Variational Multiparticle-Multihole Configuration Mixing Method

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Plan

I. **Introduction** [1]

II. **Formalism** of the variational multiparticle-multihole (mp-mh) configuration mixing method

III. **Three applications**

(1) P.Ring and P.Schuck, "The Nuclear Many-Body Problem", Springer-Verlag, 1980.

Nucleus = A interacting nucleons

(2≤A ≤270)

- **N-N interaction**
  (QCD not yet *usable*)
  - **Bare forces**
  - **In medium forces**

  (Phenomenological)

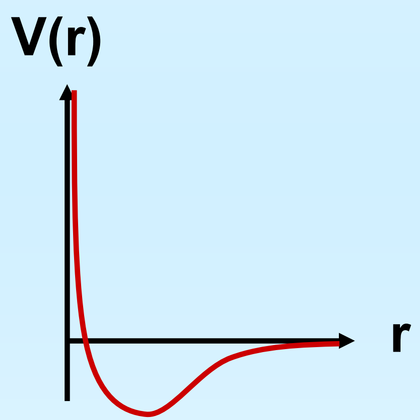
- **Many-body problem**
  - **Numerical solution of exact equations**
    A≤12-14
  - **Approximations**

N-N potential and Independent Particle Model

- **N-N potential**

"molecular potential" + spin-isospin dependence + …

Nucleonic charge g: $g^2/hc \sim 12\text{-}14$
Fine structure constant : $\alpha = e^2/hc = 1/137$



- **In nuclei**

  ✓ **Evidence for shell structure**
  Magic numbers : 2, 8, 20, 28, 50, 82, 126

  ✓ **Independent particle model works : existence of a mean field**

Current theoretical nuclear approaches

Shell model

- Inert core + valence space
- Effective interaction between valence nucleons
- Conservation of symmetries
- *All* correlations taken into account between valence nucleons

  ✓Description of all excited states

Mean field theories

- No inert core (binding energies)
- Effective force between *all* nucleons
- Symmetry breaking
- Correlations incorporated step by step

  ✓Hartree-Fock (HF)

  ✓Pairing (BCS,HFB)

  ✓Collective excitations (RPA,GCM)

Variational mp-mh configuration mixing method :

Attempt to unify the description of correlations beyond HF approximation

Variational mp-mh configuration mixing method

Theoretical point of view

- Gives a unified description of {Pairing + RPA + particle vibration} correlations on top of HF mean field theory
- Respects conservation of particle numbers and Pauli principle
- Treats on the same footing even-even nuclei, odd and odd-odd nuclei
- Can describe both ground states and excited states

Particular interesting physical cases

- K isomers
- Pairing correlations
- Light exotic nuclei

Trial wave function

Superposition of Slater Determinants (SD) corresponding to mp-mh excitations upon a given state of HF type

$$|\Psi>= A^{0p0h}_{\pi\nu}|\phi_\pi\phi_\nu>_{0p0h} + \sum_{\alpha_\pi\alpha_\nu} A^{1p1h}_{\alpha_\pi\alpha_\nu}|\phi_{\alpha_\pi}\phi_{\alpha_\nu}>_{1p1h} + \sum_{\alpha_\pi\alpha_\nu} A^{2p2h}_{\alpha_\pi\alpha_\nu}|\phi_{\alpha_\pi}\phi_{\alpha_\nu}>_{2p2h} + \ldots$$

$$|\Phi_{\alpha_\tau}>= \prod_{(kl)=1}^{m}(a_k^+ a_l)|\Phi_\tau>_{0p0h}$$

$$|\Phi_\tau>_{0p0h}= |HF>= \prod_{i=1}^{N} a_i^+|0>$$

Variational parameters :

Mixing coefficients

Single particle orbitals

Variational principle

- **Functional:** $$\mathcal{F} = E - \lambda < \Psi | \Psi >$$

$$E \quad =< \Psi | \hat{H} \quad | \Psi >=< \Psi | \hat{K} + \hat{V} | \quad | \Psi >$$

- **Determination of mixing coefficients:** $$\frac{\partial \mathcal{F}}{\partial A^*_{\alpha_\pi \alpha_\nu}} = 0$$

- **Determination of optimized single particle states:** $$\frac{\partial \mathcal{F}}{\partial \varphi_i^{\tau *}} = 0$$

Mixing coefficients

$$\frac{\partial \mathcal{F}}{\partial A^*_{\alpha_\pi \alpha_\nu}} = 0$$

Single particle states

$$\frac{\partial \mathcal{F}}{\partial \varphi_i^{\tau *}} = 0$$

$$\sum_{\alpha_\pi} A_{\alpha_\pi \alpha'_\nu} (< \phi_{\alpha'_\pi} | \hat{H}^\pi | \phi_{\alpha_\pi} > + \sum_{mn} C^\pi_{mn} < \phi_{\alpha'_\pi} | a^+_m a_n | \phi_{\alpha_\pi} >) +$$
$$\sum_{\alpha_\nu} A_{\alpha'_\pi \alpha_\nu} (< \phi_{\alpha'_\nu} | \hat{H}^\nu | \phi_{\alpha_\nu} > + \sum_{mn} C^\nu_{mn} < \phi_{\alpha'_\nu} | a^+_m a_n | \phi_{\alpha_\nu} >) +$$
$$\sum_{\alpha_\pi \alpha_\nu} A_{\alpha_\pi \alpha_\nu} < \phi_{\alpha'_\pi} \phi_{\alpha'_\nu} | \hat{V}^{\pi\nu} | \phi_{\alpha_\pi} \phi_{\alpha_\nu} > \quad = \quad \lambda A_{\alpha'_\pi \alpha'_\nu}$$

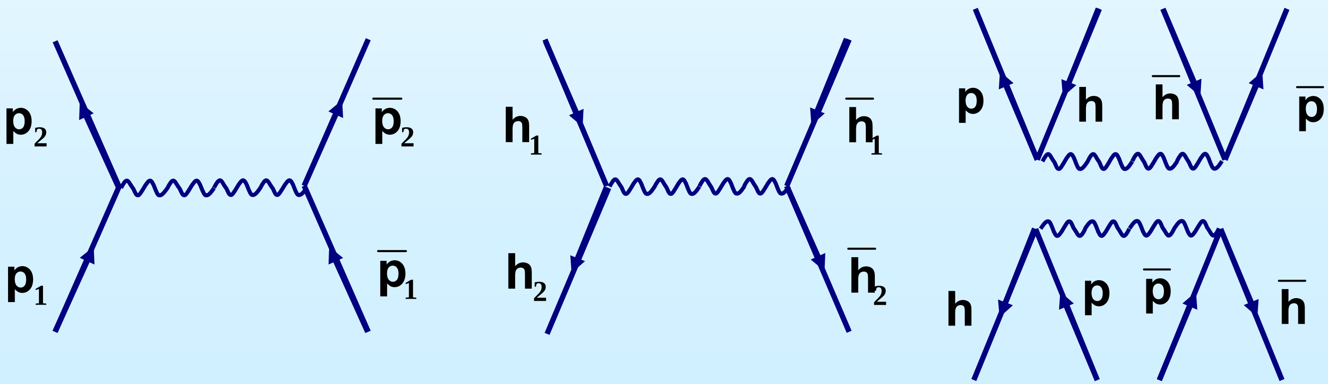
→ **self-consistent procedure**

→ **Renormalization of the HF field**

- **In the present work :** $[h[\rho], \rho] = 0$

Residual interaction

• Pairing



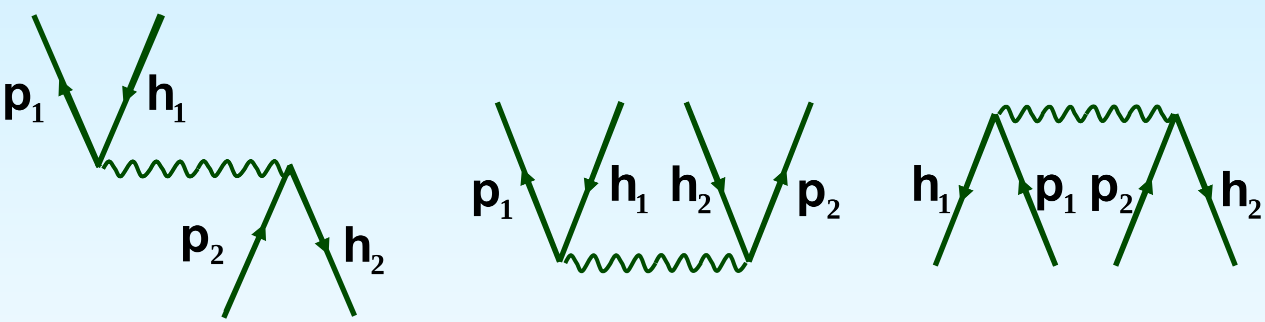
$$< p_2\bar{p}_2 \,|\, V \,|\, p_1\bar{p}_1 >$$

$$< h_2\bar{h}_2 \,|\, V \,|\, h_1\bar{h}_1 >$$

$$< p\,\bar{p} \,|\, V \,|\, h\,\bar{h} >$$

$$< h\,\bar{h} \,|\, V \,|\, p\,\bar{p} >$$

• RPA

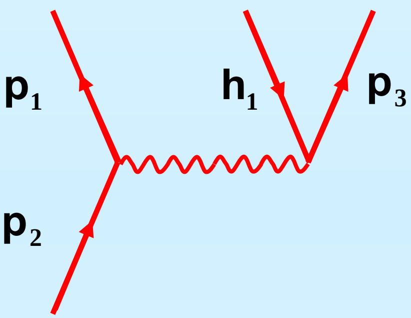


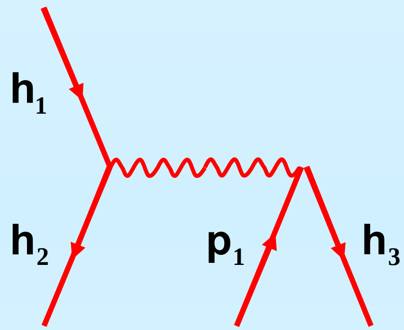
$$< p_1h_2 \,|\, V \,|\, h_1p_2 >$$

$$< p_1p_2 \,|\, V \,|\, h_1h_2 >$$

$$< h_1h_2 \,|\, V \,|\, p_1p_2 >$$

• Particle vibration coupling





$$< p_3 p_1 \,|\, V \,|\, h_1 p_2 >$$

$$< h_2 h_3 \,|\, V \,|\, h_1 p_1 >$$

Gogny phenomenological effective force [1]

$$V_{12} = \sum_{j=1}^{2} e^{-(r_1-r_2)^2/\mu_j^2}\left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right)$$ **Central**

$$+ t_3\left(1 + x_0 P_\sigma\right)\delta\left(\vec{r}_1 - \vec{r}_2\right)\left[\rho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)\right]^\alpha$$ **Density-dependent**

$$+ iW_{LS}\overleftarrow{\nabla}_{12}\delta\left(\vec{r}_1 - \vec{r}_2\right)\wedge\vec{\nabla}_{12}.\left(\vec{\sigma}_1 + \vec{\sigma}_2\right)$$ **Spin-orbit**

$$+ \left(1 + 2\tau_{1z}\right)\left(1 + \tau_{2z}\right)\frac{e^2}{\left|\vec{r}_1 - \vec{r}_2\right|}$$ **Coulomb**

- The two ranges ($\mu_{j=1,2}$= 0.7 et 1.2 fm) simulate the “molecular potential”
- Density dependence necessary for saturation
- Spin-orbit necessary for magic numbers

➡ 14 parameters adjusted on nuclear matter properties and on some stable nuclei

(1) J.Dechargé and D.Gogny, Phys.Rev. C21, 1568 (1980)

Solution of secular equation

- **Lanczos method**

  - Standard diagonalization method : CPU time increases like N^3 (N matrix dimension)

  - Adapted to the search of lowest eigenvalues, numerically efficient

  - Limitating factor for huge matrices : Lanczos vector storage

- **m-scheme** [(1)]

  - Method applied for axially deformed nuclei

  - Method for coding the Slater Determinant (with good K), the operators and storing the non zero matrix elements used in the Lanczos algorithm in shell model-type codes

  - 80% of the work = proton-neutron part

(1) R.R.Withehead, A.Watt, B.J.Cole, I.Morrison, Adv. Nucl. Phys. 9, 123 (1977)

E.Caurier and F.Nowacki, Act.Phys.Pol.B, vol. 30 (1999) 705

Calculation schemes

- **Possible truncation schemes**

  - order of excitation in the wave function (1p1h, 2p2h, …)

  - size of the single particle state space

  - cut-off energy in mp-mh configurations

- **Importance of self-consistency :**

  helps to include higher order of HF mp-mh states through "renormalization" of mean-field (ρ built with the correlated wave function)

- **Still large matrices** ⇒ Need for supercomputers → Tera10, CCRT

Dimension of matrices

- ^{16}O ground state with all correlations (including proton-neutron)

  48 neutron orbitals + 48 proton orbitals

mp-mh truncation	1p1h	2p2h	3p3h	4p4h	…
Total dimension	88	31276	5 097411	526 910280	…

- ^{100}Sn ground state with only pair excitations (without proton-neutron)

  286 neutron orbitals + 286 proton orbitals

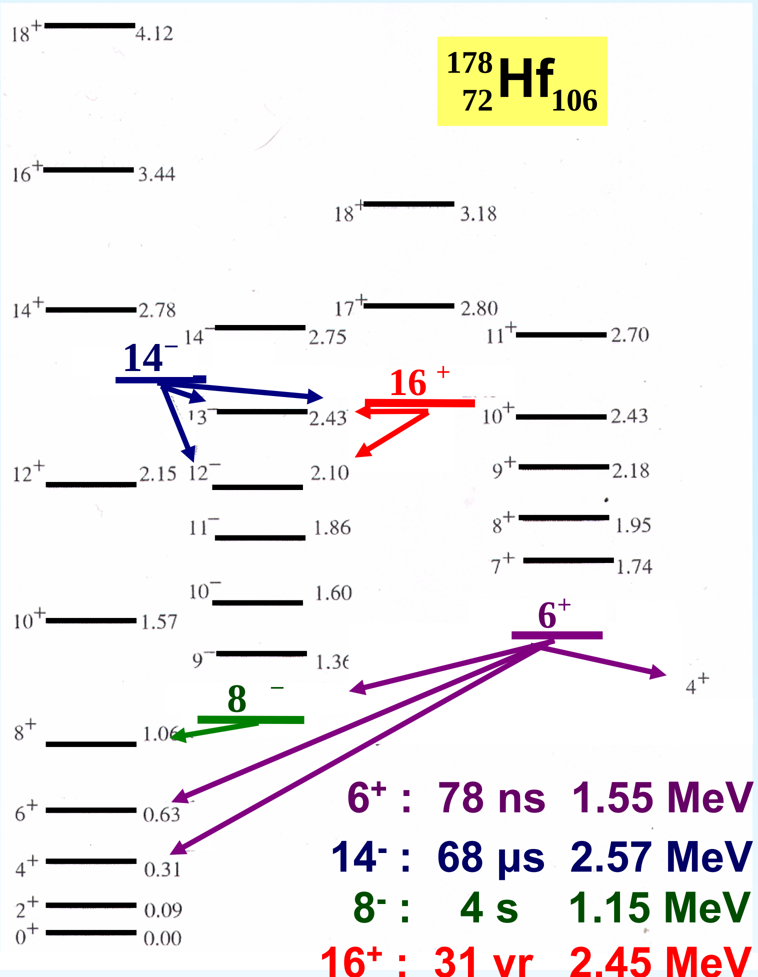
mp-mh truncation	1 pair	2 pairs	…
Total dimension	13001	62 478001	…

Number of non zero matrix elements : 5 759 422500

Number of words stored : 17 833 473518

First application – K isomers in ^{178}Hf (1)

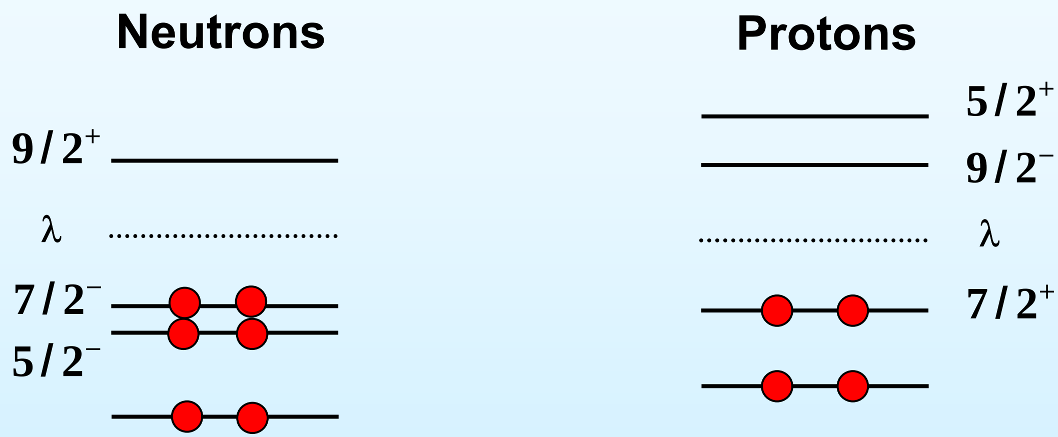
- **4 isomeric states**



- **Model assumptions**
  - mean field build with the zero range interaction Skyrme SIII
  - residual interaction : contact interaction
  - valence space : ±5 MeV around the Fermi level
  - neutron and proton are treated separately
  - no self-consistency

- **0$^+$ ground state of ^{178}Hf**
  - axially deformed nucleus
  - weak level density - weak pairing regime

(1) N.Pillet, P.Quentin and J.Libert, Nucl.Phys. A697 (2002) 141-163



	Neutron		Proton	
	HF	1 pair (>1%)	HF	1 pair (>1%)
0^+	68	21	54	36
16^+	91	3	68	24

(in %)

Isomers	mp-mh	Exp.	ε_{ph}
16+	2.59	2.45	1.484
8-	1.17 (n) 1.42 (p)	1.15	0.637 0.846
6+	1.41 (n) 2.25 (p)	1.54	1.278 1.565
14-	2.83	2.57	2.120

(in MeV)

- **Quenching of correlations in isomeric states**
- **Importance of the configuration mixing (effect on energies)**

Second application – Richardson exact solution for the Pairing hamiltonian

- **Pairing hamiltonian**

$$\hat{H} = \sum_f 2\epsilon_f \hat{N}_f - g \sum_{ff'} b_f^+ b'_f$$

$$\hat{N}_f = \frac{1}{2}(a_f^+ a_f + a_{\bar{f}}^+ a_{\bar{f}})$$

$$b_f^+ = a_f^+ a_{\bar{f}}^+$$

$$[b_f^+, b_{f'}]_+ = \delta_{ff'}(1 - 2\hat{N}_f)$$

- **Exact solution** [1]

  - Similarity between the many-fermion-pair system with pairing forces and the many-boson system with one-body forces

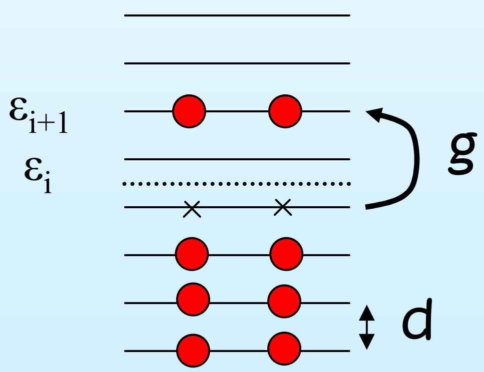
  - Exact wave function : mp-mh wave function including all the configurations built as pair excitations

  - Exact solution obtained from a coupled system of algebraic equations deduced from variational principle

➡ **Test of the importance of the different terms in the mp-mh wave function expansion (2p2h, 4p4h ...)**

(1) R.W. Richardson, Phys.Rev. 141 (1966) 949

Picket fence model

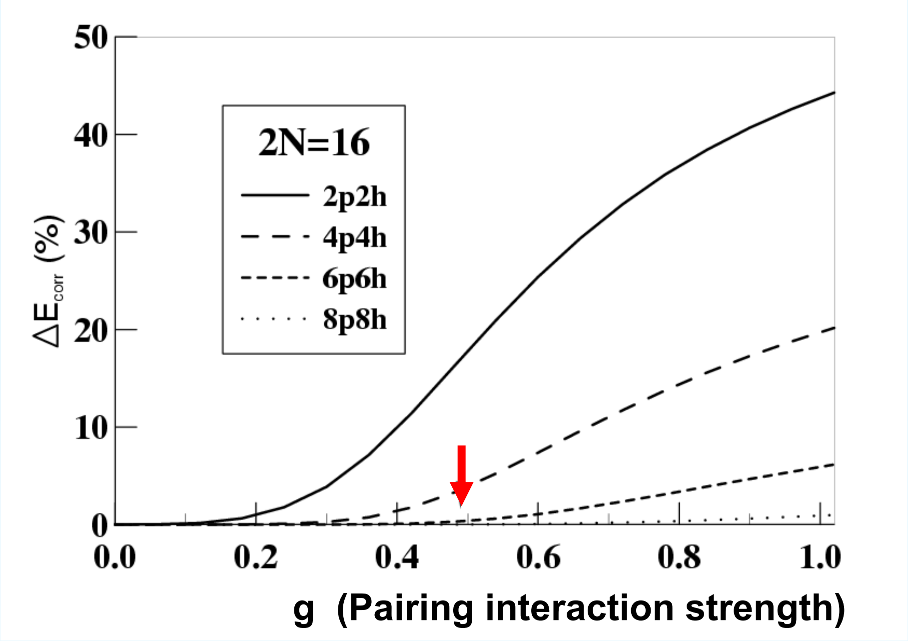


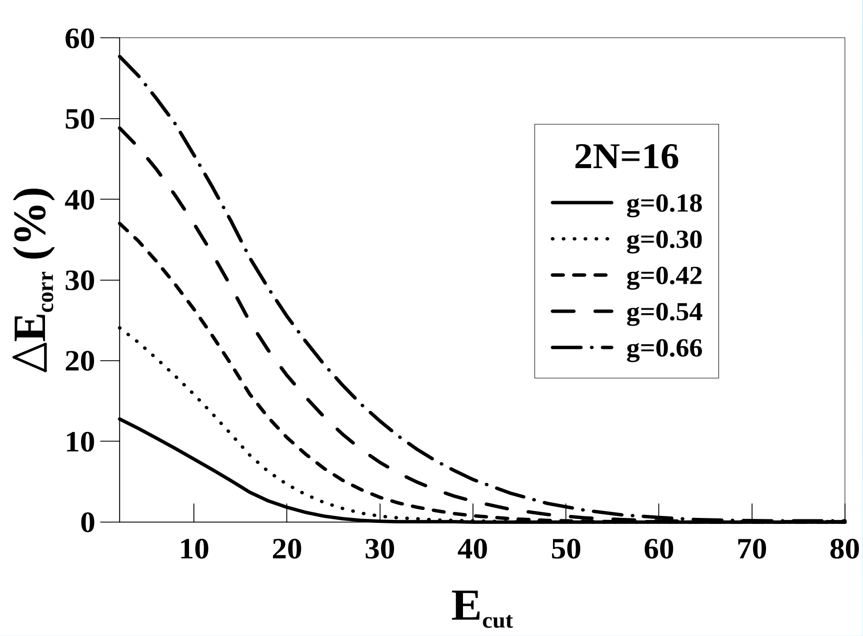
- System of 2N particles in 2N equispaced and doubly-degenerated levels
- System of identical fermions
- Constant pairing interaction strength
- Prototype of axially deformed nuclei

Ground state Correlation energy [1]

$$E_{corr}=E(g\neq 0)-E(g=0)$$

$$\Delta E_{corr} = E_{corr\,(exact)} - E_{corr\,(mp\text{-}mh)}$$



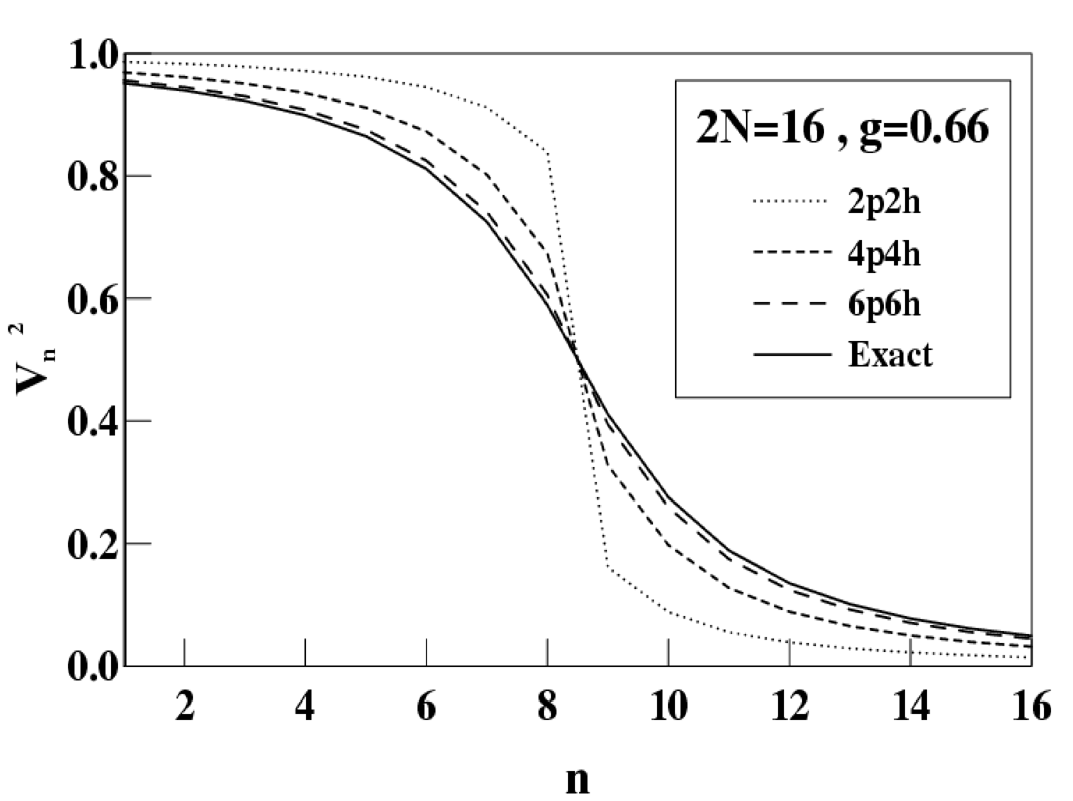


Truncation in mp-mh order of excitation

Truncation in excitation energy

(1) N.Pillet, N.Sandulescu, Nguyen Van Giai and J.-F.Berger , Phys.Rev. C71 , 044306 (2005)

Ground state occupation probabilities



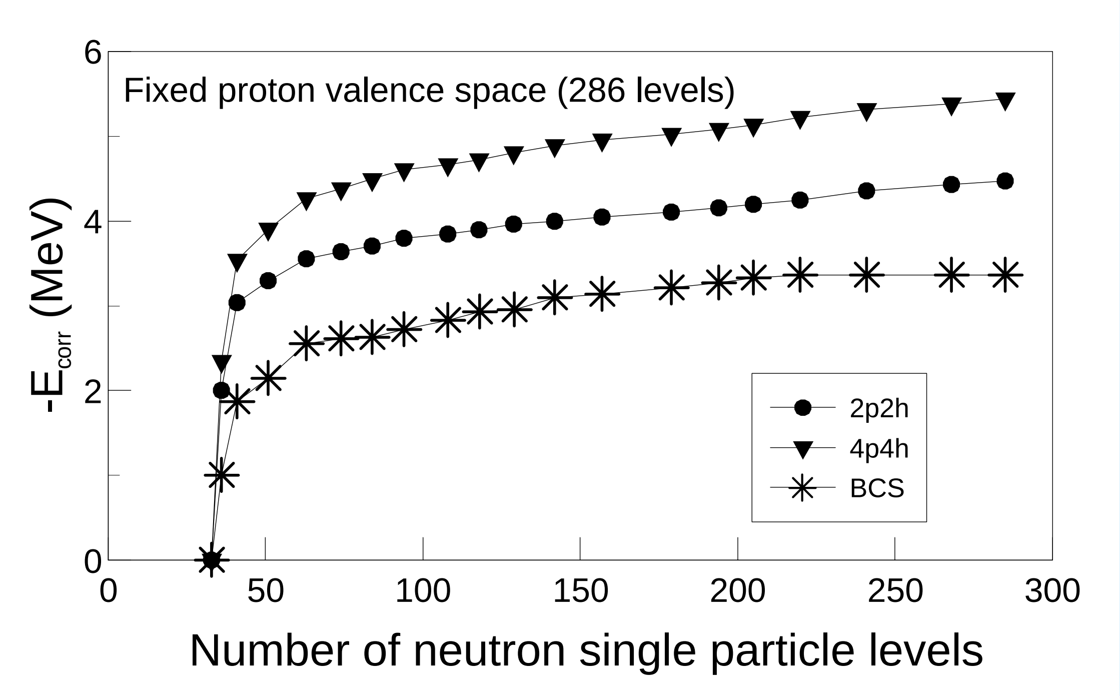
Third application-Pairing in ^{116}Sn with Gogny force [1]

- ^{116}Sn : spherical nucleus with Z=50 and N=66
- Mean field and residual parts of Hamiltonian calculated with the D1S Gogny force
- Wave function built only with pair excitations (excluding pn pairs)
- Correlation energy : $E_{cor} = < \Psi|\hat{H}[\rho]|\Psi > - < HF|\hat{H}[\rho]|HF >$

(1) N.Pillet, J.-F.Berger, E.Caurier and M.Girod, Int.J.Mod.Phys. E15, 464 (2006)

N.Pillet, J-F. Berger, E.Caurier and H.Goutte , paper under preparation.

^{116}Sn - Correlation energy



Binding energy in ^{116}Sn

Exp	:	988.683 MeV
HF	:	981.462 MeV
BCS	:	984.826 MeV
mp-mh	:	986.903 MeV

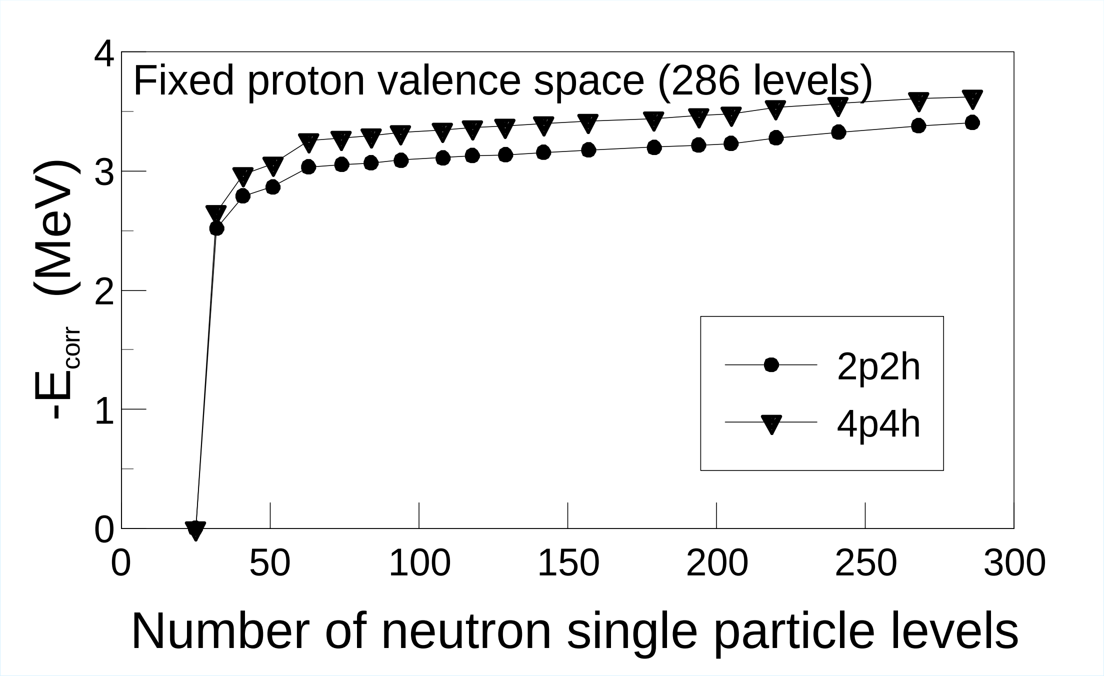
$-E_{corr}$ = {

mp-mh	5.441 MeV
BCS	3.364 MeV
difference	2.077 MeV

{ 2p2h : 4.474 MeV
4p4h : 0.967 MeV

→ need for 4p4h

^{100}Sn - Correlation energy



$-E_{corr} =$

mp-mh	3.672 MeV	
BCS	0.000 MeV	
difference	3.672 MeV	

- 2p2h : 3.397 MeV
- 4p4h : 0.275 MeV

→ 4p4h less important in ^{100}Sn

Correlated Wave Functions

(%)	HF	(1 pair)$_\nu$	(1 pair)$_\pi$	(2 pairs)$_\nu$	(1 pair)$_\nu$ (1 pair)$_\pi$	(2 pairs)$_\pi$
^{116}Sn	65.38	26.04	4.50	2.68	1.23	0.17
^{100}Sn	90.85	5.02	3.70	0.16	0.18	0.09

75 components > 0.05% → 23.2%

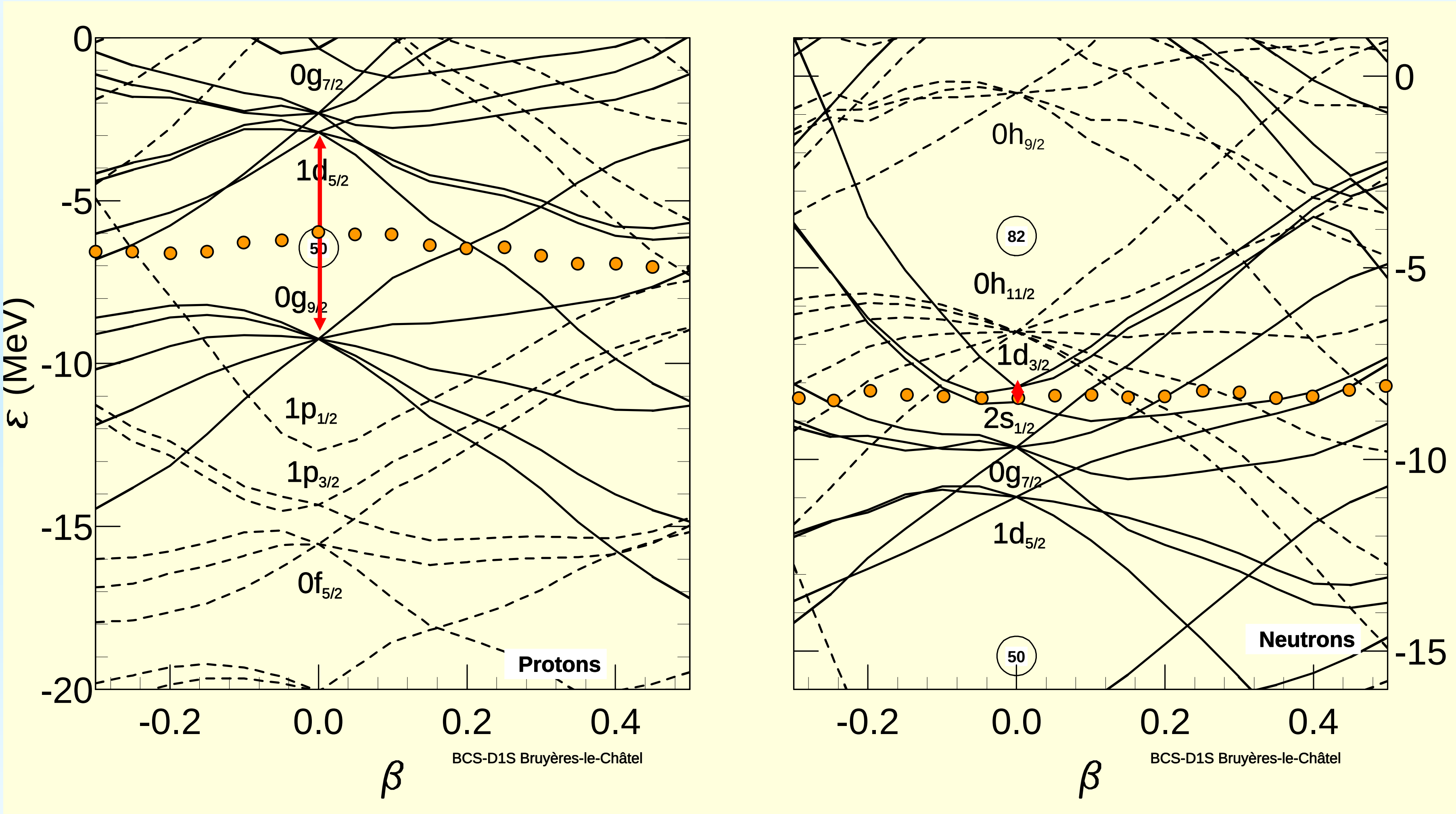
- 2 configurations 2p2h built with $1d_{3/2}$: 8.2%
- 6 configurations 2p2h built with $0h_{11/2}$: 2.5 %
- 67 configurations : 12.5%   (0.05%<x<0.3%)

(number of configurations : ~ 70 millions)

0.05% <37 components<0.1%

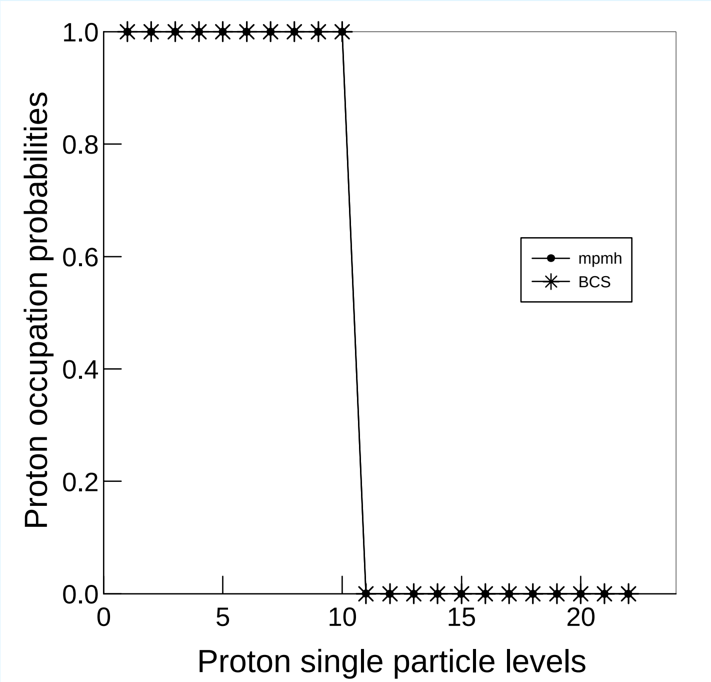
(number of configurations : 63 millions)

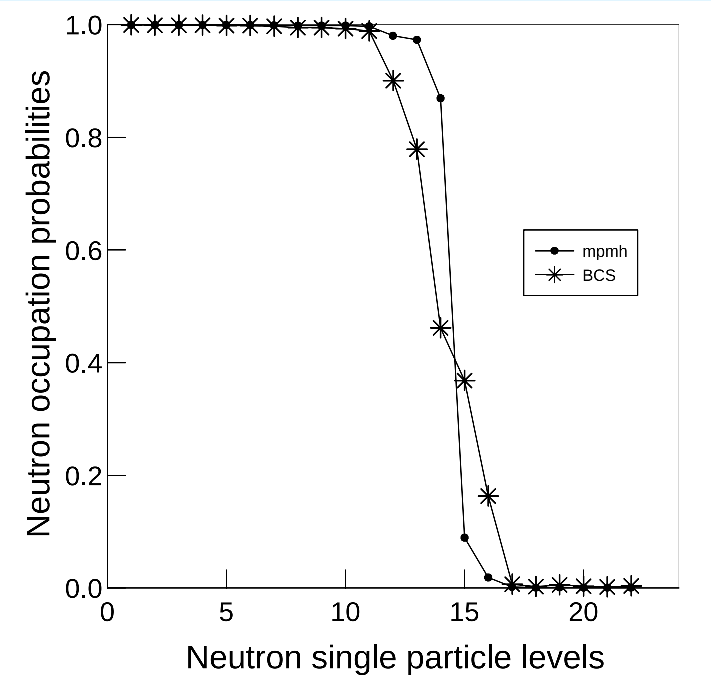
Single particle level spectrum



Single particle states occupation probabilities

- ^{116}Sn





- ^{100}Sn

No impact of correlations on occupancies !

Preliminar results - Self-consistency effect - ^{116}Sn

- Correlation energy

(MeV)	1 pair
Non self-consistent	4.474
Approximate Self-consistent	5.065

Energy gain

- Correlated wave function

(%)	HF	1 pair
Non self-consistent	87.29	12.71
Approximate Self-consistent	82.60	17.40

Summary

- **Self-consistent mp-mh approach**

  unifies the description of important correlations beyond mean field in nuclei (Pairing, RPA, Particle vibration)

  ✓ **Now tractable for medium-heavy nuclei with present computers (pairing hamiltonian)**

- **First applications to nuclear superfluidity quite encouraging**

- **Future ones : collective vibrations, exotic light nuclei**

- **Requires re-definition of effective N-N interaction in pn channels (under way)**