Covalent Binding with Neutrons on the Femto-scale

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Abstract. In light nuclei we have well defined clusters, nuclei with closed shells, which serve as centers for binary molecules with covalent binding by valence neutrons. Single neutron orbitals in light neutron-excess nuclei have well defined shell model quantum numbers. With the combination of two clusters and their neutron valence states, molecular two-center orbitals are defined; in the two-center shell model we can place valence neutrons in a large variety of molecular two-center states, and the formation of Dimers becomes possible. The corresponding rotational bands point with their large moments of inertia and the Coriolis decoupling effect (for K = 1/2 bands) to the internal molecular orbital structure in these states. On the basis of these the neutron rich isotopes allow the formation of a large variety molecular structures on the nuclear scale. An extended Ikeda diagram can be drawn for these cases. Molecular bands in Be and Ne-isotopes are discussed as text-book examples.

1. Introduction

After several decades of work on molecular orbitals in heavy ion collisions (see Ref. [1]), the important step has been taken (Ref. [2]) on defining molecular nuclear states as two body systems with covalent binding with neutron orbitals. This has been initially met with violent objection by the referees, however, the notion of valence neutrons in molecular \( \sigma \)- and \( \pi \)-orbitals soon afterwards has been established by theoretical approaches (with AMD). In the Method of Antisymmetrized Molecular Dynamics (AMD) by H. Horiuchi, Y. Kanada-En’yo, M. Kimura et al [3, 4, 5, 6] the intrinsic density distributions of the valence neutrons in molecular orbits are obtained. For the observation of stable bound molecular states the potential between the two clusters must have “molecular” character, with a repulsion at smaller distances. Best cases (see Ref.[7]) are two \( \alpha \)-particles and the \( \alpha + ^{16}\text{O} \) system, shown in Fig. 1. The repulsion at smaller distances is caused by the Pauli-principle acting as soon as a larger overlap of densities occurs.

The recent experimental work has established many molecular rotational bands in light nuclei, see Refs. [8, 9, 10], where many observables for the nuclear structure in terms of two-center molecular states has been found. In work using the \((^7\text{Li},p)\)-reactions molecular rotational bands have been established recently in the Oxygen isotopes \(^{18,19,20}\text{O}\). These are intrinsically reflection asymmetric molecules, where the rotational bands appear as parity inversion doublets. These are structures consisting of \( \alpha \)-particles, with \( ^{16}\text{O} \)- and \(^{14}\text{C}\)-cores. The intrinsically reflection asymmetric molecular states (consisting of \( \alpha \)-particles and \(^{16}\text{O}\)-cores) have been established in the \(^{21,22}\text{Ne}\)-isotopes, see Refs. [12, 14]. With these observations a diagram for nuclear molecular states based on covalent binding between strongly bound cores can be drawn, it is shown in Fig.1. Many of these states have been established in recent [10] experimental works.
2. Dimers, Be- and Ne-isotopes

The molecular structure of the Be-isotopes and Ne-isotopes are textbook examples for physical chemistry on the Femto scale, see the book by Herzberg [11]. We concentrate on these cases in the present contribution. The molecular structures for Be-isotopes can be obtained by inspecting the correlation diagram for valence neutrons and two $\alpha$-particles, shown in Fig. 2. The energy splitting of the levels starting at the larger distances is observed, these are defined by their quantum numbers of molecular structure, as described in Ref.[10]. The rotational bands give clear indications of the $\sigma$- and $\pi$-orbits, the $\sigma$-configurations produce a larger distance between the cores and give larger moments of inertia. The compilation of the rotational bands (excitation energies as function of $j(j+1)$) in the Be-isotopes is shown in Fig. 3. This figure illustrates the dependence of the moments of inertia on different configurations. The larger moment of inertia of the $(\sigma)^2$ configuration in the $K=0^+_2$ - band is clearly visible. The $K=0^-$ band starting with $J=1^-$ is a mixed $(\sigma-\pi)$-configuration.

Another important feature of molecular configurations is the Coriolis-decoupling effect in the rotational bands with $K = 1/2$, which produce the characteristic zig-zag structure seen in Fig. 3. The latter appears also in the $K = 1/2$-band in $^{21}$Ne, Fig. 6. In these cases the spin of the valence particle in a rotational band can be flipped between two projections on the symmetry axis.

It is a case of “complete” spectroscopy, all states in $^{9,10,11,12}$Be can be described with valence neutrons in two-center orbitals. We can clearly identify the configurations of the two neutrons occupying $\sigma$ or $\pi$ orbits obtained with the valence neutrons in shell model $p_{3/2}$-configurations in the He-isotopes. The mixed orbitals of two neutrons, $(\sigma \times \pi)$ in the $1^-$ states give the “distorted” wave functions. With this AMD-approach the the internal structure of states of the Be-isotopes are perfectly reproduced.

The method of Antisymmetrized Molecular Dynamics, the AMD [3, 4, 5], is the most powerful tool to illustrate the intrinsic wave functions with the molecular orbitals supporting the concept of molecular orbitals. In fact, the large variety of structures in the Be-isotopes obtained with AMD is shown in Fig. 4.

**Figure 1.** Left side: The locally (phase-)equivalent potentials describing the $\alpha-\alpha$ and the $\alpha-^{16}$O interaction, with “molecular” character, namely the repulsion at small distances. The empirical potentials (full lines) and the theoretical (dashed) are shown, from Ref.[7]. Right-side: These potentials allow the formation of various covalently bound states, as suggested in the schematic diagram (the “extended” Ikeda diagram), e.g. the formation of dimers in $^{9,10,11,12}$Be as well as in $^{20,21,22}$Ne, respectively, see Ref.[10].
Figure 2. The correlation diagram for two-center neutron orbitals in Be-isotopes. The two orientations of the $p_{3/2}$ states, leading to the formation of four (4) molecular orbitals with the quantum numbers $K$, symmetry (g,u) and parity, and gerade/ungerade-properties as indicated. The possible molecular orbitals are the $\sigma$ and $\pi$ orbits, with spatial distributions illustrated in the lower part of the figure.

Figure 3. The rotational bands of the isotopes $^{8,9,10}$Be. The band with $K=0^+$ based on the excited $J=0^+$ state in $^{10}$Be shows a slope corresponding to the larger moment of inertia of the $(\sigma)^2$ configuration. Note the strong zig-zag dependence for the $K = 1/2^+$ band in $^{9}$Be, due to the Coriolis-decoupling effect. This is also observed in $^{21}$Ne as shown in Fig. 6.
Figure 4. Overview of some intrinsic densities (not projected on parity) for the Be-isotopes $^{10,12}$Be, obtained in AMD-calculations [5]. The total densities are shown as well as the cases for protons and neutrons separately, the latter showing the distribution of the valence neutrons.

The very characteristic valence neutron distributions, which give rise to the covalent binding effect in $^{10}$Be are further shown in Fig. 5, where in addition the molecular orbital structures of $^{22}$Ne are illustrated, again $\sigma$- and $\pi$-orbits play the dominant role.

![Intrinsic densities of $\sigma$- and $\pi$-orbits for the Be-isotope $^{10}$Be, and for the $^{22}$Ne isotope, as obtained in AMD-calculations.](image)

Figure 5.

The $^{20,21,22}$Ne isotopes are further text-book examples for intrinsically asymmetric binary systems, this was recognized for the cases of $^{20,21}$Ne. The occurrence of parity splitting of rotational bands in $^{20}$Ne has already been explained in 1968 [15] by H. Horiuchi. For $^{21}$Ne with a single valence neutron unique features are observed [12]. For the $\pi$-binding in the $K = 3/2$ band, the splitting is very similar to that of $K = 0^+\text{--}^-\text{--}^+$ bands in $^{20}$Ne, the neutron densities are outside of the symmetry axis, giving space for the exchange as in $^{20}$Ne for the $K = 0^+$ states. Then there appears the parity splitting for the $K = 1/2$ bands. The extremely small energy splitting, in this case in $^{21}$Ne can be explained in the molecular orbital frame. For the neutrons in the $\sigma$-orbits the densities are concentrated on the symmetry axis, preventing an exchange along the axis, in the projection on eigenstates.

Actually in earlier work for $^{21}$Ne a systematic survey of the possible rotational bands has been made [13]. In this work the authors used mainly the deformed shell model, however, they were not able to accommodate the many negative parity states ("citation": to many states with negative parity are observed), because the number of states in the deformed shell model had been exhausted.
The concept of molecular orbitals is a powerful tool for the description of isotopes in light nuclei with neutron excess. Many more nuclei with exotic shapes as in Fig.1 can be anticipated. The chain states based on the configuration with three $\alpha$-particles (like $^{16}$C) have been recently treated explicitly, as reported at this conference.

![Diagram](Figure 6. Overview of rotational bands in $^{20−21}$Ne. For $^{20}$Ne we observe the well known parity splitting, for the two bands with $K = 0^+$. A similar splitting is observed for the $K = 3/2$ bands in $^{21}$Ne, showing a similar splitting as in $^{20}$Ne. Note the zig-zag behavior (Coriolis decoupling effect) for the $K = 1/2$ bands. The energy splitting is here only 15-20 KeV, due to the fact that the neutrons in the $\sigma$-orbit are concentrated on the symmetry axis.)

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