Microscopic Cluster Model

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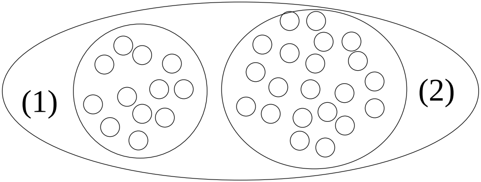
Outline

- Overview of the Theoretical Framework
- Microscopic Cluster Model Applications
  - Nuclear Astrophysics: the ^{12}C$(\alpha,\gamma)^{16}$O $E2$ cross section
  - Molecular Band in the ^{12}Be nucleus
  - Unbound system: the ^{16}B nucleus case

Overview of the Theoretical Framework

$(1) + (2) \longrightarrow (1,2) \longrightarrow \ldots$



$$A = A1 + A2$$

We approximatively solve the Schrödinger equation of a $A-$nucleon system with the Generator Coordinate Method combined with the Microscopic R-Matrix Method to determine:

- Cross Sections (Elastic, Radiative Capture, Transfer reaction, etc)
- Physical properties of the unified $(1,2)$ nucleus (Spectrocopy, etc)

Microscopic Hamiltonian

$$\mathcal{H} = \sum_{i}^{A} T_i + \sum_{i<j=1}^{A} \left(V_{ij}^{NN} + V_{ij}^{SO} + V_{ij}^{Coul} \right)$$

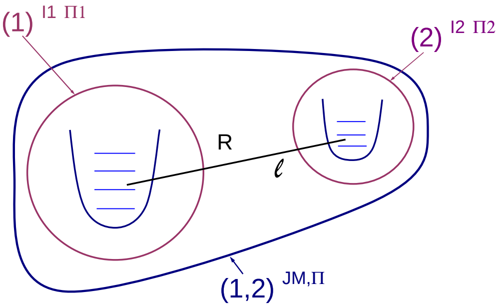
- Central part: combination of N_g Gaussian form factors

$$V_{ij}^{NN}(r) = \sum_{k=1}^{N_g} V_{0k} \exp(-(r/a_k)^2)\,(w_k - m_k P_{ij}^{\sigma} P_{ij}^{\tau} + b_k P_{ij}^{\sigma} - h_k P_{ij}^{\tau}).$$

  - Volkov, Minnesota forces - One free parameter
  - Extended Volkov Interaction - Two free parameters[2]
- V_{ij}^{SO}, Spin-Orbit force - One free parameter
- V_{ij}^{Coul}, Coulomb force - Exactly treated

[2] M.Dufour and P. Descouvemont, Nucl. Phys. **A726**, 53 (2003).

Two Cluster Model Basis State



- A Cluster is an Harmonic Oscillator Potential.
- All quantum numbers are exactly treated.
- *R*: Generator Coordinate

Resonating Groupe Method (RGM) Wave Function

In partial (JM, π) vawe, the total WF can be written as:

$$\Psi^{JM\pi} = \sum_{c\ell I} \Psi^{JM\pi}_{c\ell I} = \sum_{c\ell I} \mathcal{A} \;\; g^{J\pi}_{c\ell I}(\rho) \;\; \varphi^{J\pi}_{c\ell I}$$

- $\mathcal{A}$ is the A-nucleon antisymmetrizor.
- c labels the various channels - ($\mathbf{J} = \mathbf{I} + \ell$, $\mathbf{I} = \mathbf{I}_1 + \mathbf{I}_2$)
- $g^{J\pi}_{c\ell I}(\rho)$ are the radial functions.
- $\varphi^{J\pi}_{c\ell I} = \left[[\phi^{I_1}_c \otimes \phi^{I_2}_c]^I \;\otimes\; Y_\ell(\Omega_\rho) \right]^{JM}$, are the channel WFs.

• $\phi^{I_1}_c$ and $\phi^{I_2}_c$ are the internal WFs of (1) and (2), defined from Slater Determinants involving the two clusters.

Generator Coordinate Method (GCM) WF

In partial (JM, π) vawe, the total WF can be written as:

$$\Psi^{JM\pi} = \sum_{c\ell I} \Psi^{JM\pi}_{c\ell I} = \sum_{c\ell I} \int f^{J\pi}_{c\ell I}(R) \; \Phi^{JM\pi}_{c\ell I} dR,$$

- R is the generator coordinate.
- $f^{J\pi}_{c\ell I}(R)$ are the generator functions.

The RGM and GCM frameworks are equivalent.

- $\Phi^{JM\pi}_{c\ell I}$ are linked to the $\varphi^{J\pi}_{c\ell I}$.
- The RGM $g^{J\pi}_{c\ell I}(\rho)$ functions can be expanded over Gaussian functions.

$$g^{J\pi}_{c\ell I}(\rho) = \int f^{J\pi}_{c\ell I}(R) \, \Gamma_\ell(\rho, R) \, dR,$$

- $\Gamma_\ell(\rho, R) = \left(\frac{\mu}{\pi b^2}\right)^{3/4} \exp\left[-\frac{\mu}{2b^2}(\rho^2 + R^2)\right] i_\ell\left(\frac{\mu \rho R}{b^2}\right)$

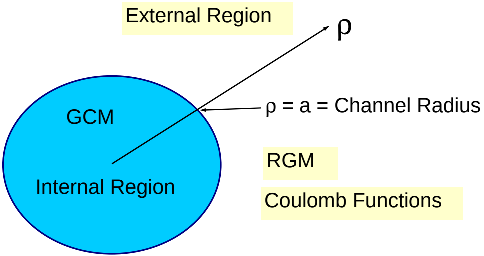
GCM - Microscopic $R-$Matrix Method (MRM)

In practice, integrals become sums over a set of generator coordinates.

$$g_{c\ell I}^{J\pi}(\rho) \approx \sum_n f_{c\ell I,n}^{J\pi}(R_n)\,\Gamma_\ell(\rho, R_n)$$

- GCM basis functions have a Gaussian asymptotic behaviour and cannot directly describe scattering states.
- $f_{c\ell I,n}^{J\pi}(R)$ are calculated by using the MRM which corrects the wrong Gaussian behaviour of the GCM functions.

The microscopic R-matrix method (MRM)



- The space is divided into two regions
- At the border defined by $\rho = a$

$$g^{int}_{c\ell I}(a) = g^{ext}_{c\ell I}(a)$$

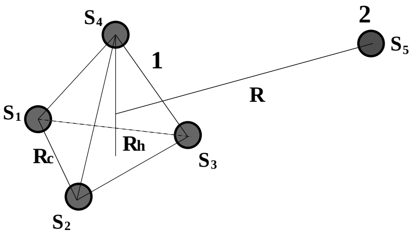
- In the external region, $g^{ext}_{c\ell I}(\rho) \propto$ Coulomb Functions

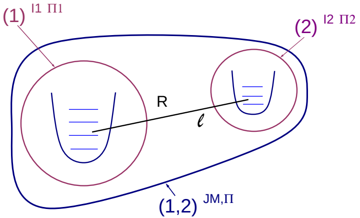
Theoretical Framework - Summary

- Unified description of bound, resonant and scattering states.
- Exact treatment of antisymmetrization: the Pauli principle is exactly treated.
- Exact center of mass separation.
- The quantum numbers associated with the colliding nuclei are restored.
- Exact asymptotic behaviour of the WFs.
- Once the interaction is fixed, the results are parameter free.

- The variational GCM basis is finite.
- Effective interactions.

How to improve the Cluster WF ?

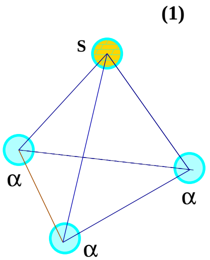




More clusters and/or more HO major shells

Multicluster model and Extended Two Cluster Model (ETCM)

Tetraedral states



Binding energies (in MeV) of one-center and four-center wave functions[3]

	Ground-State	One center	Four centers	Difference
^{12}C	0^+	-76.3	-88.	$\simeq$ -12
^{13}C	$1/2^-$	-83.7	-91.7	$\simeq$ -8
^{14}C	0^+	-96.1	-103.4	$\simeq$ -7
^{15}N	$1/2^-$	-120.7	-126.8	$\simeq$ -6
^{16}O	0^+	-140.4	-148.8	$\simeq$ -8

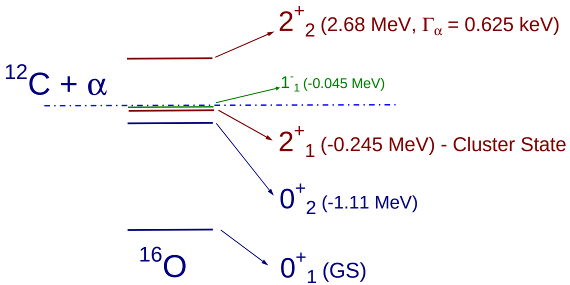
Better description as compared to a one center model.

[3] M.Dufour and P. Descouvemont, Nucl. Phys. **A650**, 160 (1996).

Application in Nuclear Astrophysics: the ^{12}C$(\alpha,\gamma)^{16}$O $E2$ cross section

- ^{12}C$(\alpha,\gamma)^{16}$O: key reaction in nuclear astrophysics
  - Determines the ^{12}C/^{16}O ratio after Helium burning
  - Uncertainties associated with the reaction rate should not exceed 20%
- Its study is a very difficult task
  - Stellar energies are very low: $E_G \approx 300$ keV
  - Charged-induced nuclear reaction take place below the Coulomb barrier $\rightarrow$ Tiny cross section
  - Experimental data are not available at astrophysical energies
  - $E1$ and $E2$ multipolarities are of equal importance
  - $E1$ are well understood
  - $E2$ are not well understood

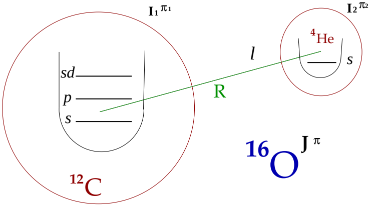
Microscopic Cluster Calculation Approach:



- $E2$ multipolarity dominated by a 2_1^+ subthreshold state at stellar energies well described as a $^{12}\mathrm{C}+\alpha$ cluster state
- Full study in[4]

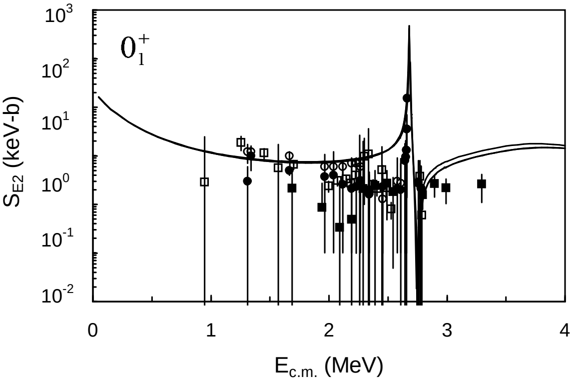
[4] M. Dufour and P. Descouvemont, Phys. Rev. **C 78 (2008) 015808**

Conditions of Calculation



- ^{12}C - (ETCM - Large Variational Basis):
- *s* shells filled, 4 p and 4 n in the *p* shells
- 225 Slater Determinants
- 23 - ^{12}C$+\alpha$ channels (I_1 from 0^+ to 4^+)
- EVI interaction
- Parameters chosen in order to reproduced the 2_1^+ and 2_2^+ energies with respect to the ^{12}C + α threshold

GCM S-factor for transitions to the ground state



- Comparaison with the latest experimental data:
  - Roters *et al.*, Eur. Phys. J. A **6**, 451 (1999).
  - R. Kunz *et al.*, Phys. Rev. Lett. **86**, 3244 (2001).
  - J. W. Hammer *et al.*, Nucl. Phys. **A758**, 363c (2005).
  - M. Assunçao *et al.*, Phys. Rev. C **73**, 055801 (2006).
- GCM-estimate of S-factor: $S(300\ \mathrm{keV}) \approx 50$ keV-b

The ^{12}C$(\alpha,\gamma)^{16}$O $E2$ cross section - Summary

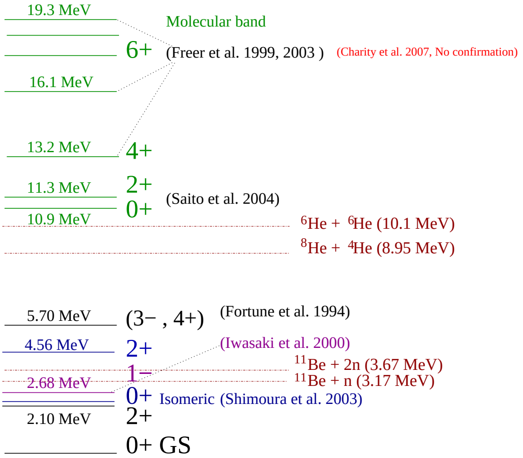
- Microscopic Cluster Calculations
  - Fundamental approach
  - Good description of the 2_1^+ subthreshold state
  - Impossible to get an exact reproduction of all the necessary spectroscopic data
- Phenomenological R-Matrix Fits
- Combination of both approaches
- To constrain the fits with the 2_1^+ ANC taken from the GCM
  - Recommended value:

$$S_{E2}(300\ \mathrm{keV}) = 42 \pm 2\ \text{keV-b}$$

Molecular band in the ^{12}Be nucleus

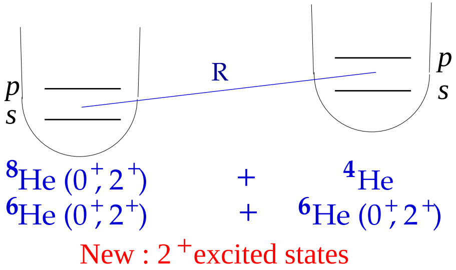
- Brief Overview of Experimental Results:

^{12}Be (Known Levels)



Other resonances but spin and parity only tentatively assigned
Widths are not measured

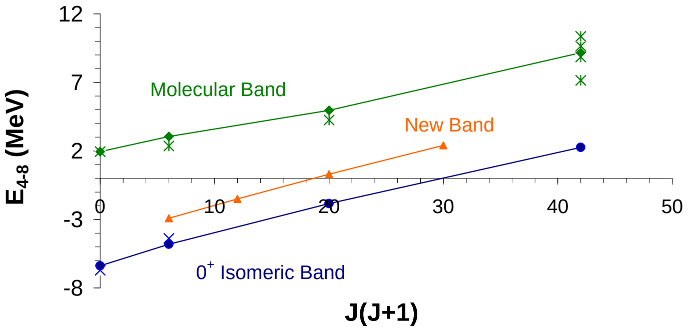
Multichannel expression of the ^{12}Be WFs



- ^{8}He$(0^+, 2^+)$+ α and ^{6}He$(0^+, 2^+)$+ ^{6}He$(0^+, 2^+)$ Channels
- EVI Force

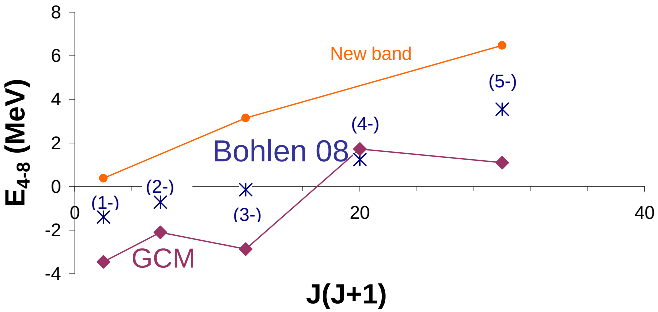
- Improvement of previous GCM investigations involving only ^{8}He(0^+) and ^{6}He(0^+) GS channels (Descouvemont and Baye in 2001).
- M. Dufour *et al.*, Nucl. Phys. **A836**, 242 (2010).

GCM - Positive parity states - Molecular band



- Our calculations support the existence of a molecular band
- 0^+_M: ($\Gamma^{GCM} = 0.365$ MeV) and clear ^{6}He(0^+)+ ^{6}He(0^+) structure.
- 0^+_2 and 2^+_2 are also well reproduced by the GCM + other states.
- We propose a new band.

GCM - Negative parity states



- $K = 1^-$ band based on the 1_1^- GCM state
- Could correspond to the tentatively assigned band of Bohlen seen in three-neutron stripping reaction on ^{9}Be

Multichannel analysis of the ^{16}B nucleus

Overview of Experimental Results:

- ^{16}B is unbound (Kryger *et al.*, Eur. Phys. J. A **6**, 451 (1999)).

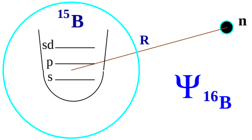
- Investigations of the low lying structure

  - Transfer reaction: ^{14}C (^{14}C,^{12}N) ^{16}B
    (R. Kalpakchieva *et al.*, Eur. Phys. J. A **7**, 451 (2000)).
  - Single-proton removal from a 35 MeV/nucleon ^{17}C beam
    (J.-L. Lecouey *et al.*, Phys. Lett. B **672**, 6-11 (2009)).

Above the ^{15}B+n threshold:

E_r	Kalpakchieva	Lecouey
(1)	0.04 ± 0.04 MeV ($\Gamma \ll 100$ keV)	0.085 ± 0.015 MeV ($\Gamma \ll 100$ keV) $\ell = 2$
(2)	2.32 ± 0.07 MeV ($\Gamma = 0.15$ MeV)	

Microscopic Wave Functions:



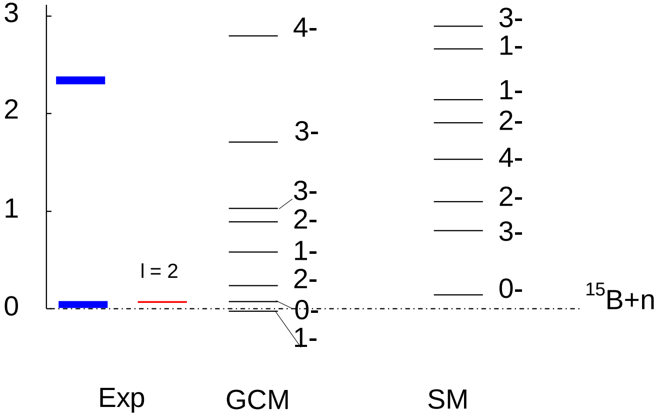
$$\Psi_{^{16}\mathrm{B}} = \Psi_{^{15}\mathrm{B}+\mathrm{n}}$$

$$\Phi_c(R) = \mathcal{A}\ \Phi_{^{15}\mathrm{B},c}(-\tfrac{1}{16}R)\ \Phi_{\mathrm{n}}(\tfrac{15}{16}R)$$

- ^{15}B: Shell Model description (1320 Slater Determinants)
  - Neutrons: s, p shells filled, 2 neutrons in the sd shell.
  - Protons: s shell filled, 3 protons in the p shells.
- ^{16}B: Cluster Model (87 channels (^{15}B + n))
  - Exact treatment of antisymmetrization.
  - Exact asymptotic behavior of the wave functions
  - Unified description of bound and resonant states.

Large Variational Basis

Results - ^{16}B spectrum



- Several resonances are obtained at low energy with the GCM
- 0_1^-, $\ell = 2$, $\Gamma = 1.26 \times 10^{-2}$ keV, consistent with Exp
- 0_1^-, $\ell = 2$, in agreement with SM calculations (Warburton *et al.* PRC **46** 923 (1992)).
- New: (1^-, $\ell = 0$) resonance at the threshold (possible GS ?)

Summary

- Unified description of bound, resonant and scattering states.
- Exact treatment of antisymmetrization: the Pauli principle is exactly treated.
- Exact asymptotic behaviour of the WFs.

- Large field of applications.
- Nuclear Astrophysics
- Light nuclei

Microscopic Hamiltonian:

$$\mathcal{H} = \sum_{i}^{16} T_i + \sum_{i<j=1}^{16} \left(V_{ij}^{NN} + V_{ij}^{SO} + V_{ij}^{Coul} \right)$$

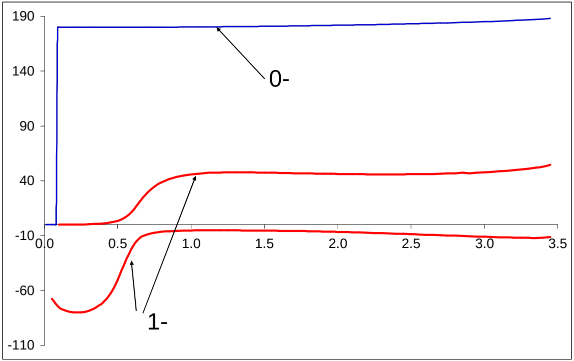
- $V_{ij}^{NN} = V_{ij}^{Volkov}$, (one free parameter: M)
- V_{ij}^{SO}, (one free parameter: S_0)

- The GCM 0_1^- is the lowest $\ell = 2$ state.
- S_0 is fixed to a typical value: $S_0 = 35$ MeV.fm^5.
- M is tuned in order to fit the GCM 0_1^- energy at ≈ 85 keV, ($M = 0.6935$).

- All the results are obtained with this interaction

Results - ^{16}B eigenphase shift

The ^{16}B resonance analysis is performed in terms of eigenphase shift.

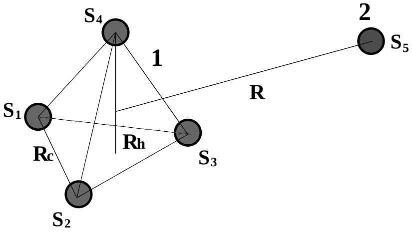


- 0_1^-: narrow resonance at $\approx$ 85 keV
- 1_1^-: resonance near the threshold
- 1_2^-: broad resonance at $\approx$ 0.6 MeV

^{16}B spectrum - Summary

- Several resonances are obtained at low energy with the GCM.
- $\ell = 2$ resonance of Lecouey *et al.* assigned to 0^- in agreement with the SM.
- 0_1^- cannot be described by the ^{15}B$(3/2-)$ + n channel.
- New: $(1^-, \ell = 0)$ state at the threshold could be the Ground-State.
- GCM: more adapted to describe resonances
  - Exact description of the asymptotic behavior of the wave functions
  - Phase shift analysis
  - Possibility to compute widths
- New experiments are needed to clarify the ^{16}B spectrum.

Multicluster Model



- ^{16}O$(\alpha,\gamma)^{20}$Ne
- ^{15}O$(\alpha,\gamma)^{19}$Ne, ^{15}N$(\alpha,\gamma)^{19}$F
- ^{13}C$(\alpha,\mathrm{n})^{16}$O, ^{16}O$(\mathrm{n},\gamma)^{17}$O
- ^{12}C$(\mathrm{n},\gamma)^{13}$C, ^{12}C$(\mathrm{p},\gamma)^{13}$N

We always get better results as compared to a simpler two cluster approach.

Combination GCM - R-Matrix Fits

- Microscopic Cluster Calculations:
  - Good description of the 2_1^+ subthreshold state
  - The Asymptotic Normalization Constant (ANC) of the 2_1^+ can be calculated with the GCM
  - *The ANC $C_{\gamma\ell}^{J\pi}$ represents the amplitude of a bound-state wave function at large distances*

$$g_{\gamma\ell}^{J\pi}(\rho) \longrightarrow C_{\gamma\ell}^{J\pi} W_{-\eta_B,\ell+1/2}(2k_B\rho),$$

where W is the Whittaker function, η_B and k_B are the Sommerfeld parameter and wave number of the bound state

  - The ANC of the 2_1^+ is linked to its reduced width γ_1
- To constrain the fits with the 2_1^+ ANC taken from the GCM

Challenge for Theoretical Calculations

- Shell Model:
- The structure of the Ground State and of the low-lying states is linked to the understanding of the breakdown of the $N = 8$ shell closure.
  - As early as in 1976, Barker pointed out the necessity to introduce non $p-$shell configurations in the wave function of the ground state in order to explain its β-decay half life.
  - Since, this point has been confirmed by several experiments and theoretical works (see e.g. Navin *et al.* PRL 2000 or Pain *et al. PRL 2006*)
- Microscopic Cluster Models:
  - Good description of cluster states such as molecular ones
  - Kanada-Enyo *et al.* 2003 (Antisymmetrized Molecular Dynamic), Ito *et al.* 2008 (molecular-like model)
  - Descouvemont and Baye (Phys. Lett B 505 2001) (Generator Coordinate Method).

0_1^- Shell Model Structure

- Shell model consideration from ^{17}C.
- Single proton removal should leave the neutron configuration of the projectile unperturbed.
- The low-lying states in ^{16}B should therefore correspond to a $\pi p3/2$ hole coupled to the ^{17}C ground state neutron configuration.
- ^{16}B ground state neutron configuration (Warburton).

$$\pi(p_{3/2})^{-1} \otimes \nu(d_{5/2})^3_{J=3/2+} + \pi(p_{3/2})^{-1} \otimes \nu(d^2_{5/2}, s_{1/2})_{J=3/2+}$$

- configuration which decays by $d-$wave neutron emission.

^{16}B Width

J^π	Γ (MeV)	(c,ℓ,I) $\theta^2_{c\ell I}$ here c refer to the ^{15}B channel
0^-_1	1.3×10^{-5}	$(5/2-,2,2)$ 3.37×10^{-2} $(3/2-,2,2)$ 1.34×10^{-3}
0^-_2	1.5	$(1/2-,0,0)$ 4.70×10^{-1}
1^-_1		$(3/2-,0,1)$ 3.26×10^{-1}
1^-_2	3.0×10^{-1}	$(3/2-,0,1)$ 1.20×10^{-1}
2^-_1	7.5×10^{-1}	$(3/2-,0,1)$ 4.92×10^{-1}
2^-_2	2.1×10^{-1}	$(5/2-,0,2)$ 2.87×10^{-1}
3^-_1	1.4×10^{-1}	$(5/2-,0,3)$ 9.79×10^{-2} $(3/2-,2,2)$ 7.60×10^{-3}
3^-_2	7.8×10^{-1}	$(5/2-,0,3)$ 3.67×10^{-1}
4^-_1	1.2	$(7/2-,0,4)$ 5.10×10^{-1} $(3/2-,2,2)$ 2.00×10^{-2}
4^-_2	8.7×10^{-1}	$(3/2-,2,1)$ 1.67×10^{-1}