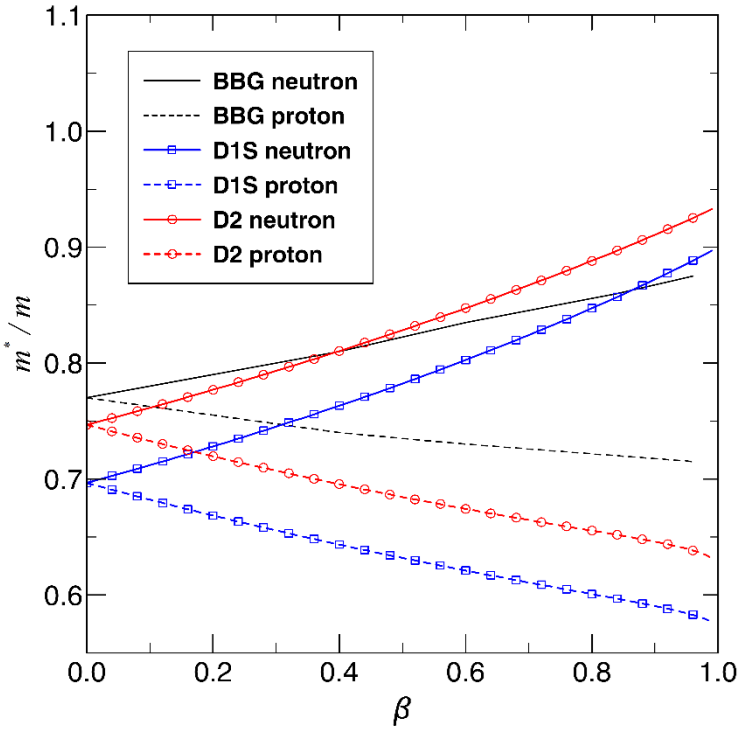
Disadvantages:

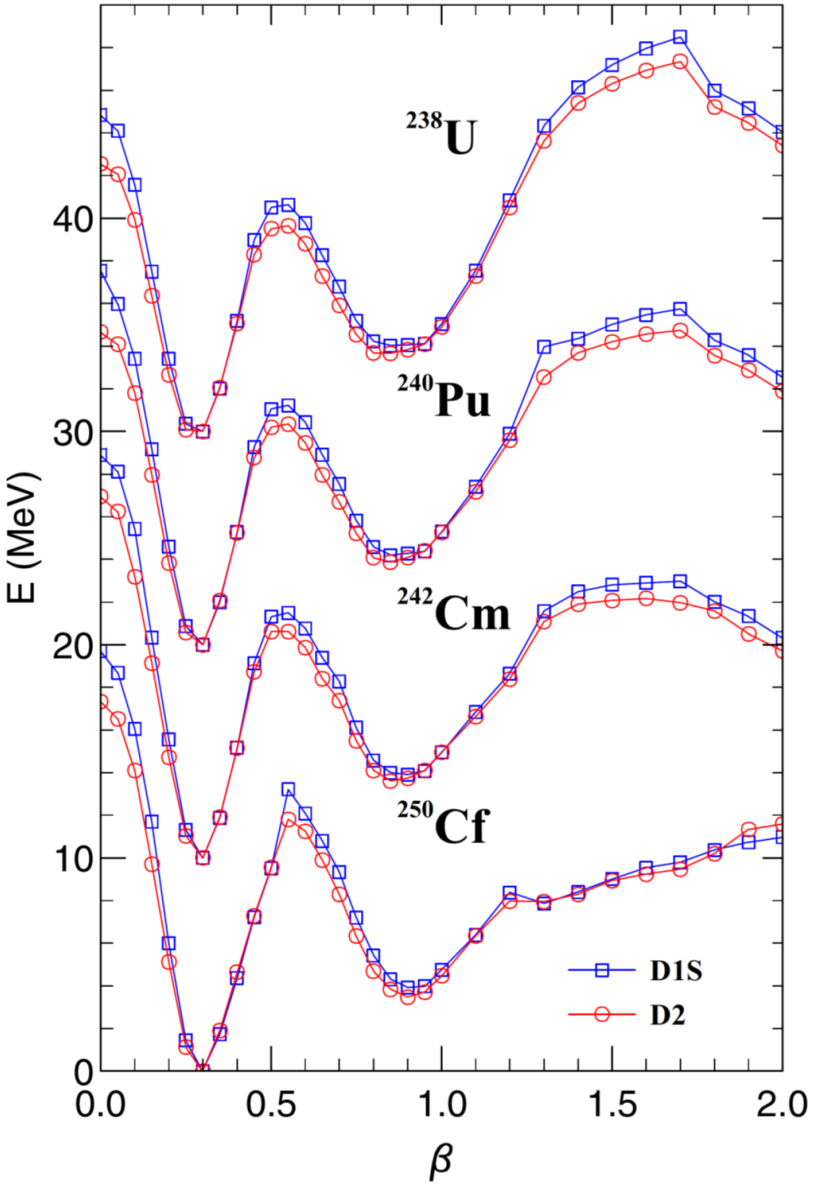
- One more system of equation for the fit (from ^{100}Sn data); abandoned new parameters set as free.

	$D2$	$D1S$	Empirical value
ρ_0(fm^{-3})	0.163	0.163	0.17 (±0.02)
E_0/A (MeV)	−16.00	−16.02	−16(±1)
K_∞ (MeV)	209	210	220 (±10)
m^*/m	0.74	0.70	0.70 (±0.05)
a_τ(MeV)	31.1	31.1	30 (±2)



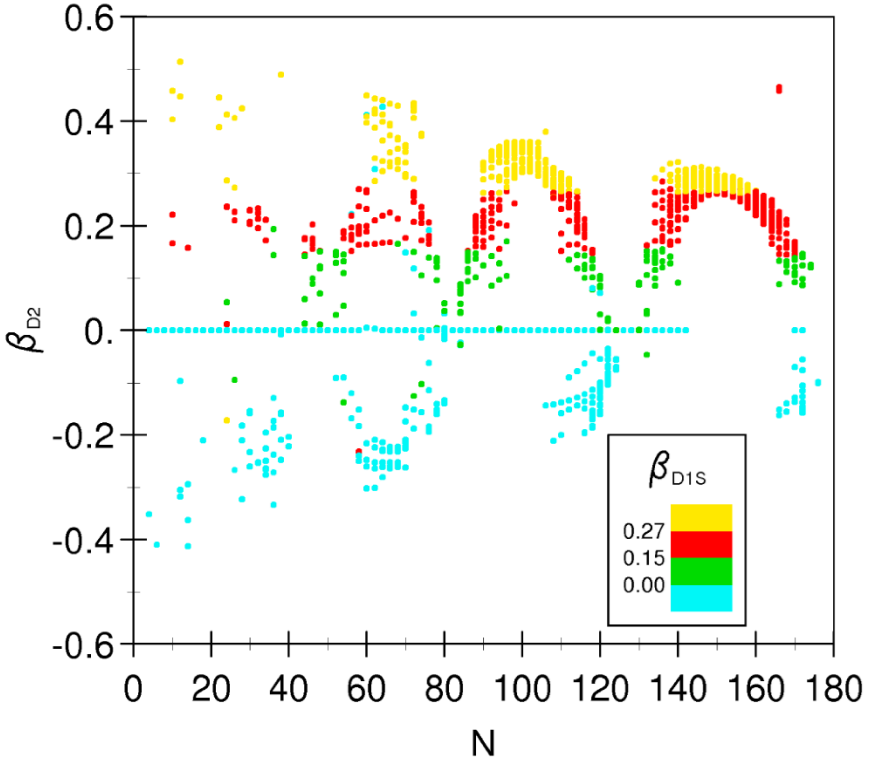
D2 IN FINITE NUCLEI

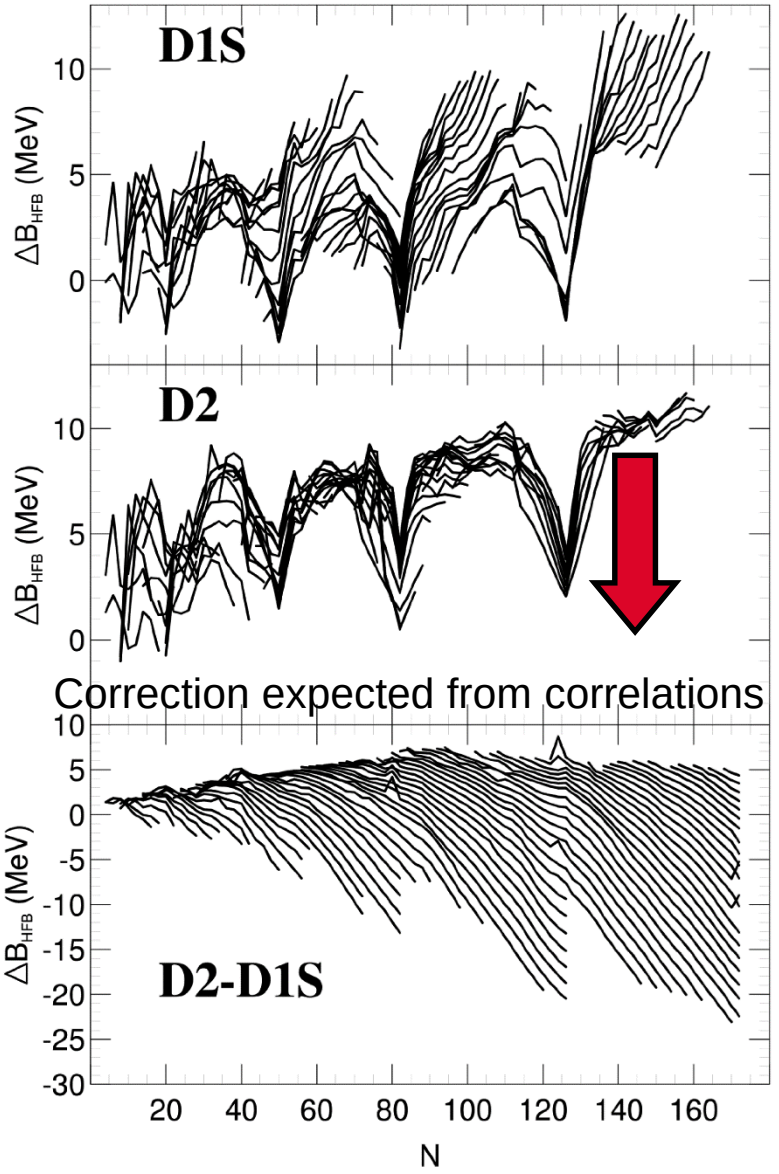




- Proton/neutron effective masses have the correct trend.
- Globally D2 is equivalent to D1S (that is pairing, deformation, masses, local OB density and radii).

D2 IN FINITE NUCLEI





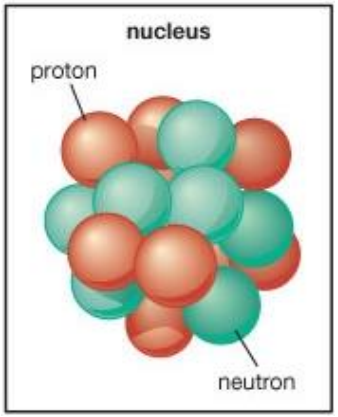
- Neutron isotopic drift is corrected by D2 (improvement due to neutron EOS).
- Axial deformation properties unchanged.

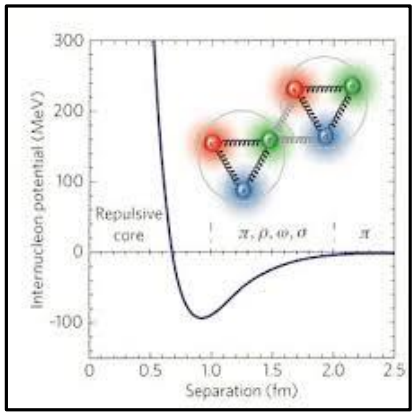
FROM RESEARCH TO INDUSTRY

MPMH TO TAILOR NUCLEAR EFFECTIVE INTERACTIONS

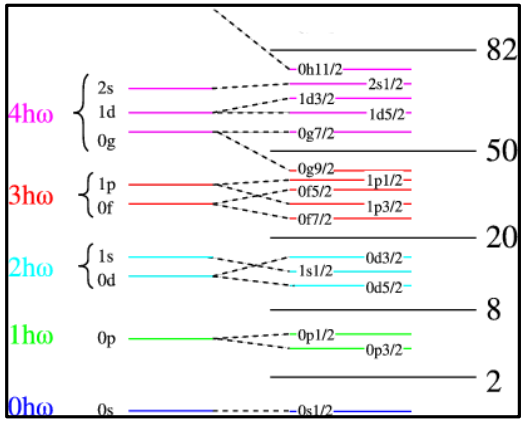
Nathalie Pillet	CEA/DAM/DIF, France
Caroline Robin	University of Washington, USA
Guillaume Hupin	IPNO, France
Marc Dupuis	CEA/DAM/DIF, France
D. Gogny	
Jean-François Berger	CEA/DAM/DIF, France
Vladimir Zelevinsky	Michigan state University, USA
Etienne Caurier	IPHC, France

GENERAL OVERVIEW





Strongly interacting system



Emergence of a mean-field
(hard core absorbed)

Two step method:

1) **Prerequisite: Existence of a mean-field as rich as possible** (HF for example)

- From phenomenological effective interaction (Gogny)
- From effective interaction derived from bare interactions (MPMH)

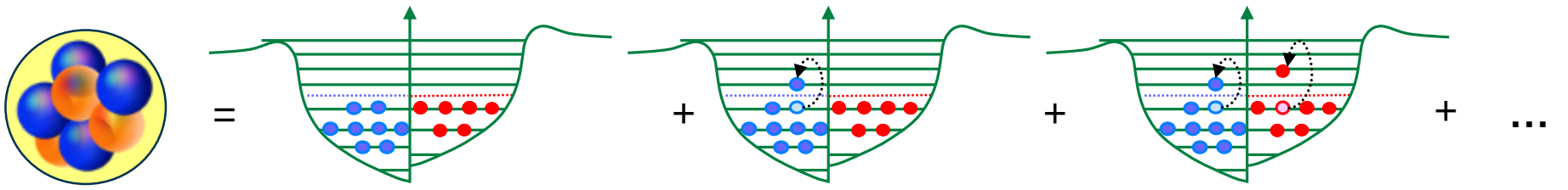
⇨ Strongly repulsive core has been avoided/treated

2) **MPMH configuration mixing: nuclear mid- (to long-) range correlations**

- Mean-field and beyond
- *Ab initio*

⇨ **At the interface of ab initio and EDF**

GENERAL OVERVIEW



Symmetries and Conservations

- Many-body wave function
- N+Z nucleons
- J conserved
- π conserved
- Fully antisymmetrized (Pauli)
- Can factorize c.m. motion

$$|\Phi\rangle = \sum_{\alpha} A_{\alpha} |\phi_{\alpha}\rangle$$

Mixing coefficients
(α : proton&neutron dependencies)

Slater determinants
α : MPMH configurations
N+Z nucleons
m-scheme: J_z, T_z
π conserved

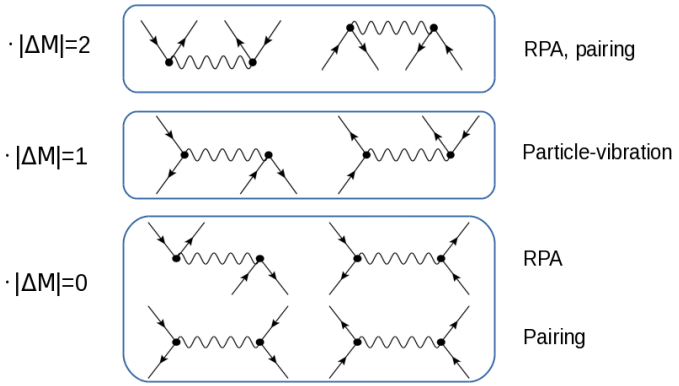
Additional properties

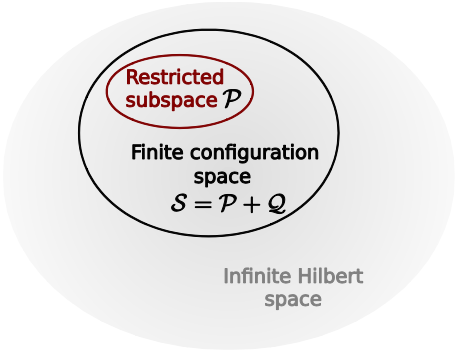
- Even-even, odd and odd-odd nuclei
- All types of nuclear long range correlations, deformations

Applications

- Structure : Excitation energies, transition probabilities, masses, radii, …
- Reactions : Inelastic nucleon and electron scattering, resonances
- Tool to test effective interactions and generate effective interactions from bare/chiral forces

GENERAL OVERVIEW



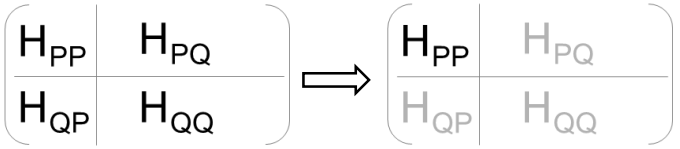


Hamiltonian (extension to three-body straightforward)

$$\hat{H} = \sum_{ij} K_{ij}\ a_i^\dagger a_j + \frac{1}{4}\sum_{ijkl} \widetilde{V}^{2N}_{ijkl}\ a_i^\dagger a_j^\dagger a_l a_k$$

Many-body wave function

- Full Hilbert space $|\Psi_{ex}\rangle$
- Truncated Hilbert space $|\Psi\rangle$



Variational principal on the total energy

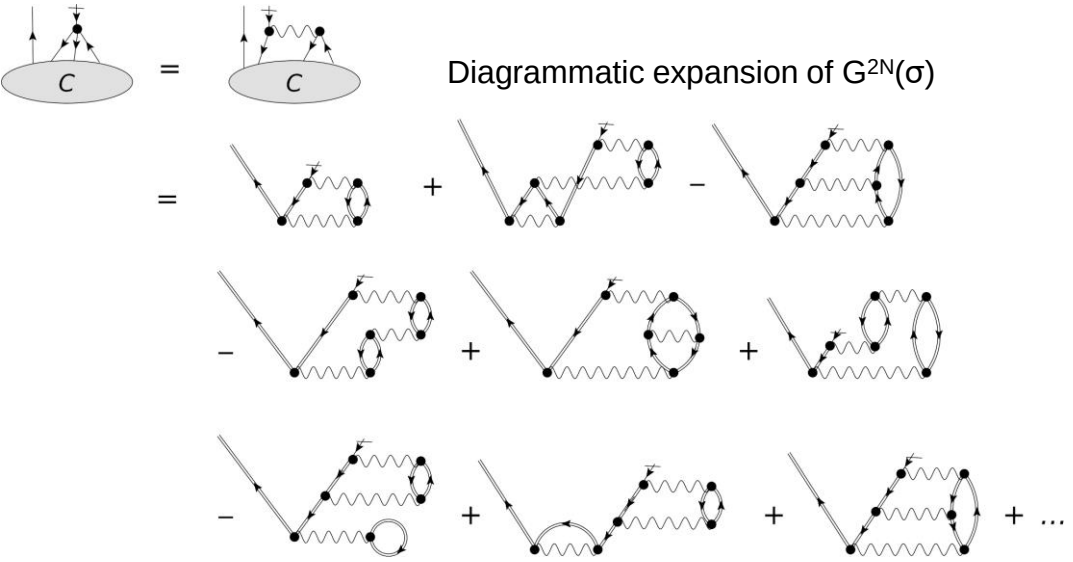
$$\mathcal{E}[\Psi_{(ex)}] = \langle \Psi_{(ex)} | \hat{H} | \Psi_{(ex)} \rangle$$

$$\delta_A \{ \mathcal{E}[\Psi_{(ex)}] - \lambda \langle \Psi_{(ex)} | \Psi_{(ex)} \rangle \} = 0 \iff \sum_\beta \langle \phi_\alpha | \hat{H} | \phi_\beta \rangle\, A_\beta = \lambda A_\alpha$$

⇒ **Mixing coefficients determined**

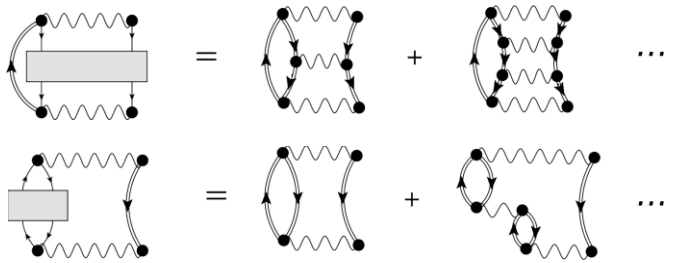
⇒ **What about orbitals?**

GENERAL OVERVIEW



Diagrammatic expansion of $G^{2N}(\sigma)$

General mean-field h(ρ)



Particular cases: Resummation of ladder and ring diagrams in $G^{2N}(\sigma)$

Link with Green's functions : Orbital equation

$$\left[\hat{h}[\rho], \hat{\rho}\right] = \hat{G}[\sigma]$$

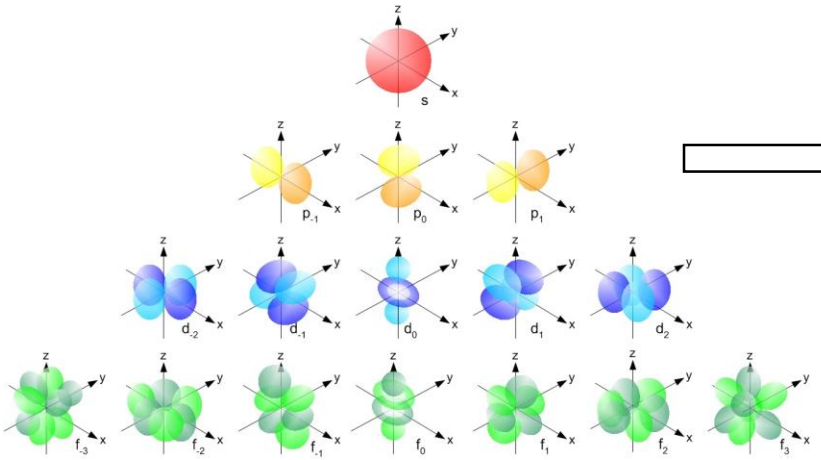
- $\hat{h}[\rho]$: General mean-field
- $\hat{\rho}$: Correlated one-body density
- $\hat{G}[\sigma]$: Connected part of the two-body density
- Source term

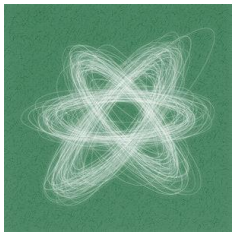
$$\hat{h}[\rho]_{ij} \equiv K_{ij} + \Gamma^{2N}[\rho]_{ij} = K_{ij} + \sum_{kl} \widetilde{V}^{2N}_{ikjl}\ \rho_{lk} \qquad G[\rho,\sigma] = F[\sigma] - F^{\dagger}[\sigma] \text{ with } F[\sigma]_{ij} = \frac{1}{2}\sum_{klm} \sigma_{ki,lm} \widetilde{V}^{2N}_{kljm}$$

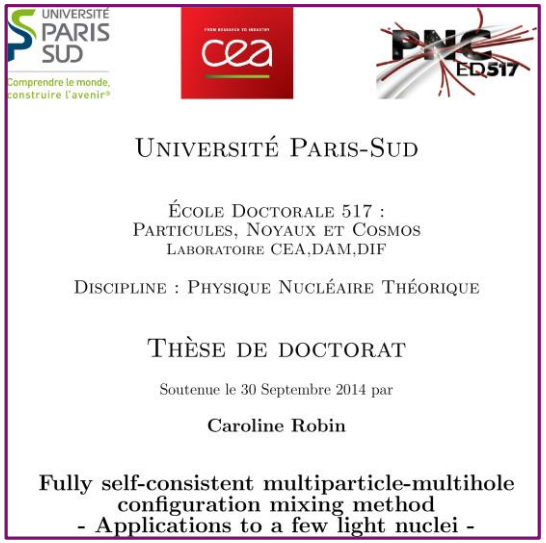
⇨ Equation automatically satisfied in the case of exact solution!

GENERAL OVERVIEW

Caroline Robin
PhD at CEA/DAM/DIF
Postdoc at WMU







UNIVERSITÉ PARIS-SUD

ÉCOLE DOCTORALE 517 :
PARTICULES, NOYAUX ET COSMOS
LABORATOIRE CEA,DAM,DIF

DISCIPLINE : PHYSIQUE NUCLÉAIRE THÉORIQUE

THÈSE DE DOCTORAT

Soutenue le 30 Septembre 2014 par

Caroline Robin

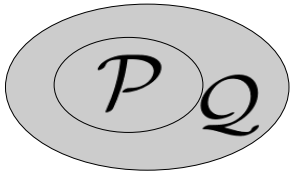
Fully self-consistent multiparticle-multihole configuration mixing method - Applications to a few light nuclei -

- **Minimization of the total energy** $\mathcal{E}[\Psi]$
  - First order variation (unitary transformation): Brillouin condition.
  - Orbital equation similar to the one derived with the exact solution but not satisfied automatically!
  - **Need to establish the consistency between one- and two-body properties by solving explicitly the orbital equation.**

$$\delta_\varphi \mathcal{E}[\Psi] = 0 \Leftrightarrow \left[\hat{h}[\rho], \hat{\rho}\right] = \hat{G}[\sigma]$$

Truncations and Symmetries

- **Truncations compatible with the conservation of the advantages of the method**
  - ✓ Conservation of symmetries
  - ✓ All types of many-body correlations and deformations
  - ✓ Even-even, odd and odd-odd nuclei
  - ✓ Full antisymmetrization (Pauli)



- **Different possible truncations ⟹ Flexibility of the MPMH configuration mixing**
  - ✓ Core+valence space
  - ✓ Excitation order of the configurations
  - ✓ Excitation energy of the configurations
    - ➢ Ideally, a combination of the truncations with the preservation of desired symmetries
    - ➢ Systematically improvable method

- **Role of the orbital equation**

Compensation for the truncations made on the wave function

Starting from a certain set of single-particle states (a^+), the orbital equation lead to a new set (b^+):

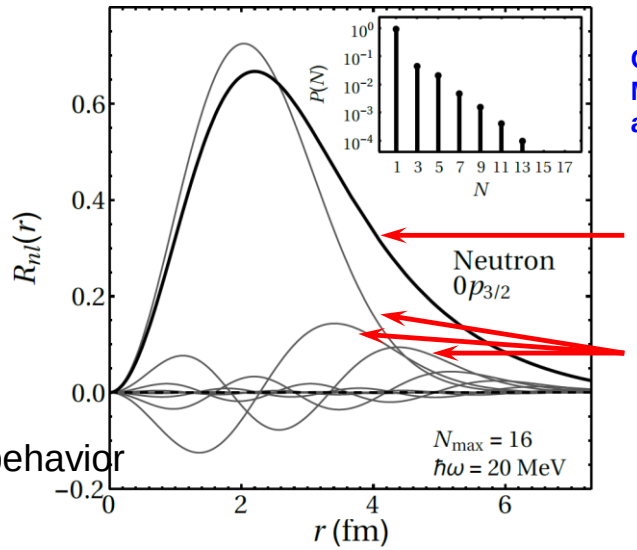
where $\hat{\Lambda} = \sum_{kl} \Lambda_{kl} a_k^\dagger a_l$

$$b_i^\dagger = e^{i\hat{\Lambda}} a_i^\dagger e^{-i\hat{\Lambda}} = \sum_j a_j^\dagger \left(e^{i\hat{\Lambda}}\right)_{ji} \equiv \sum_j a_j^\dagger \theta_{ji}$$

Under this transformation, the N-body configurations vary as

$$\begin{aligned} |\phi_\alpha\rangle \to |\phi'_\alpha\rangle &= e^{i\Lambda}|\phi_\alpha\rangle \\ &= |\phi_\alpha\rangle + \sum_{ij} \Lambda_{ij} a_i^\dagger a_j |\phi_\alpha\rangle + \sum_{ijkl} \Lambda_{ij}\Lambda_{kl} a_i^\dagger a_j a_k^\dagger a_l |\phi_\alpha\rangle + \ldots \end{aligned}$$

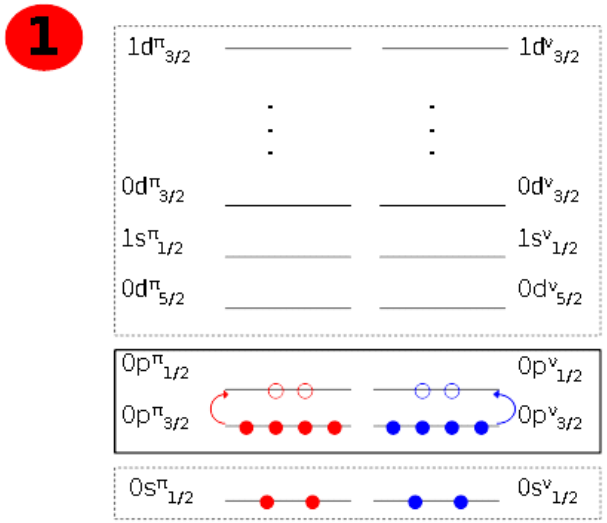
- Optimization of orbitals: Creation of MPMH excitations on top of the existing configurations
- The MPMH excitations extend to the whole single-particle basis one is considering
- Since Λ is a one-body operator, they are always built as product of 1P1H excitations

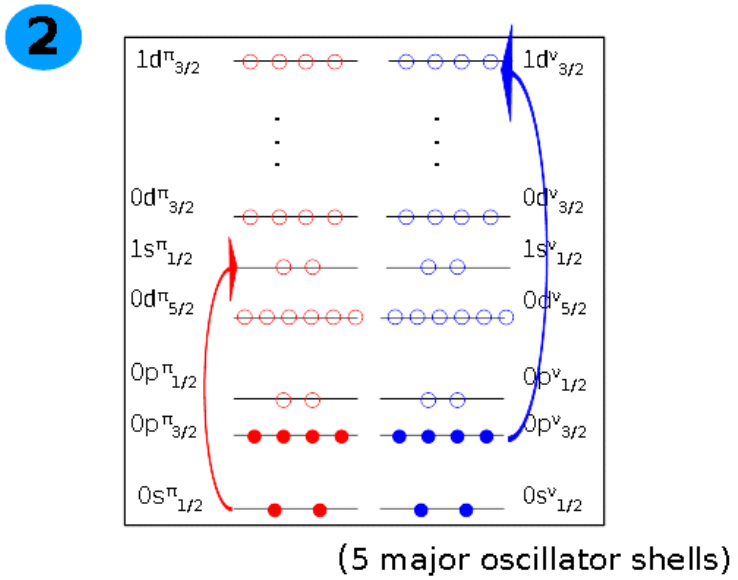


Ch. Constantinou, M. A. Caprio *et al.* arXiv:1605.04976

Illustration on the radial behavior with natural orbital basis

NUMERICAL ALGORITHM WITH ORBITAL OPTIMIZATION





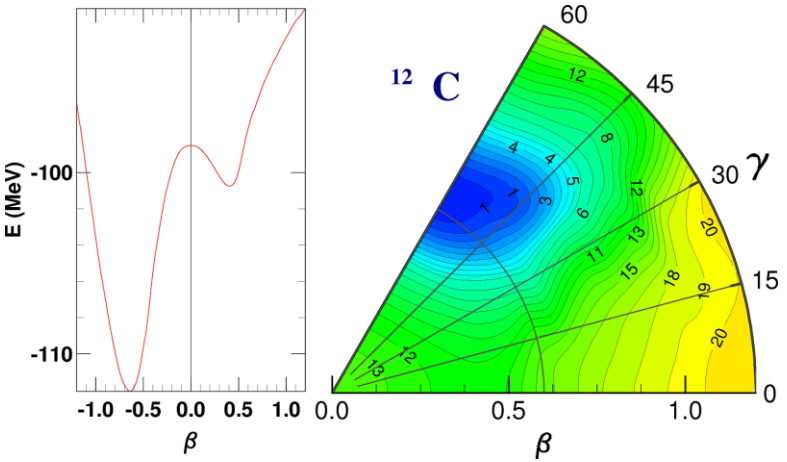
(5 major oscillator shells)

^{12}C test nucleus

Two types of truncation schemes tested:

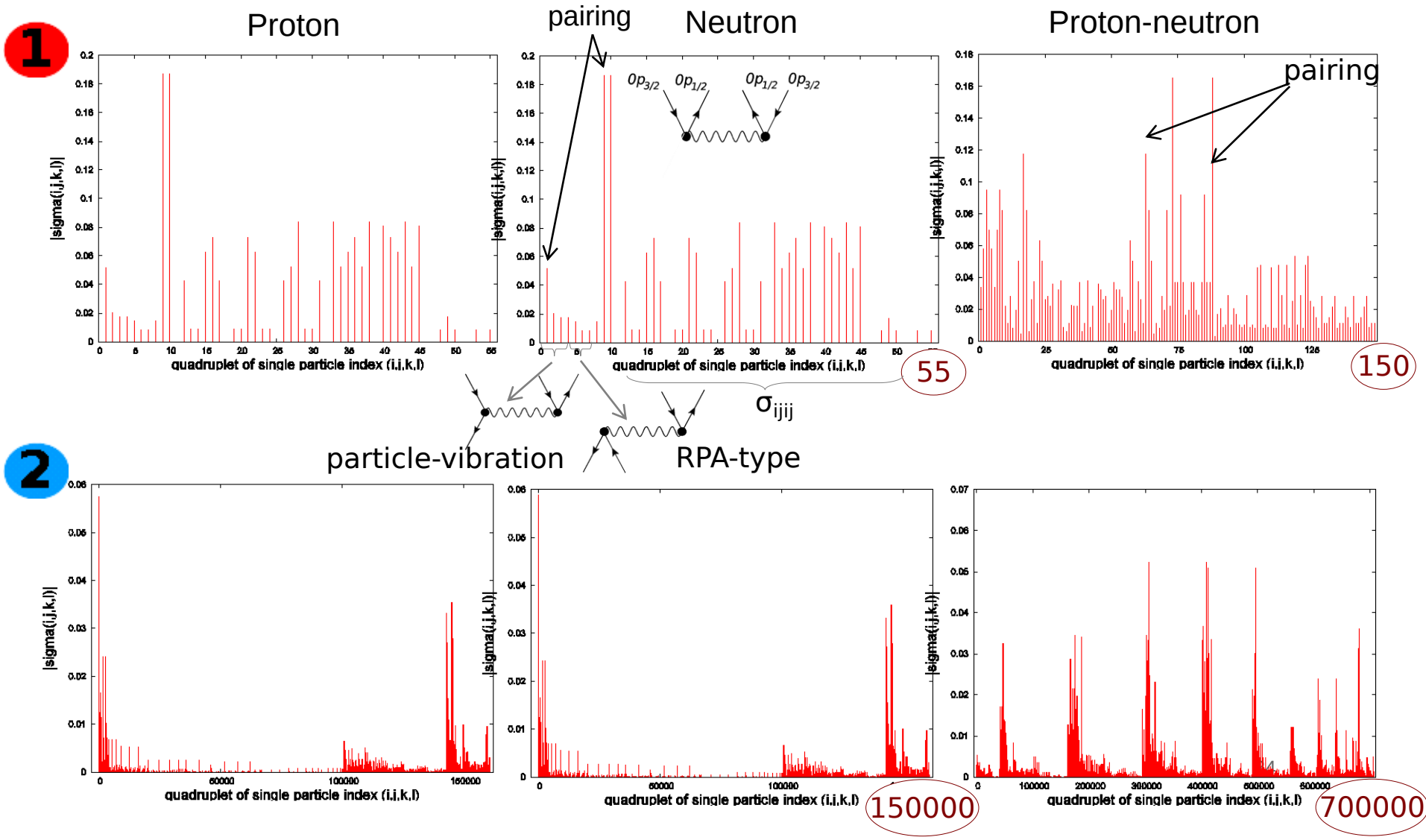
1. ^{4}He core + 0ħω valence space
   - 38 configurations
   - Natural max. excitation order: 4P4H

2. Nħω space
   - Truncation at 4P4H
   - 26 401 700 configurations



NUMERICAL ALGORITHM WITH ORBITAL OPTIMIZATION

Two-body correlation matrix σ_{ijkl}

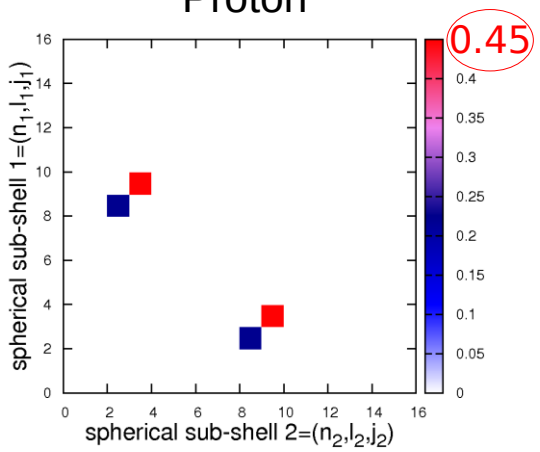


NUMERICAL ALGORITHM WITH ORBITAL OPTIMIZATION

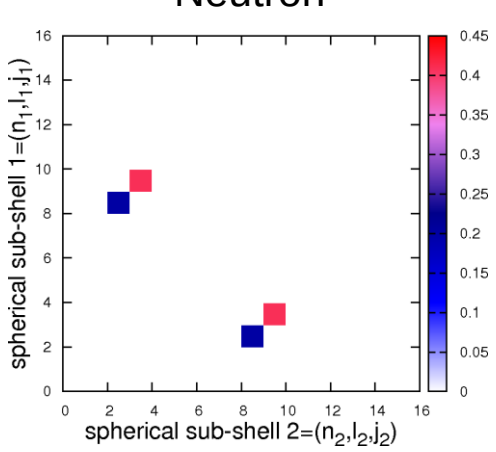
Source term $G(\sigma)_{ij}$

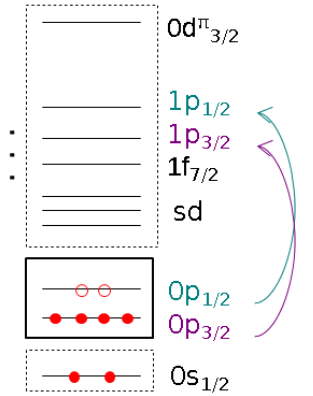
1

Proton

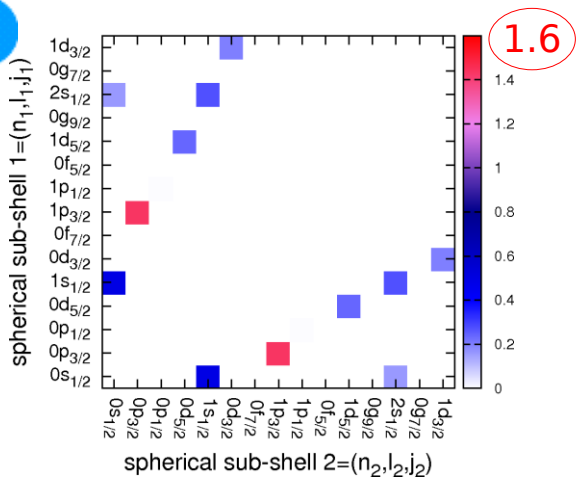


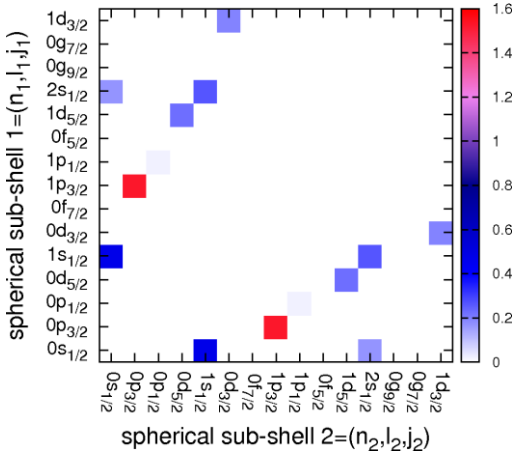
Neutron





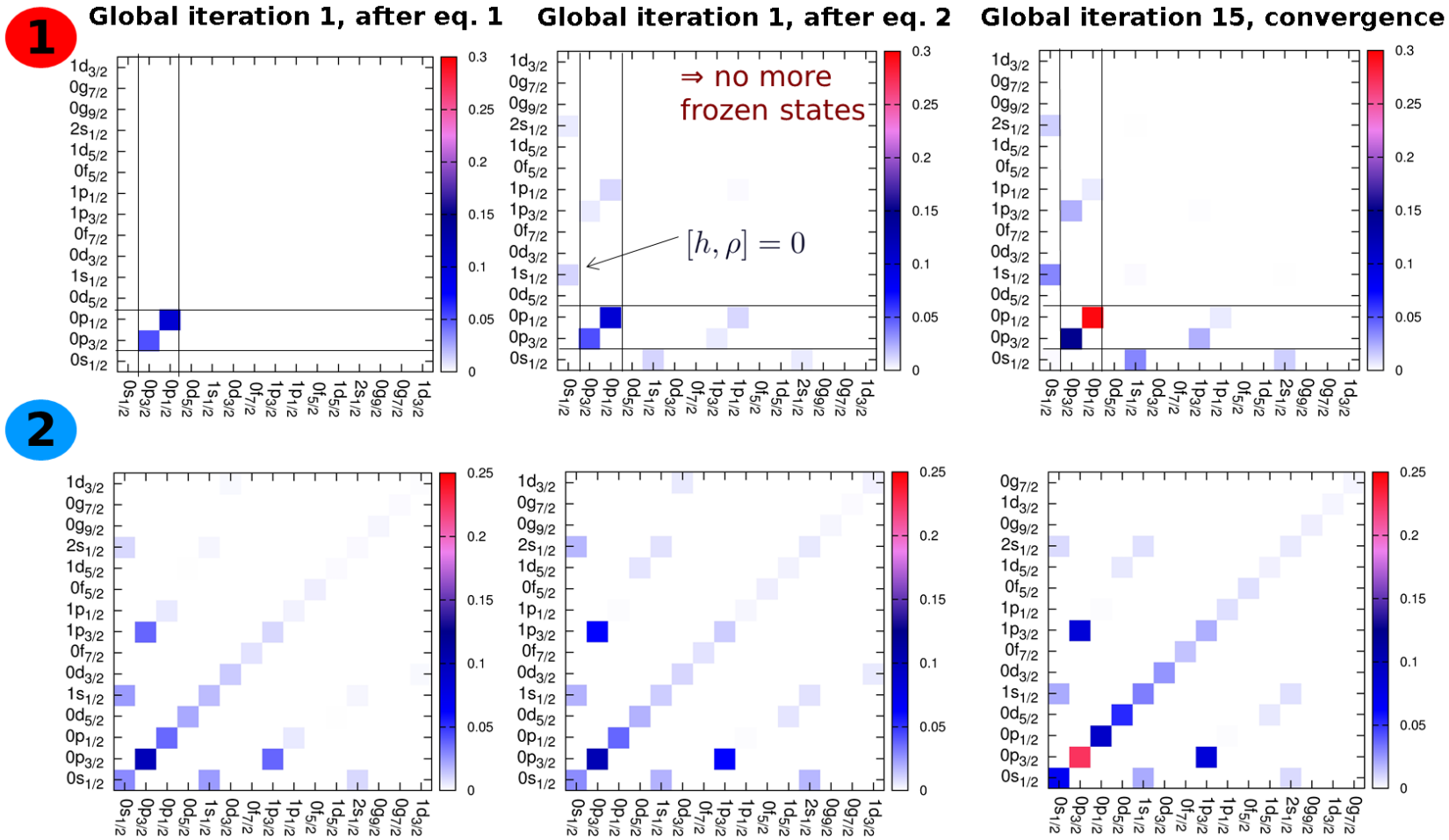
2





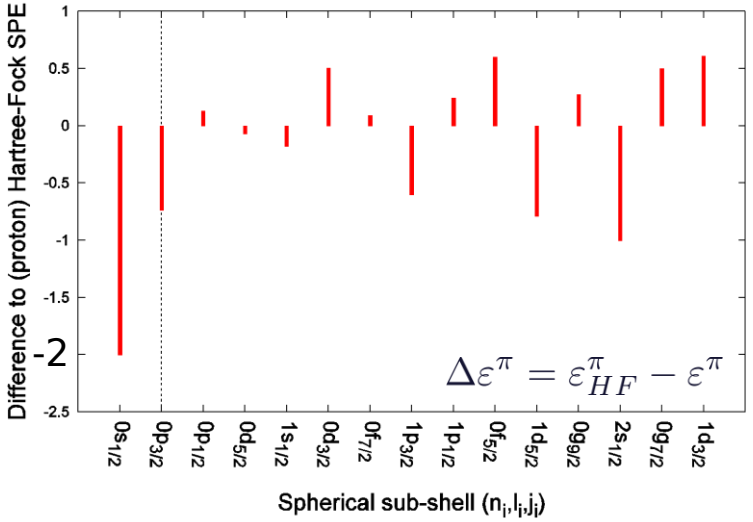
NUMERICAL ALGORITHM WITH ORBITAL OPTIMIZATION

Evolution of the one-body density: Representation of $\Delta\rho=|\rho_{HF}-\rho_{correlated}|$ in HF basis

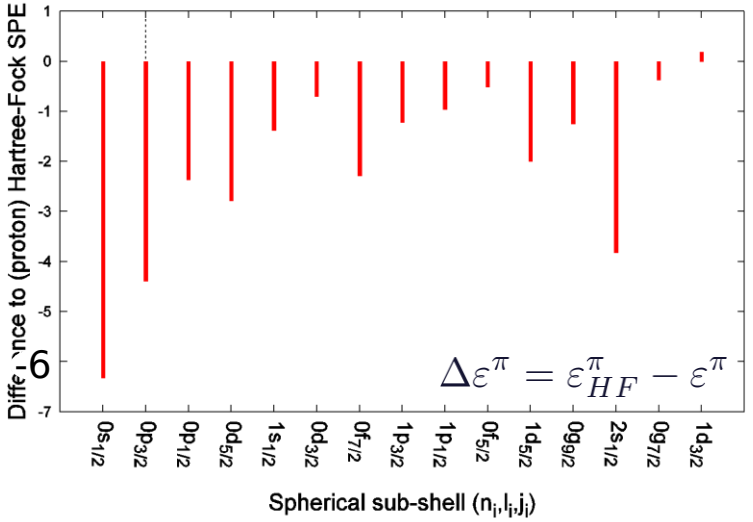


NUMERICAL ALGORITHM WITH ORBITAL OPTIMIZATION

1



2



Modifications of the single-particle energies

Eigenvalues ε of $h[\rho,\sigma]_{ij} = T_{ij} + \sum_{kl}\langle ik|\widetilde{V}|jl\rangle\rho_{lk} + \frac{1}{4}\sum_{klmn}\langle kl|\frac{\partial\widetilde{V}}{\partial\rho_{ji}}|mn\rangle\langle\Psi|a_k^\dagger a_l^\dagger a_n a_m|\Psi\rangle$ compared to ε_{HF}.

1

- Spectrum compressed by ~2.5 MeV
- 0s increased by ~2 MeV
- Gap $0p_{3/2}$-$0p_{1/2}$ (8.15 MeV) reduced by ~870 keV.

2

- Spectrum compressed by ~6 MeV
- 0s increased by ~6 MeV
- Gap $0p_{3/2}$-$0p_{1/2}$ (8.15 MeV) reduced by ~2 MeV.

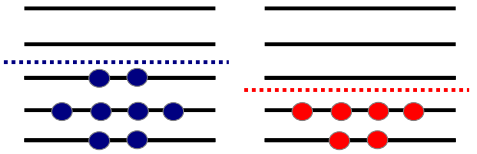
NUMERICAL ALGORITHM WITH ORBITAL OPTIMIZATION

1

Correlation energy E_{corr} (MeV)	
1^{st} equation	$1^{st}+2^{nd}$ equation
6.22	6.56

2

Correlation energy E_{corr} (MeV)	
1^{st} equation	$1^{st}+2^{nd}$ equation
61.77	62.54



Effect on the ground state

- HF binding energy: E(HF)= -92.9 MeV
- Experimental binding energy: E(HF)= -92.16 MeV

- Correlation energy: $E_{corr} = E(\Psi) - E(HF)$ (correlated state: $E(\Psi)$; Hartree-Fock state: $E(HF)$)

1

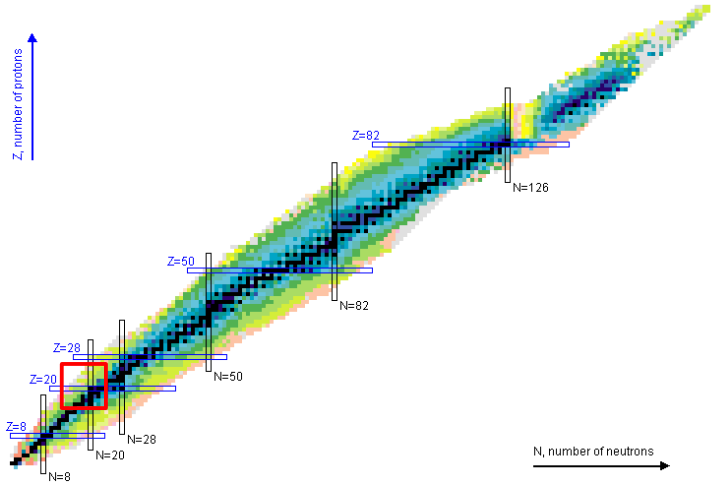
Gain 340 keV

2

Gain 770 keV

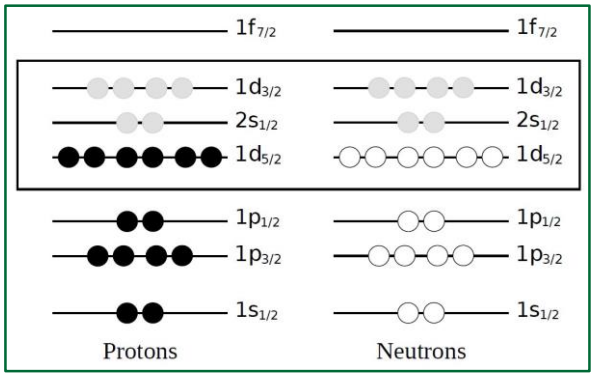
- Clear overbinding in ^{12}C!
- What is happening with the interaction, related to the truncation scheme?

VARIOUS APPLICATIONS WITH THE GOGNY FORCE



Framework:

- Even-even nuclei $10 \leq (Z,N) \leq 18$
- Truncation scheme: core of ^{16}O (non frozen) + valence



Ex: $^{28}Si \rightarrow$ 12P12H

- N_0=9 major oscillator shells

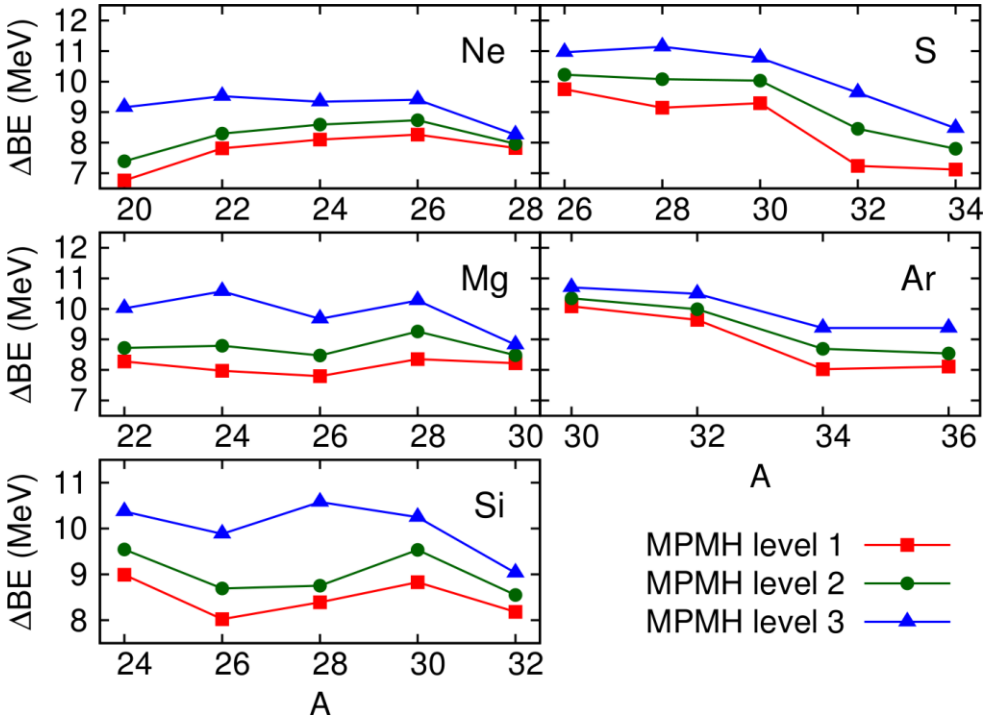
Description of ground state and spectroscopic properties

- Binding and separation energies, charge radii
- Excitation energies
- Magnetic dipole moments μ and quadrupole spectroscopic moments Q_s
- Transition probabilities B(E2) and B(M1)
- Inelastic electron and proton scattering on discrete states

⇨ How are these observables affected by the optimization of orbitals?

Ground state properties

- **Binding energy**



Average difference
- Level 1: 8.91 MeV
- Level 3: 9.84 MeV

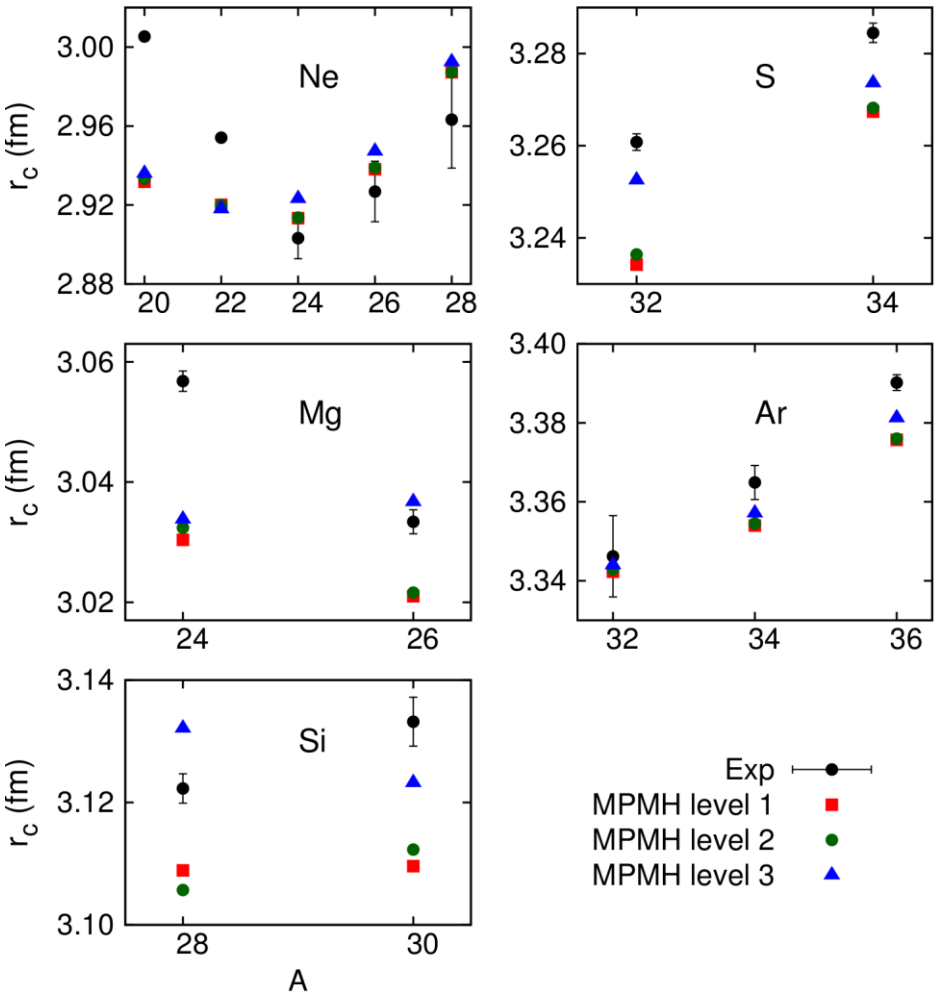
Standard deviation
- Level 1: 0.793 MeV
- Level 3: 0.789 MeV

- **Correlation energy**

	Level 1: Eq. (2) with $\rho = \rho_{HF}$, $\sigma = 0$.	Level 2: Full Eq. (2).	Level 3: Full Eqs. (2)& (3).
^{28}Ne	1.15	1.28	1.58
^{26}Ne	0.41	0.88	1.55
^{24}Ne	5.75	6.23	6.98
^{22}Ne	10.48	10.90	12.12
^{20}Ne	10.93	11.54	13.30
^{24}Mg	14.24	15.06	16.04
^{28}Si	5.89	6.25	8.08
^{32}S	3.37	4.58	5.76

VARIOUS APPLICATIONS WITH THE GOGNY FORCE

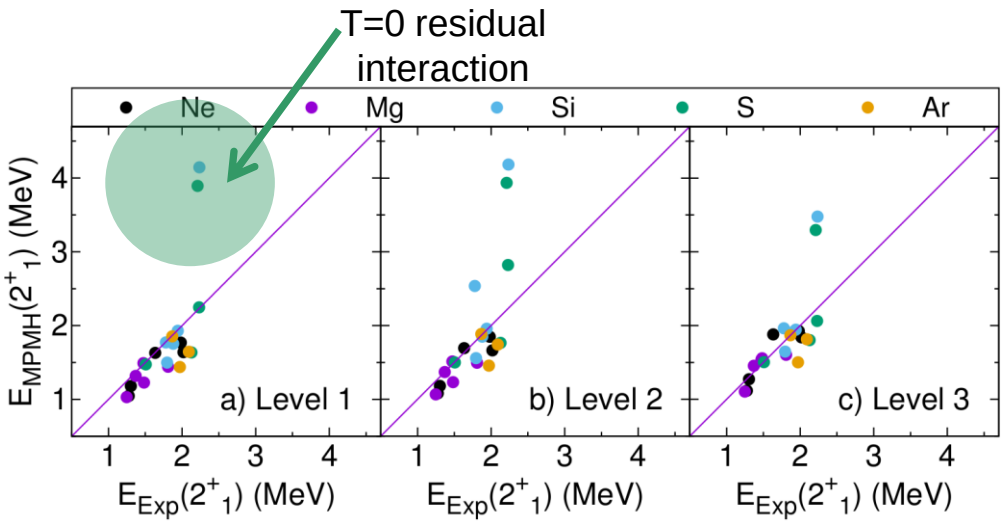
- **Charge radii**

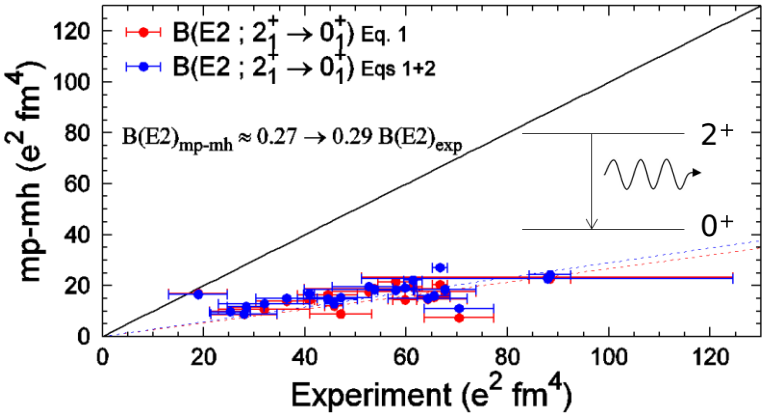


Average difference
- Level 1: 0.021 fm
- Level 3: 0.018 fm

Standard deviation
- Level 1: 0.017 fm
- Level 3: 0.018 fm

First 2^+ excited state and B(E2) transition probabilities toward the ground state





Average difference
- Level 1: 373 keV
- Level 3: 235 keV

Standard deviation
- Level 1: 517 keV
- Level 3: 323 keV

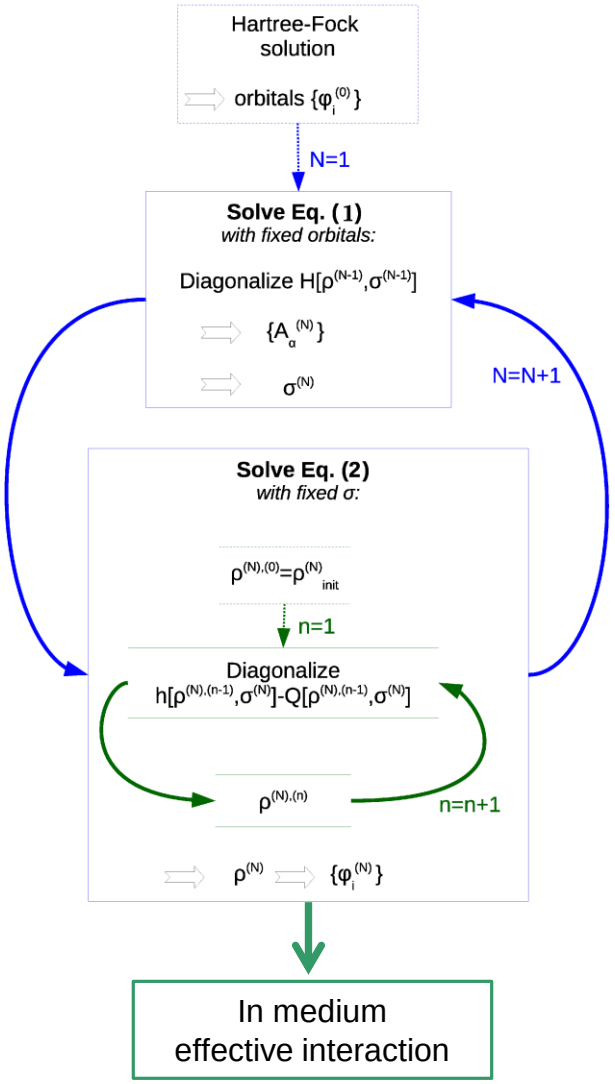
Excluding ^{30}Si and ^{30}S

Average difference
- Level 1: 226 keV
- Level 3: 142 keV

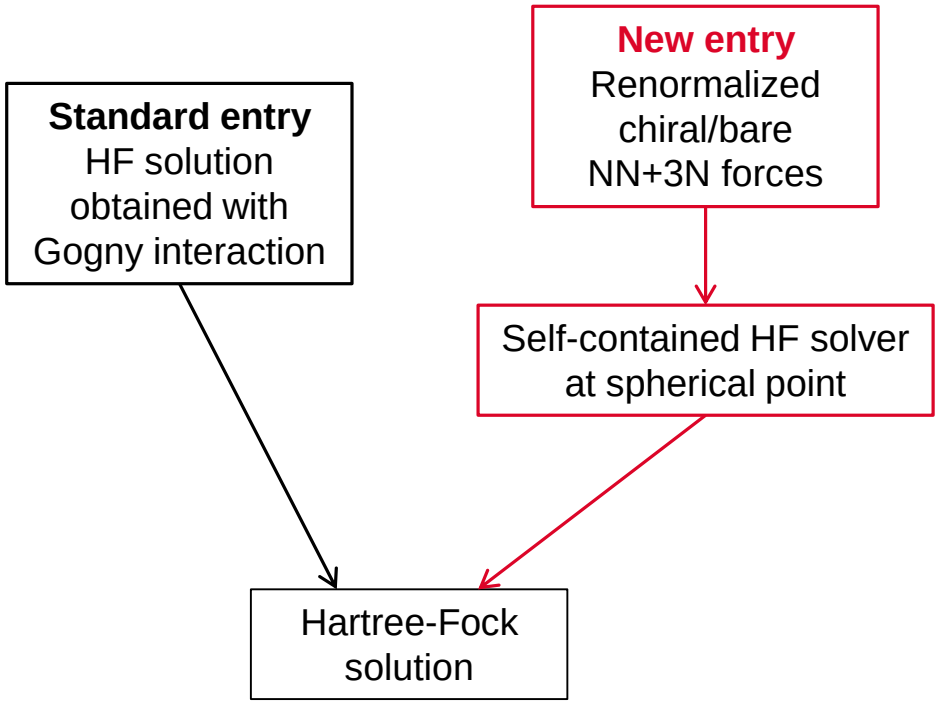
Standard deviation
- Level 1: 214 keV
- Level 3: 122 keV

- Experimental trends globally well reproduced but...
- Clear lack of collectivity due to the restricted valence space
- Little but positive effect from optimization of orbitals

IN DEVELOPMENT: MPMH AS AN AB INITIO METHOD & A TOOLS TO TAILOR EFFECTIVE INTERACTION

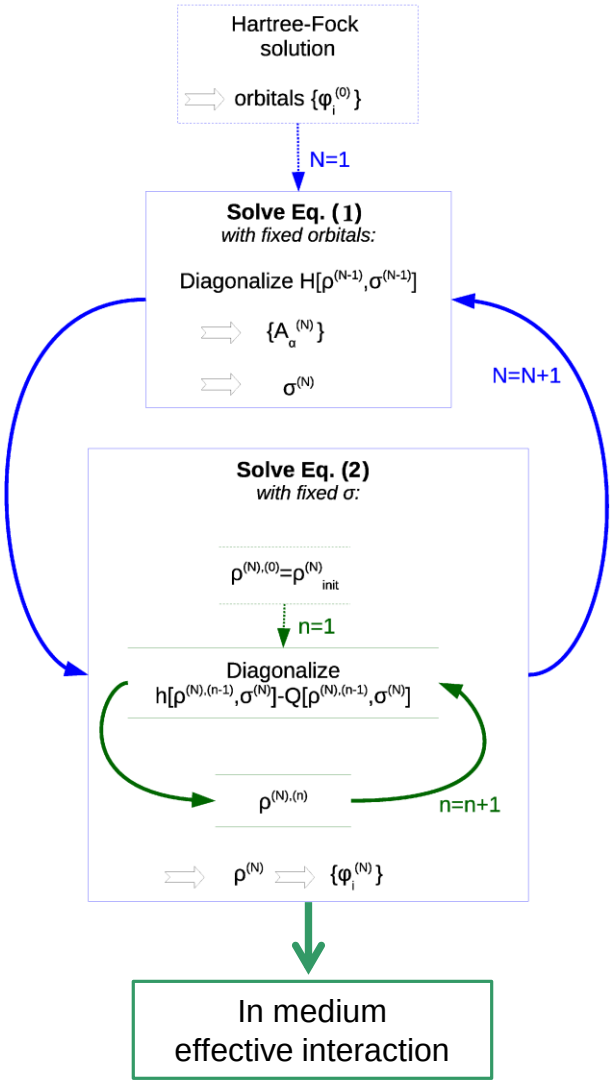


Constrained effective interaction to ab initio inputs



⟹ MPMH configurations introduced at a given order of excitation

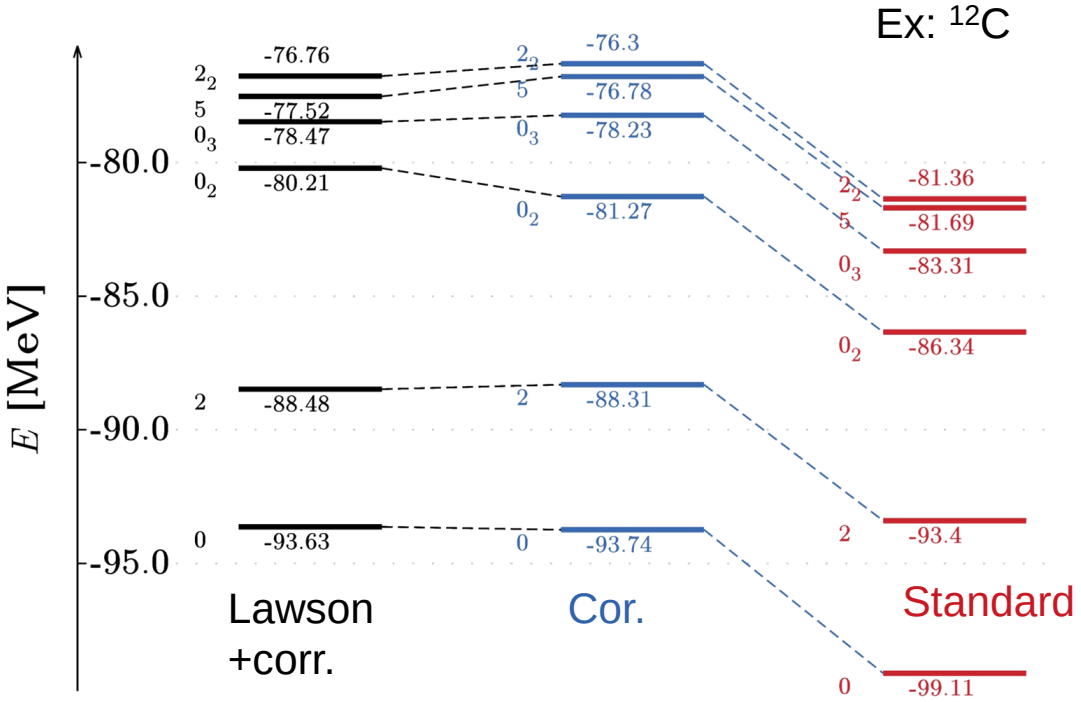
IN DEVELOPMENT: MPMH AS AN AB INITIO METHOD & A TOOLS TO TAILOR EFFECTIVE INTERACTION



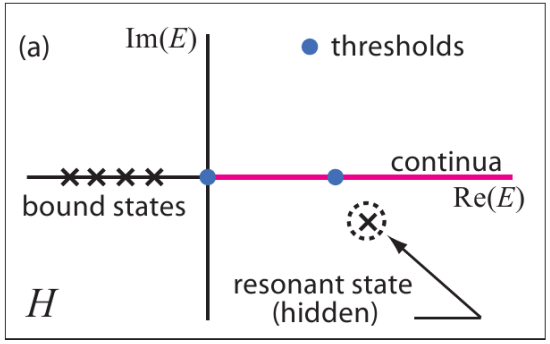
$$\mathcal{H} \rightarrow T_{\text{kin}} + T_{cor.} + V^{NN} + \beta\mathcal{H}_{\text{c.m.}}$$

Correction du centre de masse

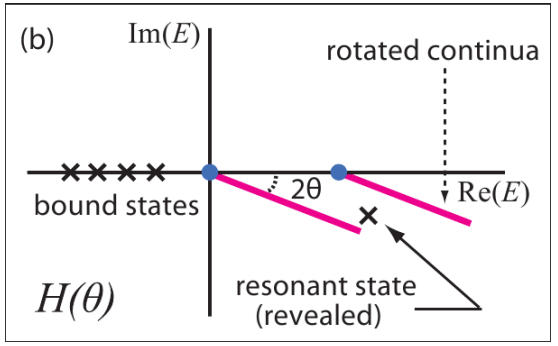
Lawson term



IN DEVELOPMENT: RESONNANCES



Complex scaling



The complex scaling and the resonance states

$$H(r) = T + V(r) \Rightarrow \begin{aligned} H(\theta) &= e^{-2i\theta}T + V\left(re^{i\theta}\right) \\ H(r) &= U(\theta)H(r)U(\theta)^{-1} \end{aligned}$$

U(θ) is a non-unitary operator of the rotation in the complex plane

Underlying Aguilar-Balslev-Combes theorem: the resonant states of the original Hamiltonian are invariant and the non-resonant scattering states are rotated and distributed on a 2θ ray that cuts the complex energy plane with a corresponding threshold being the rotation point.

Solve the Schrödinger equation in a L^2 basis (i.e. HO, MPMH orbitals…)

$$H(r,\theta)\psi(r,\theta) = (E + i\Gamma)\psi(r,\theta)$$

Energie Demi-vie

En pratique

$$\int \phi_n(r)V\left(re^{i\theta}\right)\phi^{n'}(r)r^2dr = e^{-i3\theta}\int \phi_n\left(r\bar{e}^{i\theta}\right)V(r)\phi^{n'}\left(re^{-i\theta}\right)r^2dr$$

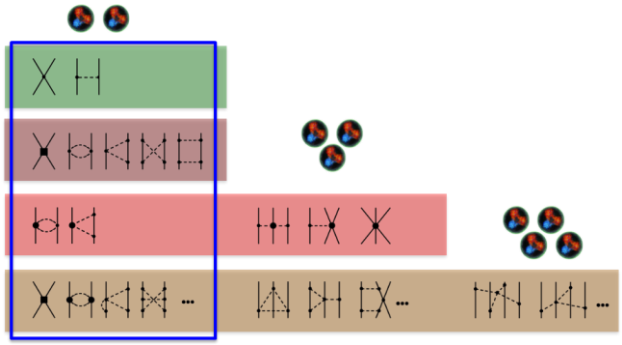
Analytic for Gaussian

IN DEVELOPMENT: RESONNANCES

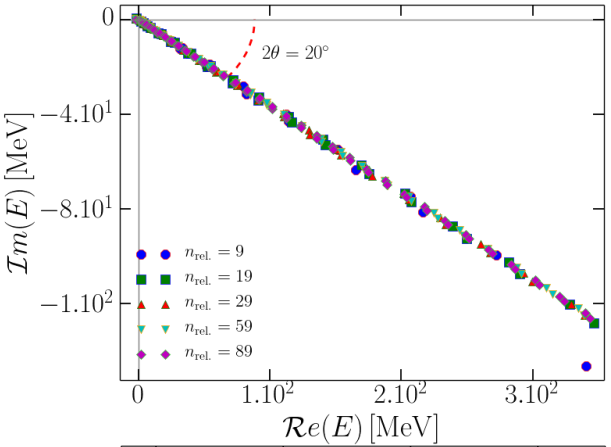
Schematic case: the deuteron

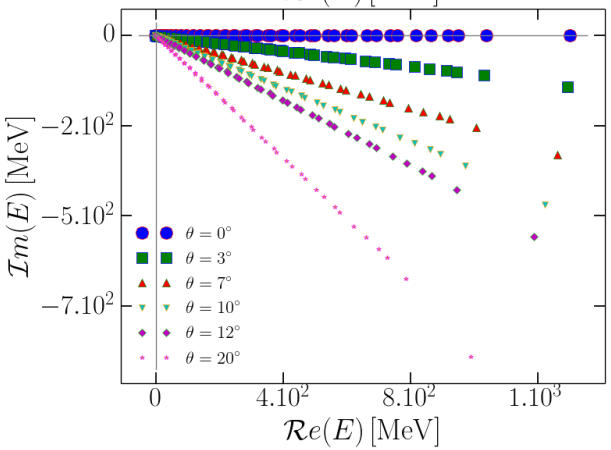
Collaboration with R. Lazauskas and J. Carbonell

- Use of an HO basis in Jacobi coordinates
- Diagonalization in the deuteron channel

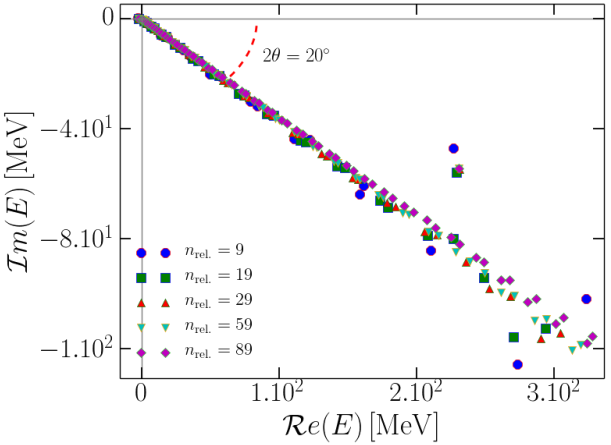


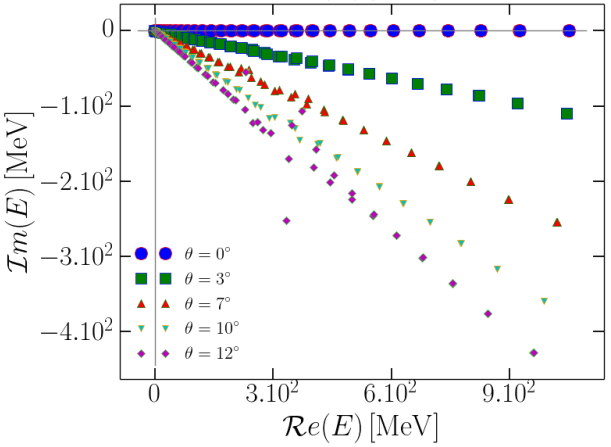
Malfliet-Tjon





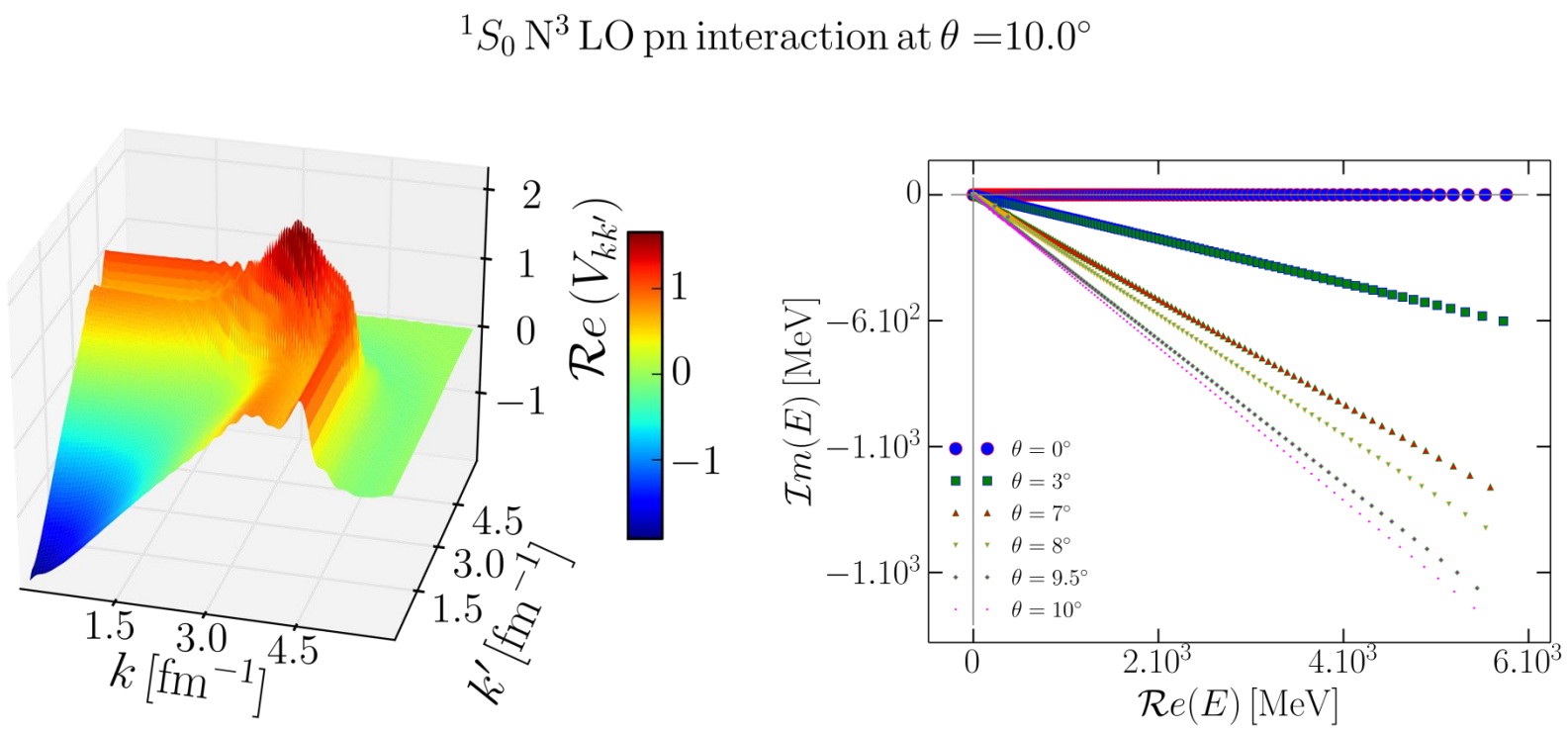
N^{3}LO





Generalization of the MPMH configuration mixing approach to symmetric non-hermitian complex matrices !

IN DEVELOPMENT: RESONNANCES



- SRG evolution requires to span a large NN basis (n_r~150). The typical scale of k is 10 fm^{-1} (V^{NN}).
- Complex scaling involves the integration of diverging polynomials (of order n) far from their zeroes.

SRG IS WORKING !

$^1S_0$ N^{3}LO pn interaction at θ =10.0° Λ_{SRG} =1.5 fm^{-1}