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A crystallographic method to investigate the presence of cluster configurations in ¹²C

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Summary. — This work presents a crystallographic approach for the investigation of the existence of cluster structures in the ground state of ${}^{12}C$, with some forecasts on its extension to other nuclei, such as ^{16}O . The model is based on outstanding analogies between the world of molecules and that of atomic nuclei: diffractive studies are indeed used to determine molecular structures and properties, and a similar approach was developed in the present work for atomic nuclei, under the assumption of the presence of regular α -cluster structures. In this work we analyzed a large database of literature data for the elastic scattering angular distributions of protons colliding on 12 C and ⁴He target nuclei in the bombarding energy range $E_p = 30$ –80 MeV, for which the de Broglie wavelength associated with the proton beam is comparable with the distance existing between the assumed α -clusters inside the nucleus.

1. – Introduction

It is well known that structures assumed by light nuclei may easily deviate from the ordinary (spherical or spheroidal) ones; this is especially evident in the case of self-conjugated nuclei, or for nuclei with a conjugated core and some excess nucleons, for the ground and for some excited states [1-4]. The presence of long-range correlations in the nuclear force, in fact, can lead to the re-organization of nucleons in bound subunits, the so-called *clusters*; such clustering aspects are enhanced for sub-units saturating spin and isospin and having a large binding energy, as seen for α -particle–like clusters. Several examples of this kind can be seen in the lightest nuclei: the ⁸Be nucleus shows a very pronounced two- α -particles cluster structure [5,6], while for some excited states of ¹²C, ¹⁶O and ²⁰Ne [7-10] a diluted α -particles gas structure can be observed. Furthermore, in C, O, Ne isotopes, the presence of extra-neutrons can lead to a stabilization of nuclear bonding, giving rise even to molecular-like structures [11-14]. The occurrence of clustered structures of those types may have crucial implications not only on the way in which atomic nuclei are commonly considered, but also on various nuclear astrophysics phenomena, such as processes and reaction mechanisms involving the nucleosynthesis of elements [15]. A hypothesis of this type was formulated for the Hoyle state of ^{12}C , which was tentatively described as a Bose-Einstein condensate of α -particles [16], along with other multi- α -particles–condensed systems, heavier than ¹²C; solid experimental evidences on these very exotic phenomena are anyway still missing [17].

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More recently, the Symmetry Group Theory [18], very well established and used in the physical chemistry field, has been applied, in the framework of the Algebraic Cluster Model (ACM) [19,20], to clustered nuclear structures such as 12 C and 8 Be, which should respectively belong to the D_{3h} and Z_2 symmetry groups. In the fashion of this theory, similarly to the geometrical description of molecules, the 12 C ground state is seen as a triangular structure of α -particles, showing the characteristic symmetry elements for the D_{3h} group: i) a three-fold main symmetry axis (C_3) , ii) three two-fold secondary symmetry axes, orthogonal to the main one and iii) a horizontal symmetry plane, which cut the three α -particles in half. In the ACM, the first 0^+ excited state of ¹²C (named the *Hoyle state*) is then seen as a *breathing mode* of the triangular ground state, *i.e.*, a triangular structure with a larger radius than that of the ground state; electron scattering experiments could be useful to have a qualitative confirmation of this idea [21]. This approach is also able to successfully reproduce, through the prevision of rotational and vibrational excitations of the fundamental triangular structures, the excited level sequences for both the ground and the Hoyle state bands [22]. Very recently, *Otsuka* and collaborators [23] performed Monte Carlo Shell Model (MCSM) calculations to estimate the occurrence of α -clustering phenomena in ¹²C ground and excited states. As a result of this study, they predicted a quite large probability of having a three- α configuration in the Hoyle state (of about 67%), while the three- α configuration for the ground state has only 6% probability of occurrence; this would make highlighting its presence from data coming from scattering or reaction experiments difficult.

The possible occurrence of a triangular structure of α -clusters in ¹²C may also be supported by the fact that it is quite difficult to describe the details of $p+^{12}C$ elastic scattering cross-section data in the 30–100 MeV projectile energy region by simply using optical model potentials with spheroidal symmetry. Deviations are still present even by performing more detailed Coupled Channel (CC) calculations [24] to describe experimental elastic and inelastic scattering data. It was suggested in refs. [25, 26] that the inclusion of a coherent scattering term, due to the presence of the triangular structure composed by the α -particles, could help to give a better reproduction of the experimental angular distributions. The inclusion of such a coherent term may be justified by the fact that, in this energy domain, the wavelength of the matter wave associated to the proton beam should be of the same order of magnitude of the characteristic distances between the clusters, r_{ij} . Theoretical calculations suggested that, for the ¹²C ground state, r_{ij} should be in the range 3.5–5.5 fm [27]; therefore, proton beams of energy in the range of 30–80 MeV impinging on ${}^{12}C$ target would have the right de Broglie wavelength to give rise to diffractive pattern effects because of coherent scattering on the α -clusters constituting the 12 C nucleus. It is therefore possible to consider that the resulting elastic scattering angular distribution $\frac{d\sigma}{d\Omega}(\theta)$ will be composed of two different contributions: the main one given by the scattering of protons on an ordinary, spheroidal, 12 C nucleus seen as a whole compact object, and the minor one, indicated as coherent contribution, given by the interference effects produced by the scattering of the proton beam by a triangular cluster structure. In the present analysis we performed a comprehensive fit of $p+$ ¹²C of elastic scattering data available in the literature by including both the spheroidal and cluster components, to describe the experimental angular distributions. Further details on the fitting procedure can be found in ref. [28]. A preliminary analysis of the same type on $p+16$ O elastic scattering data is also discussed.

2. – Model description

In the present model, we will describe the experimental angular distribution of $p+$ ¹²C elastic scattering data as the incoherent sum of two different contributions: the first one, $I(\theta)_{spher}$ will describe the scattering from the spheroidal structure; the second, $I(\theta)_{clust}$, the coherent interference pattern given by the triangular cluster structure:

(1)
$$
I(\theta)_{tot} = A \cdot I(\theta)_{sphere} + B \cdot I(\theta)_{clust}.
$$

The two contributions for $I(\theta)$ inside eq. (1) have been computed in two different ways. $I(\theta)_{spher}$ has been estimated by CC calculations based on optical model parameters, in the range of 30–50 MeV, originally taken from [24]. In the framework of this approach, the couplings which have been taken into account were those between the ground state, the 4.44 MeV (2^+) and 14.08 MeV (4^+) , all belonging to the ground state band; on the other hand, couplings of the ground with the Hoyle and the 9.64 MeV (3−) excited states were neglected, since it has already been shown [24] that their inclusion has only a very small influence on the determination of the elastic scattering cross-section. The contribution from the scattering on the clustered structure, the so-called coherent part, has been calculated by the application of the Wierl crystallographic formula [18, 29], which links the diffraction intensity $I_{clust}(\theta)$ to the scattering amplitude of protons colliding on the single α -cluster (f_i) , and to the diffraction phenomena on matter waves caused by two neighbouring clusters

(2)
$$
I_{clust}\theta = \sum_{i} |f_i|^2 + 2 \sum_{i,j}^{i \neq j} f_i f_j \cdot \frac{\sin(\mu r_{ij})}{\mu r_{ij}}.
$$

In the formula reported in eq. (2) , the scattering amplitude for a single α -cluster scattering centre has been estimated through the analysis of the cross-sections for $p+4$ He in *vacuo* elastic scattering reactions in the $E_p \approx 30{\text{meV}}$. By doing this, we performed bi-dimensional extrapolations (in both angle and energy) of experimental data obtained at several energies from the EXFOR database [30-33]. The second term in the right-hand side of the equation depends on the geometrical properties of the diffracting structure through the inter-cluster distance, r_{ij} , and also on the wavelength of the incident beam, since $\mu = \frac{4\pi}{\lambda} \sin(\frac{\theta}{2})$, where θ is the scattering angle in the centre-of-mass frame. A preliminary optimization of the (dominant) spheroidal contribution, $I(\theta)_{sphere}$, was carefully performed by performing a coupled channel fit of $p+^{12}C$ elastic scattering data available from the EXFOR database [34-40]. The starting parameters for the fit were taken from ref. [24]; the original parameters were allowed to vary within 30% with respect to the starting values. The following parameters have been fitted: the imaginary depth of the surface potential and the radius (R) and diffuseness (a) of the real and imaginary potentials. To give a further physical constraint to the parameters, together with the elastic scattering data we simultaneously fitted the reaction cross-section data reported in ref. [41].

3. – Results

In fig. 1 we report, as red dotted lines, the results of the CC fit of $p+^{12}C$ elastic scattering data at some of the investigated energies, without assuming any cluster contribution. For comparison, we reported as green dashed lines the CC calculations performed with the original parameters taken from the literature [24]. The description of the data with the improved parameters coming from the fit procedure is quite satisfactory at all the angles and for all the energies investigated; this would point out (as already mentioned)

Fig. 1. – Angular distributions for the $p+^{12}C$ elastic scattering fits reported at energies $E_p =$ 35 MeV [36], 40 MeV [26, 37], 61 MeV [39], 65 MeV [40]. In the graphs, the three dashed curves represent different fitting conditions: the spheroidal contribution with this work's optimized parameters (red dotted line) and with original parameters from [24] (green dashed line) and the cluster term only (blue dashed line). The red solid lines represent the comprehensive fit, including the contributions from the spheroidal and the coherent terms.

the dominant role of the spheroidal contribution. At backward angles, a slight difference between the fitting curves and the experimental data is present. This may be due to the presence of exchange effects, and/or compound nucleus effects which may arise in this angular region, that are not included in our simplified model. To put in light the possible presence of contributions due to the occurrence of a triangular cluster structure in ^{12}C , we performed a comprehensive fit of all the experimental data (elastic scattering and reaction cross-section) with both the spheroidal and cluster term, using as starting parameters for the spheroidal term the optimized values here discussed. In the fit procedure, we constrained the spectroscopic factors A and B to fulfill the unitary condition $A + B = 1$, meaning that phenomena other than scattering or absorption are not taken into account. The inter-cluster distance r_{ij} was left as a free parameter in the fit procedure.

In fig. 1 we plot as solid red lines the results of the global fit, and as blue dashed lines the contributions due to the coherent part. The inclusion of the coherent term brings a slight improvement in the fit (with a χ^2 value $\approx 10\%$ smaller than the fit with the spheroidal contribution only). The small improvement in the fit can be also seen from the histograms of fig. 2 (left), showing the distributions of the normalized residuals between data and fit calculations: the inclusion of the coherent contribution in the fit leads to a slightly narrower distribution. As a result of the fit procedure, it is possible to estimate, for the B parameter, an upper limit of 1% with a 99.75% confidence level, and an inter-cluster distance of $r_{ij} = 3.9 \pm 0.5$ fm in the ground state of the ¹²C nucleus. These results point out a minor contribution of the cluster configuration in the wave function of ¹²C ground state; qualitatively, the order of magnitude of both the inter-cluster distance and the B parameter are not far from the prediction of ref. [23].

A similar, but still very preliminary analysis, was performed for $p+^{16}O$ elastic scattering data. In this case, we assumed a tetrahedral configuration for the four α -particles in the ground state of ^{16}O , as recently suggested in refs. [42, 43]; the coherent term can be described by using the Wierl formula (eq. (2)) for a tetrahedral structure. The contribution due to the scattering on a spherical structure is described by optical model calculations with parameters taken from the commonly used compilation of [45]. In fig. 2 (right) we show, as a red line, the optical model calculations together with data at $E_p = 31$ MeV taken from refs. [35, 42]. The discrepancies shown at medium-to-large angles ($\theta \approx 70^{\circ} - 140^{\circ}$) cannot be easily solved with moderate variation of the optical model parameters, while the description of data becomes (qualitatively) much better if we in-

Fig. 2. – (Left) Normalized residual distribution: $\delta = \frac{\sigma_{th}(\theta) - \sigma_{exp}(\theta)}{\sigma_{exp}(\theta)}$. Green dashed line: coupled $\frac{\sigma}{\sigma_{exp}(\theta)}$. Green dashed line: coupled channels calculations with literature parameters [24]. Red dashed line: coupled channels calculations with optimized parameters. Filled histogram: both spheroidal and cluster components included. (Right) A similar analysis performed on experimental data for $p+16$ O elastic scattering at $E_p = 31 \text{ MeV}$ [35, 44], where the spherical part is described with simple optical model calculations (red line) and with the inclusion of a 2% contribution from a clustered tetrahedral structure (blue line).

clude the presence of a $\approx 2\%$ contribution due to the coherent scattering on the cluster structure; the deviation at higher angles can be attributed to the same effects discussed for the 12 C case. Starting from these preliminary analyses, more detailed investigations on the structure of 16 O are planned to be performed in the future.

4. – Conclusions

In this paper we discussed a novel approach to unveil the presence of (transient) cluster structures in the ground state of the 12 C self-conjugate nucleus based on the analysis of $p+^{12}C$ elastic scattering data at intermediate energies. The differential cross-section of elastic collisions was assumed to derive from the superposition of two contributions: a main term given by the scattering of the proton matter wave on a spheroidal structure, and a more exotic term, coming from the coherent scattering of the proton matter wave onto an equilateral triangular structure composed of three α -particles. The coherent term was treated by using the Wierl crystallographic formula in analogy with diffraction experiments on molecules. A simultaneous multi-parametric fit of a large database of scattering data at several energies allowed to obtain an estimate of the relative weights of the two contributions. A minor influence of the cluster configuration on the ground state of ¹²C has been found, compatible with an upper limit of 1\% (99.75\% CL). A larger impact of the cluster structure seems instead to be needed to describe the $p+^{16}O$ elastic scattering data, but the results are still preliminary and need to be refined with further analyses on a much larger database. It is worth noting that currently available datasets are affected by large uncertainties on the cross-section and use large angular steps, representing a limitation for the fit procedure; new experimental data could help to better disentangle the impact of the cluster contribution.

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