# Complex nuclear spectra in a new Large Scale Shell Model Approach

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Oslo 2011

# Summary

- Nuclear Shell Model
- Diagonalization methods
- A new Iterative diagonalization algorithm (APL)
- Importance sampling algorithm
- Applications to $^{134-130}Xe$

# Nuclear Shell Model

Infinite Space, **A** nucleons

$$H\psi_\alpha = E_\alpha \psi_\alpha$$

Model Space, v nucleons

$$H_{eff}\phi_\alpha = E_\alpha \phi_\alpha$$

$^{116}Sn$, $N \sim 10^7$

$^{130}Xe$, $N \sim 10^9$

$^{128}Xe$, $N \sim 10^{10}$

**Problem** : size of the Hamiltonian matrix too large as A increases

- Since **N** very large

- Standard diagonalization methods very lengthy: $t \propto N^3$

- **However**,

  1. only **n ~1** eigenstates of a given J **needed**

  2. $\{\mathbf{H_{ij}} \neq 0\} \propto \mathbf{N}$

$$\Downarrow$$

**Diagonalization algorithms** identifying the $\mathbf{H_{ij} \neq 0}$ **needed**

# Two alternative methods

-Direct diagonalization: Lanczos

Numerical Implementation: **Antoine**

E. Caurier et al. Rev. Mod. Phys. 77, 427 (2005) for review

**-Stochastic methods**: SM Montecarlo (SMMC)

S. E. Koonin, D.J. Dean, and K.Langanke, Phys. Repts. 278, 2 (1997)

Suitable for **ground state** and **strength functions.**

**MINUS sign problem**

# In between: Truncation methods

**Quantum Montecarlo diagonalization (QMCD)**

(T. Otsuka et al., Prog. Part. Nucl Phys. 46, 319 (2001) for a review)

**Samples** the **relevant** basis states **stochastically**

Problems: Redundancy, symmetries broken by the stochastic procedure.

**D**ensity**M**atrix**R**enormalization**G**roup

J. Dukelsky and S. Pittel, Rep. Prog. Phys. 67, 513 (2004)

borrowed from condensed matter

S. R. White PRL 69, 2863 (1992)

# Diagonalization algorithm

F. Andreozzi, A. Porrino, and N. Lo Iudice, J. Phys. A 35, L61 (2002)

F. Andreozzi, N. Lo Iudice, A. Porrino, J. P. G 29, 2319 (2003)

**Iterative generation of an eigenspace**

- A → Symmetric matrix representing a self-adjoint operator in an orthonormal basis

$$\{ |1\rangle, |2\rangle, \ldots, |N\rangle \}$$

- A → $\{ a_{ij} \} = \{ \langle i | \hat{A} | j \rangle \}$

- Lowest eigenvalue and eigenvector

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

# Iterative diagonalization

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \Rightarrow \quad \lambda_2 \quad | \varphi_2 > = c_1^{(2)} |1> + c_2^{(2)} |2>$$

Update $\quad \mathbf{b_3} = < \varphi_2 | \hat{A} | 3 >$

$$\begin{pmatrix} \lambda_2 & b_3 \\ b_3 & a_{33} \end{pmatrix} \Rightarrow \quad \lambda_3 \quad | \varphi_3 > = c_1^{(3)} |1> + c_2^{(3)} |2> + c_3^{(3)} |3>$$

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• • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • •

**Update** $b_N = < \varphi_{N-1} | \hat{A} | N >$

| | |
|---|---|
| $\lambda_{N-1}$ | $b_N$ |
| $b_N$ | $a_{NN}$ |

$$\lambda_N \equiv E^{(1)}$$

$$|\varphi_N> = |\Psi^{(1)}> = \sum_{i=1,N} c_i^{(N)} | i >$$

End first iteration loop

# Second iteration

Def. $|\varphi_1^{(2)}> = |\psi^{(1)}>$ $\lambda_1^{(2)} = E^{(1)}$

$\{ |\boldsymbol{\varphi}_1^{(2)}>, |1> \}$ are not linearly independent

## Generalized eigenvalue problem

$$\mathcal{D}et \left( \begin{pmatrix} \lambda_1^{(2)} & b_1 \\ b_1 & a_{11} \end{pmatrix} - \lambda \begin{pmatrix} 1 & <\varphi_1^{(2)}|1> \\ <\varphi_1^{(2)}|1> & 1 \end{pmatrix} \right) = 0$$

$$E^{(1)}, \mathbf{\Psi}^{(1)} \longrightarrow E^{(2)}, \mathbf{\Psi}^{(2)} \longrightarrow \cdots\cdots$$

# THEOREM

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

$E^{(i)} \longrightarrow E$ (eigenvalue of the matrix A)

$\mathbf{\Psi}^{(i)} \longrightarrow \mathbf{\Psi}$ (eigenvector of the matrix A)

# Simultaneous determination of v eigensolutions

The structure of the algorithm unchanged

$$\begin{pmatrix} \lambda_{j-1} & b_j \\ b_j & a_{jj} \end{pmatrix} \Rightarrow \begin{pmatrix} \Lambda_h & B_h \\ B_h^T & \tilde{\mathbf{A}} \end{pmatrix}$$

$$
\begin{array}{cccccccc}
\lambda_1 & 0 & \ldots & 0 & b_{11} & \ldots & b_{1j} \\
0 & \lambda_2 & \ldots & 0 & b_{21} & \ldots & b_{2j} \\
 & & \ldots & & & \ldots & \\
0 & 0 & \ldots & \lambda_v & b_{v1} & \ldots & b_{vj} \\
b_{11} & & \ldots & b_{v1} & a_{11} & \ldots & a_{1j} \\
b_{12} & & \ldots & b_{v2} & a_{21} & \ldots & a_{2j} \\
 & & \ldots & & & \ldots & \\
b_{1j} & & \ldots & b_{vj} & a_{j1} & \ldots & a_{jj}
\end{array}
$$

# Properties 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
- $O(N)$ operations when the sparsity of H is exploited

# Implementation: Space Decomposition

$$I = M_0 \oplus M_1 \oplus \ldots\ldots\ldots \oplus M_p$$

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

2. $\Lambda_0(v) \oplus M_1$

$$\downarrow$$

$$\Lambda_1(v) \equiv \{(E_1^{(1)}\,\psi_1^{(1)}) \;\ldots\; (E_v^{(1)}, \psi_v^{(1)})\}$$

# Sampling Procedure

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

**accepted only the |j> states fulfilling**

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

**for each $M_i$ subspace**

**$N^0$ of operations $\propto N_{sampled}$**

# Numerical Applications: $^{134-130}$Xe

- **Experimentally** Xe isotopes extensively studied
- T. Ahn et al. Phys.Lett. B **679** (2009) 19–24
- L. Coquard et al. PRC **82**, 024317 (2010)
- L. Bettermann et al. PRC **79,** 034315 (2009)
- H. von Garrel et al. PRC **73,** 054315 (2006)

An important issue:

## Mixed Symmetry States (**MSS**)

- **Theoreticaly** only $^{134}$Xe investigated
- N. Lo Iudice, Ch. Stoyanov , D. Tarpanov PRC **77**, 044310 (2008)
- K. Sieja et al. PRC **80,** 054311 (2009)

Studying $^{132}$Xe and $^{130}$Xe is a challenge

# Proton-Neutron Symmetry

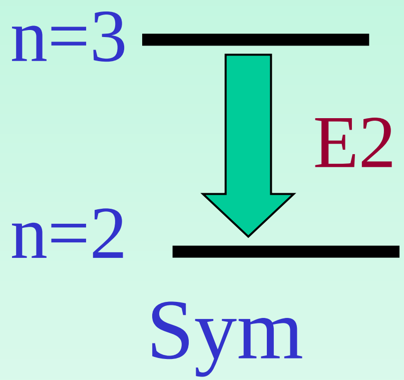
## Symmetric States

$|n, \nu\rangle_s = Q_S^n |0\rangle = (Q_p + Q_n)^n |0\rangle$

**Signature:**

$\mathcal{M}(E2) \propto Q_S$ ($\Delta n=1$)

symmetry preserving ($\Delta F=0$)



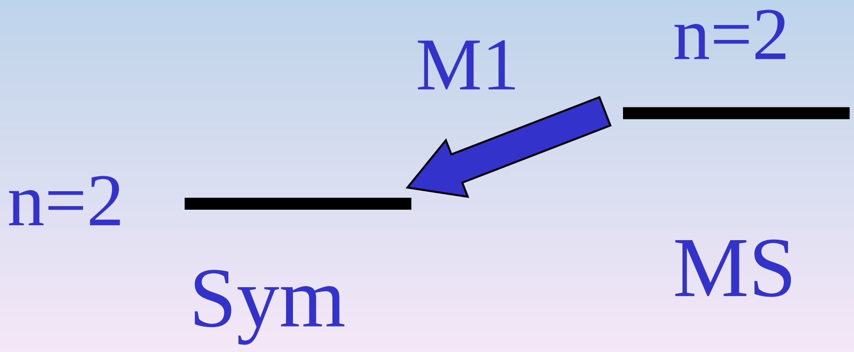

## MS States

$|n, \nu\rangle_{MS} = (Q_p - Q_n)(Q_p + Q_n)^{(n-1)} |0\rangle$

**Signature**

$\mathcal{M}(M1) \propto J_n - J_p$ ($\Delta n=0$)

symmetry changing ($\Delta F=1$)



# Numerical Applications: $^{134-130}Xe$

**Model space**: 0-hω
N=4 major shell

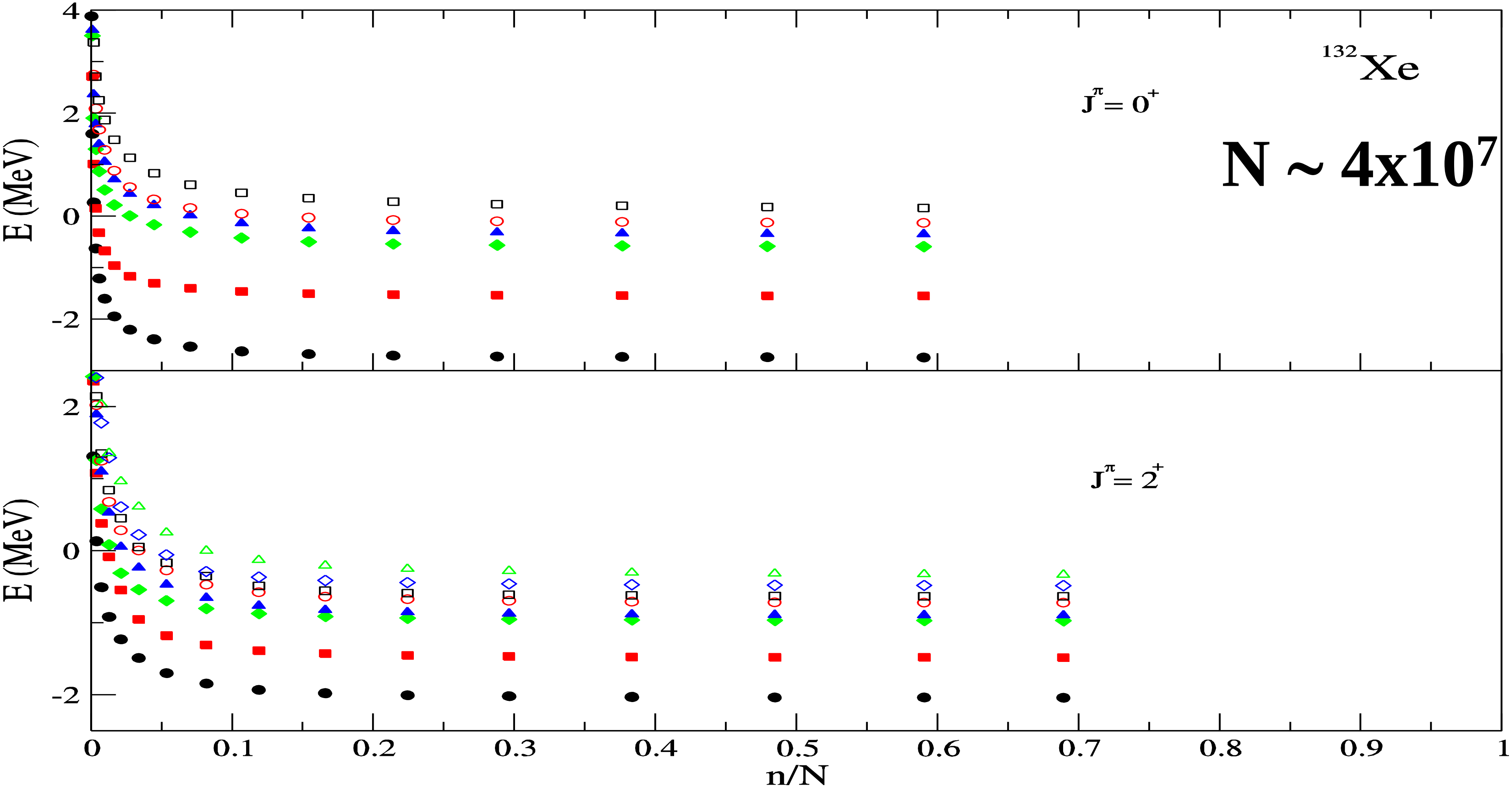
**M**≡{0g7/2, 1d5/2, 1d3/2, 2s1/2, 0h11/2}

**S.p. basis:** Nilsson

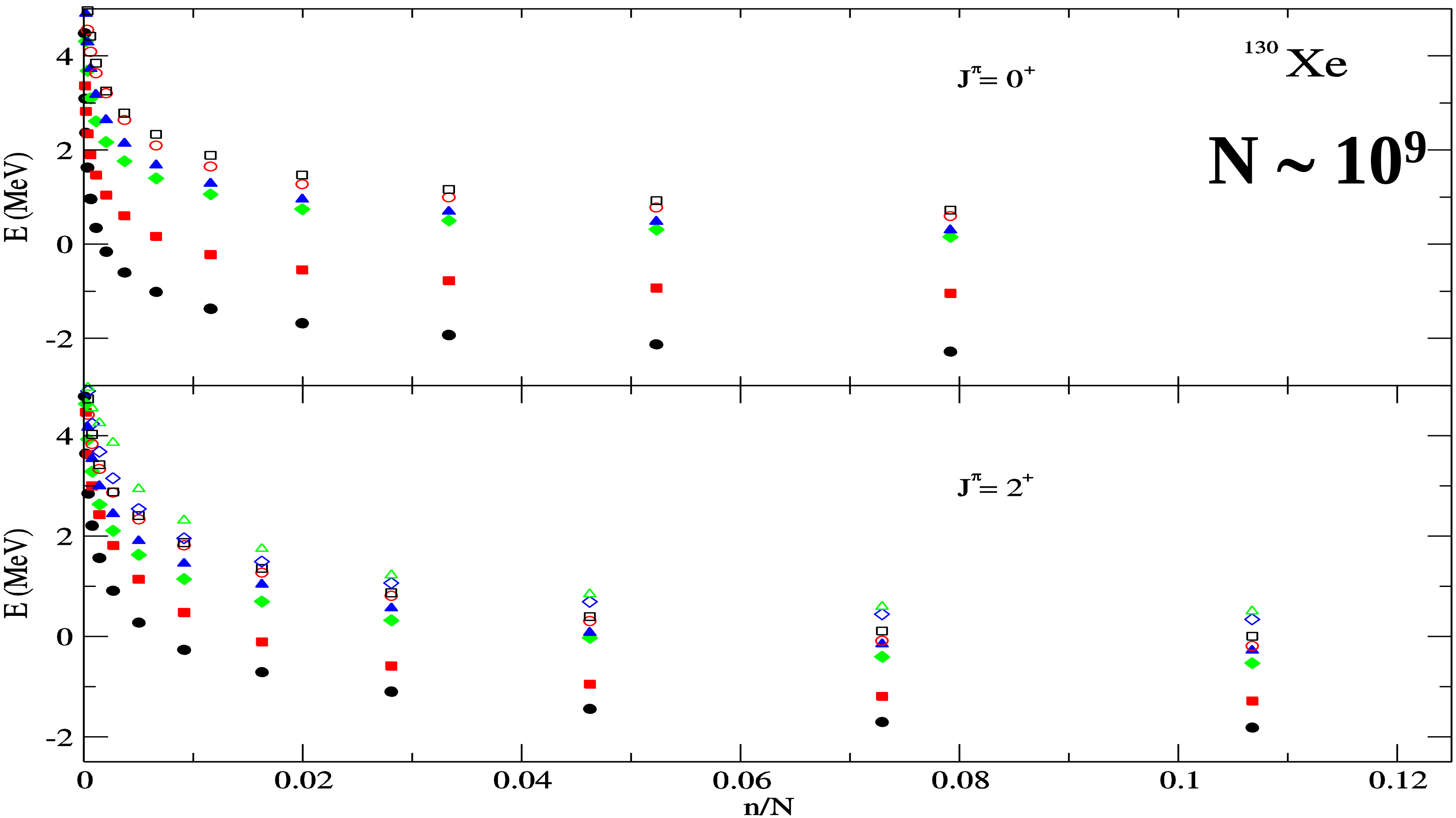
**Two-body Potential**

**G-matrix** derived from **CD-Bonn** potential

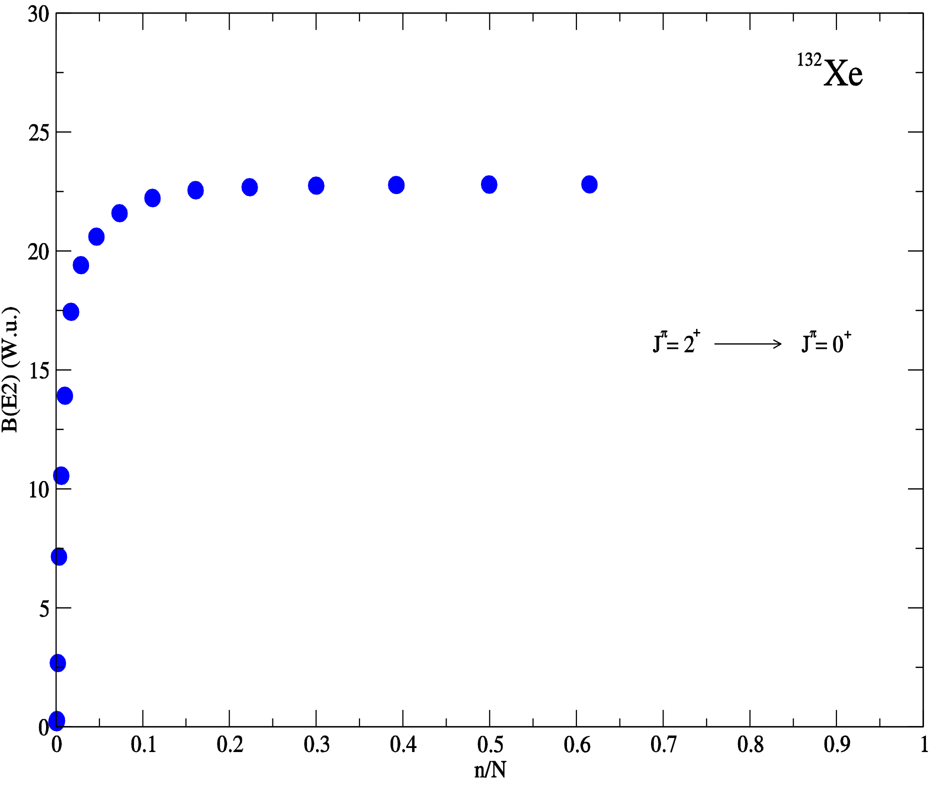
# **Convergence** properties: **Energies**

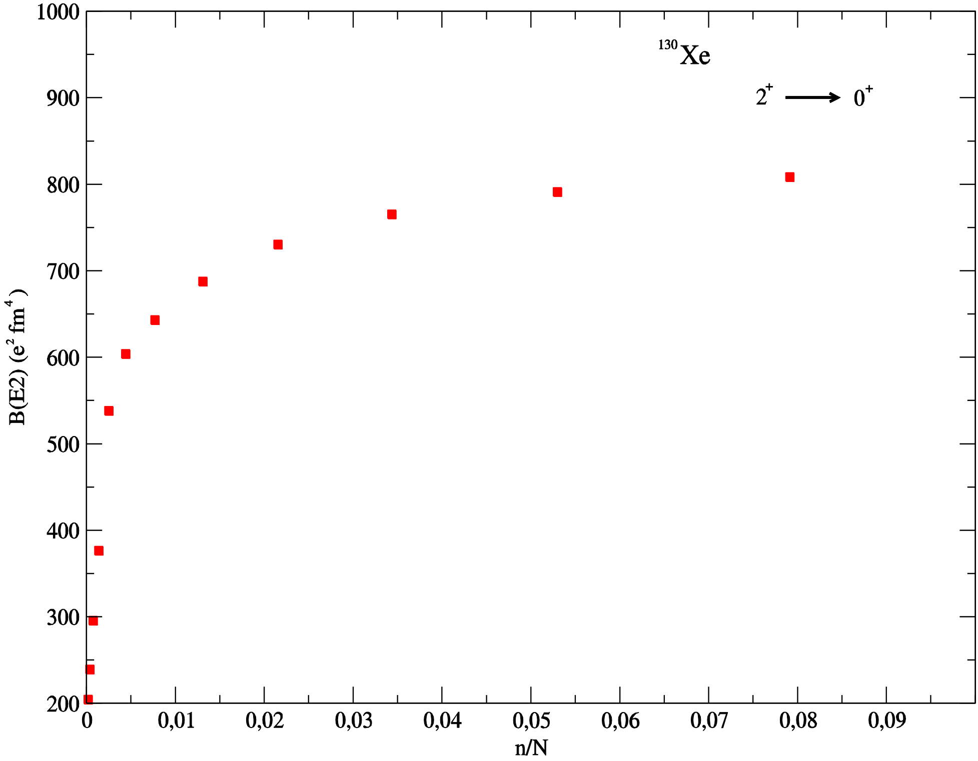


# **Convergence** properties: **Energies**

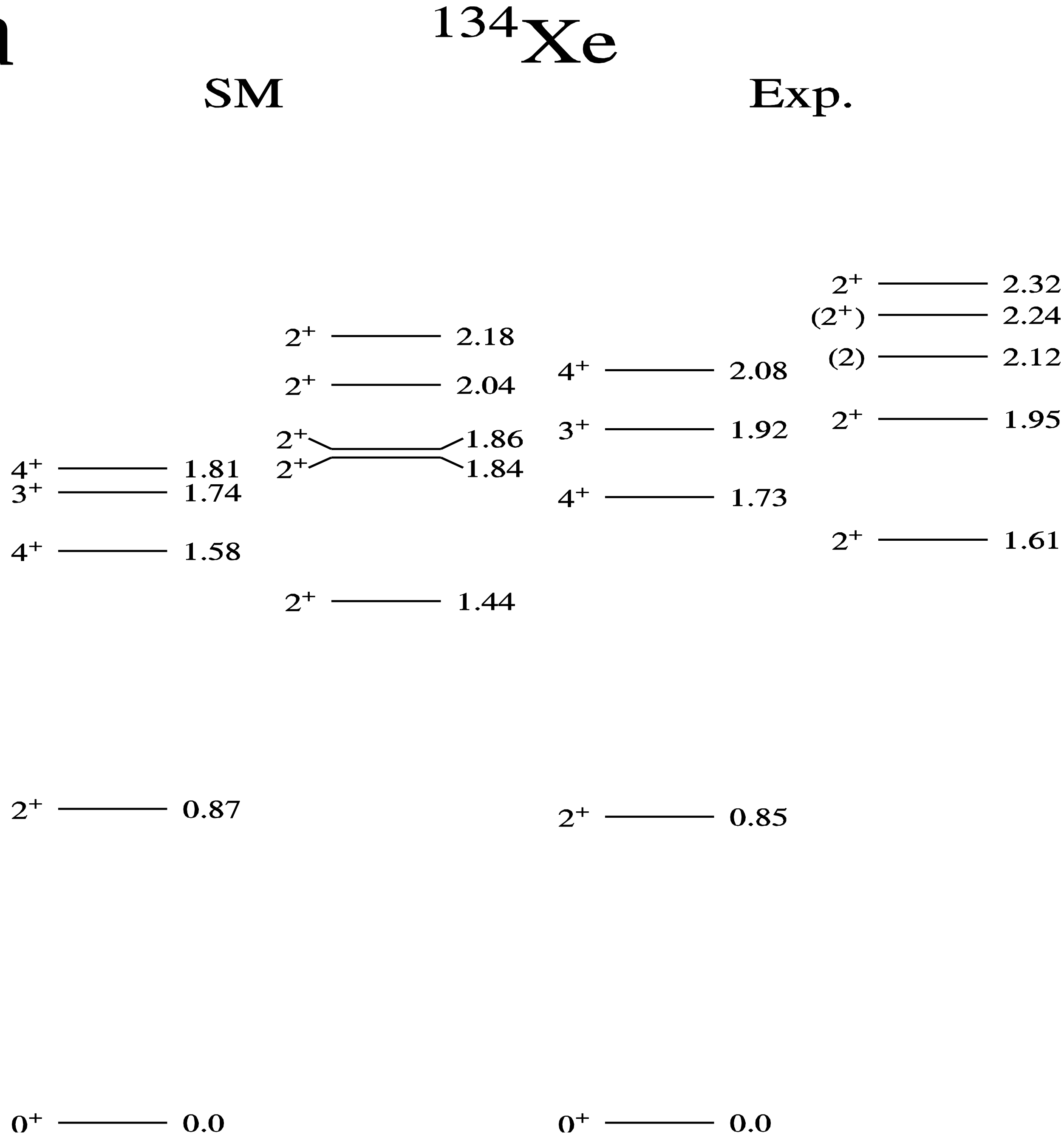


# **Convergence** properties: **B(E2)**

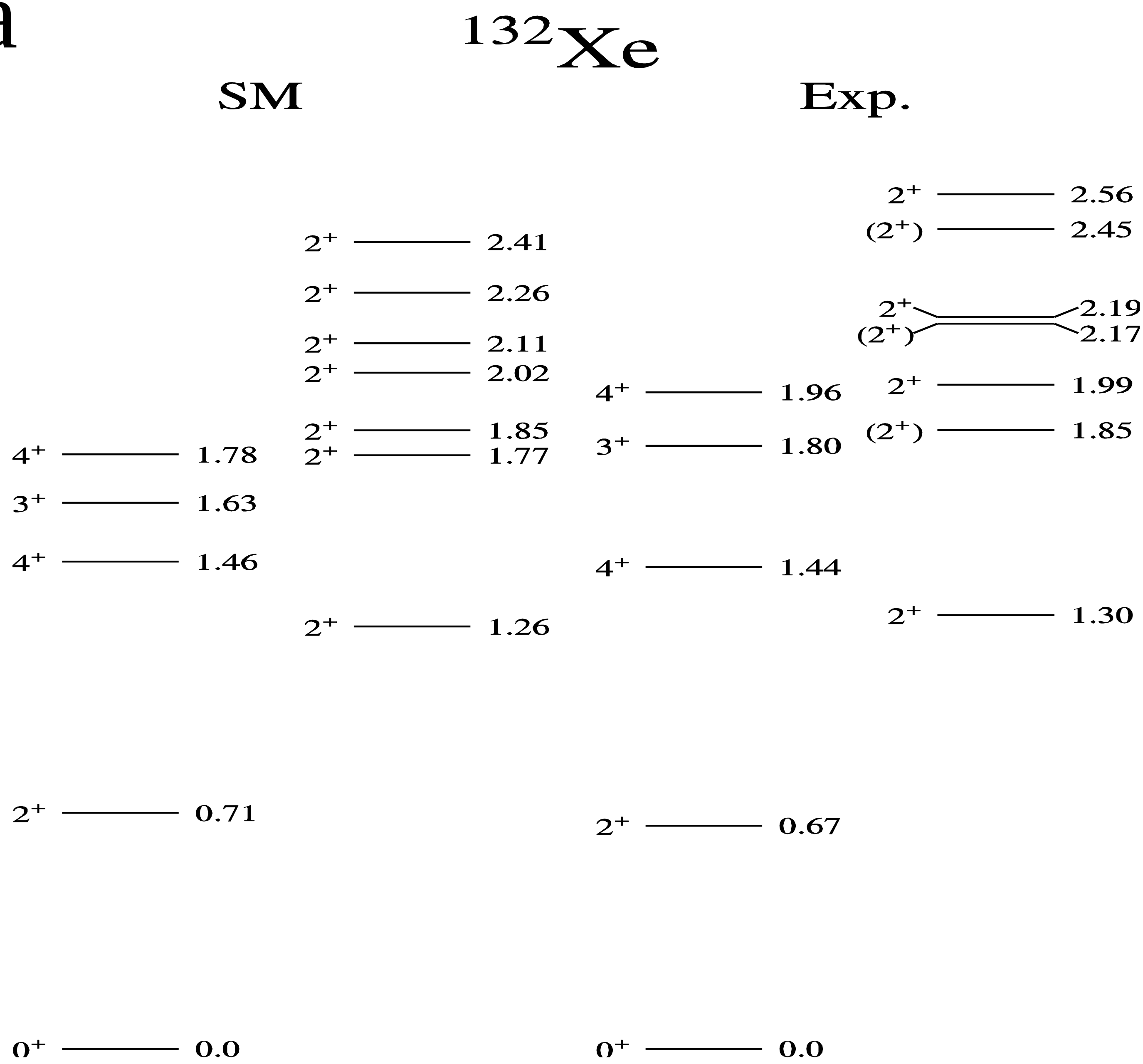


# Spectra

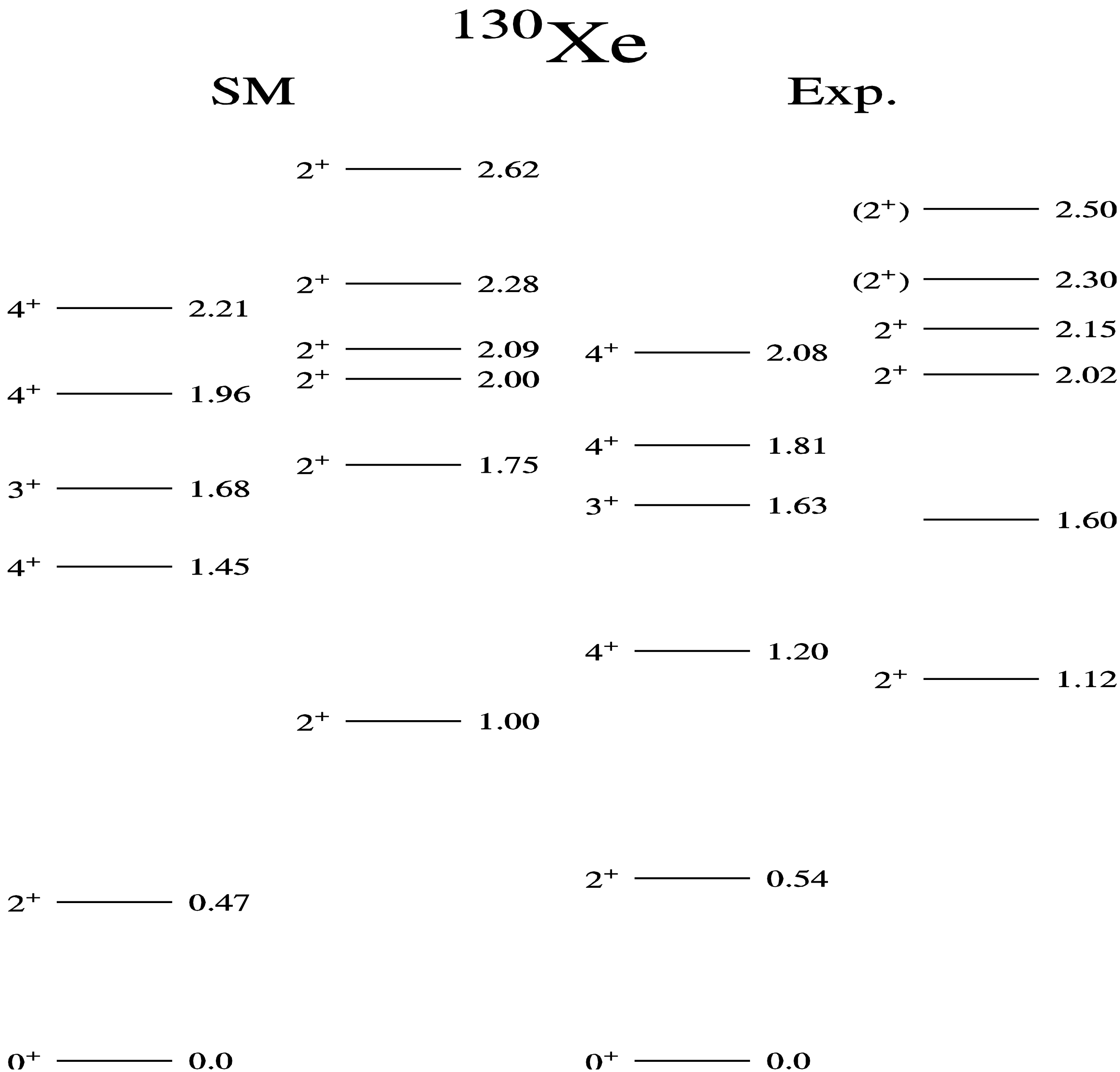

$^{134}$Xe
SM
Exp.
2+ 2.18
2+ 2.04
2+ 1.86
2+ 1.84
4+ 1.81
3+ 1.74
4+ 1.58
2+ 1.44
2+ 0.87
0+ 0.0
2+ 2.32
(2+) 2.24
(2) 2.12
4+ 2.08
2+ 1.95
3+ 1.92
4+ 1.73
2+ 1.61
2+ 0.85
0+ 0.0

# spectra



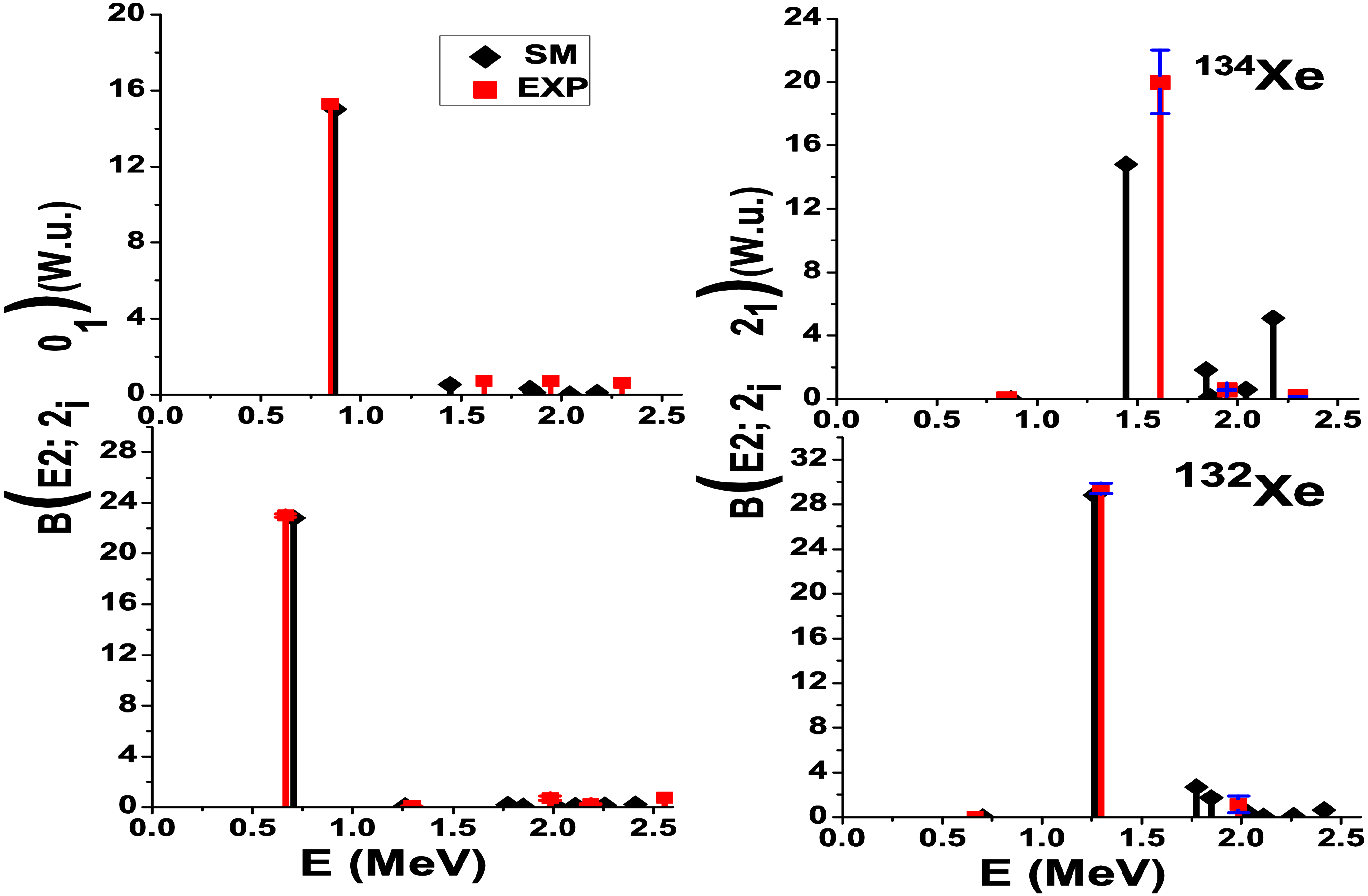
$^{132}$Xe
SM
Exp.
2+ 2.41
2+ 2.26
2+ 2.11
2+ 2.02
2+ 1.85
2+ 1.77
4+ 1.78
3+ 1.63
4+ 1.46
2+ 1.26
2+ 0.71
0+ 0.0
2+ 2.56
(2+) 2.45
2+ 2.19
(2+) 2.17
4+ 1.96
2+ 1.99
(2+) 1.85
3+ 1.80
4+ 1.44
2+ 1.30
2+ 0.67
0+ 0.0

# Spectra

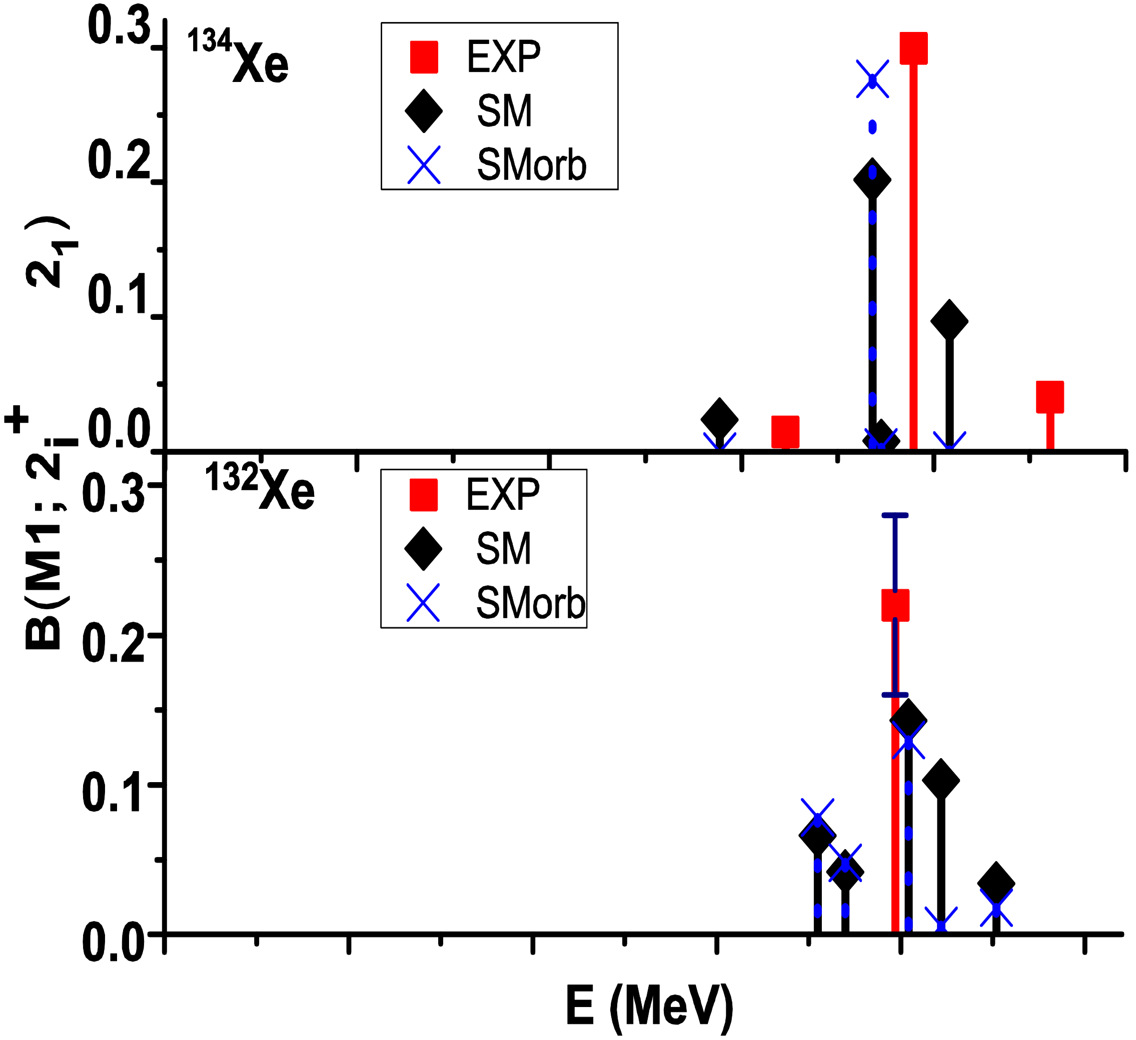


130Xe
SM
Exp.
2+ 2.62
(2+) 2.50
(2+) 2.30
4+ 2.21
2+ 2.28
2+ 2.15
2+ 2.09
4+ 2.08
2+ 2.02
2+ 2.00
4+ 1.96
4+ 1.81
2+ 1.75
3+ 1.68
3+ 1.63
1.60
4+ 1.45
4+ 1.20
2+ 1.12
2+ 1.00
2+ 0.54
2+ 0.47
0+ 0.0
0+ 0.0

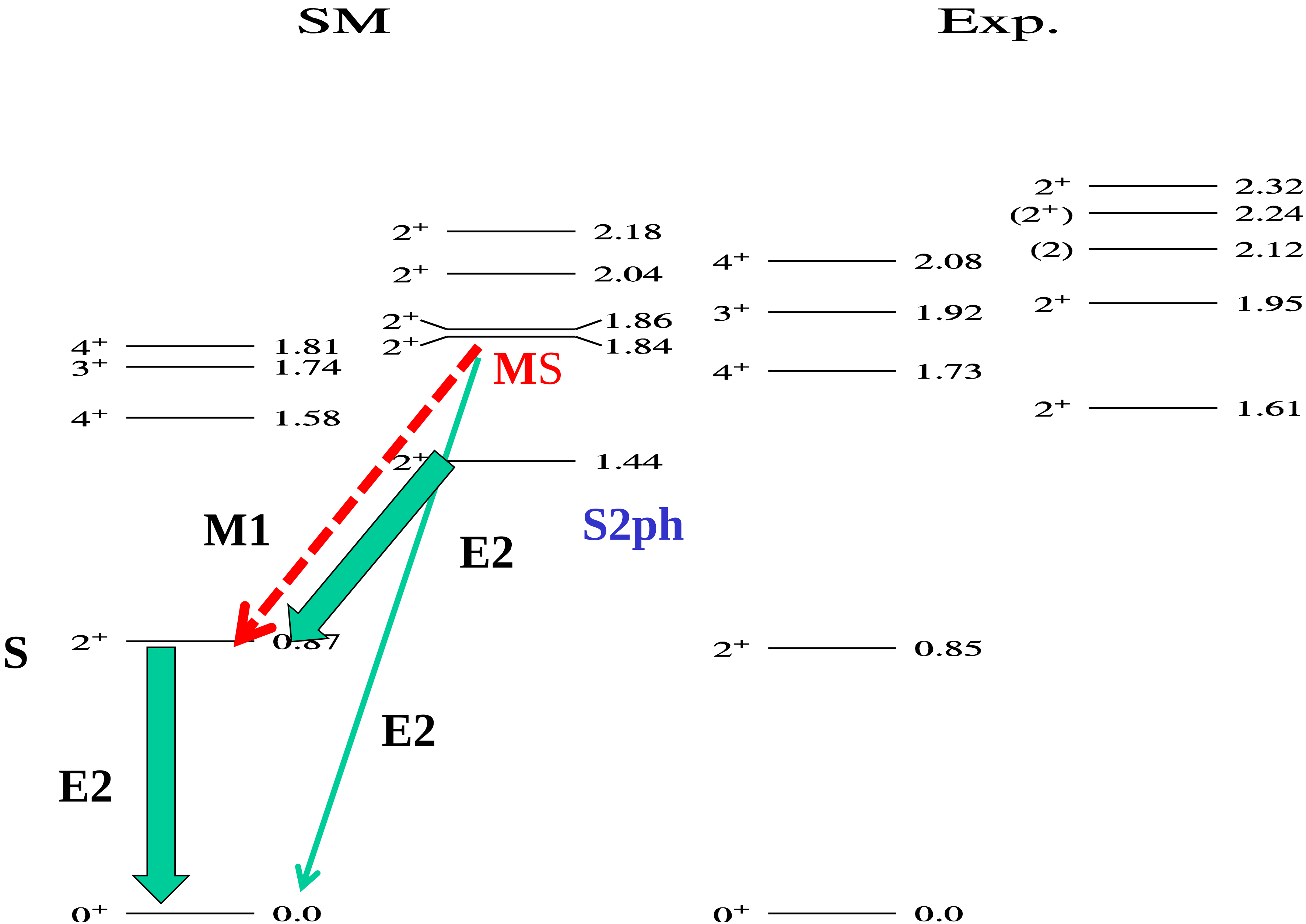
# E2 Transitions



# M1 Transitions



# $^{134}$Xe



SM
Exp.
2+ 2.18
2+ 2.04
2+ 1.86
2+ 1.84
4+ 1.81
3+ 1.74
4+ 1.58
MS
2+ 1.44
S2ph
M1
E2
S
2+ 0.87
E2
E2
0+ 0.0
4+ 2.08
3+ 1.92
4+ 1.73
2+ 0.85
0+ 0.0
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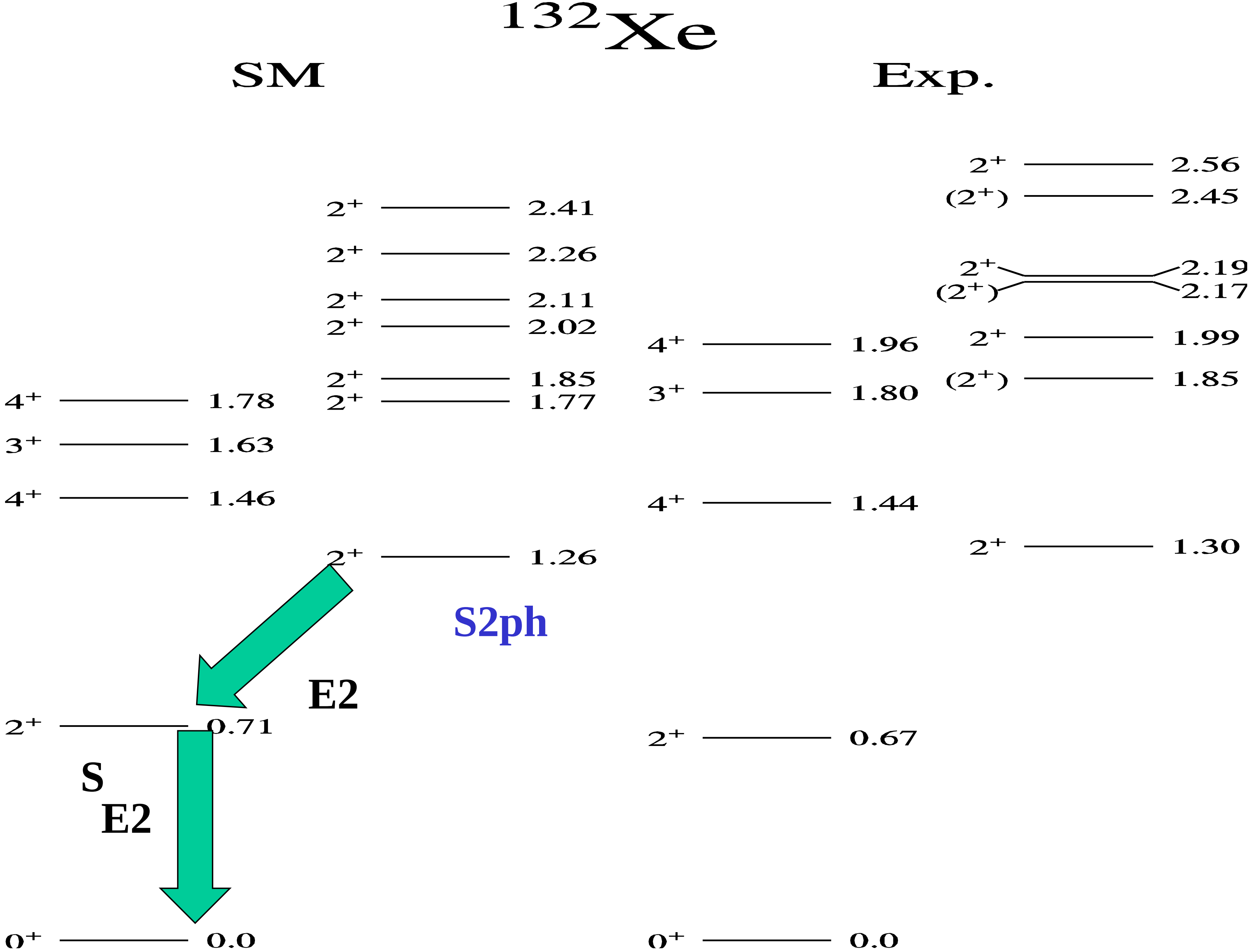
2+ 1.61



132Xe
SM
Exp.
2+ 2.41
2+ 2.26
2+ 2.11
2+ 2.02
2+ 1.85
2+ 1.77
4+ 1.78
3+ 1.63
4+ 1.46
2+ 1.26
S2ph
E2
2+ 0.71
S
E2
0+ 0.0
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(2+) 1.85
3+ 1.80
4+ 1.44
2+ 1.30
2+ 0.67
0+ 0.0

# Summary of the Xe results

- In **both** $^{134,132}$**Xe** we get

- the **first** $\mathbf{2^+_1}$ is **one-boson** p-n **symmetric**

--The **second** $\mathbf{2^+_2}$ is **two-boson symmetric**

- In $^{134}$**Xe**

- the **third** $\mathbf{2^+_3}$ is **one-boson** p-n **MS**

- In $^{132}$**Xe**

- the p-n **MS not obvious** since: B(M1) shared by two-three 2+ states

**NB: the IBM p-n symmetry is not a SM Symmetry**

# Summary

- The new   algorithm  allow us to perform large scale shell model calculations
- The convergence properties of the algorithm and the important sampling induce  an effective truncation of the space
- Future developments: Parallel code?
- Even now, it can be usefully implemented to study complex spectroscopy

Thank you