TWO-CENTER STRUCTURE IN LIGHT EXOTIC NUCLEI*

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The physics of the two-center shell model for the a-a potential and covalent valence neutrons and protons with up to 4 valence nucleons is discussed. The structure of nuclear dimers and their rotational bands is illustrated using published transfer reaction data for Be and Boron isotopes. Based on the state in 12C at an excitation energy of 7.65 MeV which is assumed to be an 3α particle chain and adding the covalent nucleons, chain states (trimers) in the system 12C* + x neutrons can be constructed.

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1. Introduction

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The two-center shell model has been established in the early times of heavy ion science [1, 2]. Numerous studies of single nucleon transfer between light nuclei have given ample evidence for the motion of nucleons in covalent two-center orbits [3, 4, 5], for example hybridisation effects, important for molecular binding and well known from atomic physics, have been observed in nuclear collisions [4, 6, 7]. However, because of the strong attraction between two nuclei at distances smaller than the Coulomb barriers, stable dimers could not be observed. The particular feature of atomic molecules, the repulsion of the core-core potentials at small distances is realised in nuclear physics only in the α-α potential, which in its local form has a repulsive core [8], and dimers can than be constructed on the basis of the a-a potential (a survey is given in Refs. [9]).

In fact it has been known since more than 15 years, that ground-states and excited states in the isotope Beryllium 9Be (and 10Be) can be described as a two center molecule (dimer), where two α-particles are bound

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by covalent neutrons. The survey of the theoretical and experimental situation which has recently been made by the author [9], shows that a wealth of experimental evidence exists also for $^{10}$Be, $^{11}$Be, and Boron isotopes, and states have been grouped into rotational bands in such a way that moments of inertia can be extracted. Based on these considerations the construction of polymers can also be envisaged; a short comment on polymers is only given here: chain states consisting of $\alpha$-particles in $4N$ nuclei has recently attracted increased attention both experimentally and theoretically [10]. After the well established structure of $^8$Be, which shows a rotational band based on a two-$\alpha$-particle structure, the second $0^+_2$ at 7.65 Mev in $^{12}$C has been proposed to be a chain of three $\alpha$-particles. Various approaches based on a cranked cluster model have confirmed that such structures exist not only in $^{12}$C, but also in other nuclei. Experimental evidence exists for example for $^{16}$O and recently also for $^{24}$Mg (see Ref. [10]). The origin of the existence of such states is the structure of the $\alpha$-$\alpha$ potential, which (in its local form) shows an attractive part and a repulsive core. Thus with the establishment of the detailed knowledge on the structure of dimers chain states, or polymers, have been predicted [9] for very neutron rich isotopes for carbon ($^{13}$C–$^{18}$C) and oxygen ($^{19}$O–$^{24}$O).

2. Dimers

2.1. Beryllium isotopes

In order to understand the structure of the Beryllium isotopes we have to discuss the properties of the two-center molecular orbitals, as they appear in a correlation diagram. In Fig. 1 we show the relevant diagram [9] for the first single particle orbits ($s_{1/2}$, $p_{3/2}$, $p_{1/2}$, $d_{5/2}$) of the separated nuclei as they are obtained from a two center shell model approach. On the left side (united nucleus limit) the well known diagram for deformed nuclei can be identified; these orbitals merge into the two-center orbitals, which are obtained by the splitting of the separated center configurations. Quantum numbers which are necessary to classify these orbitals are indicated: the projection of the spin on the molecular axis ($K$), the reflection symmetry for the exchange of identical cores (gerade (g), ungerade (u)), the parity $\Pi$, and for larger distances the classification of molecular orbitals by the angular momentum component, $\lambda$, around the two center axis — the $\sigma$, $\pi$, etc. orbitals. The population of orbitals in isotopes of $^9$Be–$^{12}$Be has to be considered at the minimum in the $\alpha$-$\alpha$ potential which occurs at a distance of approx. 3.5 fm. At smaller distance the a-a potential (in its local form) becomes strongly repulsive. The Coulomb barrier (with $r_c = 1.25$ fm) is located at $R \approx 4.0$ fm. The structure of Beryllium isotopes is determined by
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Fig. 1. Correlation diagram for nucleons in molecular orbitals in a two-center system with identical cores. The minimum of the $\alpha + \alpha$-potential is located at a distance of ca. 3.5 fm (adopted from Ref. [2]).

The binding effect of the $p_{3/2}$-neutron which forms a resonance state in $^5$He at $E_r = 0.83$ MeV. The particular binding configurations for the $p_{3/2}$-orbits correspond to the well known $\sigma$-binding (horizontal orientation of $\ell = 1$ distributions) and the $\pi$-binding (vertical orientation relative to the distance vector). The fact that these quantum number ($\sigma, \pi$) are of relevance can be seen in the configurations observed in the "model-independent" calculations of Kanada–Enyo [11], the densities of which are shown in Fig. 4.

The $3/2^{-}$ groundstate of $^9$Be corresponds here to the $K = 3/2$, $\pi$-binding orbital ($\pi_{3/2}^{-}, g$), whereas at the distance $R \approx 3.5$ fm the next excited state, the $1/2^{+}$ state corresponds to the $K = 1/2$, $\sigma$-ungerade-binding orbital ($\sigma_{1/2}^{+}, u$), and the $1/2$-state to the $K = 1/2$, $\sigma$-gerade-anti-binding orbital ($\pi_{1/2}^{+}, g$). In fact all states of $^9$Be can be explained in such a model. A detailed discussion of the molecular orbital structure, based on the linear combination of nuclear orbitals is given for the Be-isotopes by Seya, Kohno and Nagata [12].
Using the Pauli-principle for two neutrons in these orbits \((\pi^{-3/2})\) and \(\left(\sigma^{+1/2}\right)\) (or neutron and proton in a \(T = 1\) state) we fill neutrons into the molecular orbitals according to Hunds-rules discussed for example by Herzberg [13] and obtain the well established four states at excitation energies of ca. 6–7 MeV in \(^{10}\text{Be}\) with \(J^{\pi} = 0^{+}; 2^{+}; 1^{-}\) and \(2^{-}\), which form rotational bands as shown in Fig. 3. The groundstate of \(^{10}\text{Be}\) shows the perfect \((\pi^{-3/2})^{2}\) configuration (see Fig. 4), with strong gain in energy due to pairing. This state and the first excited state \(\Delta E(0^{+} - 2^{+}) = 3.36\) MeV) form an independent rotational band with a smaller deformation parameter, whereas the dimers show rotational excitations with a much larger moment of inertia \(\Delta E(0^{+} - 2^{+}) = 1.35\) MeV), see Fig. 3 and Section 3.

Fig. 2. Energy diagrams for dimers of the Beryllium isotopes. The excitation energies (and thresholds) are shown relative to the energy of the \((\alpha + \alpha + xn)\) threshold. Only the first possible isomeric two-center states are indicated (without rotational excitations) in boxes.
Fig. 2 shows the relevant information on binding energies for $^9$Be and the heavier isotopes ($^{11}$Be and $^{12}$Be). The excitation energies are shifted so as to have a common line for the relevant thresholds ($2\alpha + xn$) for all isotopes. The binding energy introduced by the addition of valence nucleons can thus be read from this line. Also the thresholds for the decay into other channels (with normal shapes) are indicated. The dimers must be considered here as shape isomers, whose band heads are predicted at the energies shown in the boxes.

Fig. 3. Excitation energies of states forming rotational bands of dimers based on $2\alpha + x$-nucleons for $^9$Be, $^{10}$Be, $^{10}$B and $^{11}$Be as function $J(J + 1)$.

We repeat here the evidence for rotational bands in $^9$Be and $^{10}$Be. This evidence [14] is based mostly on inelastic $\alpha$-scattering, ($\alpha$, $^3$He) reactions as well as ($d$, $p$) reactions on $^9$Be. In Fig. 3 the different rotational bands are summarised and their properties are discussed in Section 3.
The evidence for states in $^{11}$Be corresponding to dimers can be obtained by looking into the population of states in two neutron transfer reactions like the $^{9}$Be($t,p$) reaction. Whereas these reactions should strongly populate such dimer states, they should not be observed in the one neutron stripping on $^{10}$Be, because the ground state does not have the appropriate structure. If there is a rotational band structure based on the $^{11}$Be, $1/2^+$ ground state we must expect a similar drastic Coriolis coupling effect as for the $1/2^+$ band in $^9$Be (see Fig. 3). From the spin assignments given in the literature and from the population of the $^{11}$Be states in the $^9$Be($t,p$) reaction we can suggest the following sequence of states for the $K=1/2^+$ band: $(1/2^+, 0.0 \text{ MeV}; 5/2^+, 1.78 \text{ MeV}; 3/2^+, 2.69 \text{ MeV}; 9/2^+, 3.88 \text{ MeV} \text{ and } 7/2^+ \text{ at 6.510 MeV})$; they are shown in Fig. 3 together with the $K = 3/2^-$ band starting at 3.96 MeV. The binding energy of three covalent valence neutrons for the $K = 3/2^-$ band amounts to approximately 5 MeV. The states of the latter band are narrow and will possibly show $\gamma$-transitions, which have not yet been studied. The neutron-pair in the $(t,p)$ reaction is coupled to spin $0^+$ and most likely populates states with the $(\sigma_1/2^+u)^2$ configuration. These states show a strong relation to the most strongly populated states in the $^9$Be ($d,p$) $^{10}$Be reaction, which are the negative parity states with $J^\pi = 2^-, 3^-, 4^-$ at 6.26, 7.37 and 9.27 MeV, respectively.

For $^{12}$Be there is little information available so far. If we fill 4 neutrons into the molecular orbitals $(\pi_{3/2}^-, \sigma_{1/2}^+)$ we expect a rather compact shape for $^{12}$Be similar to $^{10}$Be$_{0,gs}$ due to the $(\sigma_{1/2}^+)^2 \times (\pi_{3/2}^-)^2$ configuration. In the two-center correlation diagram the $\sigma_{1/2}^+$ (see Fig. 1) configuration has a slope with an increasing binding energy for larger deformation (or two-center distance). Thus the fact that the moment of inertia is larger for the $^{12}$Be$_{GS}$-band ($\Delta E(2^+-0^+) = 2.10 \text{ MeV}$ compared to the $^{10}$Be$_{0}^+$-band can be understood. Starting with values of the $n$-binding energies obtained for $^{11}$Be, and assuming that the fourth neutron can contribute approximately 1.5 MeV (like in $^9$Be) the dimers in $^{12}$Be should be observed from excitation energies of approximately 4.5 MeV.

2.2. Boron isotopes

The concept of isospin tells us immediately that the dimers in the neutron rich isotopes have isospin analogues in the neighbouring nuclei (see Ref. [1]), if a proton is replaced for a neutron.

For $^{10}$B we start with the basic structure of $^9$Be. By adding a proton we can form in $^{10}$B the $T = 1$ analogue states ($T_\pi$) of the four states in $^{10}$Be*. These analogues have been identified in $^{10}$B in the excitation energy region of 6.56–7.5 MeV. An identical (to $^{10}$Be*)band is observed (Fig. 3).
Adding the proton to form the $T_<(T = 0)$ states we will have again four states as in the $^{10}\text{Be}^*$ case, and using the generalised Pauli principle the corresponding states are, $J^r = 1^+, 3^+$ for $(\pi_{3/2})^2$ and $1^-, 2^-$ for the $(\pi_{3/2})^2 \times (\sigma_{1/2}^+)$ configurations; although they may mix strongly with other $T = 0$ states they may form rotational bands. Now the nucleon-nucleon interaction is slightly more attractive and we expect that the corresponding states are lowered by ca. 2 MeV relative to the $T_>\: 1$ states.

For the $^{11}\text{B}$ nucleus there are detailed studies of ($^3\text{He}, p$) and ($\alpha, d$) reactions on $^9\text{Be}$, which could strongly populate states in $^{11}\text{B}$ with $T_>\: 3/2$ and $T_<\: 1/2$. The $T_>$ states are analogues of the states in $^{11}\text{Be}$ already discussed. The state ($T = 3/2$) at 5.24 MeV of $^{11}\text{Be}$ will be located at approximately 17.50 MeV in $^{11}\text{B}$. In fact strong transitions with narrow width have been observed in the ($^3\text{He}, p$) reaction at high excitation energy [9, 14].

The molecular structure with a strong concentration of the valence particles will strongly be influenced by the Coulomb force if neutrons are replaced by protons. Thus the mirror states in $^9\text{B}$ of the $1/2^+$ state in $^9\text{Be}$ is not observed, and some states of $^{10}\text{Be}$ at 6 MeV excitation in $^{10}\text{C}$ (see contribution by Fujiwara in these proceedings) have not been observed [15].

3. Moments of inertia and assignment of configurations to states in the isotopes $^{10}\text{Be}$ and $^{11}\text{Be}$

The moments of inertia, $\theta$, of the dimers are of course the most relevant points of information for the discussion of their shapes (in particular also the $\gamma$-ray transition probabilities between these states if they are observed). In Fig. 3 the excitation energies of states in the Beryllium and Boron isotopes are plotted in diagrams representing rotational bands. I use the simplest expression for the rotational energy for a nucleus with moment of inertia, $\theta$, as function of an angular momentum $J(K > 1/2)$: $E(J) = \hbar^2/2\theta[J(J + 1) - K(K + 1)]$. For $K = 1/2$, we use, incorporating the effect of Coriolis decoupling: $E(J) = \hbar^2/2\theta[J(J + 1) + (-)^{J+1/2}a(J + 1/2)]$, where $a$, is the Coriolis decoupling parameter. The energy in this case can also be written as $E(J) = b [(J + (1 + \sigma a/2))^2$, where $\sigma$ is the signature, $(-)^{J+1/2}$, defining the reflection symmetry of the intrinsic state.

For the $^9\text{Be}^*$ ($K = 1/2^+$) band I obtain the values $b(= \hbar^2/2\theta) = 0.35 - 0.46$ [MeV] and $a \approx 2.0$; the same $a$-value is obtained for the $K = 1/2$ band of $^{11}\text{Be}$ shown in Fig. 3 ($b$ is smaller $\sim 0.2$-0.3 MeV) ($a \approx 2.0$). This value (because it is given by $(-)^{J+1/2}(j + 1/2)$, if only one orbital is considered) must be interpreted as the fact that the original spin of the orbit, whose $K$-quantum number is considered, is $j = 3/2$. The Coriolis decoupling parameter in the two cases gives thus a strong support for the two-center correlation diagram interpretation of these states. The results
for the moments of inertia are summarized as follows:

a) For the $^9$Be, $K = 3/2^-$ and $^{10}$Be$_{GS}$ bands (and $^8$Be) values for $\hbar^2/2\theta$ are in the range of 0.5-0.6 MeV. If we use a simple formula for the moments of inertia, $(\mu R^2)$, we have for $\mu = 2.0$ and $\mu = 2.22$ and $R = r_0(2 \cdot (4)^{1/3})$ a radial distance of the two masses with $r_0 \approx 1.3$ fm. These states still have a rather compact shape. As suggested by Seya et al. [12], the ground state of $^{10}$Be ($0^+$) can be assumed to be the $(\pi_{3/2},g)^2$, $0^+$ configuration.

b) For the rotational bands of the excited dimer configurations in $^{10}$Be*, $^{11}$Be*, $^{10}$B* and $^{11}$B* we observe values for $\hbar^2/2\theta$ in the range 0.23-0.25 MeV. This means that the distance between the two $\alpha$-particles in the two-center diagram must be much larger than for the ground state bands.

For the discussion of the configurations it is important to note that the $(\sigma_{1/2},u)$ configuration crosses the $(\pi_{3/2},g)$ at ca. $R \approx 4$ fm; it has a decreasing slope (increasing binding energy) for $R > 4$ fm, whereas the $(\pi_{3/2},g)$ configuration shows an increase of the binding energy by approaching smaller distances ($R < 4$ fm) with a possible minimum at $R \approx 3$ fm. We may thus give the following interpretation of the valence neutron structure of the two $0^+$ states in $^{10}$Be (see also Ref. [9]).

$$|^{10}\text{Be}_0 + (GS)\rangle = (2.19)^{1/2}(\pi_{-3/2}g)^2_{0^+} + (0.01)^{1/2}(\sigma_{1/2}^+ u)^2_{0^+};$$

$$|^{10}\text{Be}_0 + (6.26 \text{ MeV})\rangle = a_0(\sigma_{1/2}^+ u)^2_{0^+}.$$ The other states at ca. 6 MeV energy in $^{10}$Be must have the following configurations:

$$|^{10}\text{Be}_2 + (5.958)\rangle = a_1(\pi_{-3/2}g)^2_{2^+} ,$$

$$|^{10}\text{Be}_1^- (5.960)\rangle = a_2[(\pi_{-3/2}g) \otimes (\sigma_{1/2}^+ u)]^- ,$$

and

$$|^{10}\text{Be}_2^- (6.263)\rangle = a_3[(\pi_{-3/2}g) \otimes (\sigma_{1/2}^+ u)]^- .$$

Concerning the configurations in $^{11}$Be, I can make the following assignments:

$$|^{11}\text{Be}_{3/2}^- (3.94)\rangle = (\sigma_{1/2}^+ u)^2_{0^+} \otimes (\pi_{3/2}g) ,$$

and

$$|^{11}\text{Be}_{1/2}^+ (GS)\rangle = (\pi_{3/2}g)^2_{0^+} \otimes (\sigma_{1/2}^+ u).$$
Fig. 4. Density distributions of nucleons (neutrons and protons) in the Beryllium isotopes as obtained from calculations based on antisymmetrised molecular dynamics (AMD) by Kanada–Enyo and Horiuchi (private communication). The neutron densities include those neutrons which are in the α-particles, still the covalent nature of the neutron bond is well seen. The possible molecular orbital configurations according to Fig. 1 are indicated. For $^{10}\text{Be}$ the groundstate band corresponds to the first $\pi = +$, and the $K = 1^-$ to the first $\pi = -$ states. In $^{11}\text{Be}$ the band heads with $\pi = +, -$ correspond to $K = 1/2$; the $K = 3/2^-$ as the second $\pi = -$ band is not shown.
The $K = 1/2^-$, state is suggested to have the configuration: $|^{11}\text{Be}_{1/2}^−; (0.32 \text{ MeV})⟩ = (\pi_{3/2}^−g)^2 \otimes (\sigma_{1/2}^−g)^1$. This configuration, $(\sigma_{1/2}^−g)$, appears as the next at a smaller two-center distance of ca. 3 fm, where the minimum for the $^{10}\text{Be}^+_0$ ground state is expected. This state has a spectroscopic amplitude (in the deformed shell model) for the $p_{1/2}$ structure determined from the $^{10}\text{Be} (d,p)$ reaction of $(0.63)^{1/2}$ and is thus related to $^{10}\text{Be}^+_0$ ground state; this state in $^{11}\text{Be}$ is thus much more compact in shape than the members of the $K = 3/2^−$ band in agreement with our extraction of the moments of inertia.

This discussion of the moments of inertia is strikingly confirmed by the calculations of Kanada–Enyo and Horiuchi (Ref. [11]) using the antisymmetrised molecular dynamics (AMD) approach. The AMD calculations reflect the properties of the two-center correlation diagram and the densities of the valence neutrons obtained correspond to those of the $(\pi_{3/2})$ and $(\sigma_{1/2})$-orbitals. I reproduce in Fig. 4 some density plots as they are obtained in these calculations. They are obtained from slater determinants after parity projection and represent the lowest states for a given parity (note that in Ref. [11] they are not projected on parity). The covalent nature of the valence neutrons is immediately recognised. The tentative configuration assignments are indicated. We observe also a remarkable effect, the mixing of covalent orbitals of different $\lambda$, but coupled to the same $J$ and $K$ which produces very spectacular density distributions for the case of the $\pi = (−)$ states in $^{10}\text{Be}$, an effect analogous to hybridisation [6, 7].

4. Conclusions

The present search on information on nuclear dimers in neutron rich isotopes of light nuclei is based on the concept of covalent molecular orbitals [3, 12] of neutrons. The level scheme of the Be-isotopes can almost exclusively be explained in this approach. We may expect as a general rule that clusterisation and even formation of chains (polymers) will occur for very neutron rich nuclei close to the threshold to a-particle substructures (see Refs. [9]). These states offer fascinating possibilities for studies using radioactive beam facilities in particular for $\gamma$-spectroscopy if the $\gamma$-branches can be measured.
REFERENCES