Les Matrices Géantes dans le cadre du Modèle en Couches

E. Caurier

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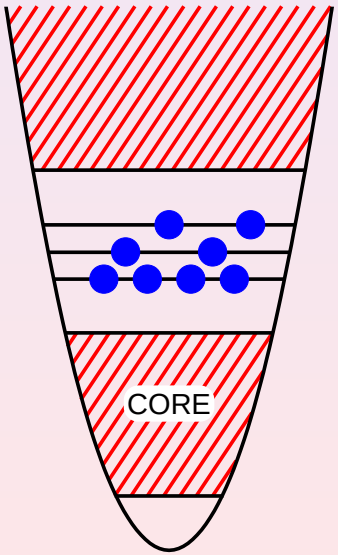
MEAN FIELD

- $H = \sum_i h_i + \sum_{i<j} V_{ij}$
- h $\longrightarrow$ harmonic oscillator +spin orbit
- V $\longrightarrow$ residual interaction
- "0$\hbar\omega$" calculations.



PERTURBATION THEORY

- Full Hilbert space $\longrightarrow$ Valence space
- $H\Psi = E\Psi \longrightarrow H_{eff}\Psi_{eff} = E\Psi_{eff}$
- $\langle\Psi|O|\Psi\rangle \longrightarrow \langle\Psi_{eff}|O_{eff}|\Psi_{eff}\rangle$

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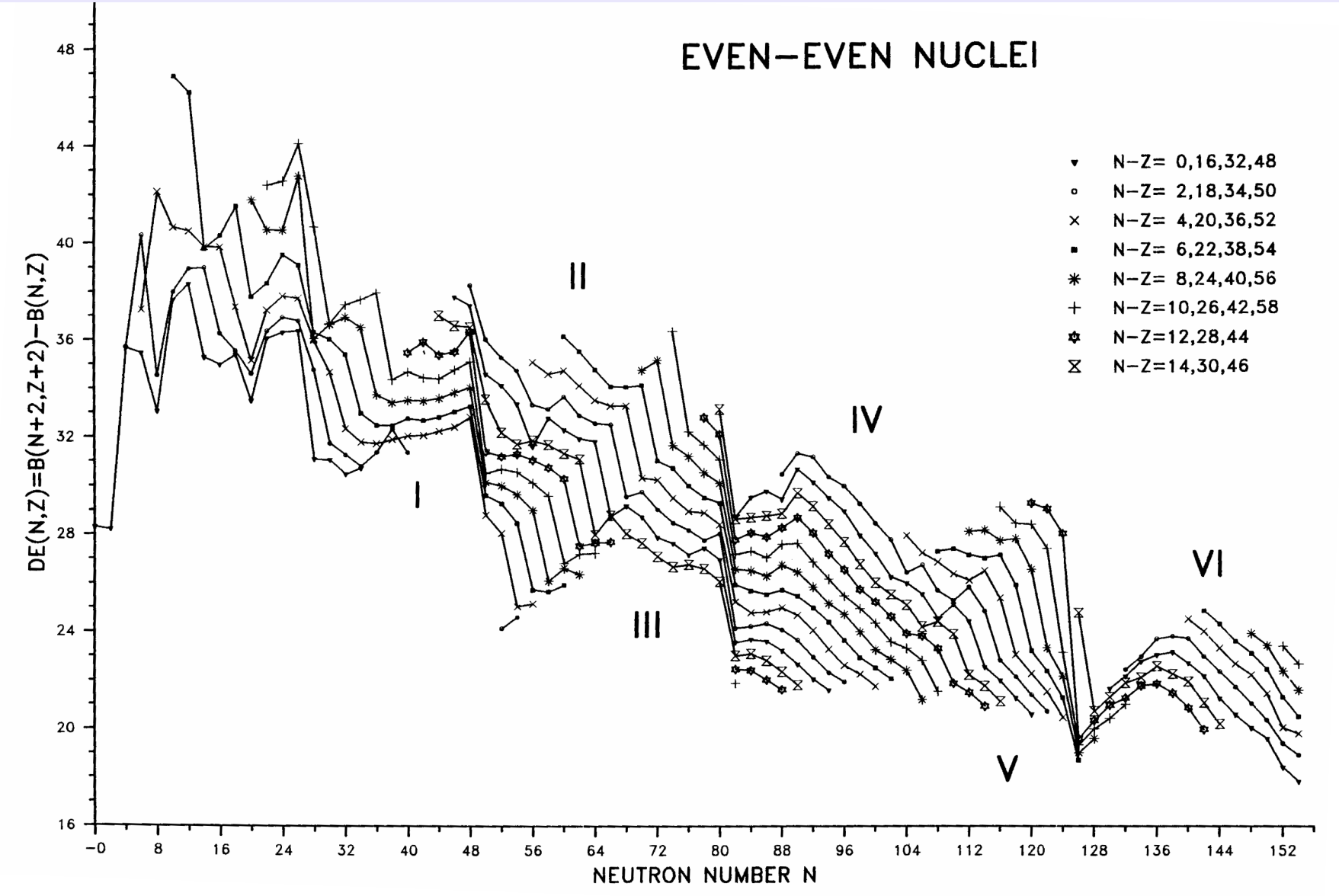
α Lines



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IN PRINCIPLE, possibility to describe SIMULTANEOUSLY

ALL the spectroscopic properties of

ALL the nuclei of the valence space.

- Energies.
- Electric and magnetic transitions.
- β decay, $\beta\beta$ decay.
- .....

BUT

- Intruder states.

- Validity of the valence space for specific spectroscopic properties ?

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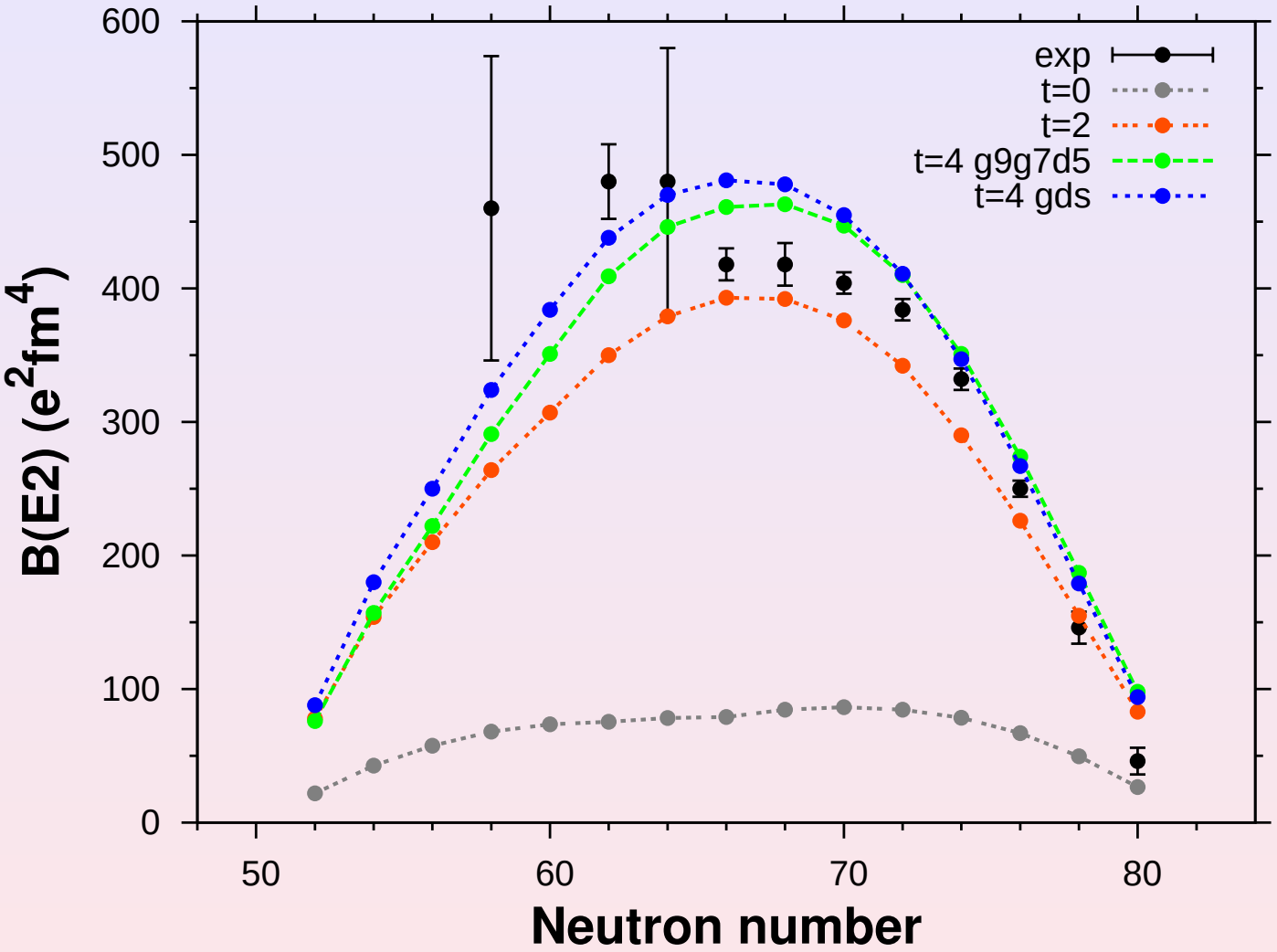
B(E2)'s in Tin isotopes



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- 1) Define a valence space
- 2) Derive an effective interaction
- 3) Build and diagonalize the Hamiltonian matrix.

Point 3) is a strong technical constraint on the choice of the valence space.

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Valence Spaces:

- $^{4}He \rightarrow^{16} O$ p shell $Dim \sim 10^{2}$
- $^{16}O \rightarrow^{40} Ca$ sd shell $Dim \sim 10^{5}$
- $^{40}Ca \rightarrow^{80} Zr$ pf shell $Dim \sim 10^{9}$

No Shell closure for $N = Z = 40 \longrightarrow {}^{80}Zr$ is a deformed nucleus.
Shell closure at N=Z=50 $\longrightarrow {}^{100}Sn$

After ^{56}Ni the $0g_{\frac{9}{2}}$ shell becomes less and less negligible.
Transition of the valence space :
$pf = 0f_{\frac{7}{2}}, 0f_{\frac{5}{2}}, 1p_{\frac{3}{2}}, 1p_{\frac{1}{2}} \longrightarrow r_3g = 0f_{\frac{5}{2}}, 1p_{\frac{3}{2}}, 1p_{\frac{1}{2}}, 0g_{\frac{9}{2}}$

r_3g space: nuclei with $28 < N, Z < 50$: $Dim \sim 10^{10}$

Description of deformed nuclei around $N = Z = 40$ needs the introduction of the $1d_{\frac{5}{2}}$ shell to get a prolate solution.but now the dimension of the space is $\sim 10^{14}$

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For Heavy nuclei spin-orbit closure N=50,82,126
Dimensions of the matrices limit strongly the domain of applicability of standard SM calculations

r_4h space: nuclei with $50 < N, Z < 82$:

- ^{112}Xe (4p+8n active particles) $Dim \sim 9.3 * 10^9$
- ^{114}Xe (4p+10n active particles) $Dim \sim 5.5 * 10^{10}$
- ^{124}Ba (6p+12n active particles) $Dim \sim 1.1 * 10^{13}$

- Few active particles (holes)
- around semi-magic nuclei

All these nuclei are spherical : seniority truncation .
^{238}U is out of reach but ^{218}U has been done. (semi-magic nucleus).

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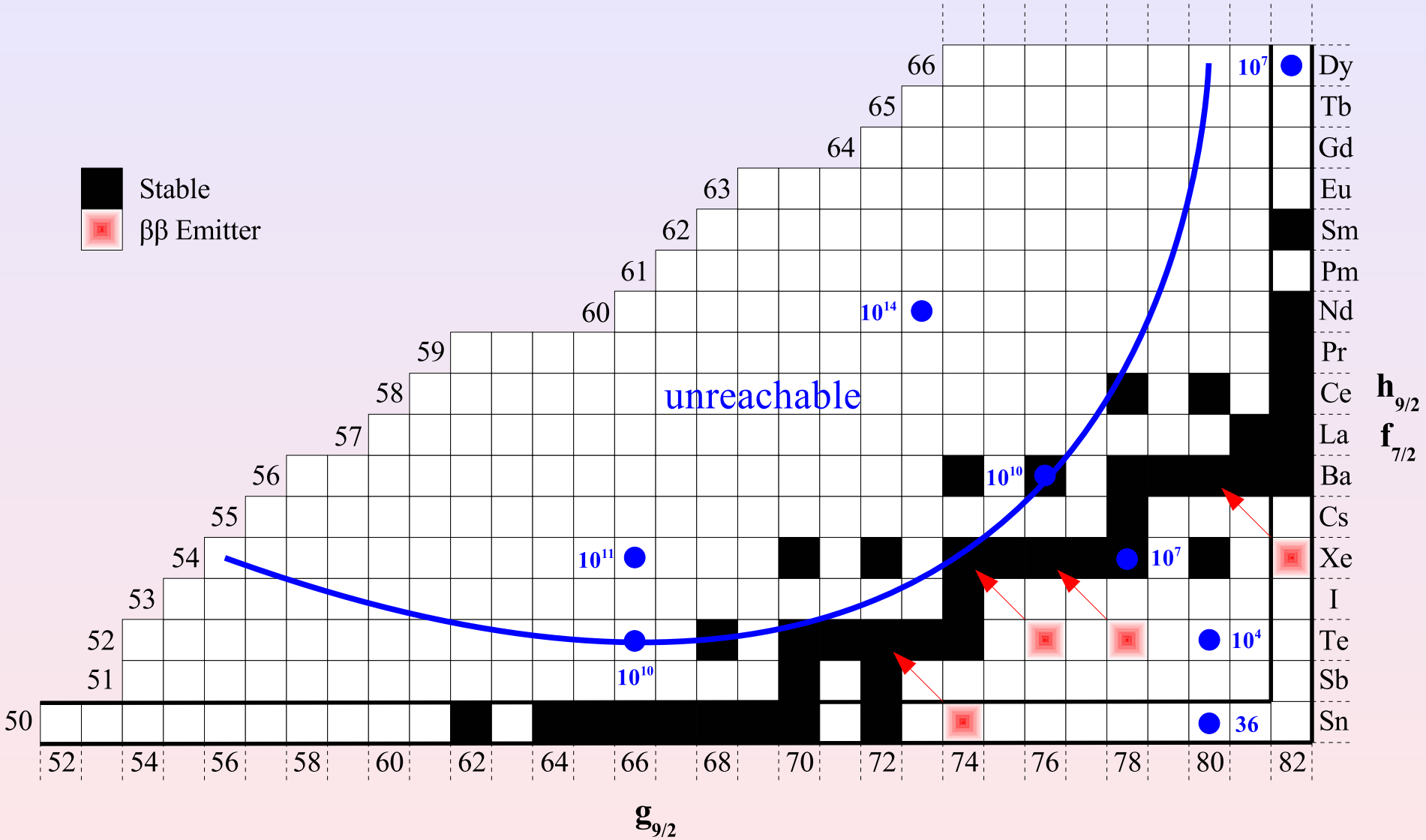
$50 \leq Z, N \leq 82$ region



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Standard valence space "$0\hbar\omega$" space.
Intruder states : introduction of some $N\hbar\omega$ states in the valence space.
Deformed and super-deformed band in ^{40}Ca:
excitations of 4 (8) particles from the *sd* to the *pf* shells .
Dimensions increase and problem of spurious states (center of mass excitaion)

in NOCORE SHELL MODEL FULL $N\hbar\omega$ space $\longrightarrow$ exact removal of the spurious center of mass states.
Convergence with N at the exact solution (comparison with GFMC results)
Limitation to light nuclei (p shell nuclei).
$N\hbar\omega = 16$ (A=6) $N\hbar\omega = 8$ (A=12,16) $N\hbar\omega = 4$ (A=22)
A=4 $N\hbar\omega = 24$ small dimension $\sim 1.2 * 10^8$ but
325 nlj shells and 5650 nljm states
$A = 48$ $Dim(N\hbar\omega = 2) \sim 2.1 * 10^8$ $(N\hbar\omega = 4) \sim 2.2 * 10^{11}$

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Diagonalization (Lanczos method)

We have a starting vector $|\mathbf{1}\rangle$, First iteration :

$$H|\mathbf{1}\rangle = E_{11}|\mathbf{1}\rangle + E_{12}|\mathbf{2}\rangle$$

Second iteration :

$$H|\mathbf{2}\rangle = E_{21}|\mathbf{1}\rangle + E_{22}|\mathbf{2}\rangle + E_{23}|\mathbf{3}\rangle$$

Third iteration :

$$H|\mathbf{3}\rangle = E_{32}|\mathbf{2}\rangle + E_{33}|\mathbf{3}\rangle + E_{34}|\mathbf{4}\rangle$$

$|\mathbf{1}\rangle$ does nor appear since $E_{31} = E_{13} = 0$
At rank N, we will get :

$$H|\mathbf{N}\rangle = E_{N,N-1}|\mathbf{N}-\mathbf{1}\rangle + E_{N,N}|\mathbf{N}\rangle + E_{N,N+1}|\mathbf{N}+\mathbf{1}\rangle$$

A new basis (Lanczos vectors) is built in which H is TRIDIAGONAL

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Diagonalization (Lanczos method)

CPU time is proportional to the number of Lanczos iterations, which is itself proportional to the number of eigenvectors that we need.
It has a small dependance with the dimension of the matrix.
(with standard method for diagonalization CPU time $\sim N^3$)

Choice of the starting vector is crucial to reduce the number of iterations: eigenvector in a smaller space.
Problems :

- storage of all the Lanczos vectors (Disk capacity)
- numerical errors can appear when the number of iterations becomes large. (orhogonality between the Lanczos vectors, quantum numbers)

note: Lanczos with J^2 operator allows to project out on states of good angular momentum.

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Lanczos Strength Function

Transition matrix elements $\langle \Psi_f | \Omega | \Psi_i \rangle$ for many final states $|\Psi_f\rangle$
β decay, pn reactions, spectroscopic factors ...

$$\Omega |\Psi_i\rangle \; = \; S_0 |\Phi_0\rangle$$

S_0^2 is the total strength and Φ_0 is the sum rule state.

Taking this Φ_0 vector to start a Lanczos calculation we get:

$$|\Phi_0\rangle \; = \; \sum_f S_f |\Psi_f\rangle$$
$$S_0 * S_f \; = \; \langle \Psi_f | \Omega | \Psi_i \rangle$$

Convergence of the strength function S_f ?

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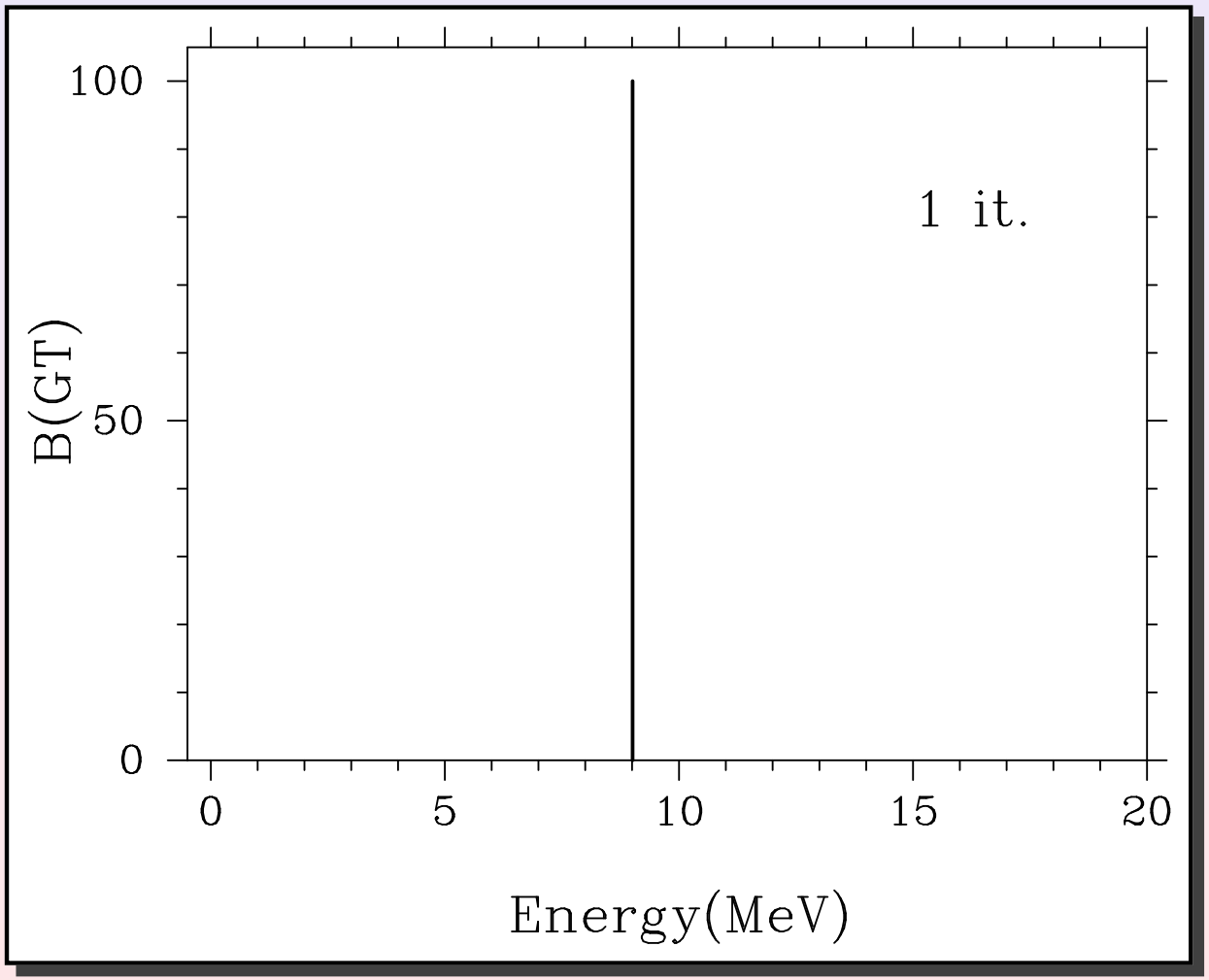
Evolution of Strength Distribution

GT Strength on ^{48}Sc



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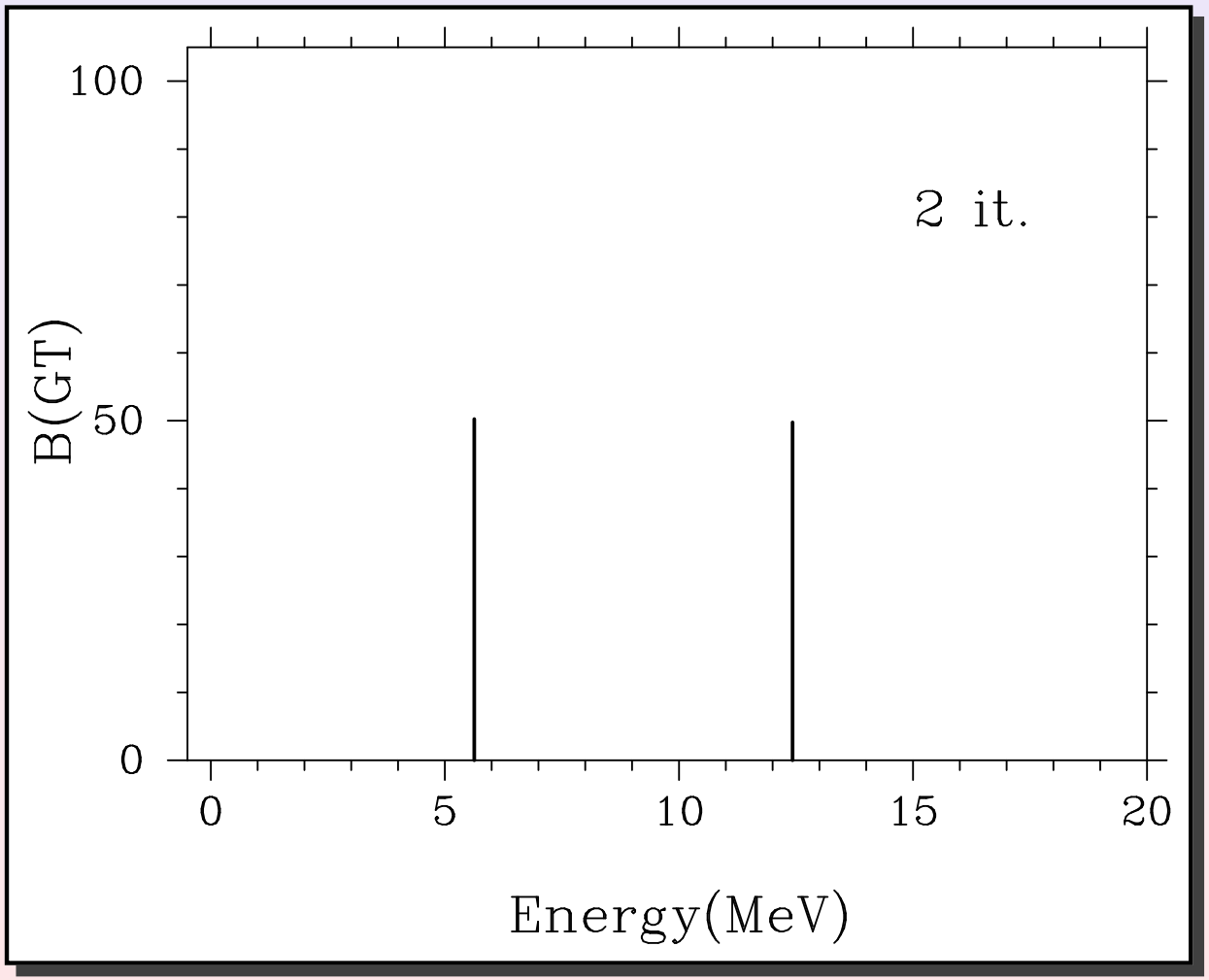

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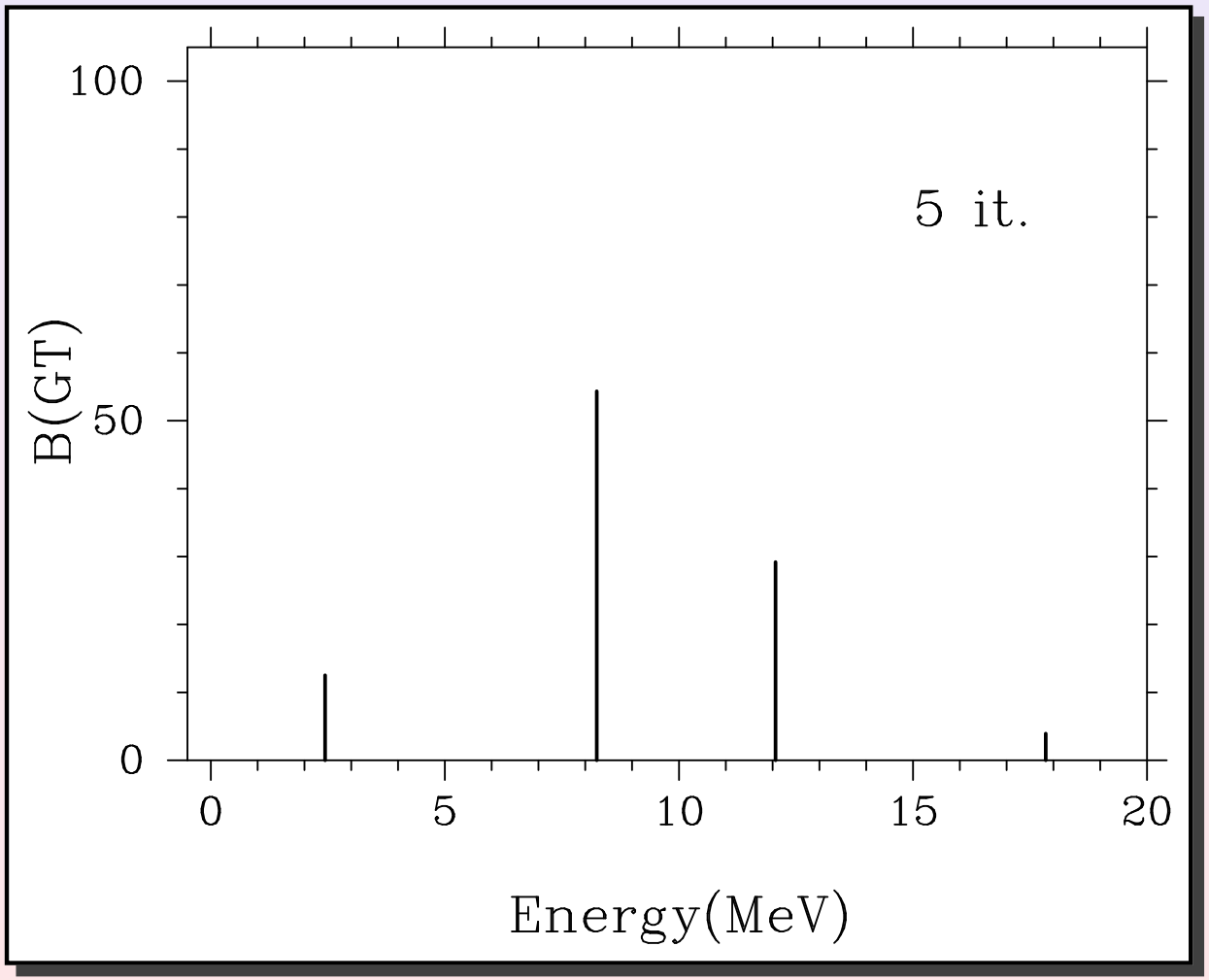

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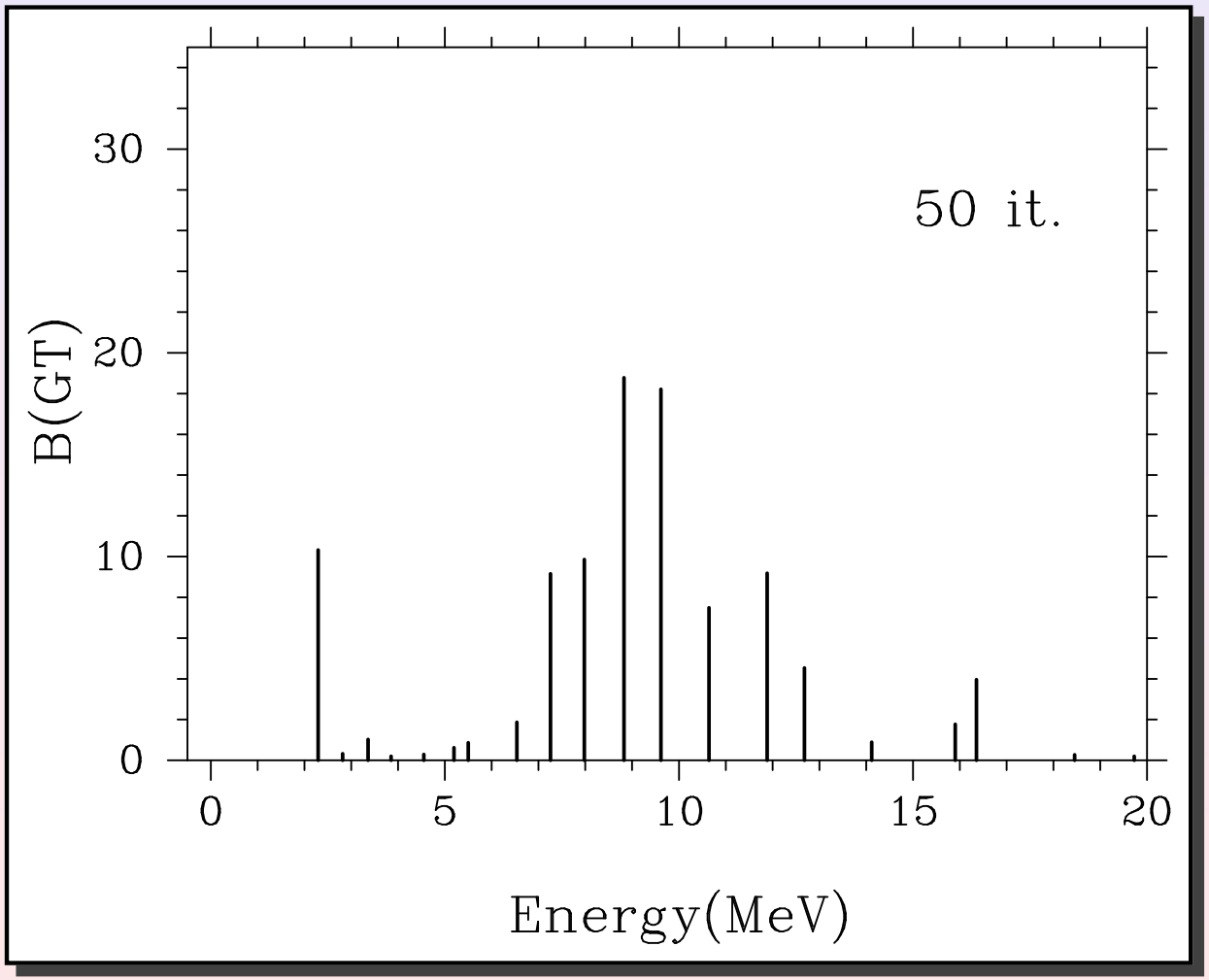

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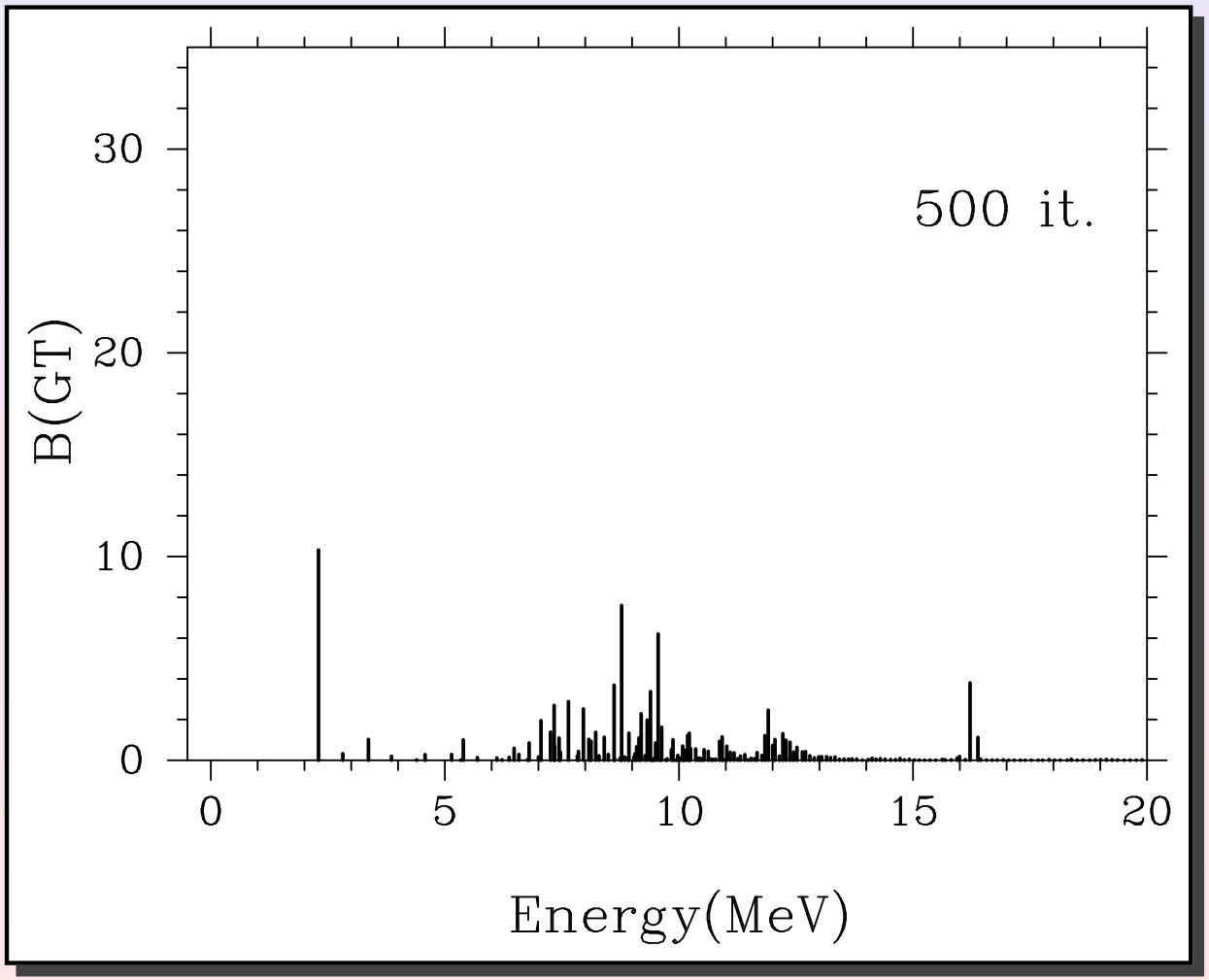

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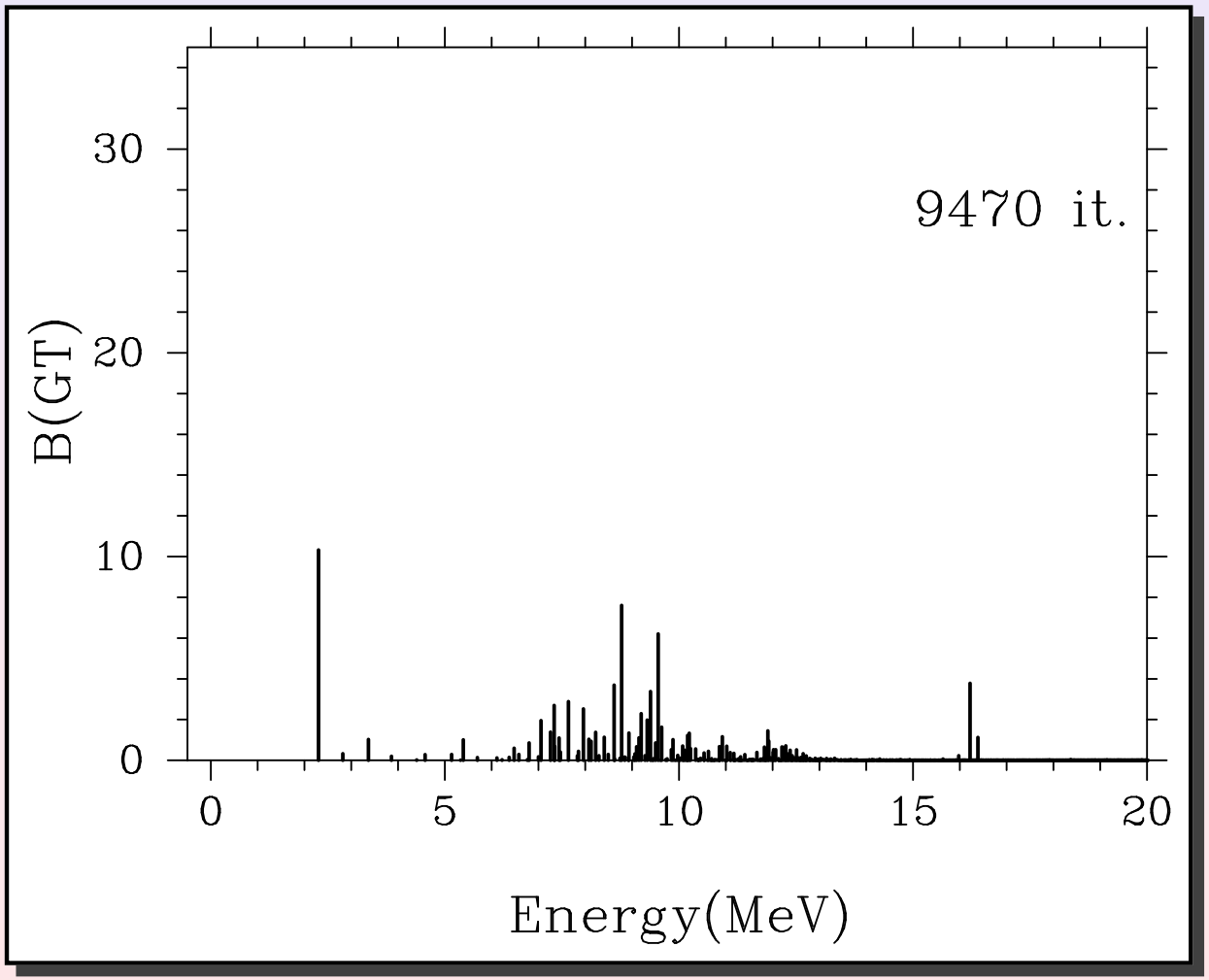

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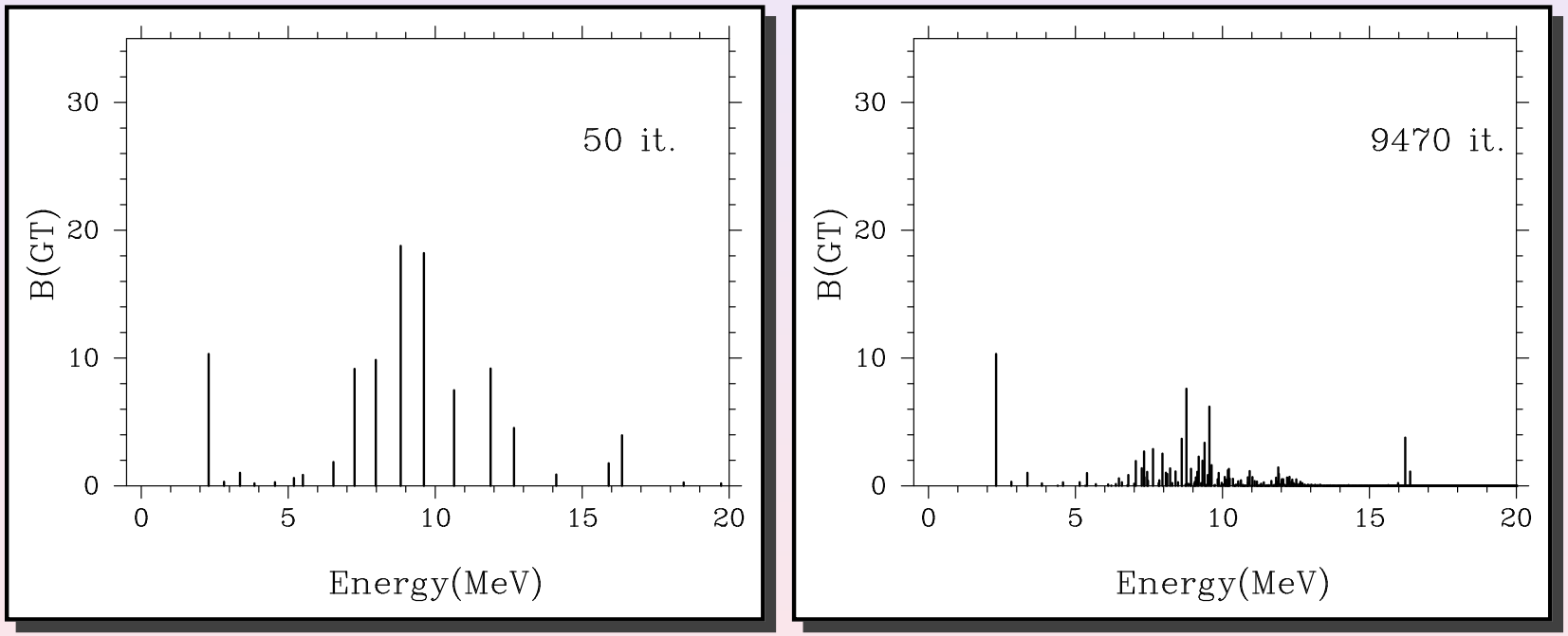

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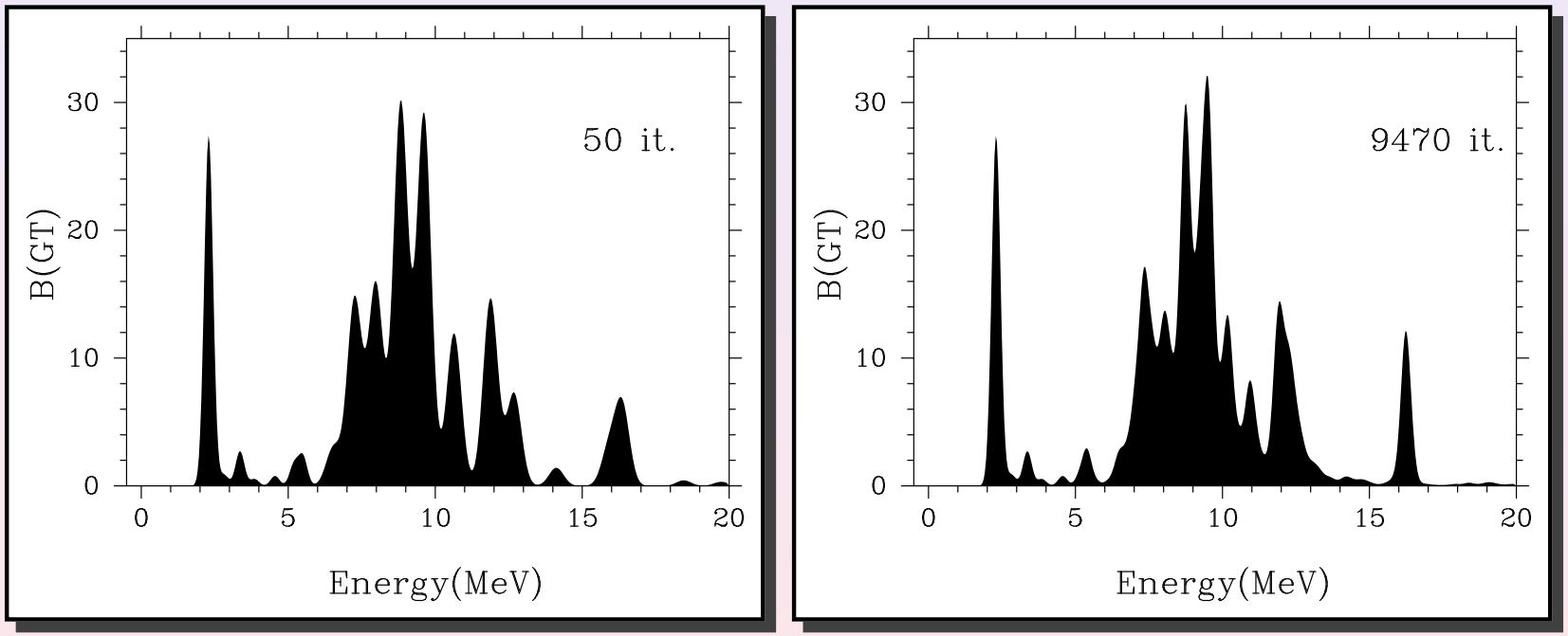

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Giant matrices

Exponential increase of the dimension with :

- N : number of individual states in the valence space.
- n : number of active particles (hole)

Number of $H_{IJ} \neq 0$ is not quadratic but $\sim$ LINEAR with the dimensions of the matrices.
However we must deal with:

GIANT MATRICES

Number of $H_{IJ} \neq 0$ too large to be precalculated AND STORED

.

They must be recalculated in the diagonalization process (Lanczos).

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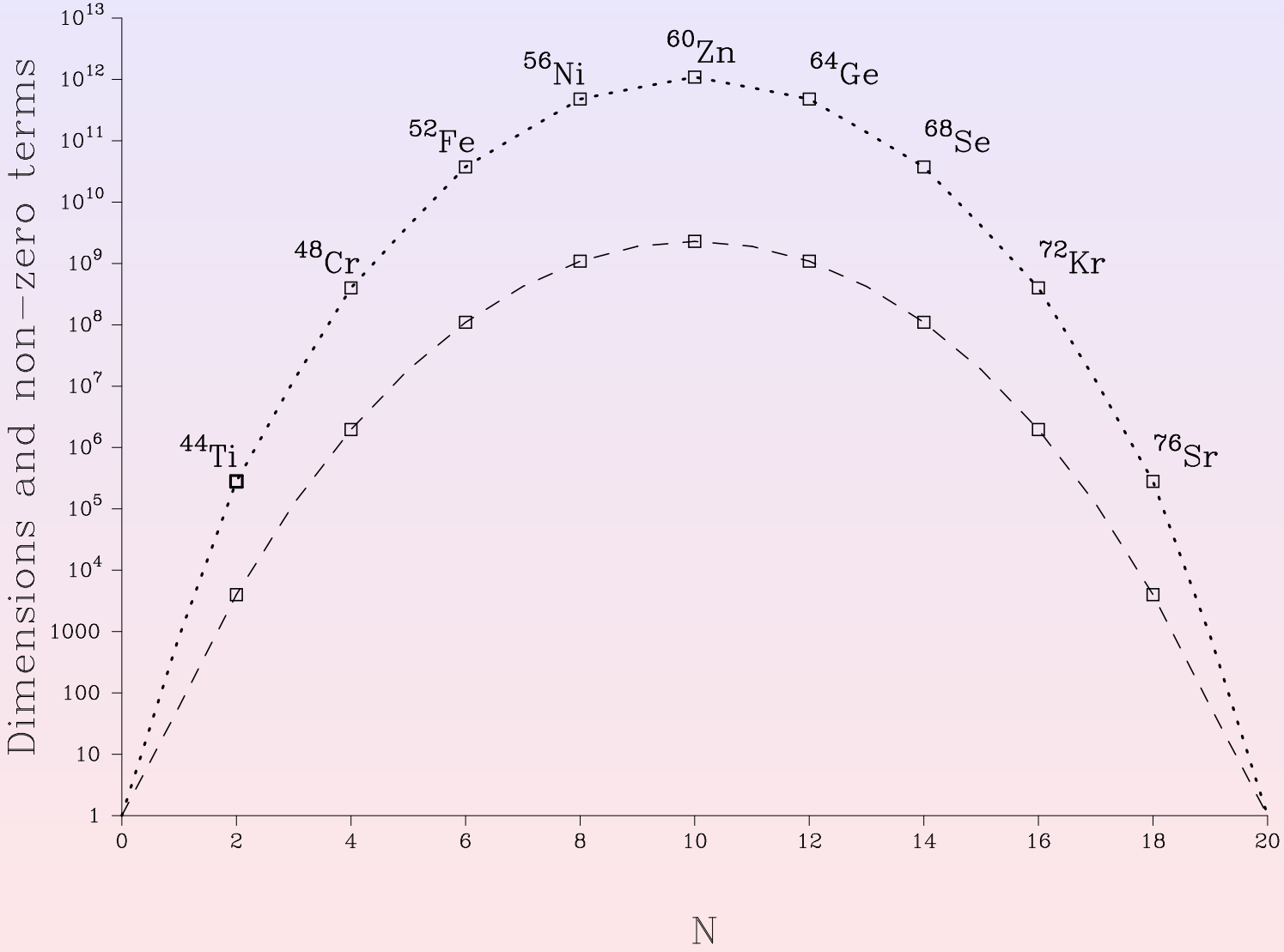
pf valence space



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Shell Model Codes

M-scheme :

The basis is composed of Slater determinants (SD)

$$|K\rangle = \prod_{i=nljm\tau} a_i^\dagger |0\rangle \; = \; a_{i1}^\dagger ... a_{iA}^\dagger |0\rangle$$

The drawback is that only J_z and T_z are good quantum numbers.
As a consequence the dimensions of the matrices are maximal:

$$\mathrm{D} \sim \binom{d_\pi}{p} \cdot \binom{d_\nu}{n}$$

- The N-body matrix elements (NBME) are very easy to calculate.
  $H_{IJ} = \pm V_{ijkl}$ (2-body matrix elements in the decoupled basis).
- The matrix is very sparse.

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Shell Model Codes

Coupled-scheme :

The wave function is written as successive coupling of one shell wave functions (c. f. p. 's) defined by $|(j_i)^{n_i} v_i \gamma_i x_i\rangle$:

$$\Big[\big[|(j_1)^{n_1} v_1 \gamma_1 x_1\rangle \; |(j_2)^{n_2} v_2 \gamma_2 x_2\rangle \big]^{\Gamma_2} \; \ldots \; |(j_k)^{n_k} v_k \gamma_k x_k\rangle \Big]^{\Gamma_k}$$

- $\vec{\Gamma}_k = \vec{\Gamma}_{k-1} + \vec{\gamma}_k$
- $v_i \equiv$ seniority i. e. number of particles non coupled by pairs to $J = 0$

- smaller dimension (especially J=0 states)
- allows truncations with seniority : heavy spherical nuclei .
- less sparse

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Limitations

M-scheme: size of the basis.

Coupled scheme: number of non-zero.

	Dimensions			$\mathcal{H}_{IJ} \neq 0$		
	M=0	$\frac{(M=0)}{(J=0)}$	$\frac{(M=0)}{(J=4)}$	M=0	$\frac{(J=0)}{(M=0)}$	$\frac{(J=4)}{(M=0)}$
^{48}Cr	$1.9\ 10^{6}$	48.	8.	$0.8\ 10^{9}$	0.6	17.
^{52}Fe	$1.1\ 10^{8}$	61.9	9.	$7.4\ 10^{10}$	2.4	83.
^{56}Ni	$1.1\ 10^{9}$	70.4	10.	$9.6\ 10^{11}$	5.	194
^{60}Zn	$2.3\ 10^{9}$	73.3	10.	$2.2\ 10^{12}$	7.	254.
^{108}Xe	$3.7\ 10^{7}$	97.	13.	$1.6\ 10^{10}$	1.1	50.
^{110}Xe	$8.5\ 10^{8}$	118.	15.	$5.2\ 10^{11}$	3.5	171.
^{112}Xe	$9.3\ 10^{9}$	135.	17.	$2.2\ 10^{12}$	8.7	436.

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M scheme

WHITEHEAD method (1977)

At each Slater Determinant K is associated an integer number W(K).
At each individual state i=nljmτ is associated a bit of this number.
This bit will be put at 1 or 0 following that the state is occupied or not.
These integer numbers W(K) are ordered .
Th Hamiltonian is written in the decoupled basis $V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$
At each Lanczos iteration the code works as it follows

- 1) Loop on K
- 2) Loop on the operators $a_i^\dagger a_j^\dagger a_k a_l$
- 3) Check bit(k)=bit(l)=1 and bit(i)=bit(j)=0 If not continue 2)
- 4) $W_0 = W(K) - bit(k) - bit(l) + bit(i) + bit(j)$
- 5) By the bisection method identify $W_0 = W(J)$
- 6) Calculate the phase (permution of the operators) and get $H_{KJ} = \pm V_{ijkl}$

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M scheme

ANTOINE SM code (1988-20..) (available on the web).
Each state of the basis is now the product of 2 Slater Determinants:

$$|K\rangle = |i\alpha\rangle$$

$i \longrightarrow$ SD for protons
$\alpha \longrightarrow$ SD for neutrons
dim(i),dim(α) $\ll$ dim(K)

^{56}Ni dim(K)=10^9 dim(i,α)=$1.25 * 10^5$

Precalculations (storage) done apart for each subspace i and α using the Whitehead Method.
The pn NBME are generated with 3 integer additions.

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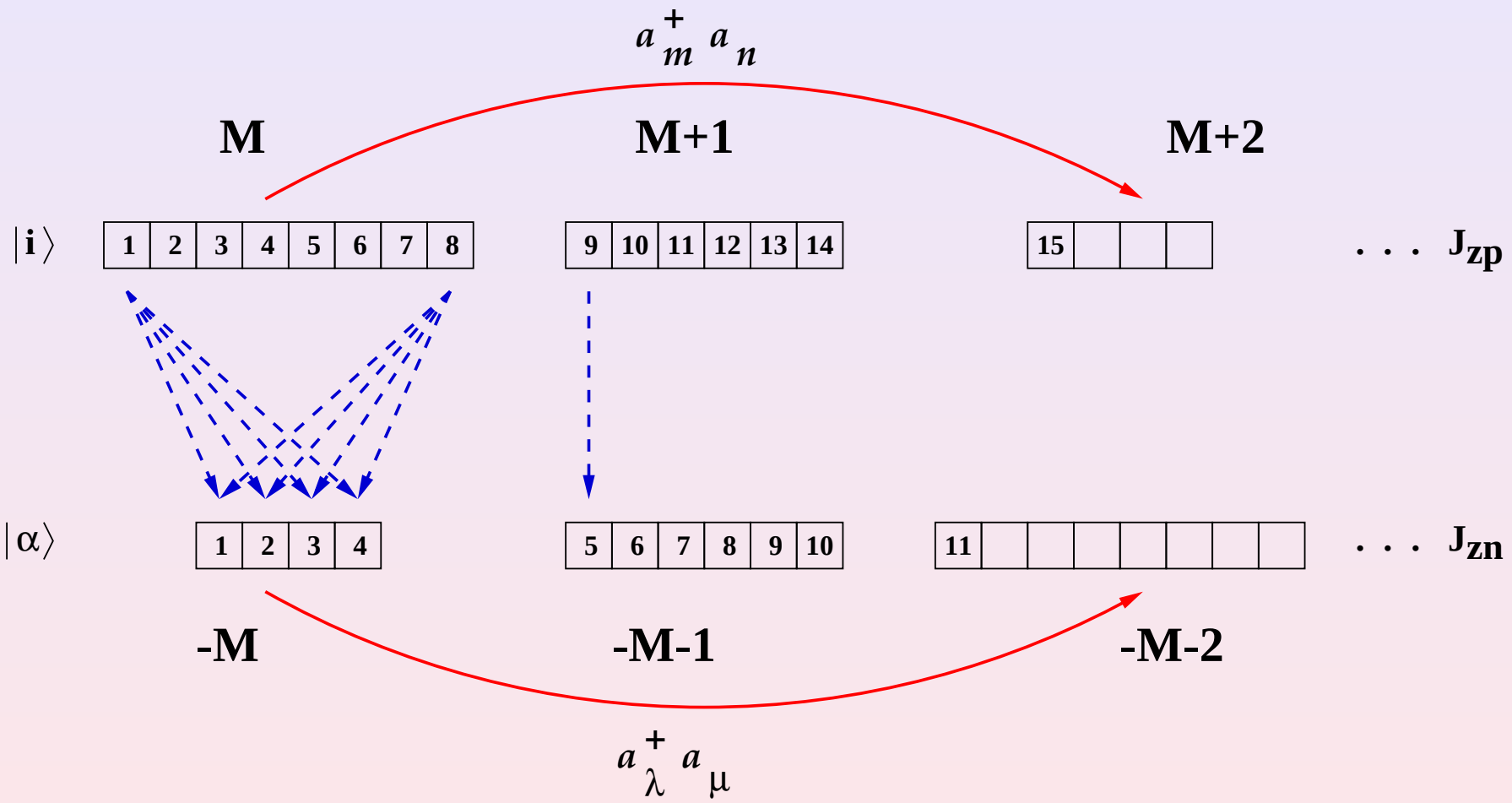
M scheme basis



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Limitations

- Disk Capacity: storage of Lanczos vectors
- RAM Memory : must contain 2 Lanczos vectors

splitting of the initial and final vectors

$$\Psi_{i,f} = \bigcup_m \Psi^m_{i,f}$$

$$\Psi^{(m)}_f = \sum_n \mathcal{H}^{(m,n)} \Psi^{(n)}_i$$

It solves the problem of the RAM memory but increases the CPU time:

- time acess to the disk
- $H(I,J)$ and $H(J,I)$ must be generated separately.

It is a natural way for parallelization .

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Coupled code

same separation of p and n subspaces $|I\rangle \equiv |i\alpha\rangle$
We have now J instead of M.

H_{nn} and H_{pp} always

$$\langle I|\mathcal{H}_{pp}|J\rangle \;=\; \langle i\alpha|\mathcal{H}_{pp}|i'\alpha'\rangle \;=\; h_{ii'}\;\delta_{\alpha\alpha'}$$

$$\langle I|\mathcal{H}_{nn}|J\rangle \;=\; \langle i\alpha|\mathcal{H}_{nn}|i'\alpha'\rangle \;=\; \delta_{ii'}\;h_{\alpha\alpha'}$$

for H_{pn} we have now generalized CFP coefficients

$$\langle I|\mathcal{H}_{pn}|J\rangle \;=\; \langle i\alpha|\mathcal{H}_{pn}|i'\alpha'\rangle \;=\; c_{ii'}\;c_{\alpha\alpha'}V(K)$$

Non-zero are generated with 3 integer additions (idem M scheme) + 2 floating multiplications.

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Coupled code

small dimensions but huge number of NBME.

natural way for parallelization : splitting of H

$$H = \sum_k H^{(k)}$$

Each processor has the initial and calculate a final vector:

$$\Psi_f^{(k)} = \mathcal{H}^{(k)} \Psi_i$$

Final vectors are added :

$$\Psi_f = \sum_k \Psi_f^{(k)}$$

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Conclusions

Progress in Computers and in Codes have allowed a strong increase of the domain of applicability of Shell Model .

Nuclei $0\nu\beta\beta$ emetters :

^{48}Ca, ^{76}Ge, ^{82}Se, ^{96}Zr, ^{100}Mo, ^{116}Cd, ^{130}Te, ^{136}Xe, ^{150}Nd

10 years ago, only ^{48}Ca could be studied with SM.
Now all of them except ^{150}Nd have been calculated .

Future goal :

- Not to reach dimensions $10^{11,12}$ but reduce the CPU time with Massive Parallelization .
  Calculation of ^{112}Xe : 15 hours (minutes !!) instead of 15 days .
- 3-body forces

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