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Search for molecular bands in ^{13}C

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Abstract. In a systematic search through experimental results for transfer reactions, inelastic excitations and other data for ^{13}C we identify states which have no simple structure related to the low-lying states of ^{12}C. We propose that these states have strong α-clustering and that they are related to chain states expected in $^{13\text{-}14}$C. The properties of these states are discussed on the basis of a molecular orbital model.

PACS. 21.10.-k Properties of nuclei; nuclear energy levels – 21.60.Gx Cluster models

1 Introduction

The neutron-rich carbon isotopes have recently been the subject of increased interest, because the observation of unique physical-shape isomers based on α-clustering is expected at high excitation energies. This feature is suggested due to the fact that molecular orbitals have been found to be very useful for the description of structures in $^{9\text{-}12}$Be isotopes [1]. These structures are based on the particular property of the $\alpha + \alpha$ potential: the local potential is very shallow and has a strong repulsion at small distances. The repulsion at small distances can be interpreted as the effect of the Pauli blocking; in the case of the $\alpha+\alpha$ potential the nucleons of the second cluster have to move up into the next major shell. The ^{8}Be nucleus is unbound, the ground state is a clear resonance at a very low energy of $E_\alpha^{\rm cm} = 92$ keV, and there are higher-lying states (resonances) with spin and parity of $J^\pi = 2^+$ and 4^+, which can be well explained within a potential model as scattering resonances. Alternatively, we can consider ^{8}Be to be the first "superdeformed" nucleus (nucleus with a deformation of 2 : 1). This nucleus is also the starting point of the Ikeda diagram of cluster nuclei [2], which has been the basis of numerous experimental studies, a survey of which can be found in ref. [3]. The heavier isotope, the ^{9}Be nucleus, has been recognised already 20 years ago as a bound nuclear three-body system, which can be understood either as a "Borromean" nucleus [4], or as the first example of a nuclear molecule consisting of two α-clusters bound by a covalent neutron [1,5–7].

The formation of covalently bound molecular structures relies not only on certain properties of the core-core potential but also on particular properties of the nucleonic molecular orbitals. The concepts of nuclear molecular orbital have often been used in scattering systems [8–11], but also specifically for the binding in beryllium isotopes [1, 5–7]. The molecular orbital model is related to the two-centre shell model (TCSM) [12], where not only valence nucleons, but all nucleons are considered. Based on the TCSM, a correlation diagram can be drawn, as shown in fig. 1, in analogy to the well-known correlation diagrams of atomic physics (see also ref. [13], p. 328).

This correlation diagram merges at small distances with the Nilsson diagram of the deformed compound nucleus. Due to the axial symmetry, projections on the z-axis appear as conserved quantum numbers. Therefore molecular configurations are classified according to the well-known quantum numbers of axial symmetric molecular states: the K-quantum number for the projection of the spin, the σ- and π-orbitals for the $m_l = 0$ and $m_l = 1$ projections of the orbital angular momentum, the parity, and the *gerade* (g) and *ungerade* (u) symmetry due to the identity of the two molecular cores. In molecular spectroscopy the concept of parity is not used, but only g and u in replacement of parity (see, *e.g.*, ref. [13], p. 318). We need both concepts independently (see ref. [8]) for the discussion of wave functions in sect. 3. With the correlation diagram we are able to discuss the structure of all states of the isotopes $^{9\text{-}12}$Be, if we consider the population of the states via molecular orbits for an α-α distance corresponding to the potential minimum [1], or to a deformation in the Nilsson model with a value of the parameter $\beta_2 \approx 0.6$.

In the compilation of ref. [1] the dimer-structure of the states of the isotopes $^{9\text{-}12}$Be has been established. In fact, due to the high binding energy of α-clusters (*ca.* 24 MeV), we can expect that strongly deformed states forming rota-

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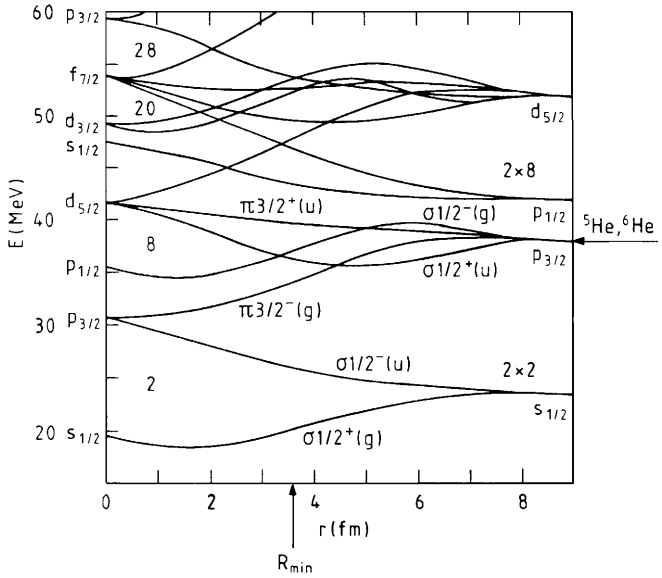

Fig. 1. Correlation diagram of molecular orbitals in a two-centre shell model picture [12]; the orbitals are labelled by their quantum numbers. r is the distance between the two centres, the arrow indicates the distance where the minimum in the $\alpha + \alpha$ potential occurs.

tional bands are observed in isotopes $^{9\text{-}12}$Be, which are determined by the properties of the valence neutrons alone. In a variety of recent experiments using stable [14–18] and radioactive [19–21] beams, rotational bands of such strongly deformed states in beryllium isotopes have been confirmed.

For the chain states of carbon isotopes, the inclusion of a third centre will introduce in the first order, as in physical chemistry, a further splitting in the basis states and a lowering of the lowest state with respect to the three-body thresholds. Another important aspect, however, will enter in the nuclear physics case because of the possible occurence of intrinsically reflection asymmetric states [22], which give rise to parity doublets (as opposed to the Be-isotopes which are reflection symmetric). Later in sect. 3 we will start the construction of the corresponding wave functions for ^{13}C-chain states.

The second 0^+ state of ^{12}C has long been considered as a 3α chain state. However, the bending mode is shown to be an important part of the wave function [23], so this state can also be described as a weak-coupling state with a $^8\mathrm{Be} + \alpha$ configuration [24]. The bending modes of the pure α-particle chains, on the other hand, may be restricted once the valence neutron bonds are added (if they correspond to a covalent-binding configuration [25,26]).

Experimental evidence for molecular states in heavier carbon isotopes is rather scarce. For the case of ^{13}C which is presented here, we will show that such evidence can be extracted from a systematic survey of the properties of all excited states of ^{13}C. There may also be some indirect indications that some states of ^{14}C can have molecular structure [1], but further experimental work is needed. Results from the recent experimental search for molecular states in ^{16}C [27,28] show that this is not going to be an easy task.

There has also been an increased interest in the theoretical description of molecular states. The method of Antisymmetrised Molecular Dynamics (AMD) [29], used by Horiuchi, Kanada-En'yo *et al.* [30–32], gave strong support for the molecular stuctures in $^{9\text{-}12}$Be. The method has also been applied to the C-isotopes [33–35]. More recent work based on the explicit use of molecular configurations has been done for Be-isotopes [36,37] and was started for C-isotopes by Itagaki *et al.* [25,26].

In sect. 2 we present a compilation of a variety of published experimental results with the aim to establish the "complete spectroscopy" of ^{13}C, which will allow us to determine the excitation energy spectra of possible strongly deformed bands in ^{13}C, *i.e.* of states which are not related to the more normal structures, *e.g.* the ^{12}C ground and first excited states. In sect. 3 we will formulate arguments for states related to the cluster states in ^{12}C, in particular to states like the three α-particle chains and to these with triangular configurations. In both cases we expect parity doublets. In subsect. 3.4 the corresponding wave functions for three-centre configurations of ^{13}C-chain states are derived and with these formulations we can make predictions for the assignments of isomeric rotational bands. Discussions, comparison with other work and conclusions are given in sect. 4.

2 Systematics of experimental results on ^{13}C

The mass 13 nuclei have been the subject of many shell-model calculations (*e.g.* [38–41]). Generally, normal- (negative) parity states in ^{13}C and ^{13}N are considered to arise from various recouplings of nine nucleons in the p-shell [38]. For the positive-parity states, use is made of the weak coupling, which exists between a nucleon in sd-shell and the ^{12}C core [42,43] (usually, only the lowest two core states are included in this model).

The level schemes of ^{13}C and ^{13}N are experimentally reasonably well determined for excitation energies up to about 9.5 MeV [44] and in this context, these two nuclei manifest the success of the simplified shell model in a striking way. Both the reduced widths and the spectrum itself lend strong support to these calculations and the mirror states in this excitation region are clearly identified (*e.g.* [45,46]).

The problems in the interpretation of states arise for the states above 9.50 MeV of excitation. Some of the experimental results still appear to be in conflict, which makes a systematisation of the data difficult. In any case it appears, that in the p-shell calculations [38] there are no candidates for the 9.90 MeV $3/2^-$, 10.75 MeV $7/2^-$, 10.82 MeV $5/2^-$ and 11.08 MeV $1/2^-$ levels. These levels are discussed to be predominantly $p^7(sd)^2$ in character and possibly arising from the coupling of two nucleons in the lowest sd-shell Nilsson orbit to the ground state ($K = 3/2$) and first excited state ($K = 1/2$) bands of an $A = 11$ core [47].

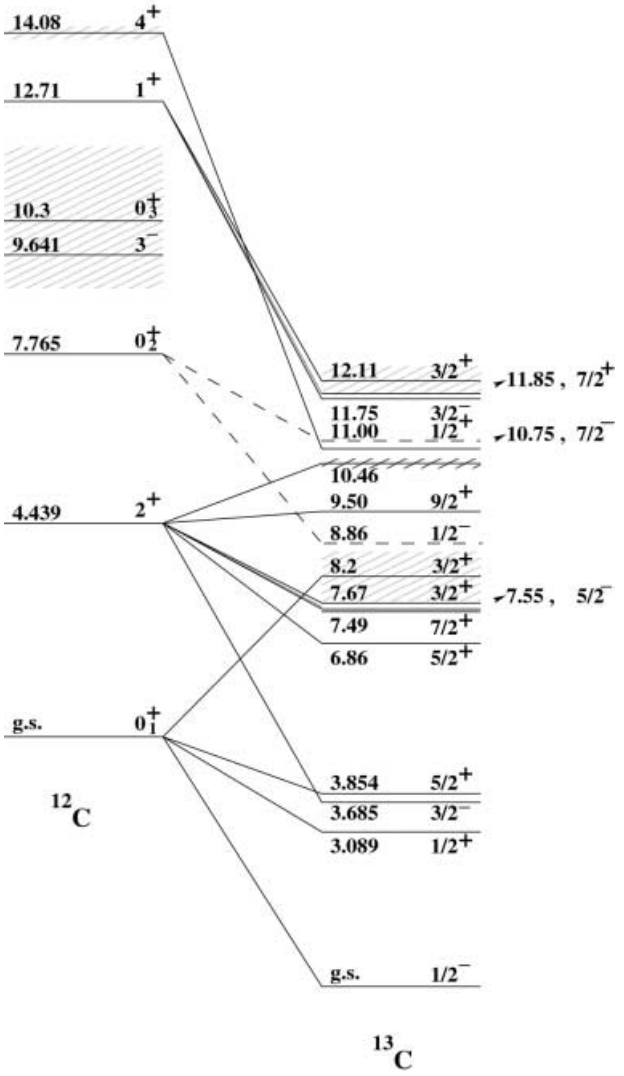

Fig. 2. Plot of energy levels for the isotopes ^{12}C and ^{13}C. States of ^{13}C have been grouped into single-particle states coupled to the indicated states of ^{12}C (except 3^-_1). The remaining states are grouped into rotational bands and shown in fig. 3. The dashed lines suggest the relation of the excited $1/2^-$ and $1/2^+$ states to the 0^+_2 (^{12}C), similar to the relation of the $1/2^-$ (g.s.) and $1/2^+$ (3.089 MeV) to the 0^+_1 (^{12}C).

Table 1. Proposed rotational bands in ^{13}C; values for Γ are taken from refs. [44,48,49].

J^π proposed	E_x (MeV)	J^π assignment in ref. [44]	Γ (keV)
$K = 3/2^-$			
$3/2^-$	9.897	$3/2^-$	26
$5/2^-$	10.818	$5/2^-$	24
$7/2^-$	12.438	$7/2^-$	336
$9/2^-$	14.13	$3/2^-$	150
$11/2^-$	16.08	$(7/2^+)$	150
$K = 3/2^+$			
$3/2^+$	11.080	$1/2^-$	≤ 4
$5/2^+$	11.950	$5/2^+$	150
$7/2^+$	13.41	$(9/2^-)$	35
$9/2^+$	15.28	$9/2^+$	
$11/2^+$	16.950	None	330

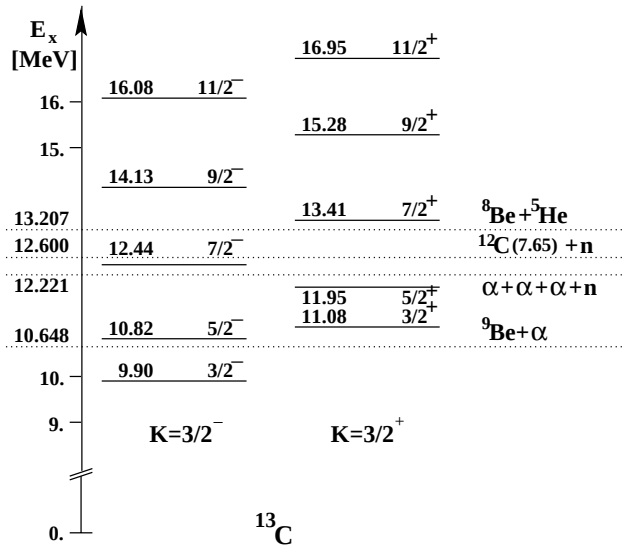

Fig. 3. Plot of energy levels of ^{13}C, which cannot be based on various compact states (g.s., 2^+_1 and 1^+_1) of ^{12}C and thus are not shown in fig. 2. The states are grouped into rotational bands with K-quantum numbers as indicated. The spin assignments are discussed in the text. Thresholds for various structure components of states in ^{13}C (mainly related to the asymptotic basis of states in the $\alpha + {}^9$Be system) are also shown.

Having in mind the excited states of ^{16}O, one can expect also in ^{13}C a significant contribution from $p^5(sd)^4$ configurations, which then naturally introduces the need for cluster models. In a weak-coupling scheme, the before mentioned states would have to be constructed with the 0^+_2 and 3^-_1 core excitations (fig. 2). Since both of these ^{12}C states cannot be explained even with the largest shell model calculations [41] and are known to be well described by the cluster models (*e.g.*, [24]), we expect similar cluster structures for the listed ^{13}C states. The available experimental data allow us to propose the existence of two molecular parity split rotational bands (given in table 1 and illustrated in figs. 3 and 4), both would correspond to a strongly deformed structure. Actually, since the underlying structure ($^9\mathrm{Be} + \alpha$ or $\alpha + \alpha + \alpha + \mathrm{n}$, see sect. 3) can be considered as intrinsically asymmetric, these bands appear as a parity doublet. The states of such structure should have large α-strength; it will be shown that they are strongly populated in reactions like $^9\mathrm{Be}(\alpha,\alpha)^9\mathrm{Be}$, $^9\mathrm{Be}(\alpha,\mathrm{n})^{12}\mathrm{C}$, $^9\mathrm{Be}(^6\mathrm{Li},\mathrm{d})^{13}\mathrm{C}$ and similar multi-nucleon transfers. Fortunately, the $^9\mathrm{Be}(\alpha,\mathrm{n})^{12}\mathrm{C}$ reaction has been of great interest for astrophysical reasons and its excitation function has been measured a number of times with an excellent resolution (*e.g.* [50,48]). These measurements give us a good basis for the identification of the states of molecular structure.

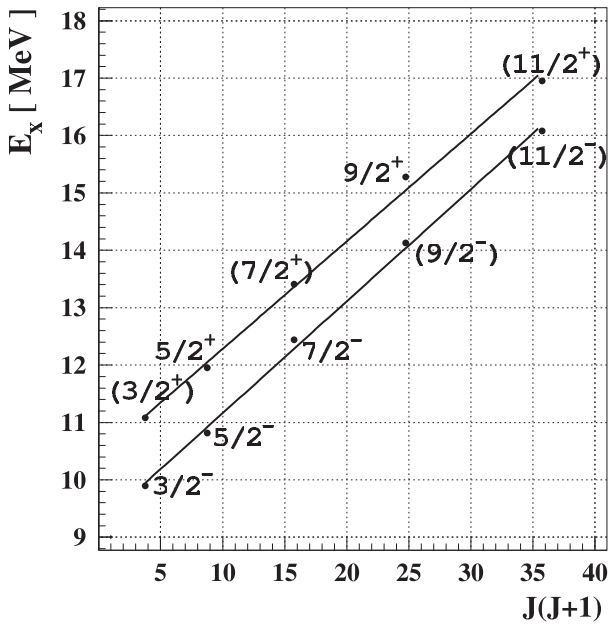

Fig. 4. Proposed rotational α-cluster bands in ^{13}C. These are states which cannot be attributed to single-particle states based on ^{12}C (g.s., 2^+_1 and 1^+_1), their energies are plotted as a function of their assumed spins, $J(J+1)$, as rotational bands with K-quantum numbers $3/2^{\pm}$ as indicated.

2.1 Rotational bands of ^{13}C

We shortly introduce here the parametrisation for the energies of the rotational bands including the Coriolis decoupling parameter, a:

$$E(J) = \frac{\hbar^2}{2\theta}\left[J(J+1) + (-)^{J+1/2}a(J+1/2)\right], \qquad (1)$$

where θ is the moment of inertia.

The internal structures of the states in ^{13}C and their moments of inertia θ can be obtained by putting the neutrons in the π- and σ-orbitals of the correlation diagram shown in fig. 1, forming the two lowest states in ^{9}Be ($3/2^-$ and $1/2^+$), at the two possible positions between the three α-particles (see sect. 3 for a more detailed discussion).

We can thus predict α-cluster states in ^{13}C with one covalent neutron, based on the two dominant molecular structures in ^{9}Be. The lowest state will form $K = 3/2$ rotational bands. In sect. 3 we will explain that the negative-parity state is the lowest, and that there must be a parity doublet for $K = 3/2$. For $K \neq 1/2$, the Coriolis coupling parameter a is usually negligibly small. The plot of the excitation energies of the states from fig. 3 as a function of $J(J+1)$ is shown in fig. 4. The agreement with eq. (1) is excellent. In the remaining part of this section we will give arguments for putting each of the states into the proposed $K = 3/2^-$ or $K = 3/2^+$ bands. We will not consider the $K = 1/2$ case also because the Coriolis decoupling may be strong and thus would make the identification of states belonging to these bands difficult. Another structural aspect of these $K = 1/2$ will be given in subsect. 2.4.

2.2 The proposed $K = 3/2^-$ band

9.897 MeV state

First we review the data focusing on the 9.897 and 11.080 MeV states. The $3/2^-$ state at 9.897 MeV of excitation is a rather narrow state (Γ = 26 keV), taking into account that it is $\approx$ 5 MeV above the threshold for neutron emission. Due to the fact that there are no other states closer than 400 keV, its spin assignment is well established (*e.g.*, [51]) and the differential cross-sections for the population of this state are easily obtained even in experiments with very bad energy resolution. One can thus see that this state is barely (or even not at all) populated in one-nucleon transfer reactions [45,52–54], but it is rather prominent in two- and three-nucleon transfer reactions [45,46,55–58] on corresponding targets, and also quite strong in α-transfer reactions on ^{9}Be [59–61]. Actually, the experimental spectroscopic strength for $^9\mathrm{Be} + \alpha \rightarrow {}^{13}\mathrm{C}$ is three orders of magnitude larger [60] than the theoretical prediction based on the $1p$ shell calculations [62]. Furthermore, both proton [63,64] and electron [47,65] inelastic scattering confirm that this level is not well described in the Cohen-Kurath model [38] (the $B(M1)$ value for the decay to the ground state is considerably smaller than those measured for any p-shell level). Also, simple models cannot properly describe ^{3}He and α inelastic scattering [66] to this state. To conclude, this is a complex state, which contains significant $2\hbar\omega$ (and probably $4\hbar\omega$, etc.) excitations in its wave functions, and which shows pronounced α-strength. The vicinity of thresholds for the $^9\mathrm{Be} + \alpha$ (10.648 MeV) and the $^{12}\mathrm{C}(0^+_2) + \mathrm{n}$ (12.600 MeV) decay, together with the above arguments, allows us to propose a strong cluster structure for the 9.897 MeV state. So we can now look for the states which form the rotational band based on it (table 1).

10.818 MeV state

The candidate for the first excited state of the rotational band is the 10.818 MeV, $5/2^-$ state. As the $3/2^-$ state, this state is only weakly populated in one-nucleon transfer reactions [45,52–54] and when resolved, it is always weaker than the 10.753 MeV state. It is not seen in proton inelastic scattering [63,64] (while the 10.753 MeV state is). Unfortunately, it is rarely clearly resolved in multi-nucleon transfer reactions; *e.g.*, in α-transfer reactions [59,60], the strongest peak in the spectrum is at $E_x \approx 10.80$ MeV, but it probably includes contributions from states at 10.753, 10.818, 10.996 and 11.080 MeV. The 10.818 MeV state is clean only in the $^{10}\mathrm{B}(^6\mathrm{Li}, {}^3\mathrm{He})^{13}\mathrm{C}$ [46] and $^{11}\mathrm{B}(^3\mathrm{He}, \mathrm{p})^{13}\mathrm{C}$ [55] reactions and in them it is stronger than the 10.753 MeV state. Although the $^9\mathrm{Be} + \alpha$ threshold is very close (at 10.648 MeV) so an α-beam of very low energy is needed, the 10.818 MeV resonance has been seen in $^9\mathrm{Be}(\alpha, \mathrm{n})^{12}\mathrm{C}$ measurements [50]. This state is also clearly seen in the $^7\mathrm{Li}(^9\mathrm{Be}, {}^{13}\mathrm{C} \rightarrow \alpha + {}^9\mathrm{Be})\mathrm{t}$ reaction [49]. Based on the arguments above, we believe that

its structure is quite different from the 10.753 MeV state, and that it can be considered as a member of the rotational cluster band.

12.438 MeV state

This $7/2^-$ state is also only weakly (if at all) populated in one-nucleon transfer reactions [45,53,54,67]. It is seen in inelastic proton scattering [63,64], but the authors conclude that "it is not the second $7/2^-$ state of Cohen-Kurath model". It is clearly seen in two-nucleon [45, 55,57] and three-nucleon [58] transfer reactions. Furthermore, it is seen in a number of $\alpha + {}^9$Be reactions: as a rather strong resonance in the $^9\mathrm{Be}(\alpha, \mathrm{n}_0)^{12}\mathrm{C}$ [48], $^9\mathrm{Be}(\alpha, \mathrm{n}_1)^{12}\mathrm{C}$ (4.44 MeV) [68], $^9\mathrm{Be}(\alpha, \mathrm{n}\gamma_{4.4})^{12}\mathrm{C}$ [69] and $^{12}\mathrm{C}(\mathrm{n}, \alpha)^9\mathrm{Be}$ [70] reactions; and also as a small peak in the $^9\mathrm{Be}(\alpha, \alpha)^9\mathrm{Be}$ [71] reaction. Also, in α-transfer reactions [59,60] this state probably corresponds to the peak listed at 12.1 MeV of excitation energy. The fact that it is not seen in the $^7\mathrm{Li}(^9\mathrm{Be}, ^{13}\mathrm{C} \rightarrow \alpha + {}^9\mathrm{Be})\mathrm{t}$ reaction [49] is probably due to the small efficiency for its detection (combined with rather small statistics and large spin). The above arguments allow us to propose that this state is not a p-shell level ($0\hbar\omega$) as proposed by Millener *et al.* [47], but the member of the proposed $K = 3/2^-$ rotational band based on the $3/2^-$ 9.897 MeV state. Note that the width of this state measured recently in the $^9\mathrm{Be}(\alpha, \mathrm{n}_0)^{12}\mathrm{C}$ reaction [48] and listed in table 1 is much bigger (336 keV) than the one (140 keV) given in the last compilation [44]. In the light of the discussion of the widths given latter in subsect. 2.6 we think that both values are acceptable.

14.13 MeV state

This state has been assigned as $3/2^-$ in ref. [44]. This assignment is based on the analysis of the $\mathrm{n} + {}^{12}\mathrm{C}$ scattering [72] and on the $^{13}\mathrm{C}(\mathrm{p}, \mathrm{p}')^{13}\mathrm{C}$ measurements [64]. In the latter work (similar to the observations for the 14.39 MeV state) the angular distribution for this state shows a maximum near 40° which indicates that it is not a low-spin state (and we propose $9/2^-$). The main argument for putting this state in the rotational band is its large α-strength. That is, it is the strongest resonance seen in $^9\mathrm{Be}(\alpha, \alpha)^9\mathrm{Be}$ [71,73] and $^9\mathrm{Be}(\alpha, \mathrm{n}_2)^{12}\mathrm{C}$ (7.65 MeV) [68] reactions (at this energy we expect $L = 4$ contributions), it is very pronounced in $^9\mathrm{Be}(\alpha, \mathrm{n}_1)^{12}\mathrm{C}$ (4.44 MeV) [68] and $^{12}\mathrm{C}(\mathrm{n}, \alpha)^9\mathrm{Be}$ [70] reactions and also clearly seen in the $^9\mathrm{Be}(^6\mathrm{Li}, \mathrm{d})^{13}\mathrm{C}$ reaction [60]. It is also seen in the $^7\mathrm{Li}(^9\mathrm{Be}, ^{13}\mathrm{C} \rightarrow \alpha + {}^9\mathrm{Be})\mathrm{t}$ reaction [49], although the efficiency for its detection was very small. A similar experiment with better statistics could help to establish its spin and show if our hypothesis is correct.

16.08 MeV state

This state has been tentatively assigned as $(7/2^+)$ in ref. [44]. It is seen in the $^9\mathrm{Be}(\alpha, \alpha)^9\mathrm{Be}$ reaction [71,73] and it is very strong in the $^9\mathrm{Be}(\alpha, \mathrm{n}_0)^{12}\mathrm{C}$ and $^9\mathrm{Be}(\alpha, \mathrm{n}_1)^{12}\mathrm{C}$ (4.44 MeV) reactions [68]. With a coupling of $L = 4^+ \otimes \mathrm{Be}(3/2^-)$, we propose the $11/2^-$ assignment for this state and as such it fits the $J(J+1)$ rule very well (fig. 4).

2.3 The proposed $K = 3/2^+$ band

11.080 MeV state

The state at 11.080 MeV is extremely narrow ($\Gamma \leq 4$ keV) with spin and parity given in ref. [44] as $1/2^-$. Its spin is assigned from a $^{15}\mathrm{N}(\mathrm{p}, ^3\mathrm{He})^{13}\mathrm{C}$ measurement [45], although the state was not resolved from the 10.996 MeV state and the DWBA-fit was not really good even when the mixture of $L = 0$ and $L = 2$ transfer was used. Also, the authors did not expect that positive-parity states could be excited in this reaction so they did not consider the possibility of $L =$ odd transfer. Later on, this assignment was questioned in a number of articles. For example, based on ^{3}He and α inelastic scattering, Peterson *et al.* [66] claim: "the DWBA-fit indicates that either the tentative $1/2^-$ spin assignment is in error or, that an unexpected selection rules eliminates the $L = 0$ cross-section expected to dominate the excitation". Collins *et al.* [63] have measured proton inelastic scattering on ^{13}C and were surprised "to observe how poorly DWBA-calculations compare with the data" (assuming $1/2^-$ spin). Yasue *et al.* [53] (based on the $^{14}\mathrm{C}(\mathrm{p}, \mathrm{d})^{13}\mathrm{C}$ reaction) found that "DWBA calculations for the 11.080 MeV state deviate from the data at backward angles" and Ohnuma *et al.* [52] have measured angular distributions for (d, p) reaction on ^{12}C ($E = 30$ MeV) but a reasonable description of the 11.080 MeV state could not be obtained by DWBA. It is interesting to note that the angular distributions for the $5/2^-$ (7.55 MeV) and $7/2^-$ (10.75 MeV) states in this last experiment have a minimum at the angle ($\theta_{\mathrm{c.m.}} \approx 45°$), where a distribution for the 11.080 MeV state has a maximum (fig. 5); this indicates that the parity of the 11.080 MeV state should be positive. Also, Knox and Lane in their R-matrix analysis of $^{12}\mathrm{C} + \mathrm{n}$ scattering claim [74] that the bad fit to the data at $E_x \approx 10.7$ MeV, "may indicate the omission from the analysis of some positive-parity states at higher excitation energies" (though they have taken into account all established positive-parity states up to $E_x = 14$ MeV).

A simple argument against the $1/2^-$ assignment comes also from the work of Davids [75]. He studied the (α, n) reaction on ^{9}Be at low energy and measured the angular distributions of neutrons (corresponding to the ground and the first excited state of ^{12}C) at α-energies from 340 to 680 keV (fig. 6). With the α-energy corresponding to the 11.080 MeV resonance, the angular distribution for the $^9\mathrm{Be}(\alpha, \mathrm{n}_1)^{12}\mathrm{C}$ (2_1^+) reaction is isotropic (as seen on the inset of fig. 6), clearly indicating a $L = 0$ decay (the interference with the background and another resonance is negligible at that α-energy). This allows only $3/2^+$ and $5/2^+$ assignments for the 11.080 MeV resonant state. The $1/2^-$ assignment needs $L = 1$ which would be rather weak (at the neutron energy as low as 1.3 MeV) and not consistent with the very strong resonance observed in the exci-

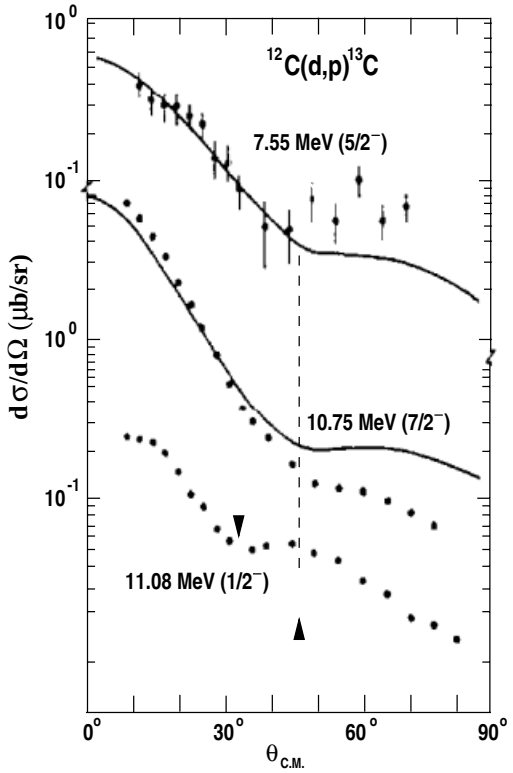

Fig. 5. Angular distributions for the population of states in ^{13}C in the ^{12}C(d,p) reaction [52]. Note the small cross-section (25 μb/sr) of the 11.080 MeV state and its shifted minimum. The (wrong!) $1/2^-$ assignment is from ref. [45].

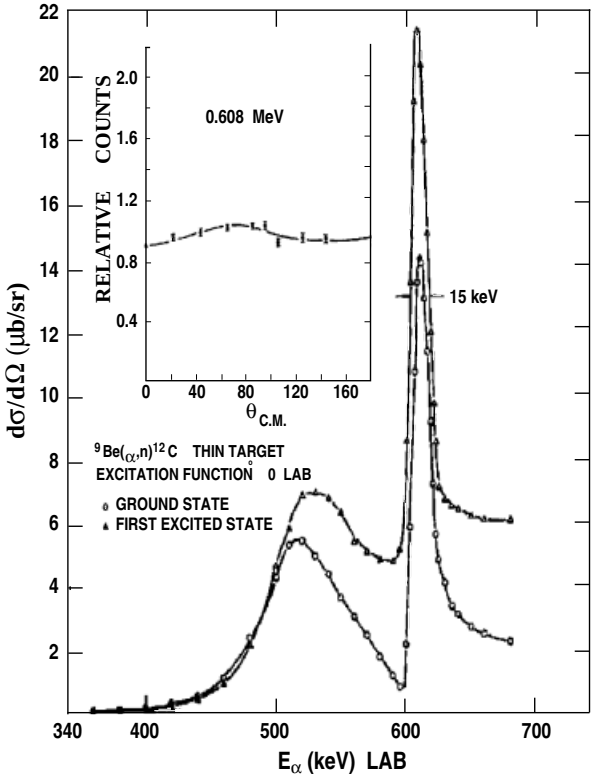

Fig. 6. Excitation functions at 0° measured for the reactions ^{9}Be$(\alpha,\mathrm{n}_0)^{12}$C and ^{9}Be$(\alpha,\mathrm{n}_1)^{12}$C (2_1^+) in the region of the 11.080 MeV state (E_α = 620 keV), together with the angular distribution for the reaction ^{9}Be$(\alpha,\mathrm{n}_1)^{12}$C (2_1^+) measured at the energy corresponding to the 11.080 MeV state (from ref. [75]). The label E_α = "0.608" MeV is due to the slightly wrong calibration in this early experiment.

tation spectrum and with its measured angular distribution. Of course, to make this argument more quantitative, one should describe the angular distribution in terms of at least four overlapping levels, but this seems to be too complex [76].

The most probable spin and parity assignment can also be found by R-matrix analysis of the resonance in the excitation spectrum of the ^{9}Be$(\alpha,\mathrm{n}_0)^{12}$C reaction [48]. The very narrow width of the resonance indicates that neutron decay goes through $L = 2$ (implying positive parity).

Based on all these arguments we can deduce firmly a spin $3/2^+$ for the 11.080 MeV state. It is consistent with its extremely narrow width (the α-decay must have at least $L = 1$, and the neutron decay has to go with $L = 2$). With this value it can be taken as the band head of the $K = 3/2^+$ rotational band (see fig. 4 and table 1).

The special structure of this state can be seen from the reactions known to populate it. It is rather weakly populated in one-nucleon transfer reactions [45,52,53], but rather prominent in two- and three-nucleon transfer reactions [45,46,55,57,58] on corresponding targets. Unfortunately, it cannot be resolved from the nearby states in the α-transfer reactions on ^{9}Be [59,60], but it is clearly seen in the ^{7}Li(^{9}Be, ^{13}C $\rightarrow \alpha + {}^9$Be)t reaction [49]. Both proton [63,64] and electron [47,65] inelastic scatterings populate this level rather weakly, as it is also the case for ^{3}He and α inelastic scattering [66]. The clearest indication of $\alpha + {}^9$Be cluster structure of this state comes from the already-mentioned measurements of the excitation function for the ^{9}Be$(\alpha,\mathrm{n}_0)^{12}$C reaction [75,50,48]; there it appears as an extremely sharp and strong resonance at $E_\alpha = 620$ keV. In conclusion, the 11.080 MeV state has a pronounced cluster structure and as such it can be taken as the head of the $K = 3/2^+$ rotational band.

11.950 MeV state

The first excited state of the $K = 3/2^+$ band would be the 11.950 MeV state with well-established spin and parity $5/2^+$ [44]. It is very close to a number of states (at 11.75, 11.85, 12.106, 12.13, 12.14 and 12.187 MeV) so it is rarely clearly resolved. One can still claim that it is only weakly seen in one-nucleon transfer reactions [45,52–54,67]. Also, it is not seen (or only very weakly) in inelastic scattering of protons, ^{3}He nuclei and α-particles. Nevertheless, it is without any doubt very strongly populated in ^{9}Be$(\alpha,\mathrm{n}_0)^{12}$C [69,48], ^{9}Be$(\alpha,\mathrm{n}\gamma)^{12}$C [69] and ^{9}Be$(\alpha,\alpha)^9$Be [71,77] reactions. So, this state is very different from the 11.85 MeV $7/2^+$ state (which is not populated in the $\alpha + {}^9$Be reactions) and it is hard to expect that these two states form a doublet as suggested

by Milliner *et al.* [47]. Since precise $^{9}\mathrm{Be}(\alpha,\mathrm{n})^{12}\mathrm{C}$ measurements [48] show that the 11.95 MeV state is the one having a large α-strength, we can also claim that this state is the one populated in the $^{9}\mathrm{Be}(^{6}\mathrm{Li},\mathrm{d})^{13}\mathrm{C}$ reaction [60] forming a peak marked with 11.90 MeV. This is supported by the results for the $^{7}\mathrm{Li}(^{9}\mathrm{Be},{}^{13}\mathrm{C}\rightarrow\alpha+{}^{9}\mathrm{Be})\mathrm{t}$ reaction [49], where a strong peak is seen at 11.950 MeV in both $\alpha+{}^{9}\mathrm{Be}$ and $\alpha+\mathrm{t}$ coincidences. All these arguments make this state a good candidate for the $5/2^{+}$ state of the proposed rotational band.

13.41 MeV state

This state has a very tentative assignment of $9/2^{-}$ [71, 44]. As all the states of the proposed bands, it is only weakly seen in one-nucleon transfer reactions [45,52–54]. On the other hand, it is always very strong in the α+^{9}Be reactions: $^{9}\mathrm{Be}(\alpha,\mathrm{n}_0)^{12}\mathrm{C}$ [69, 48], $^{9}\mathrm{Be}(\alpha,\mathrm{n}_1)^{12}\mathrm{C}$ (4.44 MeV) [68], $^{9}\mathrm{Be}(\alpha,\mathrm{n}_2)^{12}\mathrm{C}$ (7.65 MeV) [68], $^{9}\mathrm{Be}(\alpha,\alpha)^{9}\mathrm{Be}$ [71], $^{9}\mathrm{Be}(\alpha,\mathrm{n}\gamma)^{12}\mathrm{C}$ [69,78] and ^{9}Be $(\alpha,\mathrm{n}2\alpha)^{4}$He [70]. It is also strongly populated in the $^{9}\mathrm{Be}(^{6}\mathrm{Li},\mathrm{d})^{13}\mathrm{C}$ reaction [60] and in the $^{7}\mathrm{Li}(^{9}\mathrm{Be},{}^{13}\mathrm{C}\rightarrow\alpha+{}^{9}\mathrm{Be})\mathrm{t}$ reaction [49]. A final determination of its spin will show if our proposal is correct. A strong argument for the $7/2^{+}$ assignment is given by the angular distribution measured in the $^{9}\mathrm{Be}(^{6}\mathrm{Li},\mathrm{d})^{13}\mathrm{C}$ reaction [60].

15.28 and 16.95 MeV states

One can also speculate about the further members of the band. A state at 15.28 MeV has $9/2^{+}$ and as such it fits the $J(J+1)$ rule almost perfectly. Unfortunately, experimental data are very scarce, therefore we cannot say anything about its structure. The state at 16.95 MeV has not been assigned with a spin, but since it is rather strong in $^{9}\mathrm{Be}(\alpha,\mathrm{n}_0)^{12}\mathrm{C}$ [69,68] and $^{9}\mathrm{Be}(\alpha,\alpha)^{9}\mathrm{Be}$ [73] reactions, we believe that it can be the candidate for the $11/2^{+}$ member of the band. As shown in fig. 4, the $J(J+1)$ rule is very well met for the proposed states.

2.4 States with K = $1/2^{+}$ and $1/2^{-}$

In the compilation shown in fig. 2 there are two conspicuous states with spin-parity $1/2^{-,+}$ at excitation energies of 8.86 MeV and 10.996 MeV, respectively. These states must have rather unusual structure, they are barely observed in "normal" reactions. The $1/2^{+}$ state at 10.996 MeV is observed as a strong resonance in the $\alpha+{}^{9}$Be system (the only one not used in the construction of the $K=3/2^{\pm}$ bands) but never observed in "simple" reactions and does not fit into shell model considerations. Almost the same statements can be made for the $1/2^{-}$ state at 8.86 MeV which, however, cannot be populated by an $\alpha+{}^{9}$Be reaction. The inelastic scattering to this state is found to be weak but similar to the excitation to the second 0^{+} state in ^{12}C [63,64]. One suggestion is that these two states correspond to configurations of $p_{1/2}$- and $2s_{1/2}$- orbits (as for the two first states of ^{13}C), based now not on the ground state of ^{12}C, but on the second 0^{+} state, as shown in fig. 2. The distance between the two states is in both cases almost the same. We will later give arguments that these two states may also be based on a valence neutron coupled to the triangular three α-particle structure. In the frame of a $^{9}\mathrm{Be}+\alpha$ structure these configurations have to be based on the first excited state of ^{9}Be $(1/2^{+})$. The valence neutron in this case may stabilise the three-α-particle structure to a triangular shape which will give rise to a parity doublet. A similar configuration has also been recently discussed for ^{14}C at comparable excitation energy by Itagaki [26].

2.5 Mirror states in ^{13}N

It is interesting to speculate if the molecular states listed in table 1 have their mirror isospin analogues in ^{13}N. Isospin, or mirror symmetry is expected to be broken in this case, because of the peculiar differences in the Coulomb interaction in covalent configurations. Up to the excitation energy of about 10.5 MeV (in ^{13}C), the mirror states in ^{13}N were identified in two experimental papers: in the first one, the reaction $^{15}\mathrm{N}(\mathrm{p},{}^{3}\mathrm{He})^{13}\mathrm{C}$ was compared with the mirror $^{15}\mathrm{N}(\mathrm{p},\mathrm{t})^{13}\mathrm{N}$ reaction [45], and in the second paper the reaction $^{10}\mathrm{B}(^{6}\mathrm{Li},\ {}^{3}\mathrm{He})^{13}\mathrm{C}$ was compared [46] with the mirror reaction $^{10}\mathrm{B}(^{6}\mathrm{Li},\mathrm{t})^{13}\mathrm{N}$. It was found that all states up to 10.5 MeV of excitation have their mirror states clearly established. The situation is less clear for the states starting with the 10.996 MeV $(1/2^{+})$ state in ^{13}C. This state is rarely resolved from the 11.080 MeV state, and its possible mirror in ^{13}N is seen in only one reaction, $^{12}\mathrm{C}(\mathrm{p},\gamma_0)^{13}\mathrm{N}$, as a very broad resonance with spin assigned as $1/2^{+}$ or $3/2^{+}$ [79]. At higher excitation energies, some mirror states are assigned [72], but most of the states from table 1 do not have clearly established mirrors in ^{13}N. This can partially be explained, because the thresholds for decays are lower in ^{13}N by a few MeV, so all unbound states in ^{13}N have larger widths. In any case, the mirror states of those listed in table 1 are only very weakly populated in the mirror reactions, which is best seen in ref. [45]. We find that this may be another evidence that states from table 1 have molecular character. Namely, as in the case of beryllium and boron isotopes, the proton as a valence particle gives less binding and tends to shift the α-particles apart, thus finally destroying the molecular structure.

2.6 Conclusions for the ^{13}C bands

For a conclusion of this part we state that *all* levels we have proposed to form rotational bands are populated in $^{9}\mathrm{Be}(\alpha,\mathrm{n})^{12}\mathrm{C}$ reactions (except the 9.897 MeV state which is under the $\alpha+{}^{9}$Be threshold). Furthermore, there is no other state (except the 10.996 MeV state) which is strongly populated in this reaction! The same argument holds for the $^{9}\mathrm{Be}(\alpha,\alpha)^{9}\mathrm{Be}$ reaction in the energy range

where excitation functions have been measured. In addition, all proposed states are strongly populated in α-transfer reactions (though in some works the states were not resolved from their neighbours). Therefore, it can be concluded that the states in the proposed bands have pronounced $\alpha + {}^9\mathrm{Be}$ or $\alpha + \alpha + \alpha + \mathrm{n}$ clustering.

The widths of the states given in table 1 are taken from the compilation in ref. [44] and have been completed with some newer data, which suggest smaller widths for some states (for example, for the state at 11.950 MeV, the compilation by Ajzenberg-Selove gives $\Gamma = 500$ keV, Lee *et al.* [49] suggest $\Gamma = 240$ keV and Kunz *et al.* [48] give even a smaller value $\Gamma = 150$ keV). As can be seen in table 1, the states of the band do not have widths increasing with spin. We think that this fact is due to the changing decay modes of each state. For example, the $5/2^+$ state at 11.950 MeV can decay with $L = 1$ through the $\alpha + {}^9\mathrm{Be}$ channel, with $L = 2$ through the $\mathrm{n} + {}^{12}\mathrm{C}$ channel and with $L = 0$ through the $\mathrm{n} + {}^{12}\mathrm{C}\ (2^+)$ channel. The next state of this band, the $7/2^+$ state at 13.41 MeV needs two units of L more for each decay; *i.e.* $L = 3$ for the $\alpha + {}^9\mathrm{Be}$ channel, $L = 4$ for the $\mathrm{n} + {}^{12}\mathrm{C}$ channel and $L = 2$ for the $\mathrm{n} + {}^{12}\mathrm{C}$ (2^+) channel. So it is clear that the decay of the 13.41 MeV state will be hindered due to the larger L-values involved for each possible decay channel and that its width will be smaller than the that of the 11.950 MeV state. The same arguments can be applied to the discussion of the varying widths for the negative-parity band. Here the $5/2^-$ state has a smaller width than the $3/2^-$ state and the $9/2^-$ state has a smaller width than the $7/2^-$ state, the $7/2^-$ state can decay with $L = 2$ through the $\alpha + {}^9\mathrm{Be}$ channel, while the next state with $9/2^-$ needs two units more, $L = 4$, which makes its width smaller compared to the $7/2^-$ state. Still, precise measurements of widths and a more quantitative discussion would be helpful in establishing the structure of these highly excited states.

We believe we have identified two rotational bands of the same K-value but different parity. This parity splitting is the consequence of the reflection asymmetric shape, further discussed in sect. 3. Both bands have very large (and almost the same) moment of inertia: $\hbar^2/2\theta \approx 180$–$190$ keV. In table 2 we list some values of the moments of inertia of deformed bands in the same mass region. When compared with the value for the ^{12}C ground state ($\hbar^2/2\theta = 750$ keV), one can see that the moments of inertia of the bands listed in table 2 are indeed huge. In beryllium isotopes, such a strong deformation is the consequence of a large α-α distance (valence neutrons concentrated along the (α-α)-axis). The value obtained here for the ^{13}C bands, suggests a geometry corresponding to a linear-chain structure (further discussed in sect. 3).

Table 2. Molecular rotational bands in nuclei with $A = 10$–16.

Nucleus	Band head	$\hbar^2/2\theta$ (keV)	References
^{10}Be	0_2^+, 1_1^-	250	[1,14]
^{11}Be	$3/2_3^-$	230	[15,18]
^{12}Be	0_2^+	210	[16,18,19]
^{13}C	$3/2_2^-$, $3/2_3^+$	190	This work
^{16}C	0_*^+	150	Predicted in [25]

$$\Psi(^{13}\mathrm{C}^*) = \frac{1}{\sqrt{1+\Delta_n}}\Big[\,|\,(\alpha_1 \circledcirc \alpha_2 \otimes \alpha_3)\rangle \pm |\,(\alpha_1 \otimes \alpha_2 \circledcirc \alpha_3)\rangle_{3c}\Big] =$$
$$= \frac{1}{\sqrt{1+\Delta_n}}\Big[\,|\,(\alpha_1 \circledcirc \alpha_2 \otimes \alpha_3)\rangle \pm |\,(\alpha_3 \otimes \alpha_2 \circledcirc \alpha_1)\rangle_{rot}\Big]$$

Fig. 7. Schematic illustration of the equivalence of the three-centre wave function (chain states) with the neutron shared with the other two centres, with the parity projected wave function eq. (6).

The parity splitting of the two bands is not so strong as for example in the 4p-4h cases in ^{16}O or for the case of ^{20}Ne (see, *e.g.*, [80]), but it is comparable to those found in ^{19}F (see, *e.g.*, [81,82]). What makes the parity splitting in ^{13}C very special, is the fact that the negative-parity band head has a lower excitation energy, well below the α-^{9}Be threshold. We believe that this is a clear sign of the three-centre structure of our bands, as discussed in the next section.

3 Considerations on the structure of the chain states in ^{13}C

In this section we make an attempt to formulate a model for the wave function of the valence neutron in the covalently bound cluster states in ^{13}C. These wave functions can be based on the asymptotic $^9\mathrm{Be} + \alpha$ structure; in this case the strongly deformed nature of the ^{9}Be enters. By choosing a specific orientation of the ^{9}Be, we arrive at ^{13}C chain states based on the $^9\mathrm{Be} + \alpha$ structure.

Figure 7 shows schematically the construction of the three-centre (linear chain) wave function based on the $^9\mathrm{Be} + \alpha$ structure (see below) and with the spin and parity projected form. Further, a model for a three-centre structure of the ^{13}C chain state making use of the molecular orbital formulation known in physical chemistry as the Hückel method [83,84] will be given. We will find that these methods give basis wave functions of the three-centre system and we will have a natural explanation for the energies and spins of the proposed bands.

3.1 Alpha-clustering states based on the $\alpha + {}^9$Be system

As a starting point we can discuss structures of ^{13}C, which as a basic building block contain the $^4\mathrm{He} + {}^8\mathrm{Be}$ system bound by a covalent neutron. The geometry and coordinates are shown in fig. 8. This approach is similar to the work of Dufour and Descouvemont [85], who used the generator coordinate method to study the ^{13}C spectroscopy at low excitation energies. Here a particular difficulty arises due to the large (2 : 1) deformation of ^{8}Be. This fact will be reflected in the properties of the asymptotic fragment ^{9}Be and the possibility to have prolate and oblate

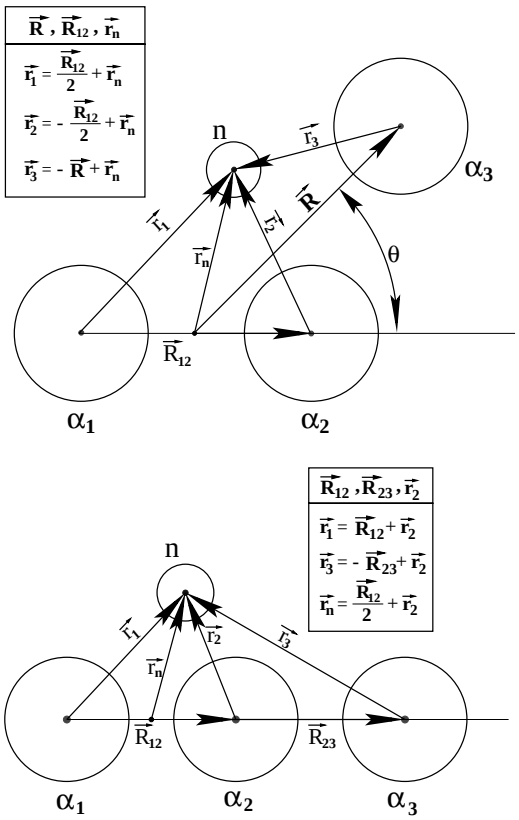

Fig. 8. Coordinates for the molecular cluster states in ^{13}C. Two solutions for the choice of the 3 independent variables are shown.

configurations in $^{12\text{-}13}$C, depending on the orientation of the distance vector between the centre of ^{8}Be and the α-particle, $\mathbf{R}(^8\text{Be-}\alpha)$. The latter can be characterised by an angle θ, with $\theta = 0°$ for prolate deformations (chain state) and $\theta = 90°$ for oblate shapes, like the ground state and possibly the first excited 0^+ state of ^{12}C. For the linear chain state we can then choose another set of independent variables, which are shown in the lower part of fig. 8.

We start with an intrinsically reflection asymmetric structure consisting of ^{5}He and ^{9}Be configurations (see fig. 7). In this approach, as in previous considerations concerning covalent neutron orbitals, the interaction of the cores is considered to be represented by a shallow local potential and antisymmetrisation between cores and valence particles is neglected. The *total Hamiltonian* $H_{\rm tot}$ can be written as follows:

$$H_{\rm tot} = T(\mathbf{R}) + T(\mathbf{r}_{n\alpha}) + T(\mathbf{r}_{\rm n\,^8Be}) + H_\alpha + H_{^8\rm Be} + V_{^8\rm Be,\alpha}(\mathbf{R},\theta) + V_{\rm n,\alpha}(\mathbf{r}_{\rm n\alpha}) + V_{\rm n,^8Be}(\mathbf{r}_{\rm n\,^8Be},\theta). \quad (2)$$

The final coordinates as shown in fig. 8 are actually $\mathbf{r}_3 = \mathbf{r}_{\rm n\alpha}$ and $\mathbf{r}_{\rm n\,^8Be} = \mathbf{r}_{\rm n}$.

Single-centre shell model states of the neutron in the sub-systems ^{5}He$(p_{3/2})$ and in the two-centre states in ^{9}Be, namely the lowest two states ^{9}Be$(3/2^-)$ and ^{9}Be$(1/2^+)$, can be used to construct the *covalent molecular wave function* for ^{13}C-cluster states.

3.2 States based on the $\alpha + {}^9$Be$(1/2^+)$ system, triangular shapes

The configurations with certain symmetries, which will be of relevance for the further discussion are the linear chain and the triangular configurations. In the latter case the angle defined in fig. 8 will be $\theta = 90°$. In this case a particular difficulty may arise if we choose the ground state of ^{9}Be$(3/2^-)$ to construct the wave function. The ^{9}Be wave function can be described by a π-orbit, in which the valence particle occupies the space spanned by the x- and y-coordinates, perpendicular to the symmetry axis (z-axis) of ^{9}Be (see, *e.g.*, ref. [25]). The third α-particle approaching along these x- or y-coordinates will thus find occupied neutron states. If the antisymmetrization between valence particles and the α is of importance, the Pauli principle will inhibit this configuration or make it energetically less favourable. The situation changes if the excited state ^{9}Be $(1/2^+)$ is chosen. In this case the valence neutron is in a σ-orbit concentrated along and on the z-axis (the symmetry axis of ^{9}Be), the x- and y-coordinates are free for the approaching third α-particle. We thus conclude that the triangular shapes will be favoured with the first excited state ^{9}Be $(1/2^+)$. The pictorial representation of fig. 7 will be changed accordingly to a configuration where the third α-particle is attached perpendicular, and a doublet with spin/parity $J^\pi = 1/2^{+,-}$ is expected. As already noted in subsect. 2.4, there may be in fact good candidates for these two states. Both states are below the ^{9}Be$(1/2^+) + \alpha$ threshold and we expect a stabilisation of the triangular shape. A corresponding configuration has been recently calculated for ^{14}C by Itagaki [26] with results in agreement for our suggestion for the mentioned ^{13}C states with $J^\pi = 1/2^\pm$.

Using the ground state, ^{9}Be$(3/2^-)$, and the arguments based on the Pauli principle, we thus expect the minimum energy in the chain configuration with the third α-particle aligned along the symmetry axis of ^{9}Be.

3.3 Alpha-clustering states based on the $\alpha + {}^9$Be$(3/2^-)$ system, linear chains

Following the arguments of the previous section the wave function for the case with $\theta = 0°$, which corresponds to the chain configurations, will now be discussed. The corresponding states in ^{12}C are expected at 7.65 MeV of excitation energy or higher (see fig. 2).

We can thus start with the following linear combinations (LCNO, $\theta = 0°$) with two choices of the phase P_C:

$$\Phi^K_{\rm LCNO,C}(\mathbf{R}, r_{\rm n}) = \frac{1}{\sqrt{(1+\delta^K_{\rm C}(\mathbf{R}))}}\big[C_1\psi_{\alpha_3}\psi_{^8\rm Be}\phi^K_{\rm n}(\mathbf{r}_3, p_{3/2}) + (-)^{P_C}C_2\psi_{\alpha_3}\psi_{^8\rm Be}\psi^K_{\rm n}(\mathbf{r}_{\rm n}, \mathbf{R}_{12}, p_{3/2})\big]. \quad (3)$$

Here we have introduced the projection K of the valence particle spin. The amplitudes C_1 and C_2 will give

a measure of the sharing of the neutron between the two asymptotic wave functions, which are now the ^{5}He($p_{3/2}$) and the two possible states in ^{9}Be; we will use only the ground state of ^{9}Be ($K = 3/2$).

For states with $K = 3/2$ we can give the wave function in a more symmetric form, where the neutron is shared in the same $p_{3/2}$ configurations between the three α-particles. The index C identifies quantities for the wave function of carbon.

The overlap of the single-particle states at the two nuclei determines the *non-orthogonality*, $\delta^K_{\rm C}(\mathbf{R})$ (eq. (4)), where the second wave function is the two-centre wave function of the valence neutron (or a deformed Nilsson orbital) given by ψ. With the coordinates written as $(\mathbf{r}_{{\rm n}\alpha} - \mathbf{R}) = \mathbf{r}_{{\rm n}\,^8{\rm Be}}$, the non-orthogonality will depend on $\mathbf{R}$:

$$\delta^K_{\rm C}(\mathbf{R}) = (-)^{P_C} \int \phi^{*K}_{p3/2}(\mathbf{r}_{{\rm n}\alpha})\psi^K_{p3/2}(\mathbf{r}_{{\rm n}\alpha} - \mathbf{R}){\rm d}\mathbf{r}_{\rm n}. \quad (4)$$

The wave function in eq. (3) corresponds to a *reflection asymmetric* state and *no intrinsic parity* is defined. We have a common symmetry axis and as *quantum numbers* the projections on this symmetry axis of the orbital (denoted as in atomic physics by σ for $m = 0$, π for $m = 1$, etc.) and total angular momenta, given by K, already introduced for the two-centre states in ^{9}Be [1].

For a more detailed discussion we give the explicit form of the ^{9}Be($3/2^-$) two-centre single-neutron wave function ψ, where the valence neutron is attached to either of the α-particles 1 or 2:

$$\psi^K_{\rm n} = \psi^K_{\rm LCNO,Be}(\mathbf{R}_{12}, r_{\rm n}) = \frac{1}{\sqrt{2(1 + \delta^K_{\rm Be}(\mathbf{R}_{12}))}} \times \left[\psi_{\alpha_1}\phi^K_{\rm n}(\mathbf{r}_1, p_{3/2}) + (-)^{p_i}\psi_{\alpha 2}\phi^K_{\rm n}(\mathbf{r}_1 - \mathbf{R}_{12}, p_{3/2})\right]. \quad (5)$$

The phase "p_i" defines the gerade, g, and ungerade, u, property of the two-centre molecular state.

The *non-orthogonality* $\delta^K_{\rm Be}(\mathbf{R}_{12})$ is now given by the overlap of the single-particle wave functions $\phi^K(\mathbf{r})$ at the two α-particles in the ^{5}He($p_{3/2}$) resonance.

Molecular states of ^{13}C with *good parity* Π, and total spin I are constructed by making the linear combinations of the reflection asymmetric shapes given by eq. (3), with a phase P and the *signature* $\sigma = (-)^{I+K}$. The total wave function now reads

$$\Psi^{I,\Pi}_{KM}(\mathbf{R}, r_{\rm n}) = N(\Delta)\left[\Phi^K_{\rm LCNO,C}(\mathbf{R}, r_{\rm n})D^I_{MK}(\omega) + (-)^{I+K+P}\Phi^K_{\rm LCNO,C}(\mathbf{R}, r_{\rm n})D^I_{M-K}(\omega)\right]. \quad (6)$$

For ^{13}C the chain states will have $K = 3/2$ and the case of *parity doublets* should be observed, like for an *asymmetric rotating "top"*. Rotational bands with levels of both parities for each spin should appear. This approach with the phase P, and phases p_1 and p_2 within the ^{9}Be wave functions, leads to three linear independent basis functions for the three cluster problem which is equivalent to the formulation of the three-centre basis function shown later. The lowest state has negative parity and the positive-parity state is obtained by a cancellation of the wave function at centre 2 (see also subsect. 3.4).

The *positive- and negative-parity bands will be split in energy*, due to a non-orthogonality Δ (illustrated in fig. 7) between the two reflected configurations.

The lowest state is obtained with a (+) phase P in the combinations of eq. (6) and a positive value of Δ with an increased binding just below the threshold for the decay into ^{9}Be($3/2^-$) + α, in agreement with the experimental observations discussed in sect. 2.

3.4 Reflection symmetric three-centre states

The wave functions for the covalent neutron of a three-centre problem can be deduced from methods known in physical chemistry as the Hückel molecular orbital method [83,84], as exemplified below.

The use of the Hückel method relies to some degree on the Born-Oppenheimer approximation, as it has been done by Fonseca *et al.* [7] for ^{9}Be. However, the most important approximation there is connected to the neglect of certain radial coupling terms, which are indeed found to be rather small.

We cite the result from quantum chemistry for a molecule with p-states at the three centres (the case of the "allyl" radical). Starting with three centres, we can use the Hamiltonian:

$$H_{\rm tot} = \sum_{i=1}^{3} T(\mathbf{r}_i) + \sum_{i=1}^{3} H_{\alpha_i} + V_{{\rm n}\alpha}(\mathbf{r}_1) + V_{{\rm n}\alpha}(\mathbf{r}_2) + V_{{\rm n}\alpha}(\mathbf{r}_3). \quad (7)$$

A linear variational calculation, using as a basis set p-orbitals ϕ_i ($i = 1, 2, 3$) at three centres, will lead to a 3×3 determinant whose roots will be molecular orbital energies. There the following matrix elements enter:

$$H_{ij} = \int \phi^*_i H_{\rm tot}\phi_j {\rm d}r, \quad (8)$$

$$S_{ij} = \int \phi^*_i \phi_j {\rm d}r. \quad (9)$$

H_{ii} is interpreted as the average energy of a neutron at the centre i experiencing a potential due to all three centres. Symmetry requires that $H_{11} = H_{33}$, H_{22} should be different but not *very* different from H_{11}. We expect the dominant part to arise from interactions with the near α-particle, the more distant α-particles playing a secondary role. Hence, one of the approximations made in the Hückel method is that all H_{ii} are equal (and usually denoted with α). Resonance or bond integrals H_{ij} between two α-particles are the overlap energies between two centres i and j. Symmetry requires that $H_{12} = H_{23}$ (usually denoted with β); between the border α-particles H_{ij} is taken to be zero ($H_{13} = H_{31} \equiv 0$). Although there is overlap

between neighbours, in the Hückel method all overlap integrals S_{ij} are taken to be zero if $i \neq j$ and one if $i = j$. So these non-orthogonality overlaps do not appear in the normalisation in the equations for the wave functions.

We have now the following wave functions, omitting to write explicitly the wave functions for the α-particles:

$$\Psi_1^K = \frac{1}{2}\left[\phi_{\rm n}^K(\mathbf{R}_{12}+\mathbf{r}_2)+\sqrt{2}\phi_{\rm n}^K(\mathbf{r}_2)+\phi_{\rm n}^K(-\mathbf{R}_{23}+\mathbf{r}_2)\right], \tag{10}$$

$$\Psi_2^K = \frac{1}{\sqrt{2}}\left[\phi_{\rm n}^K(\mathbf{R}_{12}+\mathbf{r}_2)-\phi_{\rm n}^K(-\mathbf{R}_{23}+\mathbf{r}_2)\right], \tag{11}$$

$$\Psi_3^K = \frac{1}{2}\left[\phi_{\rm n}^K(\mathbf{R}_{12}+\mathbf{r}_2)-\sqrt{2}\phi_{\rm n}^K(\mathbf{r}_2)+\phi_{\rm n}^K(-\mathbf{R}_{23}+\mathbf{r}_2)\right], \tag{12}$$

with the solution for the energies:

$$\begin{aligned} E_1 &= \alpha-\beta\,,\\ E_2 &= \quad\alpha\,,\\ E_3 &= \alpha+\beta\,. \end{aligned} \tag{13}$$

At the three centres *we do not have equal amplitudes* and we will have the eigen-energies given in eq. (13). The contours of the molecular orbitals for these wave functions of ^{13}C are schematically shown in fig. 9.

For the energetically lowest state Ψ_1^K, the valence particle is being shared by all three centres (see fig. 9), it has negative parity and its energy should be below the threshold for three α-particles and a neutron. The next state, Ψ_2^K, has positive parity (the valence particle is shifted to the borders α_1 and α_3, see fig. 9), and it is likely to be placed at the lowest threshold for the decomposition of the molecule into its clusters and valence particle. In physical chemistry it is called "non-bonding" state, because there are no π-orbitals on neighbouring centres. Overlap between π-orbitals is hindered due to the nodal plane in the middle and this structure can be relatively stable to bending. Ψ_3^K again has negative parity and must be considered as the "anti-binding" state, because of the two extra nodes in the wave function (actually nodal planes).

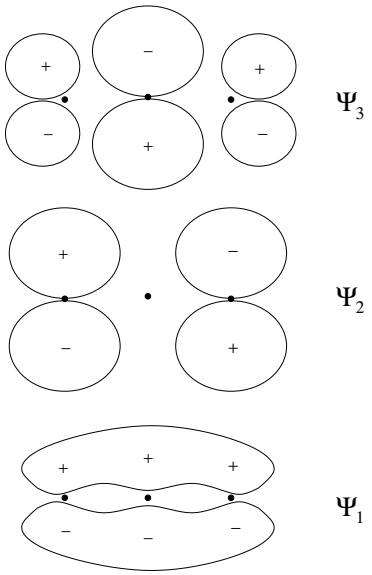

Fig. 9. Schematic illustration of molecular orbitals contours for the three-centre wave functions of ^{13}C chain states obtained by the Hückel method (figure adapted from ref. [84]).

The excitation energy would be the lowest for the Ψ_1^K state; this configuration most likely corresponds to the 9.897 MeV state. The 11.080 MeV state should correspond to the Ψ_2^K configuration which has the positive parity. The Ψ_3^K configuration should appear at even higher excitation energies and we were unable to identify corresponding states from the existing experimental data, possibly because their width is very large.

4 Discussion and conclusions

4.1 The molecular chain states of ^{13}C

In this work we suggest that parity split rotational bands based on the ^{9}Be($3/2^-$, g.s.) + α structure can be identified in ^{13}C. The band heads coincide with the two lowest states, based on the three-centre molecular orbital approach and the observed moments of inertia suggest a linear chain of three α-particles bound by a covalent neutron.

States corresponding to the ^{9}Be($1/2^+$, 1.68 MeV) + α configuration are expected to be observed as well. They should appear in the same excitation energy, however, these states will have the most stable configuration with a triangular geometry. A doublet with $J^\pi = 1/2^\pm$ observed in the spectrum of ^{13}C, states at 10.996 MeV and 8.86 MeV, is taken as candidate for this structure.

The distinction between linear and triangular shapes is here obtained by considerations of σ- and π-orbitals for the ground and first excited states of ^{9}Be, in which the valence neutron occupies two different (and orthogonal) configurations.

In future experiments a search for γ-decay branches of some of the states appears possible (especially with large γ-detector arrays) and will show if this and other states in ^{13}C or heavier isotopes have deformations as suggested here.

4.2 The molecular chain states of heavier carbon isotopes ($^{14\text{-}16}$C)

We can predict three-centre states with two covalent neutrons, which will be based on the ^{10}Be + α and ^{9}Be + ^{5} He structures. In this case band heads of isomeric states in ^{14}C should appear below these thresholds. These states will be reflection asymmetric, however, intrinsically symmetric states with good parity can be build as in the case of ^{13}C. We note that the non-orthogonality integrals may be very different from case to case. In addition parity split bands can be based on the excited states of ^{10}Be, with configurations corresponding to principal molecular orbitals structures as discussed for this nucleus: i) $(\pi)^2$, ii) $(\sigma)^2$ and iii) $(\sigma \times \pi)$. Dominant structures in ^{14}C will be based on the ground state $K = 0$ $(\pi)^2$-state, and on the excited

$K = 0$ $(\sigma)^2$-state, as well as on the $K = 1^-(\sigma \times \pi)$-state of ^{10}Be. Also interesting hybridised configurations can be expected. An alternative approach will be to discuss the structure of linear chains of ^{14}C with the three-centre basis wave functions discussed here and the corresponding configurations will be obtained by filling the neutrons into these orbits. A discussion of the spectra of excited states of ^{14}C and their structure will be given in a forthcoming publication.

For ^{15}C similarly chain states could be constructed based on the resonant sharing of a neutron between ^{10}Be and ^{4}He, namely between the lowest states of ^{11}Be and the ^{5}He resonance, or again with the three-centre basis wave functions.

The most interesting case is ^{16}C , which can have as the lowest state a very symmetric configuration with positive parity. These have been studied by Itagaki *et al.* [25], where for the mixed configuration with π- and σ-orbits a chain is obtained, that is stabilised relative to the bending mode. A study of the heavier carbon isotopes thus becomes an interesting subject. The formulation for heavier chains, with four α-particles like in $^{16+xn}$O, can also be done on the basis of Hückel's molecular orbital approach. Experimental and theoretical work on these structures is expected to give interesting results in the future.

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