## Clusters and correlations in nuclear structure and reactions

ZOOM with Tongji University－Shanghai－ 25 Nov 2021

## Lorenzo Fortunato

 Univ．Padova \＆INFN Italy| name | shape | group | $\Gamma_{v i b}$ | Patterns |
| :---: | :---: | :---: | :---: | :---: |
| linear $=$ | $\bullet-\bullet$ | $\mathcal{D}_{\infty h}$ | $A_{1 g}+A_{1 u}+E_{1 u}$ | 1叫 |
| linear $\neq$ | $\cdots$－ | $\mathcal{C}_{\infty \nu}$ | $2 A_{1}+E_{1}$ | 叫 |
| equilateral | $\theta$ | $\mathcal{D}_{3 h}$ | $A_{1}^{\prime}+E^{\prime}$ | $\xrightarrow{\text { 叫 }}$ |
| isosceles | $\theta$ | $\mathcal{C}_{2 \nu}$ | $2 A_{1}+B_{1}$ | 叫 |
| scalene | $8$ | $\mathcal{C}_{s}$ | $3 A^{\prime}$ | \U\｜ |




## Collaborators

L. Fortunato

$\qquad$

Jesús Casal (Padova and now Seville)
Jagjit Singh (Padova, Sapporo and Osaka)

Wataru Horiuchi (Sapporo)

Andrea Vitturi (Padova)

Edoardo Lanza (Catania)
Jesús Casal (Padova and now Seville)
Jagjit Singh (Padova, Sapporo and Osaka)
Wataru Horiuchi (Sapporo)
Andrea Vitturi (Padova)
Edoardo Lanza (Catania)

Outline of the presentation

* Polarized gamma beams: scenario for future measurements on the depolarization ratio for the case of 12C with triangular and more exotic structures
* Transition densities in action for 12C and 160, recent results on alpha-transfer form factors
* New insight on the structure of 29F at the border of the island of inversion


## Discrete symmetries and polarized gamma-rays in 12 C

## PHYSICAL REVIEW C 99, 031302(R) (2019)

Rapid Communications Editors' Suggestion

Establishing the geometry of $\alpha$ clusters in ${ }^{12} \mathrm{C}$ through patterns of polarized $\gamma$ rays

Lorenzo Fortunato
Dipartimento di Fisica e Astronomia "G.Galilei"-Università di Padova, via Marzolo 8, I-35131 Padova, Italy and INFN-Sez.di Padova, via Marzolo 8, I-35131 Padova, Italy
(1) (Received 13 December 2018; published 11 March 2019)

One can shoot linearly polarized gamma rays (Electric field oscillating in a given direction constant in time) of appropriate energy (tuned to match the resonances of interest) and observe the outcoming gammas of the same or different energies with a polarizer/analyzer. If the nucleus has a definite geometrical symmetry (i.e. if there is an underlying discrete group structure), very strict selection rules apply. Experimentally the polarization can be measured with another inverse Compton scattering.


## Polarized gamma-ray facilites around the globe:

Mainz Microtron MAMI (Continuous Wave, beam polarization $80 \%$, En. resol. 0.1 MeV , but energy too high 50-800 MeV)
Triangle University Higs facility (FEL type, quasi CW operation, 2-60 MeV, flux 10^8-10^9 phot./s)
ELI-NP in Romania ( $0-20 \mathrm{MeV}$, high flux, high resolution, $100 \%$ polarization)
LEPS - Japan (very high energy)
D NewSubaru

- ...
1)())|)l Ci $\begin{gathered}\text { Extreme Light Infrastructure } \\ \text { Nuclear Physics (ELI-NP) }\end{gathered}$

| Gamma beam parameter | Value |
| :---: | :---: |
| Energy [ MeV ] | 0.2-19.5 |
| Spectral density [ph/s/eV] | $0.8-4 \cdot 10^{4}$ |
| Bandwidth rms [\%] | $\leq 0.5$ |
| \#Photons/shot within FWHM bdw. | $\leq 2.6 \cdot 10^{5}$ |
| \#Photons/s within FWHM bdw. | $\leq 8.3 \cdot 10^{8}$ |
| Source rms size [ $\mu \mathrm{m}$ ] | 10-30 |
| Source rms divergence [ $\mu \mathrm{rad}$ ] | 25-200 |
| Peak brilliance $\left[\mathrm{N}_{\mathrm{ph}} / \mathrm{s} \cdot \mathrm{mm}^{2} \cdot \mathrm{mrad}^{2} \cdot 0.1 \%\right.$ bdw] | $10^{20}-10^{23}$ |
| Pulse length rms [ps] | 0.7-1.5 |
| Linear polarization [\%] | $>99$ |
| Macro repetition rate [ Hz ] | 100 |
| Number of pulses/macropulse | 32 |
| Pulse-to-pulse separation [ps] | 16 |

With the advent of the new facility in Romania, beams of high brilliance, focused, polarized gamma rays produced with Inverse Compton Scattering will become available with energies ranging from $0.2-20 \mathrm{MeV}$

## Depolarization ratio

One can measure the so-called depolarization ratio between intensities, by turning the analyzer/polarizer of 90 degrees, i.e.:

$$
\rho=\frac{I_{\perp}}{I_{\|}}
$$



Figure 8.6. Parallel and perpendicular Raman scattering.
as a tool to determine which modes are totally symmetric modes. In fact from the theory of Raman scattering

$$
\begin{array}{r}
0 \leq \rho \leq \frac{3}{4} \quad \begin{array}{l}
\text { for polarized bands } \\
\text { (symmetric modes) }
\end{array}
\end{array}
$$

$$
\rho=\frac{3}{4} \quad \text { for depolarized bands }
$$ (non-symmetric modes)



Figure 8.8. Polarized light scattering by a sphere.
even with a randomly oriented sample.

## Depolarization ratio : a chemical example $\mathrm{CCl}_{4}$

This kind of measuments of $\rho=\frac{I_{\perp}}{I_{\|}}$are absolutely standard in optical spectroscopy (where polarizers and analyzers are easy to do and handle).


Figure 2: Polarized Raman spectra of $\mathrm{CCl}_{4}$.

Depolarization ratio

Nuclear Molecule
Polarized gamma Analyzer

## Panoply of different models

(Too) many models have been proposed for 12 C where the triangle is not equilateral, isosceles, scalene or even a linear chain (Morinaga). Therefore. I have set forth to determine all possible outcomes and the patterns that can be predicted are intended as a guidance as to which configuration is right and the crucial method is clearly through measurements of the depolarization ratio in Raman-like experiments of nuclear fluorescence that will be feasible at ELI-NP or in other labs where gamma-rays are available.



FIG. 10 (Color online) $0^{+}$-projected energy surface on the $\Lambda-D$ plane for ${ }^{12} \mathrm{C}$ calculated by the AQCM. The interaction and width parameters are same as those in Ref. (Suhara et al., 2013).
antisymmetrized quasi-cluster model
container model

## Algebraic cluster model for 3 alphas

Bijker and lachello (Ann.Phys. 298, 2002) have clearly demonstrated the succesfull application of the ACM, or algebraic cluster model, to the vibrational-rotational spectrum of alpha-conjugate nuclei like 12C and 160.


Note that rotational bands DO NOT conform tothe usual quadrupole rotational bands we are used, they have a different symmetry! Rather, these are the ways in which you can spin a triangle.

FIG. 2. Comparison between the low-lying experimental spectrum of ${ }^{12} \mathrm{C}$ [12] and that calculated using Eq. (6) with $A=7.0, B$ $=9.0, C=0.7$, and $D=0.0 \mathrm{MeV}$. States with uncertain spin-parity assignment are in parentheses.


This lovely paper confirms the assignation of the 5 - state at $22.4(2) \mathrm{MeV}$ to the g.s. band of an equilater triangular structure.
Note the uncommon spin-parity of bands (the doublet 4+/4-has a natural explanation in terms of D3h symmetry!).

```
Different
geometric
arrangements of
```

Discrete
symmetry group
Precise selection
rules

## Work plan:

- Decide arrangement of N particles
- This means 3N-6 d.o.f (or 3N-5 d.o.f. for linear arrangement)
- Identify the underlying discrete group structure
- Find the character under transformations of the group $\Gamma_{3 \mathrm{~N}}$
- Subtract translations and rotations to single out character of vibrational modes $\Gamma_{\text {vib }}$
- Identify patterns of totally symmetric modes
- Check models against measures of intensities $\rightarrow$ Eureka !!

Tables in PRC 99 (2019) paper: 3 equal clusters

| name | shape | group | $\Gamma_{v i b}$ | Patterns |
| :---: | :---: | :---: | :---: | :---: |
| linear $=$ | $\bullet$-- | $\mathcal{D}_{\infty h}$ | $A_{1 g}+A_{1 u}+E_{1 u}$ | THIL |
| linear $\neq$ | -0- | $\mathcal{C}_{\infty \nu}$ | $2 A_{1}+E_{1}$ |  |
| equilateral | $\theta$ | $\mathcal{D}_{3 h}$ | $A_{1}^{\prime}+E^{\prime}$ | $\xrightarrow{\square}$ |
| isosceles | $\theta$ | $\mathcal{C}_{2 \nu}$ | $2 A_{1}+B_{1}$ | $\xrightarrow[\square]{\square}$ |
| scalene | $0$ | $\mathcal{C}_{s}$ | $3 A^{\prime}$ | $\uparrow \square \\|$ |

The number of totally symmetric peaks over total is different in each case, therefore one can disentagle the various possibilities

There might be more than just one configuration! The picture complicates a little, but not too much! One can invoke the concept of descent in symmetry ans still apply some of the rules.



| $\mathcal{D}_{\infty h}$ | $A_{1 g}+$ | $A_{1 u}+$ | $E_{1 u}$ |  | $\mathcal{D}_{\infty h}$ | $A_{1 g}+$ | $A_{1 u}+$ | $E_{1 u}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\downarrow$ | $\downarrow$ | $\downarrow$ |  |  | $\downarrow$ | $\downarrow$ | $\downarrow$ |
| $\mathcal{C}_{\infty \nu}$ | $A_{1}+$ | $A_{1}+$ | $E_{1}$ |  | $\mathcal{D}_{3 h}$ | $A_{1}^{\prime}+$ | $A_{2}^{\prime \prime}+$ | $E^{\prime}$ |
|  | $\downarrow$ | $\downarrow$ | $\downarrow$ |  |  | $\downarrow$ |  |  |
|  | $\downarrow$ |  |  |  |  |  |  |  |
| $\mathcal{C}_{2 \nu}$ | $A_{1}+$ | $A_{1}+$ | $\overbrace{B_{1}+B_{2}}$ |  | $\mathcal{C}_{2 \nu}$ | $A_{1}+$ |  | $\overbrace{A_{1}+B_{1}}$ |
|  | $\downarrow$ | $\downarrow$ | $\downarrow$ |  |  | $\downarrow$ |  | $\downarrow$ |
| $\mathcal{C}_{s}$ | $A^{\prime}+$ | $A^{\prime}+$ | $A^{\prime}$ |  | $\mathcal{C}_{s}$ | $A^{\prime}+$ |  | $A^{\prime}+A^{\prime}$ |

FIG. 4. Descent in symmetry restricted to representations of the groups that are relevant to all possible configurations of three identical particles.

## Tetrahedral shape in 16 Oxygen

Bijker, lachello
PRL 112, 152501 (2014)

| $-6^{ \pm}$ $-4^{+}$ $-3^{-}$ $-0^{+} . .$ | $\begin{aligned} & -6 \\ & -4 \\ & -3 \\ & -0 \end{aligned}$ | - - - - $\vdots$ | $\begin{aligned} & -6^{+ \pm} \\ & -5^{- \pm} \\ & -4^{ \pm} \\ & -3^{ \pm} \\ & =2^{+} \end{aligned}$ |
| :---: | :---: | :---: | :---: |
| $\begin{gathered} (000) \\ A \end{gathered}$ | (100) $A$ | $(010$ $E$ | $(001)$ $F$ |

FIG. 1. Schematic spectrum of a spherical top with tetrahedral symmetry and $\omega_{1}=\omega_{2}=\omega_{3}$. The rotational bands are labeled by $\left(v_{1}, v_{2}, v_{3}\right)$ (bottom). All states are symmetric under $S_{4}$.

## Transition densities and form factors in the triangular $\alpha$-cluster model of ${ }^{12} \mathrm{C}$

 with application to ${ }^{12} \mathrm{C}+\alpha$ scatteringA. Vitturi, ${ }^{1,2}$ J. Casal $\odot,^{1,2}$ L. Fortunato $\odot^{1,2}$ and E. G. Lanza $\odot^{3,4}$
${ }^{1}$ Dipartimento di Fisica e Astronomia "G. Galilei", Università di Padova
${ }^{2}$ I.N.F.N., Sez. di Padova, I-35131 Padova, Italy
${ }^{3}$ I.N.F.N., Sez. di Catania, I-95123 Catania, Italy
${ }^{4}$ Dipartimento di Fisica e di Astronomia "Ettore Majorana", Università Catania, Italy
(0) (Received 1 October 2019; published 21 January 2020)

Densities and transition densities are computed in an equilateral triangular $\alpha$-cluster model for ${ }^{12} \mathrm{C}$, in which each $\alpha$ particle is taken as a Gaussian density distribution. The ground state, the symmetric vibration (Hoyle state), and the asymmetric bend vibration are analyzed in a molecular approach and dissected into their components in a series of harmonic functions, revealing their intrinsic structures. The transition densities in the laboratory frame are then used to construct form factors and to compute distorted-wave Born approximation inelastic cross sections for the ${ }^{12} \mathrm{C}\left(\alpha, \alpha^{\prime}\right)$ reaction. The comparison with experimental data indicates that the simple geometrical model with rotations and vibrations gives a reliable description of reactions where $\alpha$-cluster degrees of freedom are involved.

M. Kamimura, Nucl. Phys. A 351, 456 (1981).
D. C. Cuong, D. T. Khoa, and Y. Kanada En'yo, Phys. Rev. C 88, 064317 (2013).
M. Ito, Phys. Rev. C 97, 044608 (2018).
Y. Kanada-En'yo and K. Ogata, Phys. Rev. C 99, 064601 (2019).

## Transition densities in 12C

$y(f m)$


This model assume guassian densities for each alpha particle

$$
\rho_{\alpha}(\vec{r})=\left(\frac{\alpha}{\pi}\right)^{3 / 2} e^{-\alpha r^{2}}
$$


and a total density that is the sum of three displaced alpha's

$$
\rho_{\mathrm{gs}}\left(\vec{r},\left\{\vec{r}_{k}\right\}\right)=\sum_{k=1}^{3} \rho_{\alpha}\left(\vec{r}-\vec{r}_{k}\right),
$$

which is then expanded in spherical harmonics

$$
\rho_{\mathrm{gs}}(\vec{r})=\sum_{\lambda \mu} \rho_{\mathrm{gs}}^{\lambda, \mu}(r) Y_{\lambda, \mu}(\theta, \varphi),
$$

$\left(\mathrm{fm}^{-3}\right)$
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.07
0.06
0.05
0.04
0.03
0.02
0.01
$\rho\left(\mathrm{fm}^{-3}\right)$
$\square$
0.07
0.06
0.05
0.04
0.03
0.02
0.01


Ground state band

Hoyle state band

$$
-0.05
$$

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## 路

- 00
- 20
 33

$$
\text { (on } 00 \text {---- } 20
$$

no

## Parameters phenomenologically adjusted



TABLE I. Calculated observables within the ground-state band.

| $\left\langle r^{2}\right\rangle_{0_{1}^{+}}^{1 / 2}$ | $2.45(\mathrm{fm})$ |
| :--- | :--- |
| $B\left(E 2 ; 2_{1}^{+} \rightarrow 0_{1}^{+}\right)$ | $7.86\left(e^{2} \mathrm{fm}^{4}\right)$ |
| $B\left(E 3 ; 3_{1}^{-} \rightarrow 0_{1}^{+}\right)$ | $65.07\left(e^{2} \mathrm{fm}^{6}\right)$ |
| $B\left(E 4 ; 4_{1}^{+} \rightarrow 0_{1}^{+}\right)$ | $96.99\left(e^{2} \mathrm{fm}^{8}\right)$ |

TABLE II. Quantities calculated in the present work for the Hoyle band using the values of $\beta$ and $\chi_{1}$ given in the text.

| $\left\langle r^{2}\right\rangle_{0_{2}^{+}}^{1 / 2}$ | $3.44(\mathrm{fm})$ |
| :--- | :---: |
| $B\left(E 2 ; 2_{2}^{+} \rightarrow 0_{1}^{+}\right)$ | $0.58\left(e^{2} \mathrm{fm}^{4}\right)$ |
| $B\left(E 2 ; 0_{2}^{+} \rightarrow 2_{1}^{+}\right)$ | $2.90\left(e^{2} \mathrm{fm}^{4}\right)$ |
| $B\left(E 3 ; 3_{2}^{-} \rightarrow 0_{1}^{+}\right)$ | $70.42\left(e^{2} \mathrm{fm}^{6}\right)$ |
| $M\left(E 0 ; 0_{2}^{+} \rightarrow 0_{1}^{+}\right)$ | $5.4\left(e \mathrm{fm}^{2}\right)$ |

Transition densities in 12C

## A-band



FIG. 7: Transition density for the first A-type vibration.
-00 (div. by 5) $-20-33$

$y(f m)$

$x(\mathrm{fm})$




## Transition densities $\rightarrow$ Form Factors $\rightarrow$ Coupled Channels $\rightarrow$ Cross-sections



FIG. 15. Form factors in logarithmic scale for a few inelastic excitation processes of interest. We show the nuclear, Coulomb, and total form factors.


FIG. 16. Differential cross section for the elastic scattering and the transitions $0_{1}^{+} \rightarrow 2_{1}^{+}$and $0_{1}^{+} \rightarrow 3_{1}^{+}$at $240-\mathrm{MeV}$ bombarding energy. Data are from Ref. [41] (retrieved through EXFOR).

Lots of results that I dont'have time to discuss in details. They confirm that with just a simple triangular model one catches all the gross features, not only of the nuclear structure, but also of reaction dynamics of 12 C .

## Importance of the imaginary part of the ion-ion potential


$V(r)+i W(r)$

FIG. 17. Differential cross section for the transition $0_{1}^{+} \rightarrow 0_{2}^{+}$at $240-\mathrm{MeV}$ bombarding energy. Data are from Ref. [41] (retrieved through EXFOR) and the three curves have different factors for the depth of the imaginary part as indicated in the figure.


## Extended to 160 in a tetrahedral arrangement $\rightarrow 12 C(\alpha, \gamma) 160$



## Selection rule for alpha transfer

$T_{d} \rightarrow S_{4}:$ :品 $[4] \quad[3,1] \quad[2,2]$


$$
D_{3 h} \rightarrow S_{3}: \quad \text { वロ } \quad \Phi
$$ $[3] \quad[2,1]$


[2]
A

Fig. 8 The representations of the systems with 4,3 and $2 \alpha$ particles connected by arrows corresponding to processes of induction/restriction that amounts to the addition/removal of one box from the corresponding Young diagrams

Taking into account the symmetric groups of 2-3-4 identical objects, one can up with a scheme for alpha-transfer (I mean the addition or removal of 1 alpha particle) based on Young tableaux, i.e. on the representations of those groups.

It turns out that not all of them can be connected, for instance one cannot go from the A states of 12C to the E states of oxygen, the alpha transfer should be identically zero!


Fluorine-29 stands on the coast of the island of inversion


PERSPECTIVE

## 888 <br> COMMUNICATIONS PHYSICS

https://doi.org/10.1038/s42005-020-00402-5 OPEN
The ${ }^{29} \mathrm{~F}$ nucleus as a lighthouse on the coast of the island of inversion


## Fluorine-29 stands on the coast of the island of inversion



Fig. 1 Standard ordering of shell-model energy levels and typical inversion mechanism. The $N=2$ sd-shell and the $N=3 p f$-shell with positive and negative parity $\pi$, respectively, are shown on the left in the standard ordering (states are labeled by the standard set of quantum number $n \ell_{j}$ ). Inversion occur (right) when the shell gap, $\Delta E$, associated with the filling of 20 neutrons, disappears and one level (or more) of the $N=3$ $p f$-shell gets lower than one (or more) of the levels of the $N=2 s d$-shell.


Fig. 2 Synopsis of known experimental data on ${ }^{\mathbf{2 8}, 29} \mathbf{F}$. All energies are in keV (not to scale) from refs. ${ }^{4--6,11}$. States in red are labelled by the $J \pi$ quantum numbers and energies are referred to the ${ }^{27} F+2 n$ threshold. States in blue are inferred from the ${ }^{29} \mathrm{~F}(-1 \mathrm{n})$ column of Fig. 2 of ref. ${ }^{6}$, and correspond only to the states decaying to the ground state of ${ }^{27} \mathrm{~F}$. They are labelled by the orbital angular momentum quantum number, $\ell$, when available. Energies are referred to the ${ }^{27} \mathrm{~F}+\mathrm{n}$ threshold.

## Fluorine-29 stands on the coast of the island of inversion

We had previously PRC 101, 024310 (2020) proposed 4 scenarios for the structure of the very exotic nucleus 29F, called A,B,C,D , based on the three-body hyperspherical formalism by J.Casal



Inverted

FIG. 1. ${ }^{27} \mathrm{~F}+n$ phase shifts for $d_{3 / 2}, p_{3 / 2}$, and $f_{7 / 2}$ states, corresponding to different sets (A-D). The dotted black line corresponds to $\pi / 2$

## Fluorine-29 stands on the coast of the island of inversion

## New experiments by

1) Revel, A. et al. "Extending the southern shore of the island of inversion to 28 F " PRL 124, 152502 (2020)
and then
2) Bagchi, S. et al. "Two-neutron halo is unveiled in 29F" PRL 124, 222504 (2020)


Fig. 3 Phase-shifts, $\delta$, for the ${ }^{\mathbf{2 7}} \mathbf{F}+\mathbf{n}$ system in the $\mathbf{D}^{b}$ scenario as a function of the neutron-core relative energy. Adjusting the red curve to reproduce the $d$-resonance at about 0.9 MeV , also gives the $f$-wave state (blue curve) at about 4 MeV .


Final picture ... Scenario D b


$$
\frac{d \sigma}{d \varepsilon}=\left(\alpha Z_{2}\right)^{2} \sum_{\pi \lambda \mu}\left(\frac{\Delta E}{\hbar c}\right)^{2 \lambda-2} \frac{d B}{d \varepsilon}(\pi \lambda ; \text { gs } \rightarrow \text { Cont. })\left|G_{\pi \lambda \mu}\left(\beta^{-1}\right)\right|^{2} g_{\mu}(\xi)
$$



Fig. 4 Results on ${ }^{29} \mathbf{F}$ within the new $\boldsymbol{D}^{\boldsymbol{b}}$ scenario. a Ground-state probability density of ${ }^{29} \mathrm{~F}$ as a function of the distance between the two valence neutrons $\left(r_{n n}\right)$ and that between their center of mass and the core $\left(r_{\mathrm{c}-\mathrm{nn}}\right)$. The maximum probability density corresponds to the dineutron configuration. $\mathbf{b}$ Electric dipole (E1) strength function from the ground state to continuum as a function of the ${ }^{27} F+n+n$ energy. The dashed line indicates the cumulative integral. The dash-dotted line is the corresponding Relativistic Coulomb Excitation (RCE) cross-section, scaled to the same maximum to illustrate the decreasing proportionality with the energy.

## Summary

$\checkmark$ PRC 99 (2019) I have suggested to use the highly polarized monochromatic gamma rays that will be available at ELI-NP as a tool to study the molecular vibrations of clusterized nuclei, taking as a definite example the 12C nucleus as composed of $3 \alpha$ particles. A measure of depolarization ratio could be done in a sort of Raman nuclear fluorescence experiment. This would yield precise patterns of vibrational spectra, that will correlate directly with a given geometric configuration possessing a discrete point-group symmetry.
$\checkmark$ PRC 101, 014315 (2021) We have calculated transition densities and form factors for 12C in a triangular molecular model for the g.s., A and E bands. We applied this model to $12 \mathrm{C}+\alpha$ scattering showing a very good agreement.
$\checkmark$ EPJA 57 (2021) We have extended these results to 160 in a tetrahedral arrangement and we have calculated alpha-induced reaction observables. I have found a new selection rule for alpha-transfer based on group theory.
$\checkmark$ Comm. Physics 3 (2020) and also PRC 101, 024310 (2020) We have succesfully interpreted new experimental results on the structure of 29 F indicating it lies at the border of the island of inversion.


## Università degli Studi di Padova



Dipartimento di Fisica
e Astronomia Galileo Galilei

## A few points for discussion

- if the g.s. rotational band contains the same multipolarity that one is trying to excite in the vibrational bands, this is also to be included in the above patterns.
- in principle the degree of polarization might be close to $3 / 4$ also for polarized (A) bands, therefore it might become hard to distinguish between them
- non-cluster degrees of freedom might come into play at a certain energy, thus blurring the picture
- in nuclei with a cluster structure including $t$ or $h$ clusters, the interplay with single-particle orbits around a molecular center might also be very relevant
- I guess a BEC gas would show no geometric arrangments (no equilibirum points) and would behave as an L=0 state (a sphere), thus offering only 1 such bands of A type (polarized).

DISCLAIMER for the first topic:

- It is perfectly clear to us that molecular models of nuclei are FUNDAMENTALLY DIFFERENT from molecular physics, where the Born-Oppenheimer approximation is valid and one can think of nuclear motion as a small vibration, happening only close to the minimum of a very deep potential energy surface (in molecular energy scales).
- Nuclei have large kinetic energy <T>, comparable to the potential energy <V> and the zero point motion inside the P.E.S. is a large fraction of the well depth, therefore there are LARGE FLUCTUATIONS around the equilibrium points and we SHOULD NOT EXPECT that the vibrational levels are deeply lying in the potential well, at most they can be weakly bound states, close to threshold, or more probably resonances in the continuum!
- Dispite this, it is instructive to look at

1. the normal modes, i.e. the «best» internal coordinates
2. symmetry-adapted vibrational orbitals
3. the energy scale and structure of the vibrational levels

## Nomenclature

Table II: The Mulliken symbols used to describe the symmetry species of point groups including their meaning with respect to molecular symmetry

| Mulliken Symbols of <br> Symmetry Specles (Column <br> 1 In Character Table) | Meaning |
| :---: | :---: |
| A | Symmetric with respect to principal axis of symmetry |
| $B$ | Antisymmetric with respect to principal axis of symmetry |
| E | Doubly degenerate, two-dimensional irreducible representation |
| $T$ | Triply degenerate, three-dimensional irreducible representation |
| $g$ | Symmetric with respect to a center of symmetry |
| $u$ | Antisymmetric with respect to a center of symmetry |
| 1 (subscript) | Symmetric with respect to a $C_{2}$ axis that is perpendicular to the principal axis. Where there is no such axis the subscript indicates that reflection in a ${ }_{v}$ plane of symmetry is symmetric. |
| 2 (subscript) | Antisymmetric with respect to a $C_{2}$ axis that is perpendicular to the principal axis. Where there is no such axis the subscript indicates that reflection in a ${ }_{v}$ plane of symmetry is antisymmetric. |
| , (prime) | Symmetric with respect to reflection in a horizontal plane of symmetry |
| "(double prime) | Antisymmetric with respect to reflection in a horizontal plane of symmetry |

From D. Tuschel - Spectroscopy : Molecular Spectroscopy workbench (2014)

## Tetrahedral shape in 16 Oxygen

They use a somewhat simplified notation based on the permutation (sub)groups $\mathrm{S}_{3}$ and $S_{4}$ of the full discrete groups $D_{3 h}$ and $T_{d}$ respectively, but the essence is the same.

${ }^{12} \mathrm{C}$

${ }^{16} \mathrm{O}$

Tables for 2 clusters and for 3 clusters of type $A A B$

| name | shape | group | $\Gamma_{v i b}$ | Patterns |
| :---: | :---: | :---: | :---: | :---: |
| linear AA | $\bullet \bullet$ | $\mathcal{D}_{\infty h}$ | $A_{1 g}$ | $\downarrow \square$ |
| linear AB | $\bigcirc \bullet$ | $\mathcal{C}_{\infty \nu}$ | $A_{1}$ | $\downarrow \square$ |


| name | shape | group | $\Gamma_{v i b}$ | Patterns |
| :---: | :---: | :---: | :---: | :---: |
| linear ABA | $0 \cdot 0$ | $\mathcal{D}_{\infty h}$ | $A_{1 g}+A_{1 u}+E_{1 u}$ | U1 |
| linear AAB | OO- | $\mathcal{C}_{\infty}$ | $2 A_{1}+E_{1}$ | - |
| isosceles AAB | 0 | $\mathcal{C}_{2 \nu}$ | $2 A_{1}+B_{1}$ |  |
| scalene AAB | 80 | $\mathcal{C}_{s}$ | $3 A^{\prime}$ |  |

Tables for 4clusters, only some have been worked out

| name | shape | group | $\Gamma_{v i b}$ | Patterns |
| :---: | :---: | :---: | :---: | :---: |
| linear aaa | $0-0-0$ | $\mathcal{D}_{\infty h}$ | $2 A_{1 g}+E_{1 g}+E_{4 g}+A_{1 u}+E_{1 u}$ | 2/6 |
| linear aba | $\cdots-\infty$ | $\mathcal{D}_{\infty h}$ | $2 A_{1 g}+E_{1 g}+A_{1 u}+E_{1 u}$ | $2 / 5$ |
| square $\mathrm{a}^{4} \mathrm{~b}^{2}$ |  | $\mathcal{D}_{4 h}$ | $A_{1 g}+B_{1 g}+B_{2 g}+B_{2 u}+E_{u}$ | 1/5 |
| kite $\mathrm{a}^{4} \mathrm{bc}$ |  | $\mathcal{D}_{2 h}$ | $2 A_{g}+B_{1 g}+B_{1 u}+B_{2 u}+B_{3 u}$ | 2/6 |
| centered eq. triangle $\mathrm{a}^{3} \mathrm{~b}^{3}$ |  | $\mathcal{D}_{3 h}$ | $A_{1}^{\prime}+2 E^{\prime}+A_{2}^{\prime \prime}$ | 1/4 |
| rectangle $\mathrm{a}^{2} \mathrm{~b}^{2} \mathrm{c}^{2}$ |  | $\mathcal{D}_{2 h}$ | $2 A_{g}+B_{1 g}+A_{u}+B_{2 u}+B_{3 u}$ | 2/6 |
| tetrahedron $\mathrm{a}^{6}$ |  | $\mathcal{T}_{d}$ | $A_{1}+E+T_{2}$ | $1 / 3$ |
| uneq. tetrah. $\mathrm{a}^{3} \mathrm{~b}^{3}$ |  | $\mathcal{C}_{3 \nu}$ | $2 A_{1}+2 E$ | 2/4 |
| wedge $\mathrm{a}^{4} \mathrm{~b}^{2}$ |  | $\mathcal{D}_{2 d}$ | $2 A_{1}+B_{1}+B_{2}+E$ | 2/5 |
| 2 triangles at $90^{\circ} \mathrm{a}^{5} \mathrm{~b}$ |  | $\mathcal{C}_{2 \nu}$ | $3 A_{1}+A_{2}+B_{1}+B_{2}$ | 3/6 |

One might gather information on polarization due to alpha particles' substructures

