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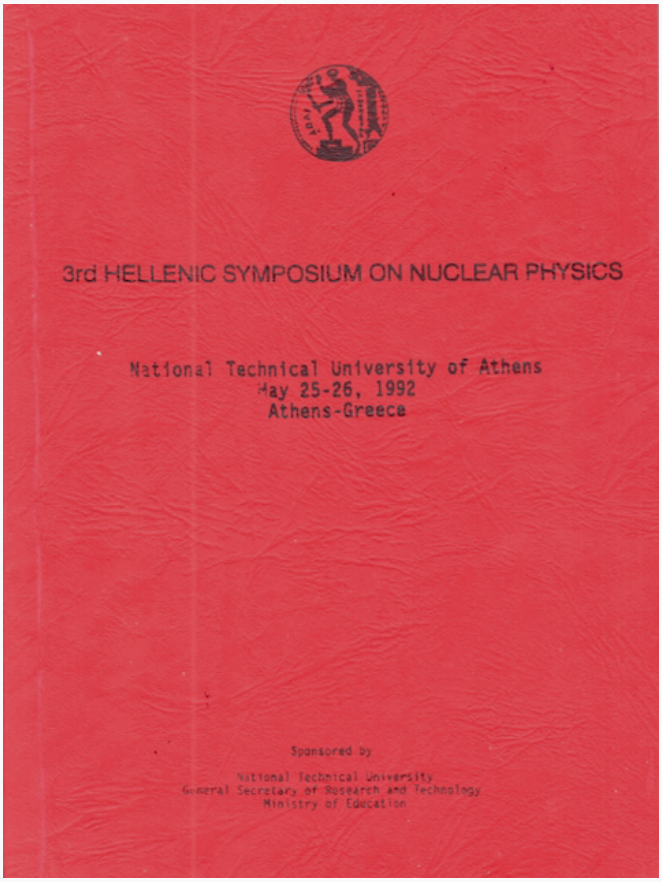


# Light mixed alkali microclusters

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# LIGHT MIXED ALKALI MICROCLUSTERS

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## Abstract

A quantum cluster approach for light mixed microclusters, composed of neutral alkali atoms and considered as atomic fermion clusters, is introduced.

## 1. Introduction

Microclusters consist of two atoms up to several thousands of isolated atoms of any chemical element (or mixture of elements). Their properties substantially differ from those of the same element in bulk, in such a way that one can consider microclusters as a new state of matter beyond solids, liquids, gases and plasma, i.e., as a fifth state of matter.

Besides the academic community, industries intensively work on microclusters due to many expected applications, e.g., in catalysis, in surface covering, in studies of the stage between two phases, etc. The field of clusters is indeed interdisciplinary and its researchers come from chemistry, crystallography, solid state, atomic, nuclear, plasma, surface physics, etc.

Experimental methods applied for the production of microclusters include supersonic expansion of vapors of the specific element, bombardment of a metal surface by ions, use of liquid metal sources, etc. The theoretical

models in the field of clusters come from chemistry (usually considering electron orbital interactions for given atomic positions each time), from solid state and atomic physics (i.e., different jellium models of free electrons resulting from delocalization of valence electrons of the constituent atoms), and from nuclear physics (where atoms or their ions are taken as atomic fermions or atomic bosons depending on the odd or even number of their electrons, respectively).

In general, the study of microclusters tends to create a new branch of physics -- a branch of few and many but not too many particles, of which atomic and nuclear physics and the physics of microclusters will be a part.

## 2. Clusters of mixed neutral alkali atoms

It is considered that under proper experimental conditions (i.e., small number of particles, low temperature, etc.) delocalization of the valence electrons does not occur and thus the constituent atoms remain neutral. Under these conditions the jellium model, which presupposes delocalization of the valence electrons, is not applicable and the alkali atoms (possessing one valent electron per atom) behave like atomic fermions [1,2].

It has been found that clusters of mixed neutral alkali atoms (e.g., $Na_nK_m$) very much resemble the atomic nucleus [3] (e.g., of n protons and of m neutrons) and thus their theoretical treatment can take place in a model analogous to nuclear shell model [1,2]. The results of this model become closer to reality if the central potential considered is not common for all particles (as usually assumed in nuclear physics), but common only for the particles of a particular shell. Thus, magic numbers and other properties of this kind of

clusters result as properties of atomic fermions in a shell-dependent, strongly non-local potential [4,6].

The purpose of the present paper is to show that the concept of fermionic behavior for neutral alkali atoms is of general validity, e.g. even for clusters with few atoms, i.e., for the cases where we do not have enough atoms to form shells. Mixed alkali dimers are taken as examples to demonstrate the model.

The approach applied, at present, is semiclassical. Quantum mechanics is introduced through the uncertainty principle and the relative orbiting of the constituents, but the Schrödinger equation is not used.

## 3. Two-atomic-fermion model

In the model the atoms at the ground state and the low energy excited states are represented by hard spheres (permitting no overlapping among each other), which are considered opaque, i.e., hiding any interior structure. Thus, while the atoms, assumed as atomic fermions, are considered confined in the whole cluster volume according to the uncertainty principle, in addition, they have a certain probability of exhibiting collective behavior of their spheres.

The study proceeds by examining the properties of all characteristic modes of motion of the quantum cluster. These modes for the dimer are shown in Fig. 1 (a)-(c). Specifically, in this figure the two atoms are confined in the volume shown (broken line) and, in addition, they have a certain probability of exhibiting collective rotation, i.e. around their common center of mass in mode (a), of the sphere 1 around sphere 2 in mode (b) and vice versa in mode (c). In all modes the atom spheres are considered in contact and the volume of the atom confinement is defined as the spherical envelope of

the space specified by their possible collective rotation (broken line). The radii of these envelopes are: mode (a) $R_a = (r_1 + r_2)/2 + r_1$, mode (b) $R_b = (r_1 + r_2) + r_1$ and mode (c) $R_c = (r_1 + r_2) + r_2$.

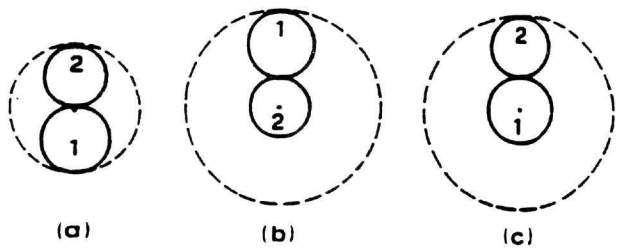


Fig. 1 Modes of collective rotation of neutral alkali dimers.

## 4. Calculations and discussion

In the present paper we deal with four observables of a mixed alkali dimer, namely, spin, binding energy (B.E.), d-state admixture (x) to the predominant s-state of the dimer ground state, and r.m.s. charge radius.

Since each neutral alkali atom possesses spin 1/2, the two neutral atoms in the mixed alkali dimer couple their spins to a total (dimer) spin J equal either to 0 or 1. Given that the various alkali atoms differ substantially both in size and mass, they are distinguishable. Therefore the Pauli principle is applicable separately to each kind. Thus, the quantum states are occupied by each component independently. The combination which reflects the ground state properties is determined by the least energy of the two fermion system. In the particular case of a mixed alkali dimer, each alkali atom in the ground state can be in one of the states $|n\ell m_\ell m_s> = |100 \pm \frac{1}{2}>$ and consequently the energetically favored spin combination leads to a total spin J=1, which might

be the most probable value of the total spin of the dimer. However, an experimental verification is called for.

The effective potential between the two atoms is taken to be of the form

$$V = \frac{A}{r^{12}} - \frac{B}{r^{6}}. \tag{1}$$

It is noted that this is a simplification, since for a detailed investigation additional effects should be considered [7].

The part of kinetic energy due to the confinement of the two atoms in volume of radius $R_{max}$ is totally attributed to the s-state of the dimer and is written

$$T_s \geq (\frac{\hbar^2}{2mR_s^2})*2, \tag{2}$$

where $R_S = (r_1 + r_2)+r_1$. The sizes of the atom spheres $r_1$ and $r_2$ may come from [8].

Provided that the two alkali atoms differ in size, the relative motion is meaningful. The part of kinetic energy due to relative motion of the two atoms is totally attributed to the d-state of the dimer and is written

$$T_d = \hbar^2 \ell(\ell+1)/2m < R_d^2 >, \tag{3}$$

where $< R_d^2 >^{1/2}$ is the classical orbit of the sphere number 2 given by the relation:

$$< R_d^2 >^{1/2} = [(r_1 + r_2)^2 + < r_2^2 >]^{1/2}. \tag{4}$$

Thus, the total kinetic energy for the dimer can be expressed as follows

$$T = (1-x)T_s+(x)T_d\ , \tag{5}$$

where x is the d to s-state admixture.

The binding energy (B.E.) for the dimer is written

$$\text{B.E.} = V-T. \tag{6}$$

For the charge root mean square radius of the dimer we obtain

$$\begin{aligned} <r^2>_{ch}^{1/2} &= <r^2>_s^{1/2}(1-x)+<r^2>_d^{1/2}(x) \\ &= \sqrt{0.6}[(r_1+r_2)+r_2](1-x)+[(r_1+r_2)^2+<r_2^2>]^{1/2}(x), \end{aligned} \tag{7}$$

where $<r^2>_s^{1/2}$ is estimated by assuming a uniform charge distribution in the volume of Fig. 1(c).

Finally, the magnetic moment of the dimer $\mu$ is given by the expression

$$\mu = (\mu_1+\mu_2)-\frac{3}{2}(\mu_1+\mu_2-\frac{1}{2})(x), \tag{8}$$

where $\mu_1 = \mu_2 = \sqrt{n(n+2)}$, n being the number of the unpaired electrons. That is for alkali n=1. Thus expression (8) becomes in this case:

$$\mu = 2\sqrt{3}-3(\sqrt{3}-\frac{1}{4})(x) \tag{9}$$

## 5. Concluding remarks

Unfortunately, due to lack of information about the parameters A and B of potential (1), it is not possible at present to obtain numerical results for the observables of the dimer. It is interesting, however, that the present very simplified quantum cluster approach (even though the present model is perhaps less elegant than other existing approaches [9-13]) leads to very good results of all observables of the deuteron, which is the nuclear analogue of the atomic dimer [14].

The advantage of the present work is that finite and not point particles, together with their relative motion, are employed. All numerical values depend on these finite sizes. The different size between sphere 1 and sphere 2 is supported by the literature [8] and helps us to conceptualize the nature of the d-state of the dimer. It is due to this difference that a relative motion between the two atom spheres is meaningful in the dimer. Due to this relative motion, the volume of confinement of the two particles increases (Fig. 1) and the related kinetic energy decreases (8).

The present paper underlines the necessity of investigating the experimental conditions (method of production, critical size and temperature, etc.) under which alkali atoms remain neutral (no delocalization of their valence electrons) and thus behave like atomic fermions, a fact responsible for many novel properties bringing atomic cluster physics parallel to nuclear physics. The fact that this approach gives encouraging results for the deuteron [14] makes it promising for the case of the atomic clusters, where in this paper the mixed alkali dimers are taken as an example.

Finally, the present paper underlines the idea that new as yet unobserved properties of alkali microclusters should be investigated. Perhaps the most important of them are the orbiting properties of atoms implying a series of properties due to orbital angular momentum, i.e. definite spin properties, independent particle and collective modes of excitation of individual species, etc. For an experimental verification of such properties, nuclear methods should be employed.

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