Nuclear pair correlations from multiparticle-multihole configuration mixing

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"Nuclear pair correlations probed via proton-induced transfer and knock-out reactions"

6-8 February 2013, Saclay

1. Formalism
2. Description of pairing within the mp-mh configuration mixing
3. Two-neutron S_{2n} and two-proton S_{2p} separation energies
4. Perspectives for pair transfer reactions

Objectives

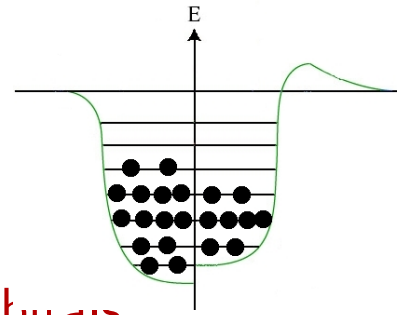
- **Inclusion of nuclear long range correlations beyond MF**
  - Pairing, RPA-type, GCM-type, Particle-Vibration coupling
- **Symmetry preserving approach**
  - Exact conservation of particle numbers (contrary to HFB)
  - No violation of Pauli principle (contrary to RPA/QRPA/2RPA)
  - Conservation of angular momentum
- **No inert core**
- **Low-lying spectroscopy**
  - Description of **ground states** + **excited states**
  - Unified description of **even-even** + **odd** + **odd-odd** nuclei
- **Reaction applications**
  - Inelastic scattering on discrete states
  - Two-nucleon transfer reactions

Formalism

(N. Pillet, J.-F. Berger, E. Caurier, PRC 78, 024305 (2008))

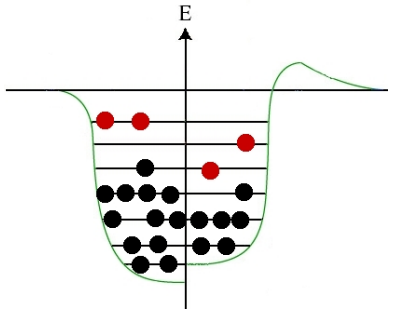
- **Static and non-relativistic**
- **Trial wave function:** Superposition of Slater determinants

$$|\Psi\rangle = \sum_{\alpha_\nu,\alpha_\pi} A_{\alpha_\nu,\alpha_\pi} \quad |\Phi_{\alpha_\nu}\rangle \otimes |\Phi_{\alpha_\pi}\rangle$$



- **2 unknown quantities:** The mixing coefficients A and the orbitals

  $\Rightarrow$ Use of the **variational principle** for their determinations



- **Energy Density Functional**

$$\mathcal{F}(\rho) = \langle\Psi|\widehat{H}(\rho)|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle - \sum_i \lambda_i Q_i$$

  - $\widehat{H}(\rho) = \widehat{T} + \widehat{V}(\rho)$ with $\widehat{V}(\rho) \equiv$ **Gogny effective interaction** + Coulomb
  - $\widehat{T}$ and $\widehat{V}(\rho)$ with 1 and 2-body center of mass corrections
  - Prescription for the one-body density entering $\widehat{V}(\rho)$: $\rho = \langle\Psi|\hat{\rho}|\Psi\rangle$

First variational equation $\Rightarrow$ Mixing coefficients A

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

- **Non-linear secular equation**

$$\Rightarrow \sum_{\alpha'_\pi \alpha'_\nu} \mathcal{H}_{\alpha_\pi \alpha_\nu, \alpha'_\pi \alpha'_\nu} \; A_{\alpha'_\pi \alpha'_\nu} = \lambda A_{\alpha_\pi \alpha_\nu}$$

  - The Hamiltonian matrix

$$\mathcal{H}_{\alpha_\pi \alpha_\nu, \alpha'_\pi \alpha'_\nu} = \langle \phi_{\alpha_\pi} \phi_{\alpha_\nu} | \; \widehat{H}(\rho) \; + \sum_{mn\tau} \mathcal{R}^\tau_{mn} \; a^+_{\tau m} a_{\tau n} \; | \phi_{\alpha'_\pi} \phi_{\alpha'_\nu} \rangle$$

  - The rearrangment terms

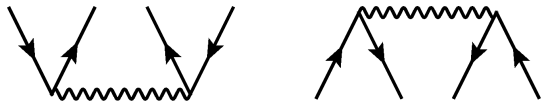
$$\mathcal{R}^\tau_{mn} = \int \varphi^*_{\tau m}(\vec{r}, \sigma) \varphi_{\tau n}(\vec{r}, \sigma) \sum_{ijkl} \; \langle ij | \frac{\partial V(\rho)}{\partial \rho(\vec{r})} | \widetilde{kl} \rangle \; \langle \Psi | a^+_i a^+_j a_l a_k | \Psi \rangle \; d^3\vec{r}$$

- **Residual interaction**

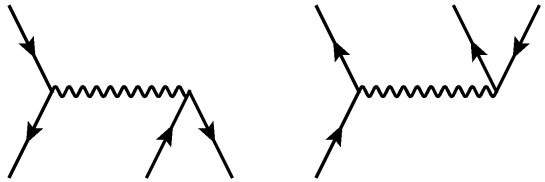
  two-body matrix elements + one-body rearrangement terms

- **Residual two-body matrix elements** $\langle \phi_{npnh} | V(\rho) | \phi_{mpmh} \rangle \equiv \langle ij | V(\rho) | kl \rangle$

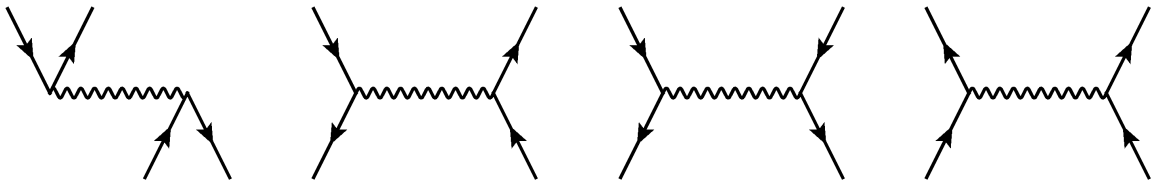
  - $|n - m| = 2 \Rightarrow$ Pairing, RPA



  - $|n - m| = 1 \Rightarrow$ Particle-vibration



  - $|n - m| = 0 \Rightarrow$ RPA, Pairing, more general



Second variational equation $\Rightarrow$ Orbitals

$$\frac{\partial \mathcal{F}(\rho)}{\partial \varphi_i^*} = 0$$

- PhD work of C. Robin (since October 2011)
- **Orbital equations $\equiv$ Inhomogeneous Hartree-Fock equations**

$$\Rightarrow [\ h(\rho,\sigma),\ \rho\ ]_{rs} = G_{rs}(\sigma)$$

  - A few definitions

    $\rightsquigarrow\ \sigma_{ij,kl} = \langle\Psi|a_i^+ a_k^+ a_l a_j|\Psi\rangle - \rho_{ji}\rho_{lk} + \rho_{jk}\rho_{li}$

    $\rightsquigarrow\ G_{rs}(\sigma) = \frac{1}{2}\left(\sum_{imn}\langle im|V(\rho)|\widetilde{rn}\rangle\sigma_{is,mn} - \sum_{imn}\langle ms|V(\rho)|\widetilde{ni}\rangle\sigma_{ri,mn}\right)$

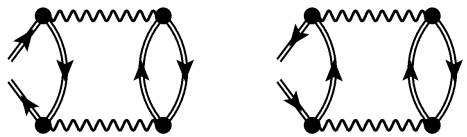
    $\rightsquigarrow\ \{r,s\} \equiv \{p,p\},\{h,h\}$ *or* $\{p,h\}\ \in$ the entire single particle basis

  - Automatically satisfied if the entire Hilbert space is taken into account!
  - Similar to the dynamical equation linking the 1-body and the 2-body Green functions at the limit of equal times

Complementary variational equations

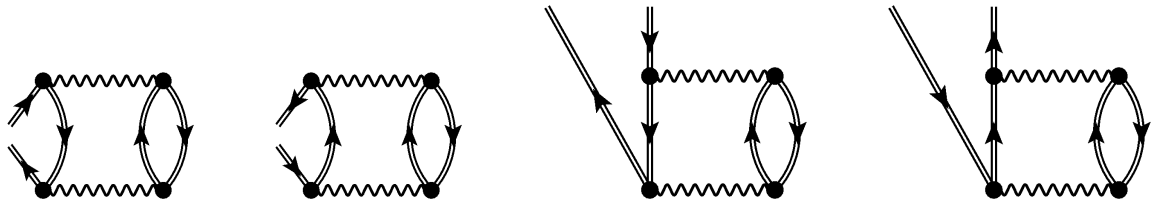
Example: Wave function with only excitations of pairs $(2n)$p-$(2n)$h

- **Perturbation theory - Correction to the wave function**
  - Zero order : $|0p0h\rangle$
  - First order : $|2p2h\rangle$
  - Second order : $|1p1h\rangle$, $|2p2h\rangle$, $|3p3h\rangle$
- **Second order corrections to ρ**
  - First variational equation ($\rho = \langle\Psi|\hat{\rho}|\Psi\rangle$)



$\Rightarrow$ External lines $\equiv$ single particle states implied in the mixing ("active orbitals")

  - Second variational equation ($\rho_{ij} = G_{ij}(\sigma)/(\epsilon_i - \epsilon_j)$)



$\Rightarrow$ External lines $\equiv$ all single particle states of the basis

$\Rightarrow$ The last two diagrams $\equiv$ Introduction of 1p-1h excitations in the wave function

Fully Self-Consistent solution

- **Non-linear secular equation + Orbital equation**

$$\sum_{\alpha'_\pi \alpha'_\nu} \mathcal{H}_{\alpha_\pi \alpha_\nu, \alpha'_\pi \alpha'_\nu} \; A_{\alpha'_\pi \alpha'_\nu} = \lambda A_{\alpha_\pi \alpha_\nu} \quad + \quad [\; h(\rho,\sigma),\; \rho \;]_{rs} = G_{rs}(\sigma)$$

- **Non-linear problem $\Rightarrow$ Iterative procedure**
  - Starting point: HF calculation
  - Solution of the non-linear secular equation
  - Until convergence
    - $\rightsquigarrow$ Determination of σ from $|\Psi\rangle$
    - $\rightsquigarrow$ Determination of ρ
    - $\rightsquigarrow$ Determination of the new $h(\rho,\sigma)$
    - $\rightsquigarrow$ Solution of the secular equation
- **Numerical details**
  - Diagonalization of $\mathcal{H}$ accomplished using the very efficient technique developed for large scale SM calculations by E. Caurier
  - Tractable with the advent of Supercomputers

General considerations

- **Exactly solvable model of pairing Hamiltonian (Picket fence model)**
  - 2N particles in 2N equispaced and doubly-degenerate levels
  - Pairing Hamiltonian

$$\widehat{H}_{pair} = \sum_{f=1}^{2N} \epsilon_f (a_f^+ a_f + a_{\bar{f}}^+ a_{\bar{f}}) - g \sum_{f=1}^{2N} \sum_{f'=1}^{2N} a_f^+ a_{\bar{f}}^+ a_{\bar{f}'} a_{f'}$$

  - **Exact solution**

$$|\Psi^{exact}\rangle \equiv |\Psi^{mp-mh}\rangle = \prod_{i=1}^{N} B_i^+ |0\rangle$$

Configurations in the *mp-mh* functions $\equiv$ multiple excitations of nucleon pairs

- Collective pair B_i^+:

$$B_i^+ = \sum_{j=1}^{N} \frac{1}{2\epsilon_j - E_i} a_j^+ a_{\bar{j}}^+$$

- Eigen energies E_i:

$$1 - 2g \sum_{j(\neq i)=1}^{N} \frac{1}{E_j - E_i} + g \sum_{j=1}^{N} \frac{1}{2\epsilon_j - E_i} = 0$$

General considerations

- **Link with the BCS and Projected BCS approach on particle numbers**
  - BCS wave function

$$|BCS\rangle_\tau = \mathcal{N}_\tau e^{B_\tau^+}|0\rangle_\tau$$

  - BCS collective pair B_τ^+

$$B_\tau^+ = \sum_{j>0} tg\theta_{\tau j} b_{\tau j}^+$$

    with $b_{\tau j}^+ = a_{\tau j}^+ a_{\tau \bar{j}}^+$

  - Projected BCS wave function with 2N particles

$$|PBCS\rangle_\tau \propto (B_\tau^+)^N |0\rangle$$

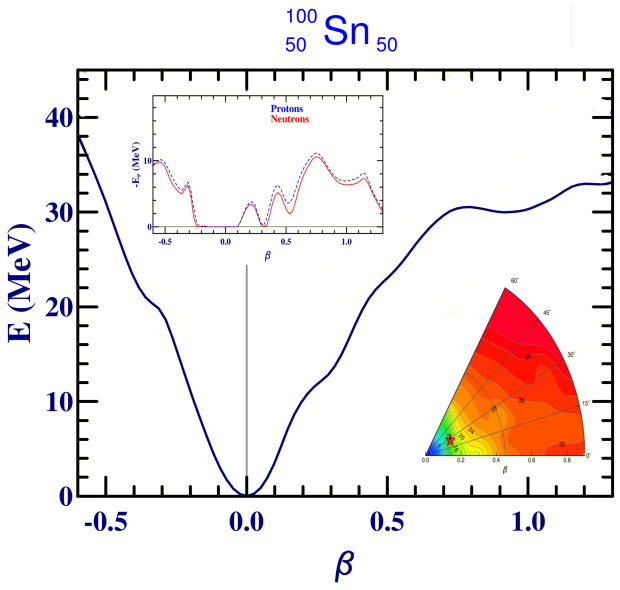
$$\Rightarrow |PBCS\rangle_\tau = \mathcal{N}'_\tau \sum_{n=0}^{\infty} \sum_{\substack{0<p_1<\ldots<p_n \\ 0<h_1<\ldots<h_n}} \frac{tg\theta_{\tau p_1}\ldots tg\theta_{\tau p_n}}{tg\theta_{\tau h_1}\ldots tg\theta_{\tau h_n}} . \prod_{k=1}^{n} (b_{\tau p_k}^+ b_{\tau h_k}) \, |HF\rangle$$

Pairing in Sn isotopes within the *m*p-*m*h configuration mixing

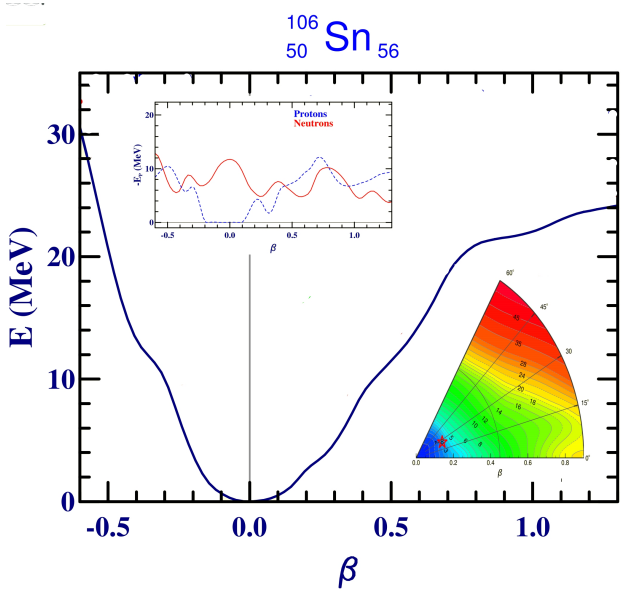
- **N. Pillet**, J.-F. Berger, E. Caurier, PRC 78, 024305 (2008)
- Reduced correlated *m*p-*m*h wave function
  - Usual pairing-type correlations
    - No residual proton-neutron interaction $\Rightarrow A_{\alpha_\nu \alpha_\nu} = A_{\alpha_\nu} A_{\alpha_\pi}$
    - Ground states of even-even Sn isotopes $\Rightarrow |\Psi\rangle_{0^+} = |\Psi_\nu\rangle_{0^+} . |\Psi_\pi\rangle_{0^+}$
  - Configurations include excited pairs of nucleons
    - One pair: two nucleons in time-reversal states
- Investigation of pairing correlations in weak, medium and strong regimes
  - Study of ^{100}Sn, ^{106}Sn and ^{116}Sn ground states
  - D1S Gogny interaction

HFB CALCULATIONS WITH D1S GOGNY FORCE

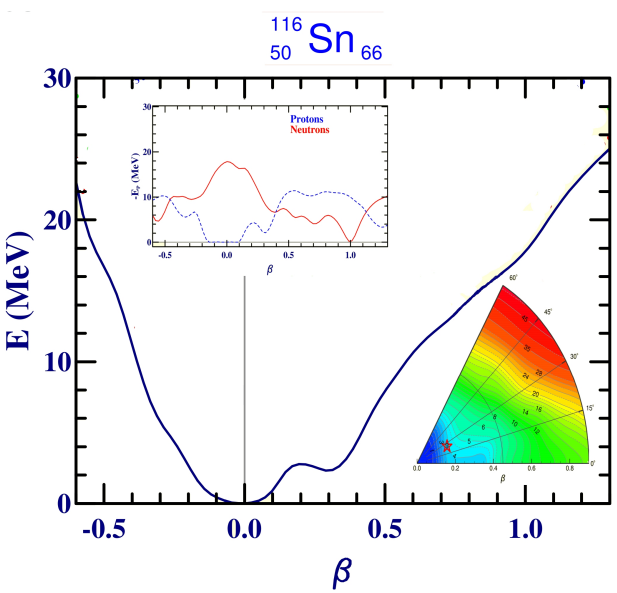
Weak Pairing



Medium Pairing



Strong pairing



- **Correlation energy** $E_{corr} = \langle \Psi | \hat{H}(\rho) | \Psi \rangle - \langle HF | \hat{H}(\rho) | HF \rangle$

  - **Taking into account the first variational equation** (frozen orbitals)
  - **Total and neutron correlation energies - Comparison to BCS**

Nucleus	$\lvert E_{corr}^{total} \rvert$	$\lvert E_{corr}^{neutron} \rvert$	$\lvert E_{corr}^{BCS} \rvert$
^{100}Sn	3.67	1.90	0.00
^{106}Sn	4.62	2.88	1.37
^{116}Sn	5.44	3.74	3.25

$\Rightarrow$ Contribution due to protons: $\simeq$ 1.7 MeV (in BCS: 0 MeV)

$\Rightarrow$ Contribution due to neutrons:

- Non zero in ^{100}Sn (contrary to BCS)
- Always larger than in the BCS approximation

- ^{100}Sn 1 pair: 3.397 MeV 2 pairs: 0.275 MeV
- ^{116}Sn 1 pair: 4.474 MeV 2 pairs: 0.967 MeV 3 pairs: 0.070 MeV

$\Rightarrow$ Results consistent with those of the picket fence model

- **Structure of correlated wave functions**

$$T(i_\pi, j_\nu) = \sum_{\alpha_\nu \alpha_\pi} |A_{\alpha_\nu \alpha_\pi}|^2$$

  - **Taking into account the first variational equation** (frozen orbitals)
  - **Components of the correlated wave function** (in percentage)

Nucleus	$T(0,0)$	$T(0,1)$	$T(1,0)$	$T(0,2)$	$T(1,1)$	$T(2,0)$
^{116}Sn	65.38	26.04	4.50	2.68	1.23	0.17
^{106}Sn	67.44	25.29	3.63	2.54	0.99	0.11
^{100}Sn	90.85	5.02	3.70	0.16	0.18	0.09

  $\Rightarrow$ ^{116}Sn is the most correlated nucleus

  $\Rightarrow$ Configurations with one excited neutron pair are the most important

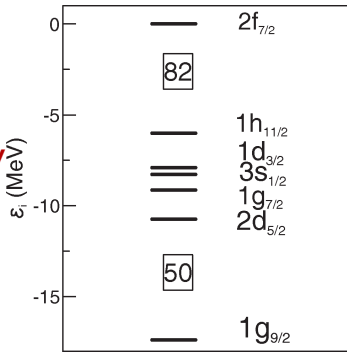
  - **Dominant configurations for the three Sn isotopes**
    - ^{116}Sn $3s_{1/2} \rightarrow 1d_{3/2}$ and $3s_{1/2} \rightarrow 1h_{11/2}$
      Total number of configurations: 81 502684
    - ^{106}Sn $2d_{5/2} \rightarrow 1g_{7/2}$
      Total number of configurations: 69 861184
    - ^{100}Sn No dominant configuration
      Total number of configurations: 62 946676

- **Approximate renormalization of orbitals**
  - **Taking into account the second variational equation** $[h(\rho),\ \rho] \approx 0$
  - **Structure of correlated wave functions**

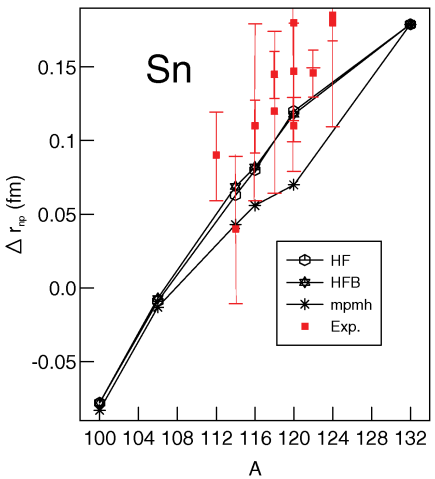
Nucleus	$T(0,0)$	$T(0,1)$	$T(1,0)$	$T(0,2)$	$T(1,1)$	$T(2,0)$
^{116}Sn	42.09	44.28	3.00	8.43	2.09	0.11
^{106}Sn	62.90	28.65	3.54	3.62	1.17	0.11
^{100}Sn	88.19	6.36	4.74	0.27	0.29	0.15

$\Rightarrow$ Strong variations in ^{116}Sn: the 2p-2h configurations are dominant

$\Rightarrow$ Reason: reduction of the neutron gap $3s_{1/2} - 1h_{11/2}$ by $\simeq$ 400 keV



  - **Neutron skin**



- Neutron skin $\Delta r_{np} = r_n - r_p$
- In strongly correlated isotopes $\Rightarrow$ Decrease of neutron radii
- Reason: Fall of the neutron $1h_{11/2}$ in the potential
  Reduction of $1h_{11/2}$ radius

$\Rightarrow$ RPA-type correlations should increase Δr_{np}

Investigation of two-body spatial pairing correlations

- Correlated part of the two-body density

$$\langle \psi^+(\tilde{\mathbf{r}}_1, \mathbf{s}_1)\psi^+(\tilde{\mathbf{r}}_2, -\mathbf{s}_2)\psi(\tilde{\mathbf{r}}_2, -\mathbf{s}_2)\psi(\tilde{\mathbf{r}}_1, \mathbf{s}_1)\rangle$$

  - In the Hartree-Fock-Bogoliubov approach

$$\kappa(\vec{r}_1 s_1, \vec{r}_2 s_2)\kappa^*(\vec{r}_1 s_1, \vec{r}_2 s_2)$$

    with $\kappa(\vec{r}_1 s_1, \vec{r}_2 s_2) = \langle \psi(\vec{r}_1, s_1)\psi(\vec{r}_2, s_2)\rangle$ pairing tensor

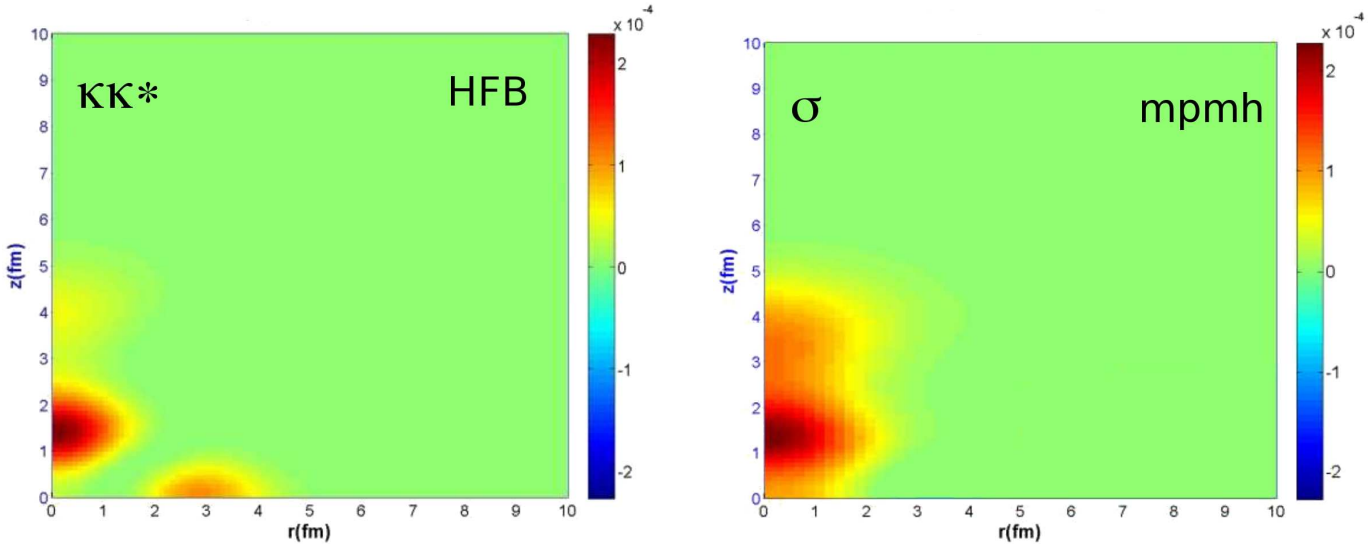
    N. Pillet, N. Sandulescu, P. Schuck, PRC 76, 024310 (2007).
    N. Pillet, N. Sandulescu, P. Schuck, J.-F. Berger, PRC C81, 034307 (2010).

  - In the *mp-mh* configuration mixing approach

$$\sigma(\vec{r}_1 s_1, \vec{r}_1 s_1, \vec{r}_2 - s_2, \vec{r}_2 - s_2)$$

Application to ^{52}Ca (D1S Gogny interaction)

- Non-local properties (C. Caizergues and N. Pillet, unpublished, 2010)



- Increase of pairing collectivity in the surface (*mp-mh* configuration mixing)
  $\Leftarrow$ Increase of parity mixing
- Importance of the conservation of particle numbers!
- Expected effects on pair transfer cross sections

Two-neutron S_{2n} and two-proton S_{2p} separation energies

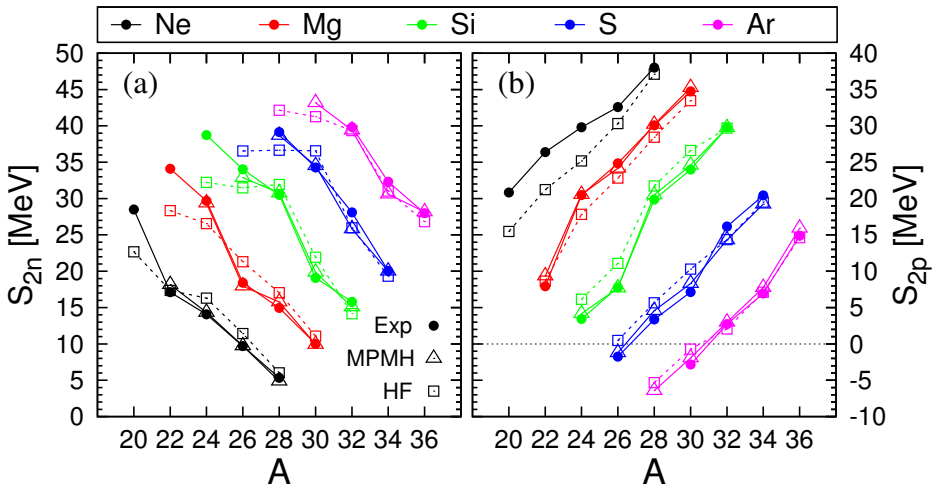
- Important observables for two-nucleon transfer reactions

  $\Rightarrow$ Theoretical S_{2n} and S_{2p} have to be calculated with enough accuracy

- Definitions

$$S_{2n}(N,Z) = BE(N,Z) - BE(N-2,Z)$$
$$S_{2p}(N,Z) = BE(N,Z) - BE(N,Z-2)$$

- Applications in *sd*-shell nuclei (Talk of J. Le Bloas)



Mean value of the difference to experiment:

$S_{2n}(HF)$=0.1MeV/S_{2n}(mpmh)=-0.24MeV, $S_{2p}(HF)$=0.5MeV/S_{2p}(mpmh)=0.29MeV

Corresponding dispersions:

$S_{2n}(HF)$=1.99MeV/S_{2n}(mpmh)=0.83MeV, $S_{2p}(HF)$=1.96MeV/S_{2p}(mpmh)=0.86MeV

J. Lebloas, N. Pillet, J.-M. Daugas, M. Dupuis et *al.*, article in preparation

Pair overlap functions for two-nucleons transfer reactions

- Starting from the two-body Green function noted G_2,

$$G_2 = \langle \Phi_0 | T\{\Psi(t_1)\Psi(t_3)\Psi^\dagger(t_2)\Psi^\dagger(t_4)\} | \Phi_0 \rangle$$

with $|\Phi_0\rangle$ the exact g.s. of the system with A nucleons and energy E_0.

  - Two particle bound states $\Rightarrow t_1 = t_3$ and $t_2 = t_4$
  - Restriction to $t_1 > t_2$ ($t_1 < t_2$ can be done in a similar way)
  - Introducing a closure relation,

$$\Rightarrow G_2 = \sum_n \langle \Phi_0 | \Psi(t_1)\Psi(t_1) | \Phi_n \rangle \langle \Phi_n | \Psi^\dagger(t_2)\Psi^\dagger(t_2) | \Phi_0 \rangle$$

with $|\Phi_n\rangle$ the eigensolutions of the system with A+2 nucleons and energy E_n.

- A few definitions
  - Excitation energy $\omega_{no} = E_n - E_0$
  - Chemical potential

$$\begin{aligned} E_0(A+1) - E_0(A) &= E_0(A) - E_0(A-1) = \mu \\ E_0(A+2) - E_0(A) &= E_0(A) - E_0(A-2) = 2\mu \end{aligned}$$

$$\Rightarrow \omega_{no} = 2\mu + \xi_{n0} \qquad (5\text{-}1)$$

- Transition amplitudes

$$G_2 = \sum_n e^{i(2\mu+\xi_{n0})(t_1-t_2)} \sum_{\alpha\beta\gamma\delta} (\eta_n)^T_{\alpha\beta} (\zeta_n)_{\gamma\delta}$$

  - One has used the Heisenberg representation of the field operators

$$\Psi^\dagger(t) = \sum_\alpha a^\dagger_\alpha(t) = \sum_\alpha e^{iHt} a^\dagger_\alpha e^{-iHt}$$

  - Expressions of transition amplitudes

$$(\eta_n)_{\alpha\beta} = \langle \Phi_n | a_\alpha a_\beta | \Phi_0 \rangle$$

$$(\zeta_n)_{\gamma\delta} = \langle \Phi_n | a^\dagger_\gamma a^\dagger_\delta | \Phi_0 \rangle$$

- Pair form factors

$$\sum_{\alpha\beta} (\eta_n)_{\alpha\beta} = \sum_{\alpha\beta} \langle \Phi_n | a_\alpha a_\beta | \Phi_0 \rangle$$

$$\sum_{\gamma\delta} (\zeta_n)_{\gamma\delta} = \sum_{\gamma\delta} \langle \Phi_n | a^\dagger_\gamma a^\dagger_\delta | \Phi_0 \rangle$$

- How the non-locality is incorporated in pair transfer reaction models?