

Establishing the geometry of α clusters in ^{12}C through patterns of polarized γ rays

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Linearly polarized monochromatic beams of γ rays, that will be available at the ELI-NP facility, will open up the way to nuclear fluorescence experiments aimed at measuring the depolarization ratio of the outgoing photons. This is the ideal tool to clearly discriminate among the various proposed geometric configurations for α -cluster nuclei, such as ^{12}C in a model-independent way. For this nucleus, all possible outcomes have been enumerated in this Rapid Communication, and the predicted theoretical patterns of intensities will serve as a guide for the conclusive experimental identification of its nuclear molecular structure.

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The purpose of this Rapid Communication is to present a method to ascertain the nature of the geometrical shape of clusterized nuclei by extending group-theoretical methods that are heavily used in molecular Raman spectroscopy and adapting them to the nuclear domain. In particular, the promises of the ELI-NP facility, that is currently under construction, to deliver beams of almost monochromatic tunable (in the 0–20-MeV range) highly intense and highly polarized γ rays allows us to propose an application of those techniques aimed at solving the mystery of α clustering in ^{12}C (and other nuclei [1–3]) with a conceptually simple experiment. Several theoretical models have been proposed along the years to unravel the structure of the all-important carbon nucleus that have either focused on the whole spectrum or focused just on the properties of the Hoyle state or of the ground state. Let us mention a few of them: as early as 1937 Wheeler was reasoning with molecular models and with the idea of a triangular configuration of α particles in the nucleus of ^{12}C [4], in 1956 Morinaga proposed a linear chain of 3α particles as a possible structure for the Hoyle state [5]. Both the conventional shell model for p -shell nuclei and more recent *ab initio* models, such as the no-core shell model [6,7], provide valuable insight on the microscopic structure but are, at present, unable to reproduce all the features of this nucleus associated with the strong α clusterization, despite the tremendous computational efforts and the success in neighboring systems or the correct reproduction of some of the observed states. It seems that state-of-the-art nucleon-nucleon interactions still miss some important ingredient that explains the formation of clusters inside a nucleus. Other approaches, such as antisymmetrized molecular dynamics [8], fermion molecular dynamics [9], and nuclear effective field-theory lattice calculations [10] often predict slightly bent linear structures (or, that is the same nonequilateral triangles). Other approaches have relied on descriptions of ^{12}C as a Bose-Einstein condensate gas of α particles [11]. The equilateral triangle shape was, very convincingly to my view, re-proposed within the algebraic cluster model (ACM) by Bijker and Iachello [12,13]. This

model provides a group-theoretical construction of rotational and vibrational states of an equilateral triangle with three α particles at the vertices that is based on the $U(7)$ dynamical symmetry and contains the D_{3h} point group as a subgroup of $SO(3)$. Therefore, in a single formalism, the vibrational energies and rotational bands are adapted to the discrete symmetry. Not only the success of this elegant model in reproducing the spectral features is overwhelming, but also a spectacular prediction of a 5^- state at high excitation energy has been duly confirmed in experiments [14]. Already more than 50 years ago, Blatt and Weisskopf [15] warned us against taking the rigid molecularlike models too seriously, preferring a sort of liquid or dynamical view of α clusters in nuclei. The ACM mentioned above, being based on general algebraic grounds, circumvents some of these obstacles. Another model worth mentioning at this point is the semimicroscopic algebraic cluster model [16–18] where the role of the Pauli principle is emphasized, and the conclusions point toward a triangular structure, even though it does not support the vibrational interpretation of the Hoyle state as a breathing mode.

Despite all of these approaches and others on which I will not dwell, a direct proof of the exact shape is not yet available, and the correctness of one model (i.e., of a geometric configuration and the underlying symmetry) over the others only comes from the relative success in reproducing energy levels, electromagnetic form factors, and transition rates [19,20]. It is the aim of the following to show how the measurement of the depolarization ratio can discriminate among the various possibilities. The independent method that is suggested here is new to nuclear physics as testified, for example, by the recent paper [21] where a lucid review of the interplay of single-fermion and cluster dynamics is given, but no agreement can be found among different models.

I will now briefly recall the elements of the Raman effect, that was conceived and is now commonly employed in the realm of molecular physics, and I will then reformulate it in the language of nuclear molecules to provide a series of theoretical patterns that can be used in experiments with

polarized γ beams to definitely rule out or rule in certain symmetries (and the corresponding models).

The history of Raman spectroscopy and its far-reaching applications are too rich and long to be summarized in this Rapid Communication (see, for example, Ref. [22]), but one can say that, whenever electromagnetic radiation of a given frequency is shined at a sample, this might absorb it and reemit the same frequency (elastic or Rayleigh scattering) or a set of different frequencies (inelastic or Raman scattering¹) that reflect the inner workings of the molecular vibrational and rotational states. The detailed structure of the energy levels is a fingerprint that reveals information on the geometric arrangement of the charges inside the molecule and how they respond to an external electric field, i.e., its polarizability (that is a rank-2 tensor). The spatial configuration of atoms in a molecule links very deeply with the mathematical description provided by discrete point groups, that give a formal, powerful, and straightforward interpretation of the measured properties and the selection rules. In particular, the connection of Raman spectroscopy with a polarimeter, obtained through the acquisition of spectra through a polarizer that works as an analyzer set along or perpendicular to the polarization axis allows for measuring the depolarization ratio $\rho = I_{\perp}/I_{\parallel}$, i.e., the ratio of intensities measured along the perpendicular and parallel directions.

This ratio is the key quantity that allows the underpinning of totally symmetric modes [23], and thus it gives a precise spectroscopic clue as to whether a certain molecule possesses a given shape, according to the underlying vibrational representation of the discrete point group. Let us be more specific: There exist a set of rules on how randomly oriented samples give off radiation such that the intensity emitted from states belonging to totally symmetric representations² are polarized along the plane of the initial polarization, giving off less and less radiation (down to zero, but not necessarily) on the perpendicular plane, whereas all other nontotally symmetric modes give off exactly 3/4 less radiation on the perpendicular plane than on the parallel plane. These topics are very clearly summarized in Ref. [24], and they are very familiar to any spectroscopist [22,23],

$$0 < \rho < 3/4, \quad \text{totally symmetric states} \rightarrow \text{polarized,}$$

$$\rho = 3/4, \quad \text{other symmetric states} \rightarrow \text{depolarized.}$$

A band or a state of the first type is called polarized, whereas all other cases of nontotally symmetric states are called depolarized. In experiments with a certain error in the measurements, there is still a marginal possibility that ρ does not differ significantly from 3/4 also in the first case, but this is improbable in practice.

Now the nuclear molecules made of α particles, even though the Born-Oppenheimer approximation is most certainly not valid and large kinetic energy fluctuations are

¹I will leave aside the distinction between Stokes and anti-Stokes lines as it is inessential to the present discussion. Nuclei do not show appreciable thermal populations of excited levels.

²The symmetric representations take various names in different groups: $A, A', A_1, A_g, A'_1, A_{1g}, \dots$, etc.

name	shape	group	Γ_{vib}	Patterns
linear =		$D_{\infty h}$	$A_{1g} + A_{1u} + E_{1u}$	
linear \neq		$C_{\infty v}$	$2A_1 + E_1$	
equilateral		D_{3h}	$A'_1 + E'$	
isosceles		C_{2v}	$2A_1 + B_1$	
scalene		C_s	$3A'$	

FIG. 1. This table enumerates the possible shapes of a nuclear molecule made out of three α 's, their underlying point-group symmetry, and the characters of the normal modes of vibration (with totally symmetric modes highlighted). The last column shows the schematic predicted patterns for depolarization ratios (intensity vs energy, not to scale). The white and black histograms represent parallel and perpendicular intensities.

present in nuclei, are also prone to acquire a certain polarizability under the influence of the external electric field of the incoming polarized radiation. Then, depending on whether the latter has enough energy to excite a given mode, they might absorb it and reemit it, and the depolarization ratio of the emitted radiation is determined by the character of the vibration. Coming now to the application that I want to discuss, one can enumerate all possible classes of molecules that might arise from three α particles, and this brings us to the first two columns of the table in Fig. 1. The three particles can be on a line at the same distance between one another, thus giving a linear centrosymmetric configuration, whose geometry is left unaltered by the operations of the $D_{\infty h}$ dihedral group. Or the particles, although still on a line, might have different distances, thus giving a noncentrosymmetric arrangement, associated with the noncentrosymmetric group $C_{\infty v}$. In principle, there is no reason why three identical particles should take different distances on the right or on the left, but I want, for the sake of generality, to take all possibilities into account. On the other hand, if the particles are not on a line, they will form a triangle. The most symmetric (and most probable, unless one has a reason to suppose that the mutual interaction is affected by some other noncentral effect) is the equilateral triangle with group D_{3h} . This is the group of the six operations $\{E, 2C_3, 3C_2, \sigma_h, 2S_3, 3\sigma_v\}$ (i.e., identity, rotations around various axes, reflections, and improper rotations) that leave invariant the equilateral triangle. Another possibility is that the triangle is isosceles (with any apex angle between 0 and π but not $\pi/3$) with group C_{2v} or even that the triangle is scalene with C_s group. This is the simplest possible, being made up only of identity and reflection on the horizontal plane $\{E, \sigma_h\}$. Note that $D_{3h} \supset C_{2v} \supset C_s$ upon a proper identification of the axes' names.

Note that bent configurations are already contained in Fig. 1 under isosceles triangles (if the arms have the same

length) or under scalene triangles (if the arms have unequal lengths).

By taking $N = 3$ particles, one should find $3N - 5 = 4$ normal modes of vibration for linear configurations and $3N - 6 = 3$ for planar configurations. Albeit trivial by well-known methods of molecular physics, such as the tabular method [23], the laborious job of working out all the vibrational characters is not derived here but merely summarized in the fourth column of Fig. 1 where the Mulliken notation has been used. For each group, the totally symmetric representation, i.e., the one that is made of +1 characters for each operation of the group, has been highlighted in red. Remembering that A -type modes are singly degenerate, whereas E -type modes are doubly degenerate, one notes that the number of symmetric modes over totally symmetric modes is $1/4$, $2/4$, $1/3$, $2/3$, and $3/3$ respectively, that is, *for each symmetry, one can expect a given pattern, and these all differ from each other*. Now, in actual experiments, measuring intensities as a function of energy, one sees the doubly degenerate modes as one peak, therefore one should correct the previous theoretical statement into a practical recipe: $1/3$, $2/3$, $1/2$, $2/3$, and $3/3$ where, unfortunately, the linear noncentrosymmetric arrangement and the isosceles triangle do show the same number of polarized peaks over total peaks. Despite this concurrence, there are anyway four mutually exclusive possibilities, depicted schematically in the last column of Fig. 1 where the white histograms represent the intensity along the parallel direction and the black histograms represent the intensity along the perpendicular direction: From white to black, depolarized bands go to $3/4$, and polarized bands typically go to something between 0 and $3/4$ as already stated. Note that each peak should have its own intensity and energy and the patterns are to be intended only as a scheme of what will be observed. This method is *independent* of the actual values of the eigenstates or of the absolute and relative intensities of the transitions, and this easy measurement is definitely worth a try.

There is one possible complication to the neat picture described above, that might arise from the fact that the nucleus is not necessarily described by the same geometry in all of the excited bands, it might, for instance, be triangular in the ground state and become linear or bent in some excited states. Stated another way, the possibility that potential-energy surfaces (PESs) pertaining to different geometries might come

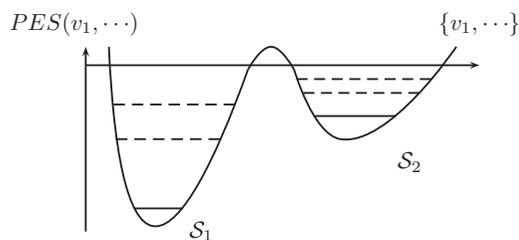


FIG. 2. Schematic of the PES, depending on the relevant variables of the potentials v_1, \dots (in general, multidimensional). More than one minimum, belonging to different symmetries, $S_{1,2}$ might be present, with its own set of excited states (bandheads shown with dashed lines).

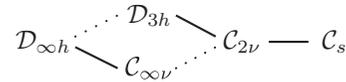


FIG. 3. Group-subgroup chain relations.

low enough to intersect with the lowest-energy curve is not to be discarded (and this would signal the presence of noncentral terms in the $\alpha - \alpha$ potential). This is depicted schematically in Fig. 2.

In this case, the rules outlined above should be connected depending on group-subgroup chain relations, see Fig. 3, using the tables of correlations between representations as in Fig. 4. This table is not complete (see Ref. [23]) but contains only the representations that occur in the normal modes (therefore sometimes there are slashed correspondences, that can be eliminated), and it should be read as follows: A representation, that behaves with certain characters under the operations of a larger group, behaves with characters belonging to some other representation of the smaller group.

The schematic in Fig. 2 does not necessarily point towards rigid models (even though it depicts the vibrations as bound states): The geometrical requirements and the rules are there also for states lying in the continuum; only the bars of the last column of Fig. 1 will correspond to resonances with finite widths rather than to narrow states.

Another issue worth mentioning at this point is as follows: What would happen to a BEC state of 3α particles? A BEC is a coherent superposition of bosons collapsed to the ground state, therefore it is a $L = 0$ state from which radiation should be scattered in a single polarized way.

Clearly all of the above is valid under the hypotheses that ^{12}C has an α -cluster structure and that the α 's are to be taken as elementary constituents. Therefore, these considerations are limited to energies low enough that the fermionic nature of the α 's does not come into play (I would guess somewhat below 20 MeV). In addition, nuclear molecules are very different from chemical molecules because the kinetic-energy fluctuations around the equilibrium points might be as large as the nucleus itself, whereas in molecules they are small vibrations, and the energy scales of vibrations and rotations do not decouple through the Born-Oppenheimer approximation as happens for atomic systems. These words of caution, however, do not affect the nature of symmetry: A discrete point-group symmetry is there even if the oscillations are large, provided that the geometry remains compatible.

$D_{\infty h}$	$A_{1g}+$	$A_{1u}+$	E_{1u}	$D_{\infty h}$	$A_{1g}+$	$A_{1u}+$	E_{1u}
	\downarrow	\downarrow	\downarrow		\downarrow	\downarrow	\downarrow
$C_{\infty v}$	A_1+	A_1+	E_1	D_{3h}	A'_1+	A''_2+	E'
	\downarrow	\downarrow	\downarrow		\downarrow	\downarrow	\downarrow
C_{2v}	A_1+	A_1+	$B_1 + B_2$	C_{2v}	A_1+	$A_1 + B_1$	
	\downarrow	\downarrow	\downarrow		\downarrow	\downarrow	
C_s	$A'+$	$A'+$	A'	C_s	$A'+$	$A'+ A'$	

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

In conclusion, it is suggested that a nuclear fluorescence experiment whereby the intensity of γ radiation emitted from an excited molecular cluster structure is measured along two perpendicular directions can be compared against a few enumerable theoretical patterns that can be traced back to different geometric point-group symmetries of the nuclear molecule. This gives a final and neat answer, independent of energies, transition rates, and the like, to the question that

arises from the puzzling plethora of interpretations that have been given on the α -cluster structure of ^{12}C . This method can easily be extended to other cluster structures with different numbers of particles or with different types of clusters.

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