SHELL MODEL AND SPECTROSCOPIC FACTORS

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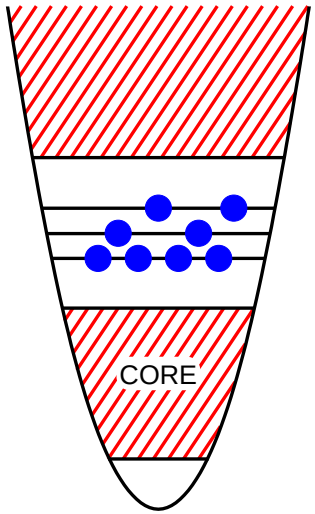

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Outline

- Le champ moyen du noyau. Les facteurs spectroscopiques dans le modèle de particules indépendantes.
- Les corrélations nucléaires de courte portée.
- Interactions effectives; Espaces de valence.
- Le hamiltonien monopolaire.
- Les derives monopolaires.
- Les corrélations nucléaires; appariement et quadrupole.
- Les facteurs spectroscopiques dans le cadre du modèle en couches.
- Fragmentation des facteurs spectroscopiques due aux correlations.
- Examples de fragmentation dans des noyaux presque magiques.
- Applications a des noyaux riches en neutrons
- Les noyaux déformés

The Independent Particle Model

The basic idea of the IPM is to assume that, at zeroth order, the result of the complicated two body interactions among the nucleons is to produce an average self-binding potential. Mayer and Jensen (1949) proposed an spherical mean field consisting in an isotropic harmonic oscillator plus a strongly attractive spin-orbit potential and an orbit-orbit term. Later, other functional forms were adopted, *e.g.* the Woods-Saxon well

The usual procedure to generate a mean field in a system of N interacting fermions, starting from their free interaction, is the Hartree-Fock approximation, extremely successful in atomic physics. Whatever the origin of the mean field, the eigenstates of the N-body problem are Slater determinants *i.e.* anti-symmetrized products of N single particle wave functions.

The Independent Particle Model

In the nucleus, there is a catch, because the very strong short range repulsion and the tensor force make the HF approximation based upon the bare nucleon-nucleon force impracticable.

However, at low energy, the nucleus do manifest itself as a system of independent particles in many cases, and when it does not, it is due to the medium range correlations that produce strong configuration mixing and not to the short range repulsion.

Does the success of the shell model really "prove" that nucleons move independently in a fully occupied Fermi sea as assumed in HF approaches? In fact, the single particle motion can persist at energies in fermion systems due to the suppression of collisions by Pauli exclusion (Pandharipande et al., RMP69)

Brueckner theory takes advantage of the Pauli blocking to regularize the bare nucleon- nucleon interaction, in the form of density dependent effective interactions of use in HF calculations or G-matrices for large scale shell model calculations.

The Independent Particle Model

The wave function of the ground state of a nucleus in the IPM is the product of an Slater determinant for the Z protons that occupy the Z lowest states in the mean field and another Slater determinant for the N neutrons in the N lowest states of the mean field

In second quantization, this state can be written as:

$$|N\rangle \cdot |Z\rangle$$

with

$$|N\rangle = n_1^\dagger n_2^\dagger \dots n_N^\dagger |0\rangle$$

$$|Z\rangle = z_1^\dagger z_2^\dagger \dots z_Z^\dagger |0\rangle$$

It is obvious that the occupied states have occupation number 1 and the empty ones occupation number 0

Spectroscopic factors

Lets denote the nucleon creation and annihilation operators by $a^\dagger$ and a, and consider the ground states of the systems of A-1, A, and A+1 nucleons, then,

$$|A\rangle = a_1^\dagger a_2^\dagger \ldots a_A^\dagger |0\rangle \text{ and, trivially}$$

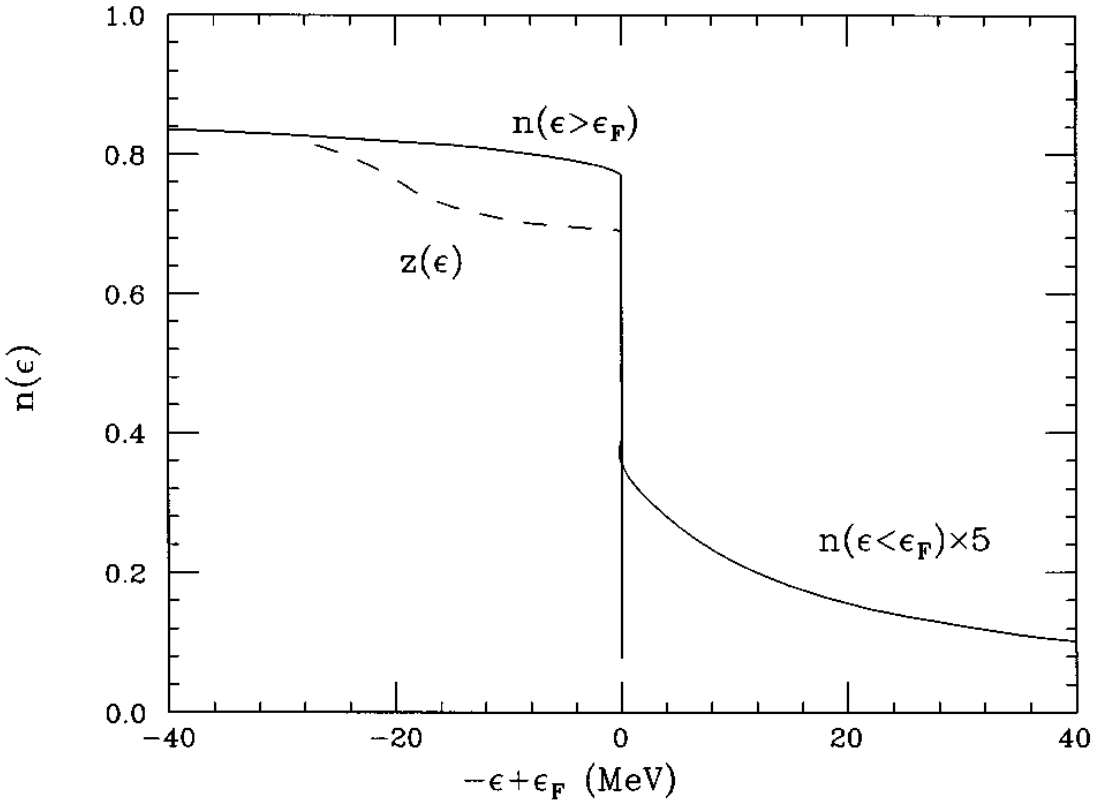
$$\langle A+1|a_{A+1}^\dagger|A\rangle = 1 \;\; ; \;\; \langle A+1|a_{\neq A+1)}^\dagger|A\rangle = 0$$

$$\langle A-1|a_{A-1}^\dagger|A\rangle = 1 \;\; ; \;\; \langle A-1|a_{\neq A-1)}^\dagger|A\rangle = 0$$

the expectation values of the operators $a^\dagger$ and a between the states of the nuclei with A+1 and A, and A-1 and A, give the spectroscopic amplitudes for stripping and pick-up reactions. The spectroscopic factors are the squares of this amplitudes with some angular momentum coefficients. When correlations are included, the spectroscopic amplitudes depart from their 0 or 1 values. The knowledge of the spectroscopic factors make it possible to learn about the structure of the mean field and the role of correlations.

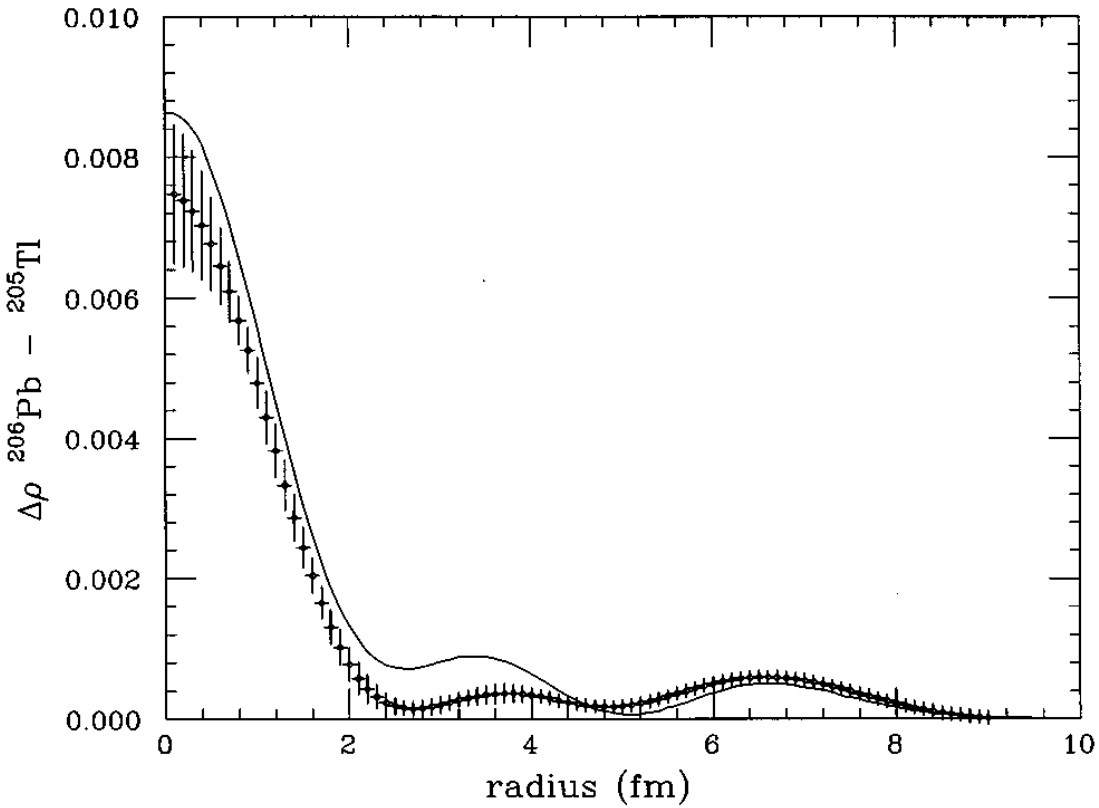
Spectroscopic Factors and the Meaning of the Shell Model

Dilution of the Spectroscopic strength by the bare N-N interaction.
Results for nuclear matter.



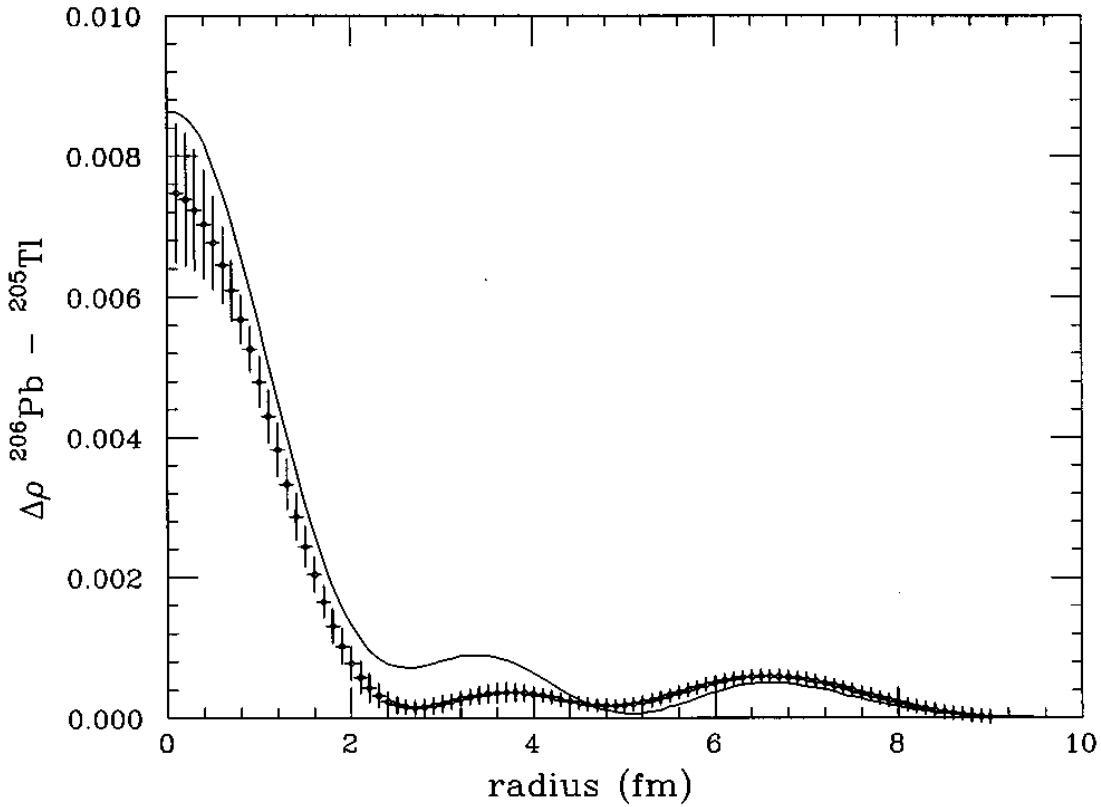
If we had a system of non interacting fermions, the figure would be just a step function with occupation 1 below the Fermi level and 0 above

Spectroscopic Factors and the Meaning of the Shell Model



In spite of that, the nuclear quasi-particles resemble extraordinarily to the mean field solutions of the IPM, as can be seen in the classical example of the charge density difference between ^{206}Pb and ^{205}TI, measured in the electron scattering experiments of Cavedon *et al, 1982*

Spectroscopic Factors and the Meaning of the Shell Model



The shape of the $3s_{1/2}$ orbit is very well given by the mean field calculation. To make the agreement quantitative the calculated density has to be scaled down by the occupation number

To know more, Read the article " Independent particle motion and correlations in fermion systems"

V. R. Pandharipande, I. Sick and P. K. A. deWitt Huberts, RMP 69 (1997) 981.

The Interacting Shell Model (ISM)

Is an approximation to the exact solution of the nuclear A-body problem using effective interactions in restricted spaces

The effective interactions are obtained from the bare nucleon-nucleon interaction by means of a regularization procedure aimed to soften the short range repulsion. In other words, using effective interactions we can treat the A-nucleon system in a basis of independent quasi-particles

A Shell Model calculation amounts to diagonalizing the nuclear hamiltonian in the basis of all the Slater determinants that can be built distributing the valence particles in a set of orbits which is called valence space. The orbits that are always full form the core.

The three pillars of the shell model

- The Effective Interaction
- Valence Spaces
- Algorithms and Codes

E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves and A. P. Zuker. "The Shell Model as a Unified View of Nuclear Structure", RMP 77 (2005) 427.

Making the Effective Interaction Simple

The effective shell model interaction appears sometimes as a long list of meanigless numbers; the two body matrix elements of the Hamiltonian.

Without loosing the simplicity of the Fock space representation, we can recast these numbers in a way full of physical insight, following Dufour-Zuker rules

Any effective interaction can be split in two parts: $\mathcal{H} = \mathcal{H}_m$(monopole) $+ \mathcal{H}_M$(multipole). $\mathcal{H}_m$ contains all the terms that are affected by a spherical Hartree-Fock variation, hence it is responsible for the global saturation properties and for the evolution of the spherical single particle energies

The Monopole Hamiltonian

$$\mathcal{H}_m = H_{sp} + \sum \left[\frac{1}{(1+\delta_{ij})} a_{ij}\, n_i (n_j - \delta_{ij}) \right.$$

$$\left. + \frac{1}{2} b_{ij} \left(T_i \cdot T_j - \frac{3 n_i}{4} \delta_{ij} \right) \right].$$

The coefficients a and b are defined in terms of the centroïds:

$$V_{ij}^T = \frac{\sum_J V_{ijij}^{JT} [J]}{\sum_J [J]}$$

as: $a_{ij} = \frac{1}{4}(3V_{ij}^1 + V_{ij}^0)$, $b_{ij} = V_{ij}^1 - V_{ij}^0$, the sums run over Pauli allowed values.

The Monopole Hamiltonian

The evolution of effective spherical single particle energies with the number of particles in the valence space is dictated by $\mathcal{H}_m$. In the case of identical particles the expression reads:

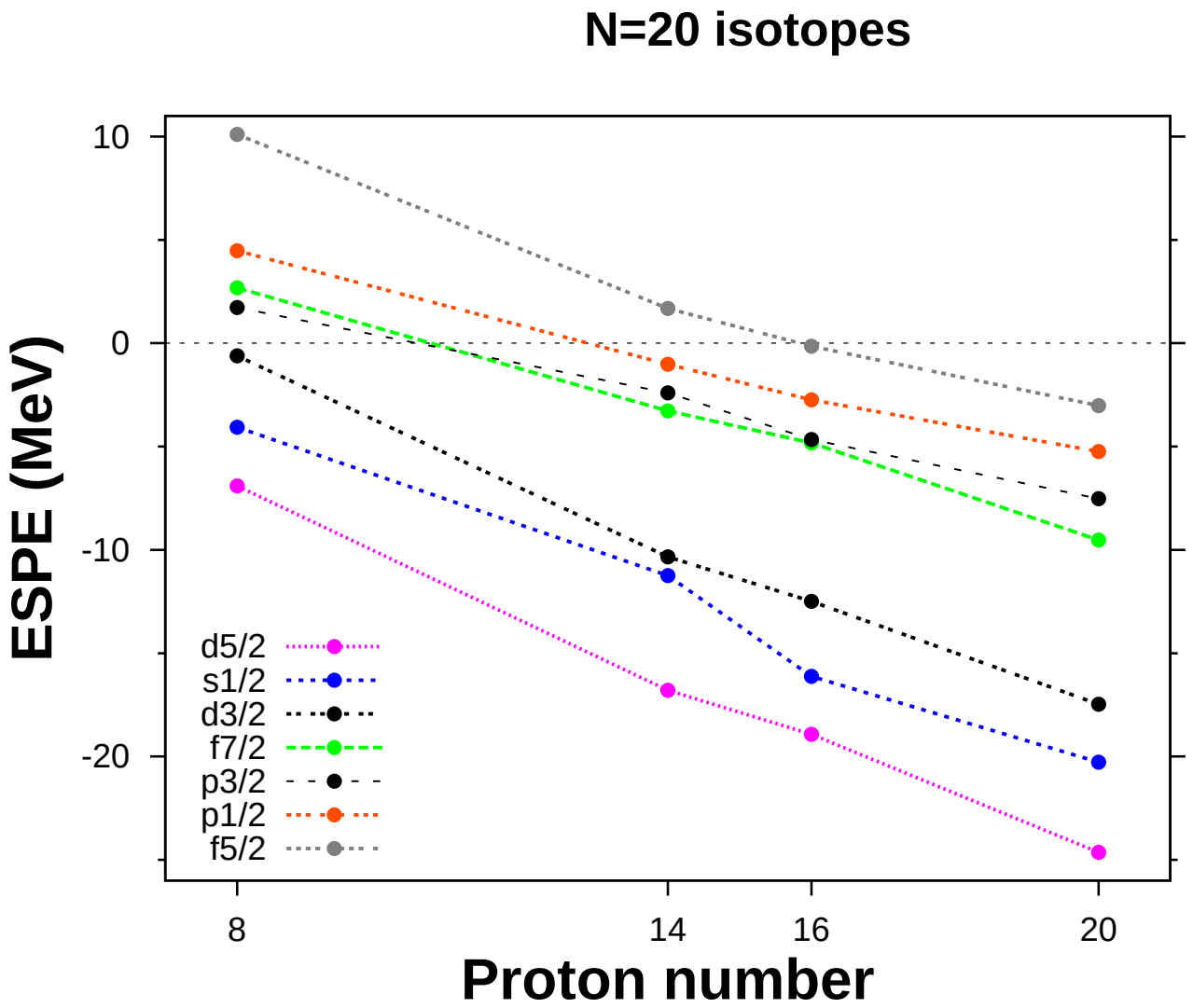
$$\epsilon_j(n) = \epsilon_j(n=1) + \sum_i V_{ij}^1 n_i$$

The monopole hamiltonian $\mathcal{H}_m$ also governs the relative position of the various T-values in the same nucleus, via the terms:

$$b_{ij} \quad T_i \cdot T_j$$

Even small defects in the centroids can produce large changes in the relative position of the different configurations due to the appearance of quadratic terms involving the number of particles in the different orbits.

The Drift of the Single Particle Energies



The Multipole Hamiltonian

$\mathcal{H}_M$ can be written in two representations, particle-particle and particle-hole:

$$\mathcal{H}_M = \sum_{r\leq s, t\leq u, \Gamma} W^{\Gamma}_{rstu} Z^{+}_{rs\Gamma} \cdot Z_{tu\Gamma},$$

$$\mathcal{H}_M = \sum_{rstu\Gamma} [\gamma]^{1/2} \frac{(1+\delta_{rs})^{1/2}(1+\delta_{tu})^{1/2}}{4} \omega^{\gamma}_{rtsu} (S^{\gamma}_{rt} S^{\gamma}_{su})^0,$$

where Z^{+}_{Γ} (Z_{Γ}) is the coupled product of two creation (annihilation) operators and S^{γ} is the coupled product of one creation and one annihilation operator.

$$Z^{+}_{rs\Gamma} = [a^{\dagger}_r a^{\dagger}_s]^{\Gamma} \text{ and } S^{\gamma}_{rs} = [a^{\dagger}_r a_s]^{\gamma}$$

The Multipole Hamiltonian

The W and ω matrix elements are related by a Racah transformation:

$$\omega^{\gamma}_{rtsu} = \sum_{\Gamma} (-)^{s+t-\gamma-\Gamma} \left\{ \begin{array}{ccc} r & s & \Gamma \\ u & t & \gamma \end{array} \right\} W^{\Gamma}_{rstu}[\Gamma],$$

$$W^{\Gamma}_{rstu} = \sum_{\gamma} (-)^{s+t-\gamma-\Gamma} \left\{ \begin{array}{ccc} r & s & \Gamma \\ u & t & \gamma \end{array} \right\} \omega^{\gamma}_{rtsu}[\gamma].$$

The operators $S^{\gamma=0}_{rr}$ are just the number operators for orbits r and $S^{\gamma=0}_{rr'}$ the spherical HF particle hole vertices. Both must have null coefficients if the monopole hamiltonian satisfies HF self-consistency.

The Multipole Hamiltonian

The operator $Z^{+}_{rr\Gamma=0}$ creates a pair of particle coupled to J=0 (or coupled to L=0 and S=0, or in a state of zero total momentum). Therefore the terms

$$Z^{+}_{rr\Gamma=0} \cdot Z_{ss\Gamma=0}$$

represent different pairing hamiltonians, whose specificities determine the values of the matrix elements $W^{\Gamma=0}_{rrss}$

The Multipole Hamiltonian

The operators S^{γ}_{rs} are typical multipole vertices of multipolarity γ. For instance, $r = s$, γ=(L=0,S=1) produces a $(\vec{\sigma} \cdot \vec{\sigma})$ term which is the main component of the residual interaction in mixed droplets of 4He-3He

The terms S^{γ}_{rs} γ=(J=2,T=0), that appear in the $(Q \cdot Q)$ interaction that is responsible for the existence of deformed nuclei, are specially large and attractive when $j_r - j_s$=2 and $l_r - l_s$=2.

Collectivity in Nuclei

The widespread presence of nuclei with deformed shapes is a conspicuous manifestation of the importance of the quadrupole-quadrupole terms in the nuclear multipole hamiltonian. Nuclear superfluidity (and the shift of the mass parabolas in even isobaric multiplets, and many other effects) signal also the importance of the pairing terms.

For a given interaction, a many body system would or would not display coherent features at low energy depending on the structure of the mean field around the Fermi level.

Universality of the Multipole Hamiltonian

Indeed, a careful analysis of the effective nucleon-nucleon interaction in the nucleus, reveals that the multipole hamiltonian is universal and dominated by BCS-like isovector and isoscalar pairing plus quadrupole-quadrupole and octupole-octupole terms of very simple nature $(r^\lambda Y_\lambda \cdot r^\lambda Y_\lambda)$

Interaction	particle-particle		particle-hole		
	JT=01	JT=10	$\lambda\tau$=20	$\lambda\tau$=40	$\lambda\tau$=11
KB3	-4.75	-4.46	-2.79	-1.39	+2.46
FPD6	-5.06	-5.08	-3.11	-1.67	+3.17
GOGNY	-4.07	-5.74	-3.23	-1.77	+2.46
GXPF1	-4.18	-5.07	-2.92	-1.39	+2.47
BONNC	-4.20	-5.60	-3.33	-1.29	+2.70

Mean Field *vs* Correlations; Nuclear needles and superconductivity

An attractive pairing interaction in an electron gas at T=0 produces the superconducting phase transition

The quadrupole-quadrupole interaction left alone –*i.e.*– if the monopole hamiltonian is negligible, would produce nuclear needles.

Magic nuclei are spherical despite the strong quadrupole-quadrupole interaction, because the large gaps in the nuclear mean field at the Fermi surface block the quadrupole correlations

The isotropic harmonic oscillator has SU(3) symmetry. The quadrupole operators are generators of this group and the Casimir of the group contains the quadrupole-quadrupole interactions. Therefore the states of lower energy are those with maximal deformation compatible with the Pauli principle.

The spin orbit interaction breaks the SU(3) symmetry, but other SU3 variants emerge when there are favorable orbits around the Fermi level, like Pseudo-SU3 or Quasi-SU3.

The Effective Interaction(s): Key aspects

The evolution of the spherical mean field in the valence spaces. What is missing in the monople hamiltonian derived from the realistic NN interactions, be it through a G-matrix, V_{low-k} or other options? Most probably three body forces whose need seems already well established. Some claim that they could be reducible to simple monopole forms, a kind of density dependence, or more precisely, occupation number dependence

The multipole hamiltonian does not seem to demand major changes with respect to the one derived from the realistic nucleon-nucleon potentials

Algorithms and Codes

Algorithms include Direct Diagonalisation, Lanczos, Monte Carlo Shell Model, Quantum Monte Carlo Diagonalization, DMRG etc. There are also a number of different extrapolation ansatzs

The Strasbourg-Madrid codes can deal with problems involving basis of 10^{10} Slater determinants, using relatively modest computational resources

The most popular "flaws" of the standard ISM description

- Quadrupole effective charges are needed (But their value is universal and rather well understood)
- Spin operators are quenched by another universal factor which relates to the regularization of the interaction, the same effect of the short range correlations that shows up in the (e, e') and $(e, e'p)$ experiments
- Not all the regions of the nuclear chart are amenable to a SM description yet

Physics Goals

Description of the nuclear correlations in the laboratory frame

Changing magic numbers far from stability: The competing roles of spherical mean field and correlations

Precision Spectroscopy toward larger masses

Double β decay, the key to the nature of the neutrinos, the absolute scale of their masses and their hierarchy

Nuclear Structure and Nuclear Astrophysics

Spectroscopic factors

The spectroscopic factors are defined as:

$$S(j,t_z) = \frac{\langle J_f\, T_f\, T_{zf} || a^{\dagger}_{jt_z} || J_i\, T_i\, T_{zi} \rangle^2}{2J_f + 1}$$

where the matrix element is reduced in angular momentum only; j and t_z refer to the spin and third isospin component of the stripped nucleon.

Spectroscopic factors

Imagine we start on doubly magic ^{48}Ca. The states

$$|r_{jt_z}\rangle = a^{\dagger}_{jt_z}|^{48}\mathrm{Ca\ gs}\rangle$$

are not, except in the non-interacting case, eigenstates of the Hamiltonian for ^{49}Sc or ^{49}Ca. The strongest the correlations, the farther they are. Therefore, to calculate $S(j, t_z)$ we overlap $|r\rangle$ with the physical states in the final nucleus. In practice, we just take $|r\rangle$ as starting vector for a sequence of Lanczos iterations. The total spectroscopic factor is the norm of the state $|r\rangle$

Spectroscopic factors

The excitation energies of the starting vectors, $e_r = \langle r|H|r\rangle - \langle f|H|f\rangle$, (in MeV)

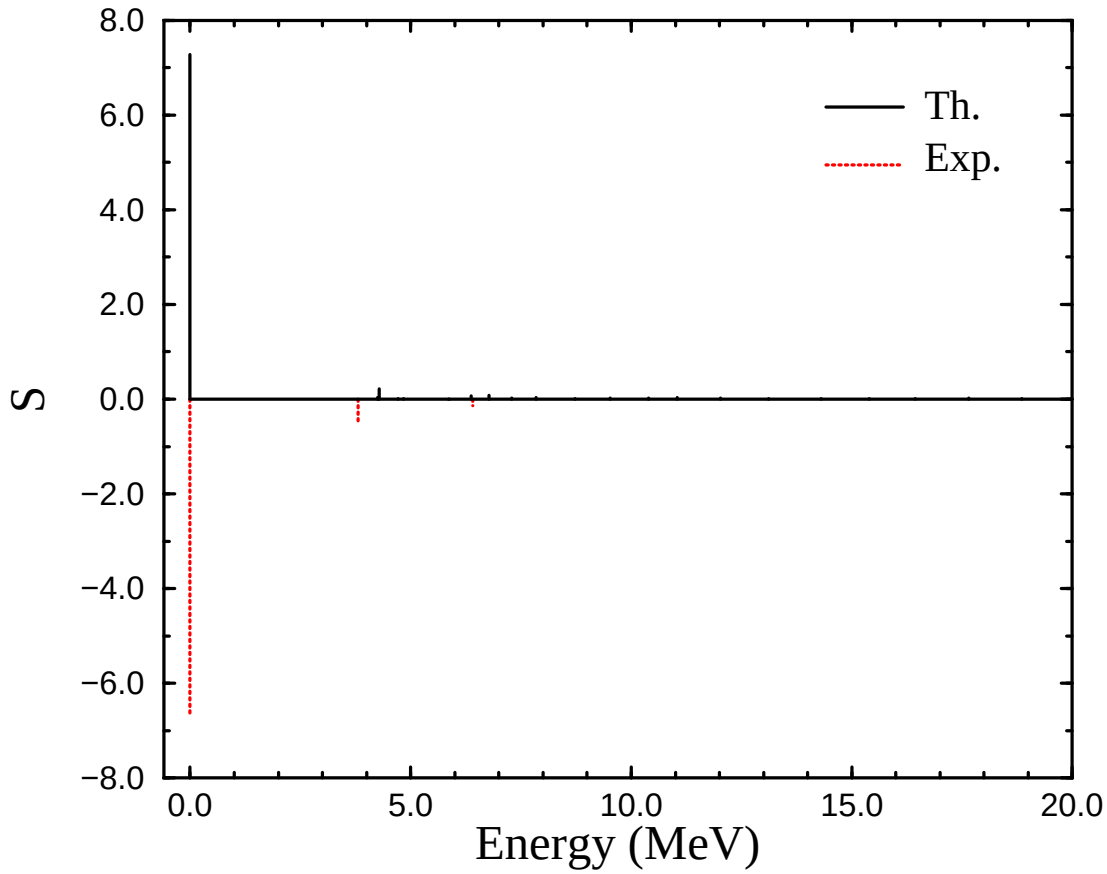
$$e_{p_{3/2}} = 4.54 \quad e_{p_{1/2}} = 5.99 \quad e_{f_{5/2}} = 5.76$$

are almost identical to the monopole prediction.

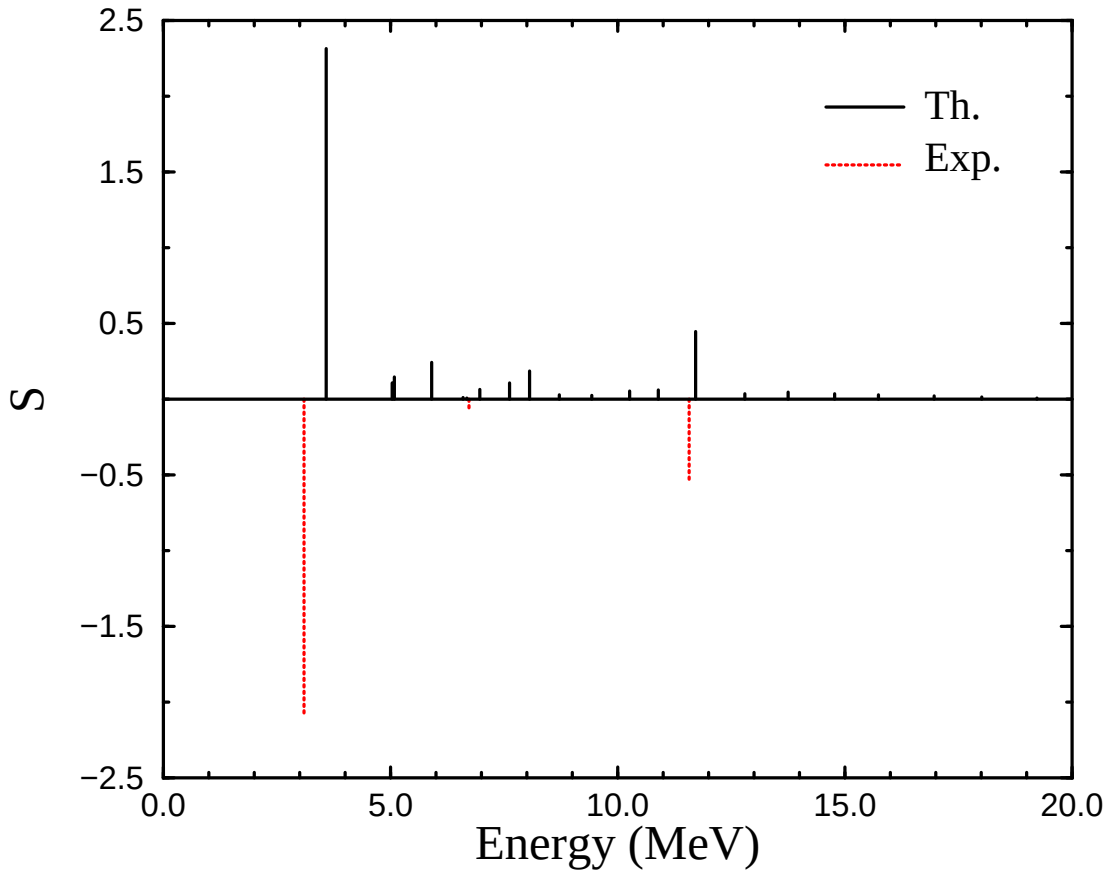
$$\epsilon_{p_{3/2}} = 4.58 \quad \epsilon_{p_{1/2}} = 5.99 \quad \epsilon_{f_{5/2}} = 5.66$$

a result readily explained by the weakness of the ground state correlations in ^{48}Ca. By the same token the sum rules for $(2j+1)S(j,t_z)$ are very close to their theoretical maximum, $(2j+1)$. Indeed, the sum rule is actually quenched by a factor of about 0.7 because of the short range correlations that take us out of the model space.

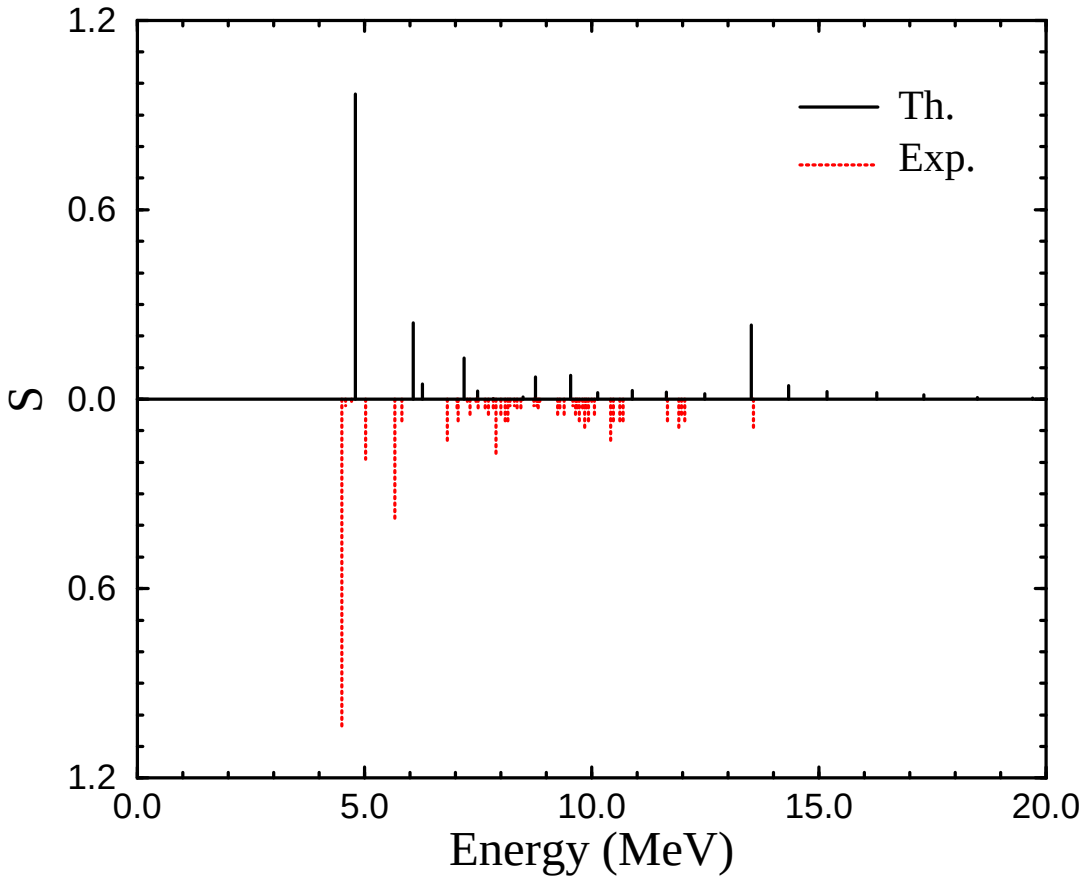
Stripping on $^{48}Ca \rightarrow {}^{49}Sc$ $0f_{7/2}$



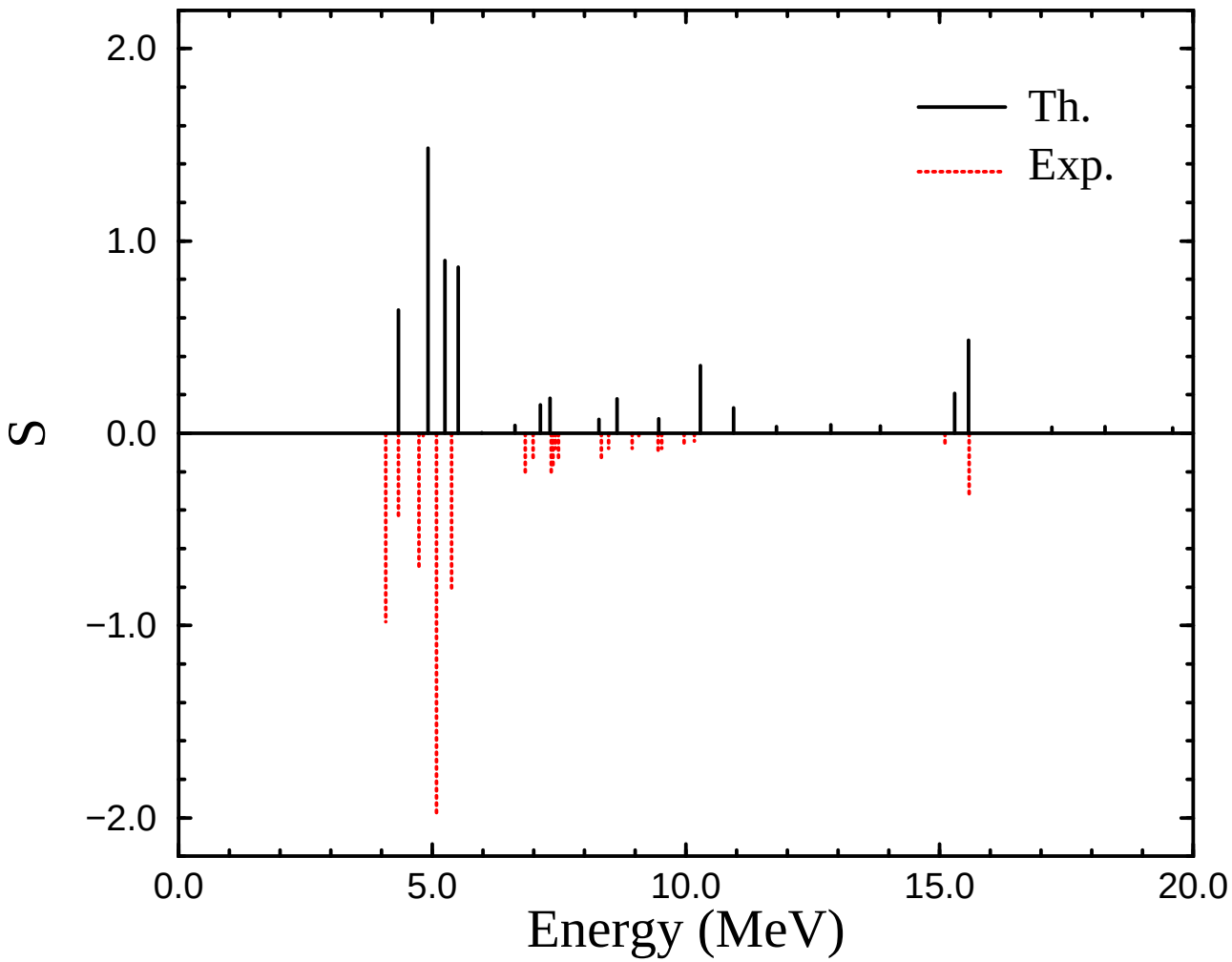
Stripping on $^{48}Ca \rightarrow {}^{49}Sc$ $1p_{3/2}$



Stripping on $^{48}Ca \rightarrow {}^{49}Sc$ $1p_{1/2}$



Stripping on $^{48}Ca \rightarrow {}^{49}Sc$ $0f_{5/2}$



Spectroscopic factors and correlations; ^{48}Ca *vs* ^{46}Ar

The correlations act in two ways:

- Shifting strength from the particle to the hole channel.
- Fragmenting the strength into many states

For the neutron stripping on ^{48}Ca and ^{46}Ar the situation is as follows:

orbit	strength	
f7/2	0.025(Ca)	0.136(Ar)
p3/2	0.982(Ca)	0.793(Ar)
p1/2	0.987(Ca)	0.966(Ar)
f5/2	0.984(Ca)	0.969(Ar)

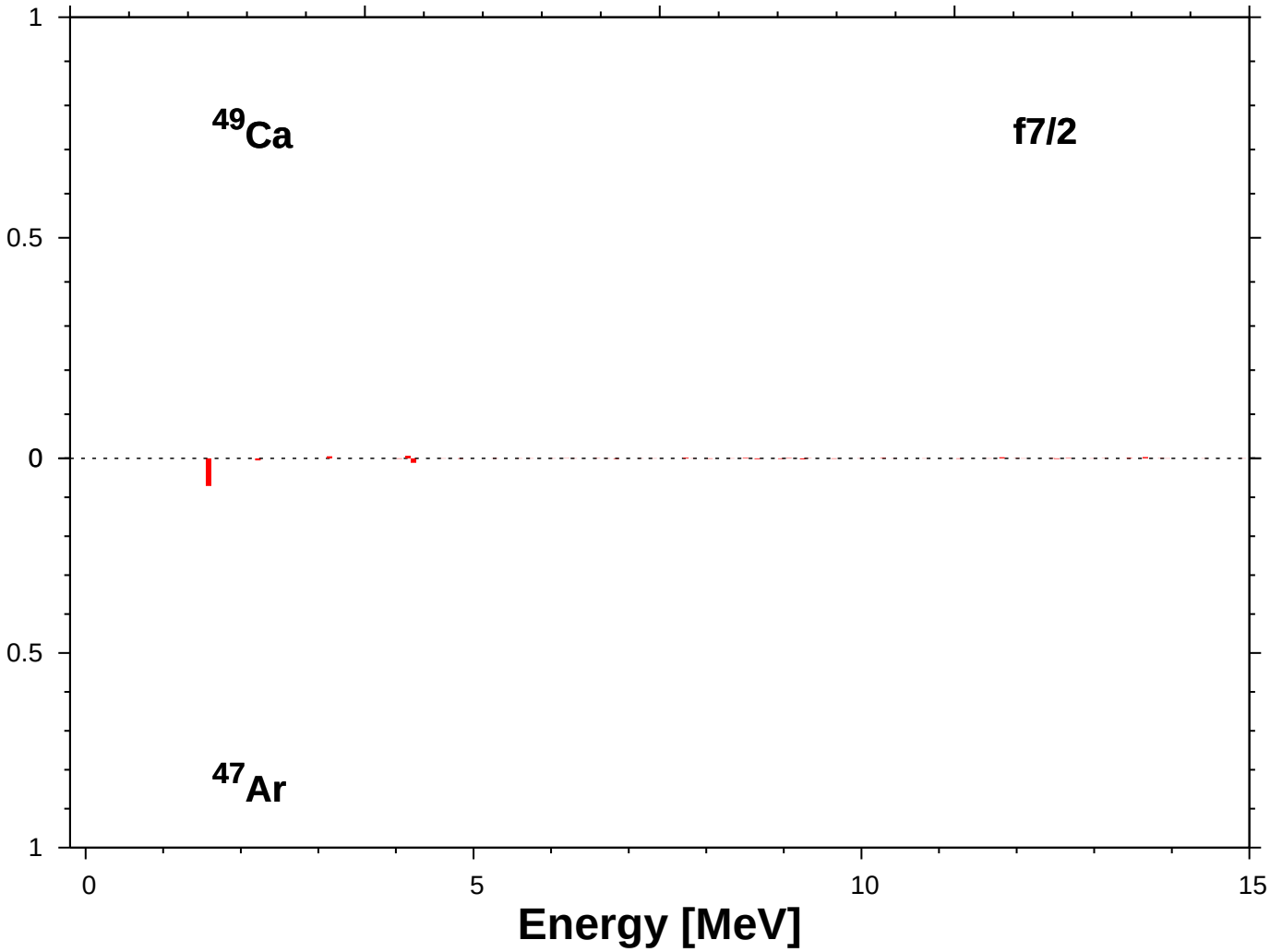
Spectroscopic factors and correlations

In the presence of correlations, when the single particle strength is fragmented, one can still have an idea of the bearings of the underlying mean field, constructing equivalent single particle energies

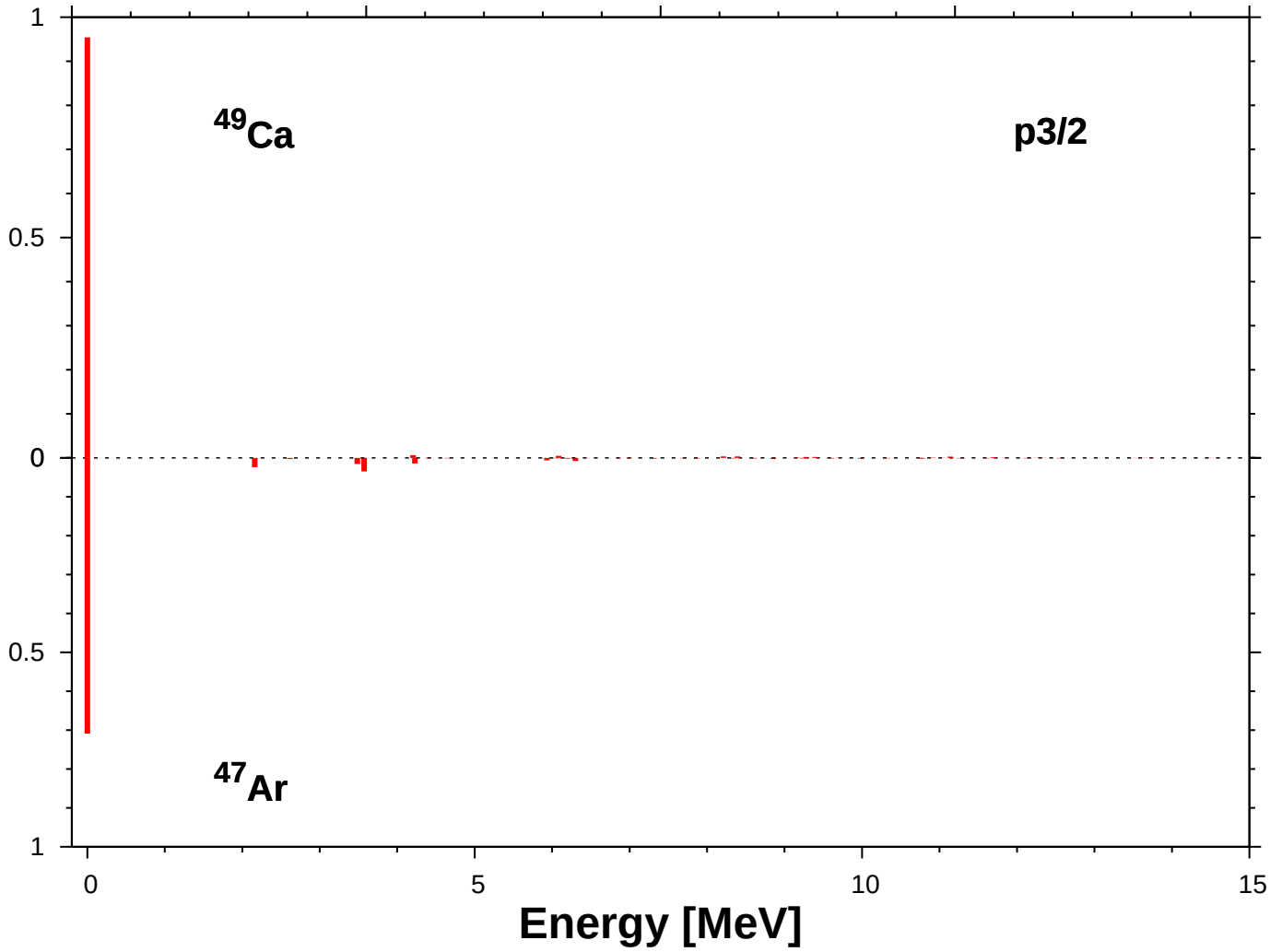
$$\epsilon_j = \frac{\sum_n (E_0 - E_n^-) S_n^- + \sum_m (2j+1)(E_0 - E_m^+) S_m^+}{(2j+1)}$$

$$\sum_n S_n^- + (2j+1) \sum_m S_m^+ = 2j+1$$

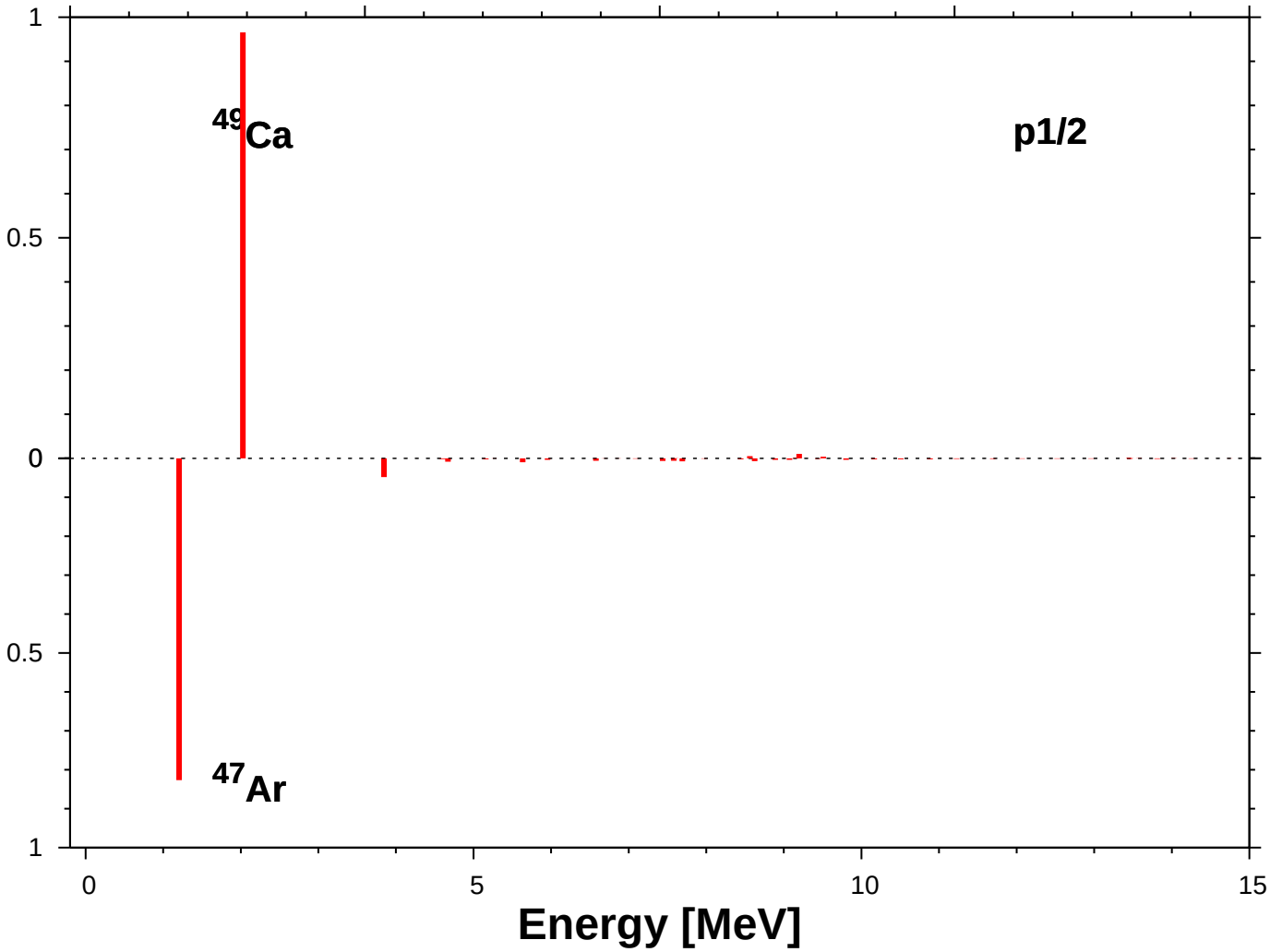
Stripping on $^{48}Ca \rightarrow {}^{49}Ca$, and $^{46}Ar \rightarrow {}^{47}Ar$; $0f_{7/2}$



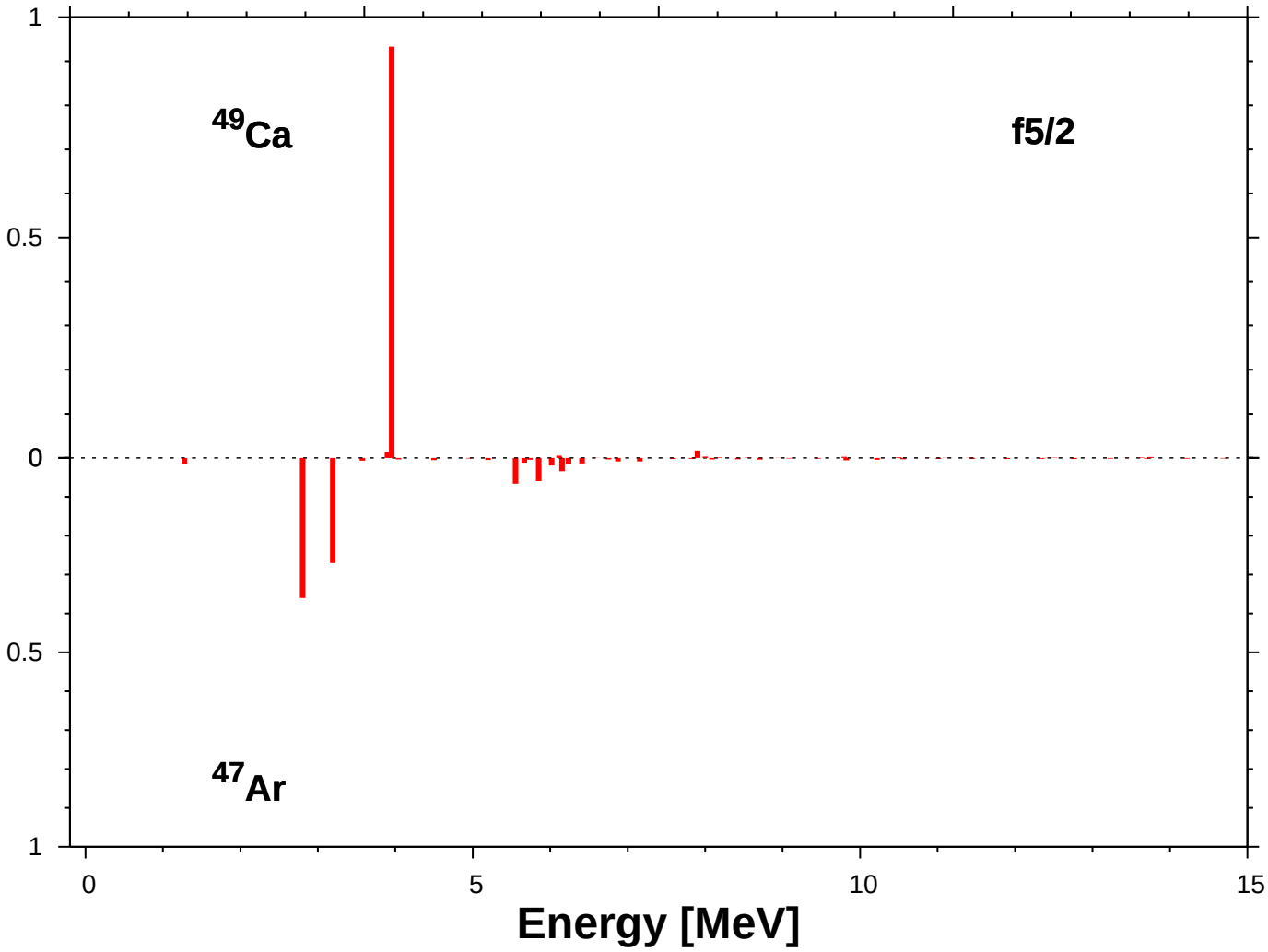
Stripping on $^{48}Ca \rightarrow {}^{49}Ca$, and $^{46}Ar \rightarrow {}^{47}Ar$; $1p_{3/2}$



Stripping on ^{48}Ca $\longrightarrow$ ^{49}Ca, and ^{46}Ar $\longrightarrow$ ^{47}Ar; $1p_{1/2}$

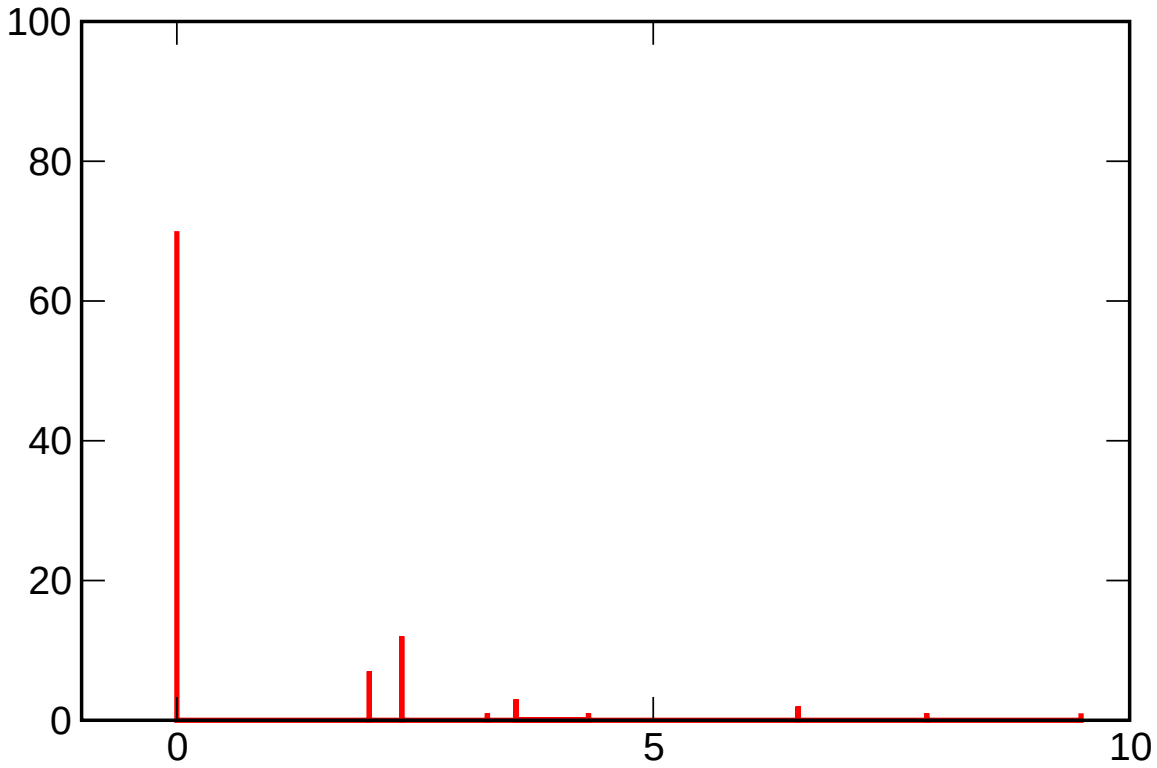


Stripping on ^{48}Ca $\longrightarrow$ ^{49}Ca, and ^{46}Ar $\longrightarrow$ ^{47}Ar; $0f_{5/2}$



Deformed nuclei; Stripping on $^{48}Cr \longrightarrow {}^{49}Cr$

In deformed nuclei, much of the particle strength goes to the hole channel, for instance in ^{48}Cr we have only 0.585 of $0f_{7/2}$ strength instead of 1.0 in the single particle limit. In addition the strength is fragmented among several states. The lowest $7/2^-$ state in the figure belongs to the K=5/2 ground state band of ^{49}Cr which has β=0.3.



Deformed nuclei; Stripping on $^{48}Cr \longrightarrow {}^{49}Cr$

Most of the $0f_{5/2}$ strength (0.96) remains in the particle channel. But now the fragmentation is much stronger. Notice that the ground state $J^{\pi} = 5/2^{-}$ does not have any $0f_{5/2}$ strength.