Large Scale Shell Model Calculations with a New Algorithm

D. Bianco

Naples

F. Andreozzi

N. Lo Iudice

A. Porrino

F. Knapp

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Currently adopted methods

- Direct Diagonalization: Lanczos:Antoine (E. Caurier et al. Rev. Mod. Phys. 77, 427 (2005) for short review)
- Stochastic methods: Monte Carlo (C.W. Johnson et al. PRL 92), suitable for ground state. *Minus sign* problem.
- Truncation methods:

- Importance Sampling: Quantum MC (M. Honma et al. PRL 95) selects the relevant basis states.

--Density Matrix Renormalization Group (DMRG) (J. Dukelsky and S. Pittel, Rep. Prog. Phys. 67, 513 (2004)

Iterative diagonalization algorithm

A. Andreozzi, A. Porrino, and N. Lo Iudice J. Phys. A 02

- Let $I = \Sigma\, |i\rangle\langle i|$

$$A\ (= A^{\dagger})\ \equiv \{\, a_{ij}\,\} = \{\, \langle\, i\, |\, \hat{A}\, |\, j\, \rangle\, \}$$

In our case A=H

$$A \equiv \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots\cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & a_{24} & \cdots\cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdots\cdots & a_{3N} \\ a_{41} & a_{42} & a_{43} & a_{44} & \cdots\cdots & a_{4N} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \\ a_{N1} & \cdots & \cdots & \cdots & \cdots & a_{NN} \end{pmatrix}$$

Goal:

Determine the lowest **eigenvalue** and **eigenvector**

- ***1° iteration loop***

$n_0 << N$

$v < n_0$

$$A_0 = \begin{pmatrix} a_{11}\ a_{12}\ a_{13} & \ldots . a_{1n_0} \\ a_{21}\ a_{22}\ a_{23} & \ldots . a_{2n_0} \\ a_{31}\ a_{32}\ a_{33} & \ldots . a_{3n_0} \\ \ldots\ldots\ldots\ldots\ldots\ldots & \\ a_{n_0 1} \ldots\ldots\ldots\ldots & a_{n_0 n_0} \end{pmatrix} \Rightarrow \Lambda_0 = \begin{pmatrix} \lambda_1 & 0 & \ldots . & 0 \\ 0 & \lambda_2 & \ldots\ldots & 0 \\ \ldots\ldots & & \ldots & \\ 0 & \ldots\ldots\ldots & & \lambda_v \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} \Lambda_0 & B_{01} \\ B_{10} & A_1 \end{pmatrix} \qquad A_1 = \begin{pmatrix} a_{(n_0+1)(n_0+1)} & \ldots\ldots & a_{(n_0+1)n_1} \\ \ldots\ldots\ldots\ldots\ldots\ldots & & \\ \ldots\ldots\ldots\ldots\ldots\ldots & & \\ a_{n_1(n_0+1)} & \ldots\ldots & a_{n_1 n_1} \end{pmatrix}$$

$b_{ij} = \langle j|A|\varphi_i\rangle \qquad i=1,v \qquad j= n_0+1, n_1$

- ***1° iteration loop***

$$\begin{pmatrix} \Lambda_0 & B_{01} \\ B_{10} & A_1 \end{pmatrix} \Rightarrow \Lambda_1 \Rightarrow \begin{pmatrix} \Lambda_1 & B_{12} \\ B_{21} & A_2 \end{pmatrix} \Rightarrow \Lambda_2 \Rightarrow$$

$$\Rightarrow \cdots\cdots\cdots\cdots \Rightarrow \begin{pmatrix} \Lambda_{n-1} & B_{(n-1)n} \\ B_{n(\,n-1)} & A_n \end{pmatrix} \Rightarrow \Lambda_n$$

$$\Lambda_n \equiv E^{(1)}, \qquad |\varphi_N> = |\,\Psi^{(1)}> = \sum c_i^{(1)}\,|\,i> \quad i = 1, N$$

End first iteration loop

- ***2° iteration loop***

$$\begin{pmatrix} E_0^{(1)} & B_0 \\ B_0 & A_0 \end{pmatrix} \Rightarrow E_1^{(1)} \Rightarrow \begin{pmatrix} E_1^{(1)} & B_1 \\ B_1 & A_1 \end{pmatrix} \Rightarrow E_2^{(1)} \Rightarrow$$

$$\Rightarrow \cdots\cdots\cdots\cdots \Rightarrow \begin{pmatrix} E_n^{(1)} & B_n \\ B_n & A_n \end{pmatrix} \Rightarrow E^{(2)}$$

$E^{(2)}$, $\qquad | \Psi^{(2)} > = \sum c_i^{(2)} | i > \quad i = 1, N$

End 2° iteration loop

Iteration loops

$E^{(1)}, \Psi^{(1)}$ $E^{(2)}, \Psi^{(2)}$ .... $E^{(i)}, \Psi^{(i)}$ .....

THEOREM

If the sequence $E^{(i)}$ converges , then

$$E^{(i)}\, \Psi^{(i)} \longrightarrow E\, \Psi = H\, \Psi$$

Features of the algorithm

- Easy implementation
- Variational foundation
- Robust

  - Convergence to the extremal eigenvalues

  -- Numerically stable and ghost-free solutions

  --Orthogonality of the computed eigenvectors

- Fast : $O(N^2)$ operations
- But not enough!

M-scheme

- **Virtue** : Construction of H matrix very easy.
- **Shortcoming**: the basis dimensions become huge.
- **Remedy: H is sparse in the m scheme**

M-scheme Implementation

i. Preliminaries

❖ **Sort** $\{j_1^{n1} \ldots j_m^{nm}\}$ (≡ partitions) $n_1 + \ldots n_i + \ldots n_m = v$

(according to **increasing energies)**

❖ Choose D

$$\mathbf{I_d} = \Sigma^d |i\rangle\langle i| = \Sigma^d \; | j_1^{n1} \ldots j_m^{nm} \rangle \langle j_1^{n1} \ldots j_m^{nm} |$$

Property

$$J_k \; | j_1^{n1} \ldots j_m^{nm} \rangle \; \in D$$

❖ **New Hamiltonian**

$$\mathbf{H_J = H + c} \, [\hat{\mathbf{J}}^2 - J(J+1)]$$

ii. Space decomposition

$$\mathbf{I} = \mathbf{M_0} \oplus \mathbf{M_1} \oplus \ldots\ldots\ldots \oplus \mathbf{M_p}$$

Property

$|i>_i \subset \mathbf{M_i}$ $\longrightarrow$ $H\ |i>_i \subset \mathbf{M_{i-1}} \oplus \mathbf{M_i} \oplus \mathbf{M_{i+1}}$

iii. Starting iteration

M_0 $\longrightarrow$ $\Lambda_0(v) \equiv \{(E_1^{(0)}\ \psi_1^{(0)})\ \ldots\ (E_v^{(0)},\ \psi_v^{(0)})\}$

$H\ \psi_k^{(0)} \subset \mathbf{M_0} \oplus \mathbf{M_1}$

$\downarrow$

$\Lambda_0(v) \oplus M_1$ $\longrightarrow$ $\Lambda_1(v) \equiv \{(E_1^{(1)}\ \psi_1^{(1)})\ \ldots\ (E_v^{(1)},\ \psi_v^{(1)})\}$

iii. Iterative process

$\Lambda_0(v) \oplus M_1 \longrightarrow \Lambda_1(v) \longrightarrow$

$\cdots\cdots\cdots$

$\longrightarrow \Lambda_{i-1}(v) \oplus M_i \longrightarrow \Lambda_i(v) \longrightarrow$

$\cdots\cdots\cdots$

$\longrightarrow \Lambda_{(p-1)}(v) \oplus M_p \Rightarrow \boxed{\Lambda_p(v) \equiv \{(E_1, \psi_1) \ldots (E_v, \psi_v)\}}$

Analogy: real space (Wilson) e density matrix (White) renormalization group

Importance Sampling

$$\varepsilon_1 > \varepsilon_2 > \ldots\ldots > \varepsilon_{p-1} > \varepsilon_p$$

$$M_0 \longrightarrow \Lambda_0(v) \equiv \{(E_1^{(0)}\,\psi_1^{(0)}) \;\ldots\; (E_v^{(0)}, \psi_v^{(0)})\}$$

1. $|\langle \Psi_k^{(0)}|H|j\rangle|^2 / (a_{jj} - E_k^{(0)}) > \varepsilon_1 \longrightarrow |j\rangle \subset M_1^{(\varepsilon)}$

$$\downarrow$$

$$\Lambda_0(v) \oplus M_1^{(\varepsilon)} \longrightarrow \Lambda_1^{(\varepsilon)}(v)$$

$$\downarrow$$

2. $|\langle \Psi_k^{(1)}|H|j\rangle|^2 / (a_{jj} - E_k^{(1)}) > \varepsilon_2$

$$\downarrow$$

$$\boxed{|j\rangle \subset M_2^{(\varepsilon)} \subset M_1 \oplus M_2}$$

Importance Sampling: Iterative process

$M_0 \longrightarrow \Lambda_0(v)$

$\Lambda_0(v) \oplus M_1^{(\varepsilon)} \longrightarrow \Lambda_1^{(\varepsilon)}(v) \longrightarrow$

$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$

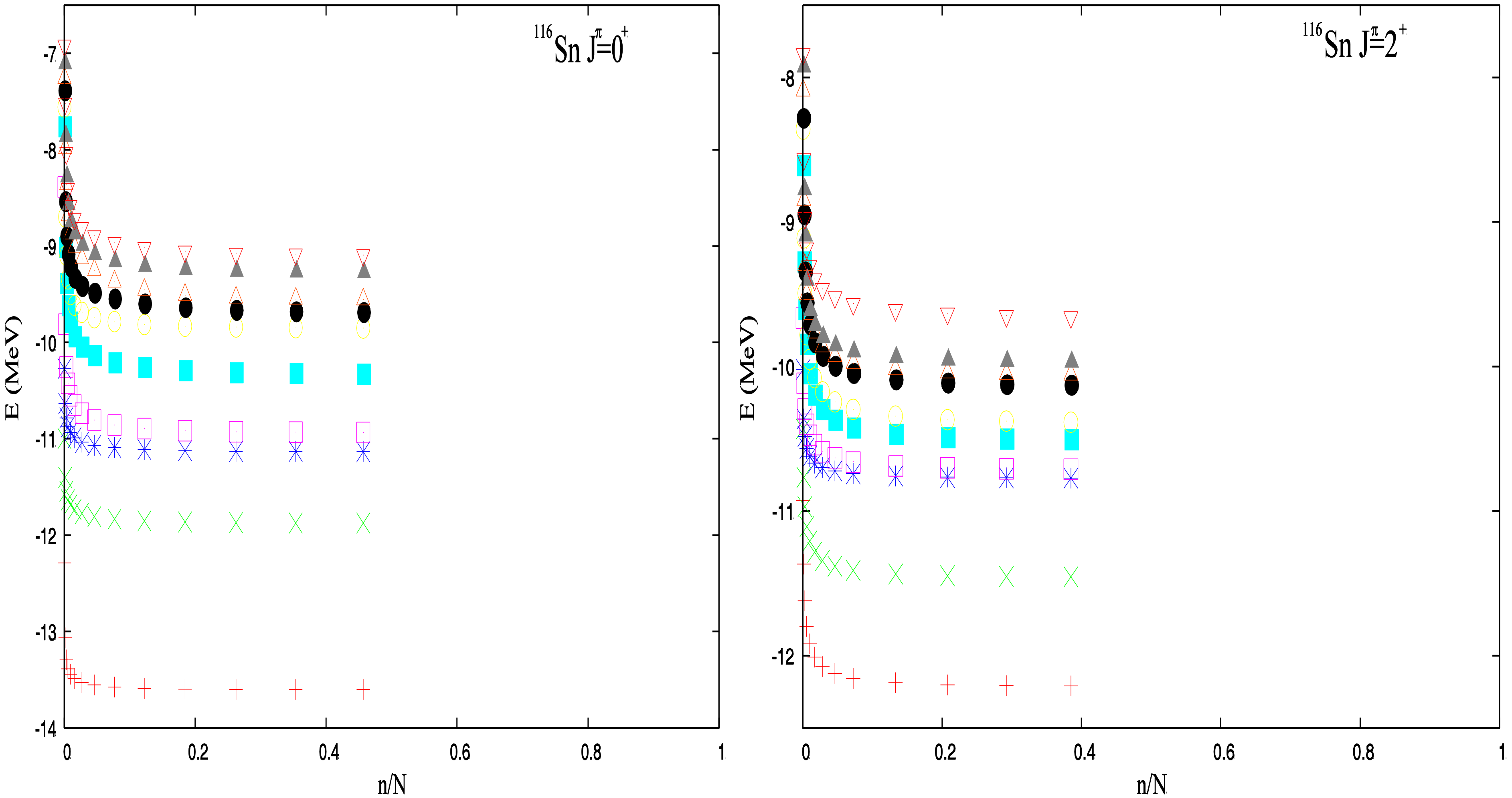
$\longrightarrow \Lambda_{i-1}^{(\varepsilon)}(v) \oplus M_i^{(\varepsilon)} \longrightarrow \Lambda_i^{(\varepsilon)}(v)$

$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$

$\longrightarrow \Lambda_{p-1}^{(\varepsilon)}(v) \oplus M_p^{(\varepsilon)}$

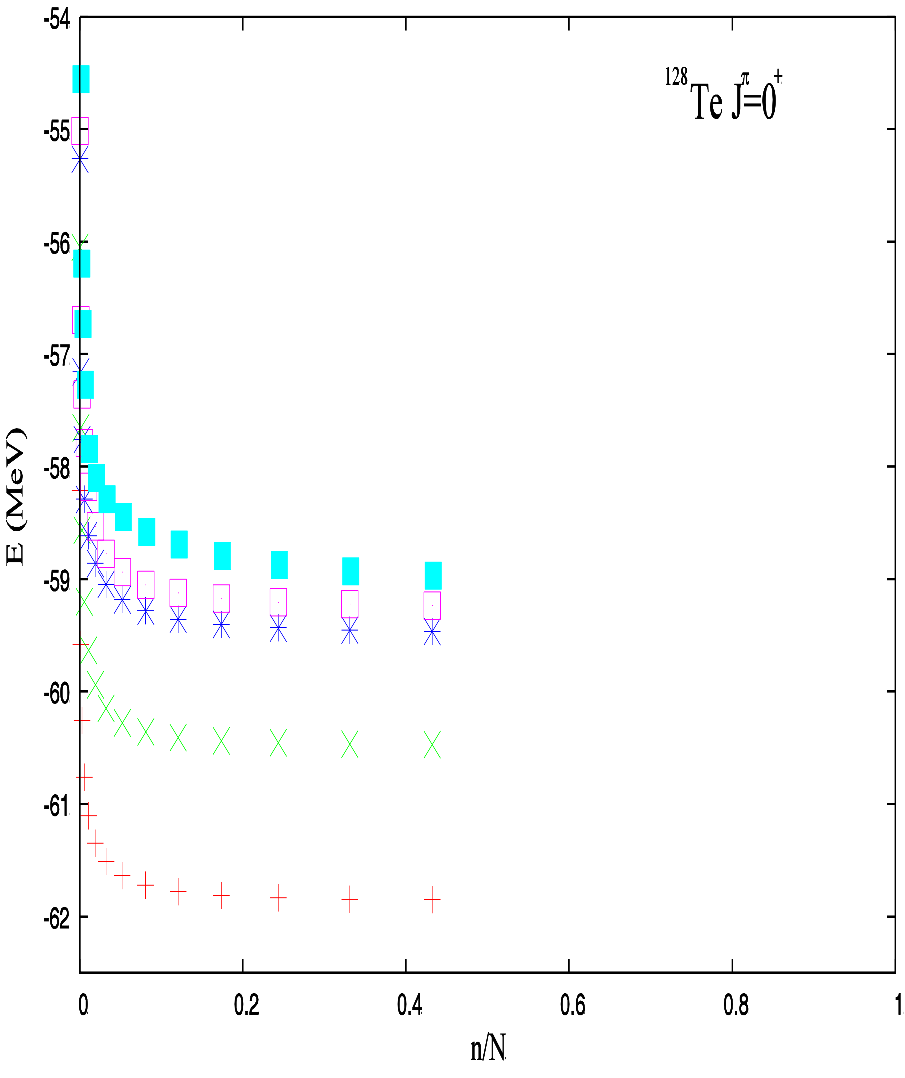
$$\Lambda_p^{(\varepsilon)}(v) \equiv \{(E_1^{(\varepsilon)}, \psi_1^{(\varepsilon)})\ldots(E_v^{(\varepsilon)}, \psi_v^{(\varepsilon)})\}$$

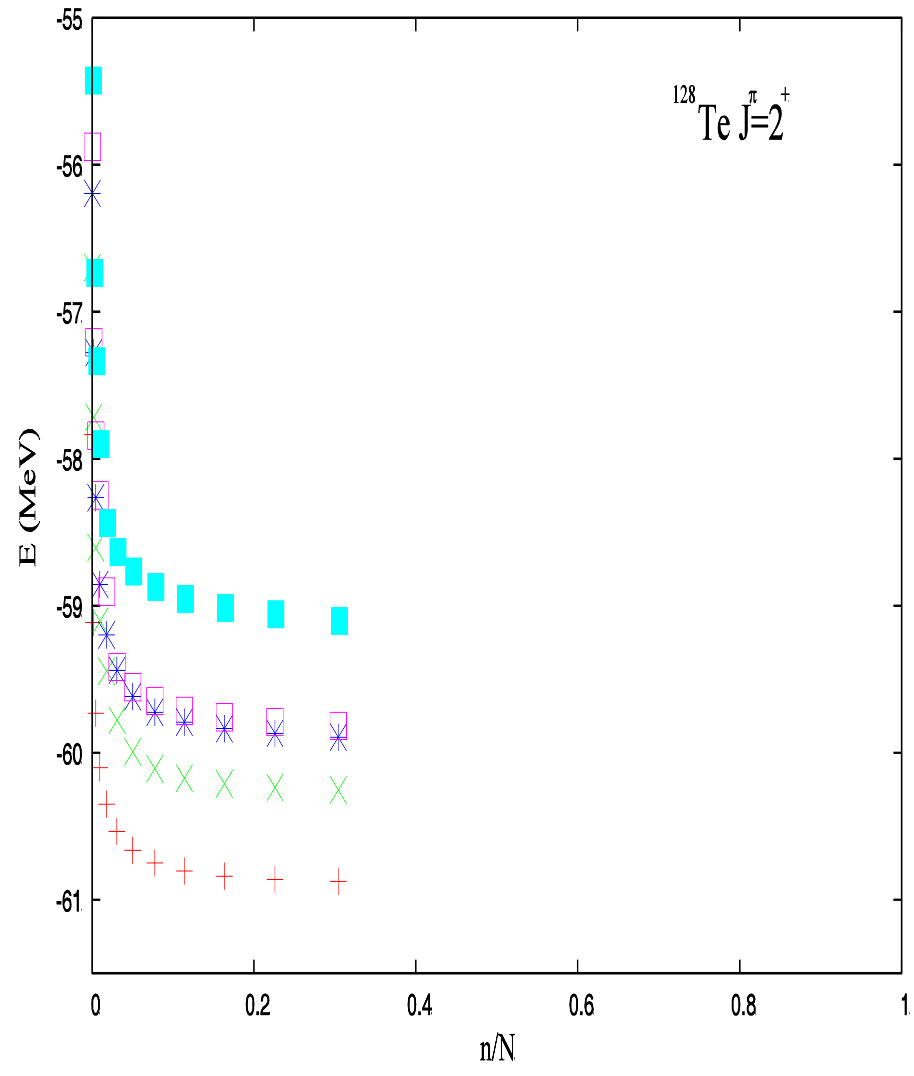
Convergence properties: Eigenvalues



Semimagic nucleus: ^{116}Sn

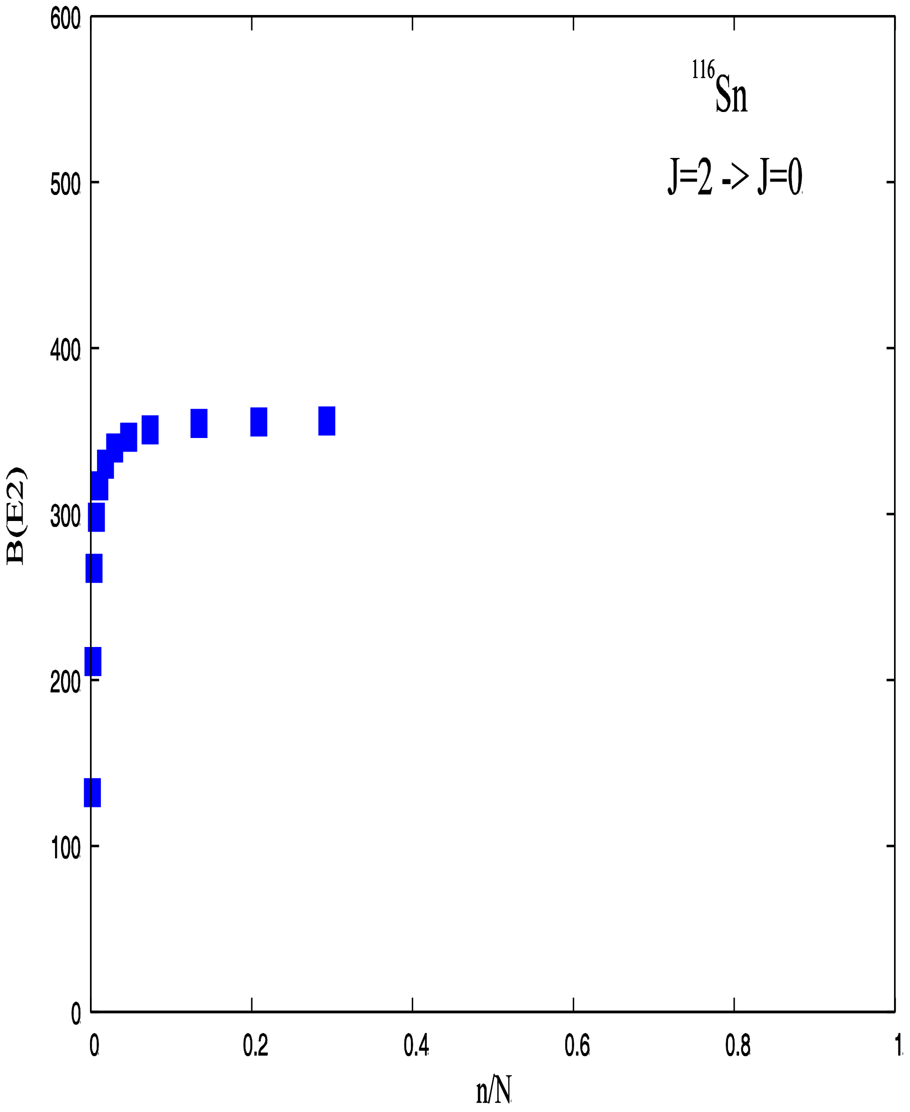
Convergence of Eigenvalues

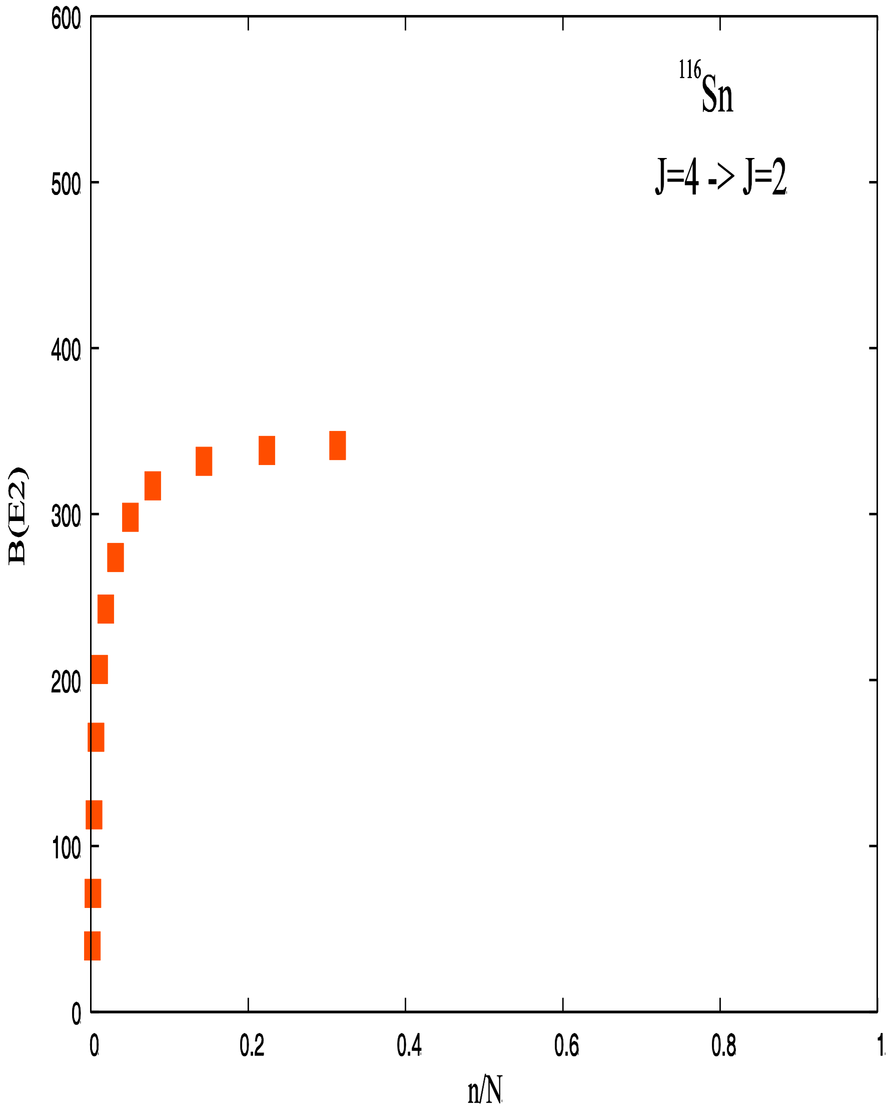




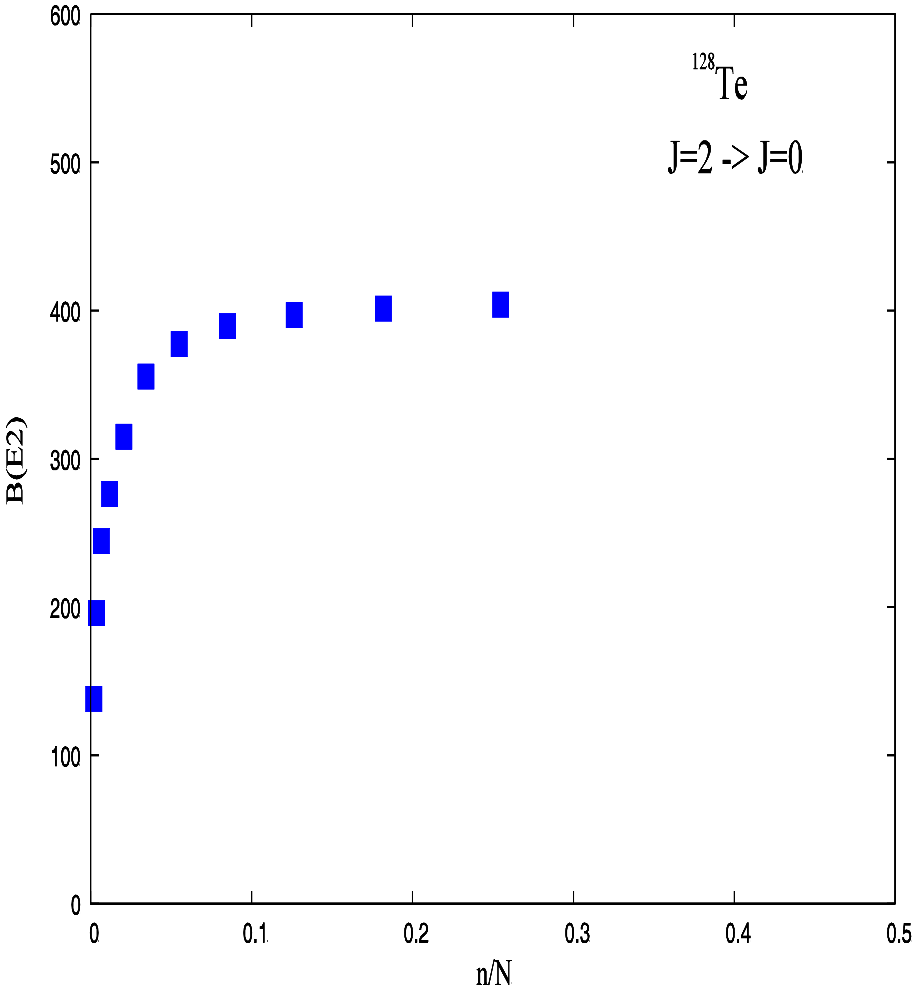
Open shell Nuclei : ^{128}Te

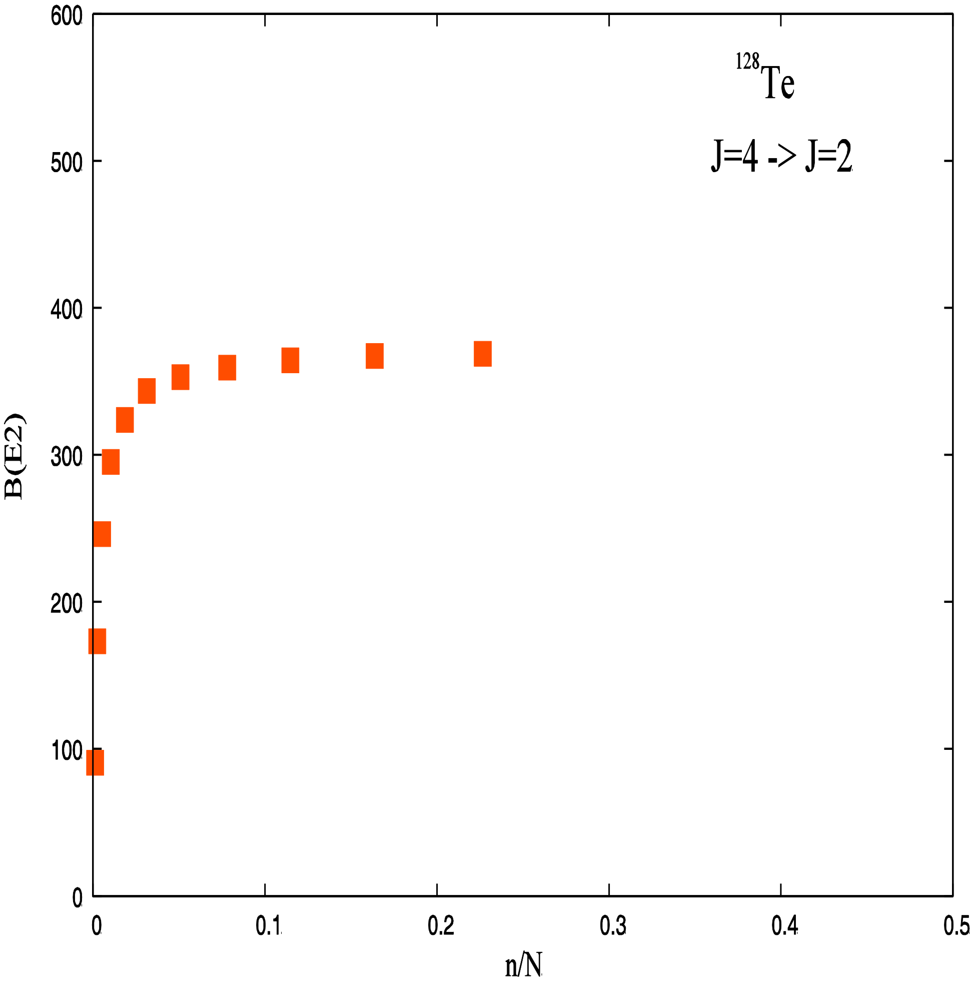
Convergence of B(E2): ^{116}Sn



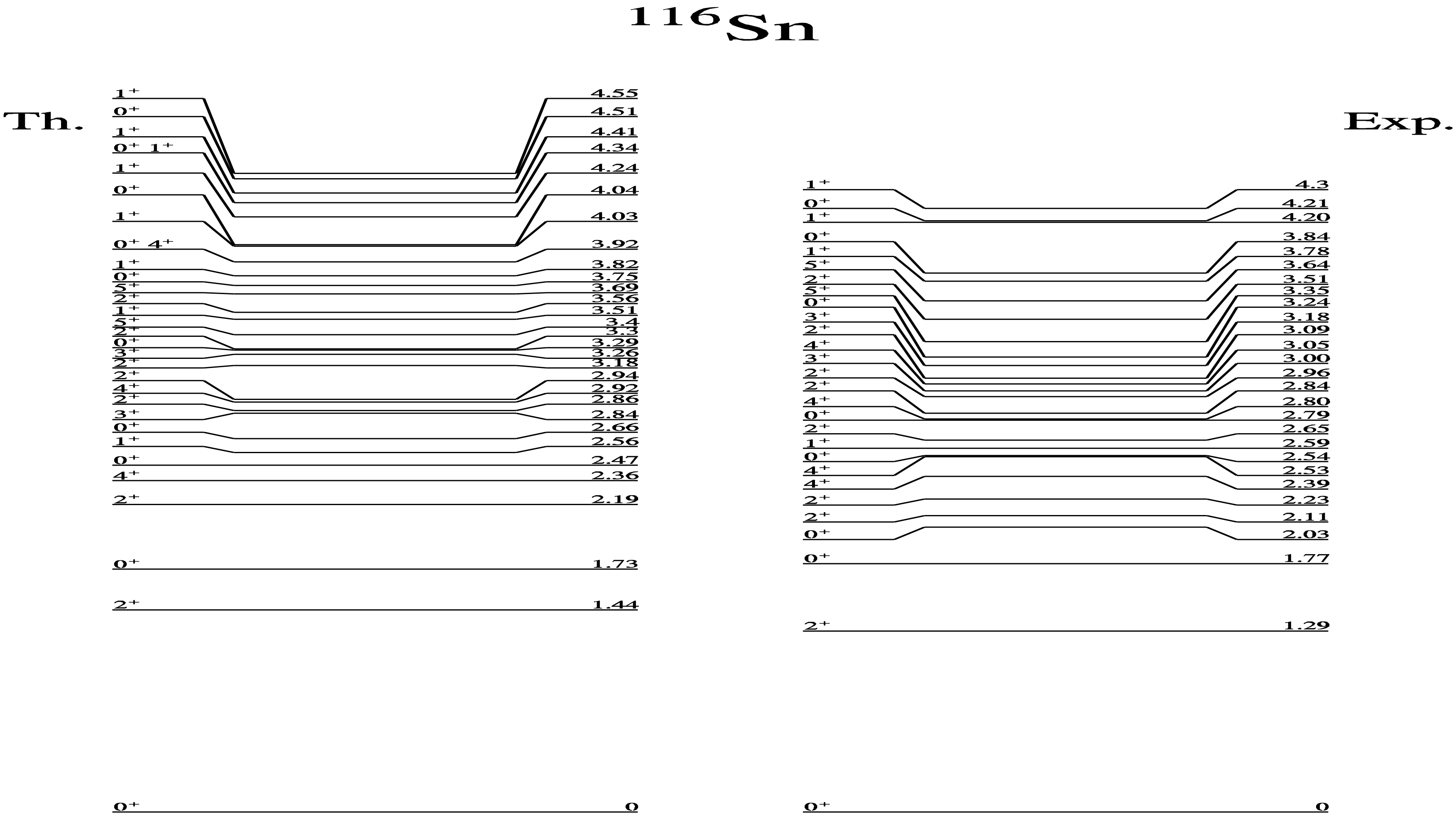


Convergence of B(E2): ^{128}Te





Spectra



116Sn
Th.
Exp.
1+ 4.55
0+ 4.51
1+ 4.41
0+ 1+ 4.34
1+ 4.24
0+ 4.04
1+ 4.03
0+ 4+ 3.92
1+ 3.82
0+ 3.75
5+ 3.69
2+ 3.56
1+ 3.51
5+ 3.4
2+ 3.3
0+ 3.29
3+ 3.26
2+ 3.18
2+ 2.94
4+ 2.92
2+ 2.86
3+ 2.84
0+ 2.66
1+ 2.56
0+ 2.47
4+ 2.36
2+ 2.19
0+ 1.73
2+ 1.44
0+ 0
1+ 4.3
0+ 4.21
1+ 4.20
0+ 3.84
1+ 3.78
5+ 3.64
2+ 3.51
5+ 3.35
0+ 3.24
3+ 3.18
2+ 3.09
4+ 3.05
3+ 3.00
2+ 2.96
2+ 2.84
4+ 2.80
0+ 2.79
2+ 2.65
1+ 2.59
0+ 2.54
4+ 2.53
4+ 2.39
2+ 2.23
2+ 2.11
0+ 2.03
0+ 1.77
2+ 1.29
0+ 0

Conclusions

- The algorithm is simple, robust and has a variational foundation
- Once endowed with the importance sampling,

a) it keeps the extent of space truncation under strict control

b) It reaches saturation very early

c) it allows for extrapolation to exact eigensolutions

THANK YOU