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Molecular bond effects in the fusion of halo nuclei

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We consider the effect of the long tail of the neutron distribution in the fusion of halo nuclei. We show that for relative separations on the order of the halo size, the exchange of the valence neutrons between the two nuclei is responsible for an effective attractive potential which decreases the Coulomb barrier and increases the fusion cross sections dramatically.

The interest in the field of very neutron-rich nuclei of low-Z elements began in 1965 with the discovery [1] of ^{8}He in fission and the measurement of its half-life when produced in a high-energy nuclear reaction [2]. With the discovery of ^{11}Li, ^{12}Be, ^{14}B, and ^{15}B the advantages of high-energy nuclear reactions for the production of exotic nuclei became evident [3]. One of the most interesting features of some neutron-rich nuclei is the long tail of the valence neutron distributions which has been inferred from measurements of total reaction cross sections and of momentum distribution in fragmentation reactions [4,5]. This long tail is due to the low binding energies of the valence neutrons, which causes their wavefunctions to extend to large distances from the neutron core.

In this paper we discuss the effect of sharing the valence neutrons between two core nuclei, as opposed to the fusion of one halo nucleus with a heavier nucleus discussed earlier in the literature [6]. Even though to be specific we consider the case of fusion of ^{11}Li + ^{9}Li at low energies, our results could be applicable to the fusion of any two such nuclei, e.g. ^{6}He + ^{4}He system. The less bound the nucleus is, the larger is the magnitude of the effect we are going to study here. Therefore, since ^{11}Li is the least bound nucleus so far known, considering the ^{11}Li + ^{9}Li system gives us an upper limit of the magnitude of the effect. The ^{11}Li nucleus can be considered as a core of ^{9}Li with a rms radius of approximately 2.4 fm surrounded by a halo consisting of two neutrons with a rms radius of approximately 6 fm [4,5]. Since the valence neutrons are very loosely bound, when a ^{9}Li nucleus comes within a distance of 12 fm from a ^{11}Li nucleus the valence neutrons can jump back-and-forth around the two ^{9}Li cores. As we shall see this effect lowers the barrier energy, increasing enormously the fusion probability. In this case one would form a ^{20}C nucleus, which existence based on the production by collisions of high energy protons on uranium is uncertain [3].

Our calculations are not intended to be very accurate, since we are more interested in showing the magnitude of the effect and predicting its consequences. Thus, we use a schematic treatment to deduce the attractive potential due to the exchange of the valence nucleons among the cores. We use the Bohr–Oppenheimer approximation which is well known in molecular physics [7]. We denote this potential by molecular bond energy since we shall deduce its magnitude by using the same concepts as in the theory of molecular bonding.

The initial step is to calculate the wavefunctions for the valence neutrons. For ^{11}Li we take a simple shell model. It is known that correlations among the valence neutrons are essential to explain the binding of ^{11}Li (for a review see, e.g., refs. [8,9]). However, the shell model wavefunctions are good enough for our purposes. We find the $0p_{1/2}$ wavefunctions by solving the shell model for a single-particle potential of the form

$$U(r) = \left(V_0 + V_{so}\,(\boldsymbol{l}.\boldsymbol{\sigma})\,\frac{1}{r}\,\frac{d}{dr}\right) \times\left[1 + \exp\left(\frac{r-R}{a}\right)\right]^{-1}, \quad (1)$$

with $R = 3.3$ fm, depth $V_0 = -26.5$ MeV and diffuseness $a = 0.67$ fm and a spin-orbit term with parameters $R_{so} = 3.3$ fm, $V_{so} = -15.5$ MeV and $a_{so} = 0.67$ fm, respectively. This potential yields a $0p_{1/2}$ neutron orbital in ^{11}Li with binding energy equal to 0.15 MeV and rms radius of 5.8 fm. The single-particle description adopted here is not completely unrealistic since calculations [9] of the ^{11}Li ground-state based on the solution of the Bethe–Goldstone equation showed that it is mainly composed (about 77%) of $0p_{1/2}$ states. In this way the separation energy of the two valence neutrons add to 0.3 MeV, which is about the same as the experimental value.

When a ^{9}Li nucleus is at a distance of $\sim$12 fm from a ^{11}Li the total attractive nuclear potential experienced by the valence neutrons as a function of the distance from the ^{9}Li cores is less than their binding energies. This means that they can oscillate back-and-forth between the two ^{9}Li cores. This situation lowers the total energy of the system as in the case of a molecular bond between atoms. As in the atomic approach to molecular bond, we assume that in an almost static situation the wavefunction of the system is given by a linear combination of the wavefunctions when the neutrons are bound either to the core A or to the core B (Bohr–Oppenheimer approximation). That is,

$$\Psi = A\,\Psi_A + B\,\Psi_B, \quad (2)$$

where Ψ_A and Ψ_B represent the states in which the valence neutrons are either in one nucleus or in the other, respectively. We do not consider the situation in which only one of the neutrons is in each nucleus because a ^{10}Li nucleus is particle unstable.

The nuclear Hamiltonian for the two-core plus two-neutron system is given by

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V_a(r_{1a}) + V_b(r_{1b}) + V_a(r_{2a}) + V_b(r_{2b}), \quad (3)$$

where r_{ia} (r_{ib}) means the position of nucleon i with respect to the core a (b). Since the two-core plus two-neutron system has a plane of symmetry perpendicular to the axis joining the two cores, the eigenfunctions must be either symmetric or antisymmetric with respect to reflections. This means that $A = \pm B$. As in the case of molecular physics, the wavefunction with $A = B$ has a lower energy eigenvalue than the one with $A = -B$. This is because, with $A = B$ the neutron wavefunctions are larger in the region between the two ^{9}Li cores where the combined mean field is stronger. Because of symmetry we also have

$$\langle A|\mathcal{H}|A\rangle = \langle B|\mathcal{H}|B\rangle = \mathcal{H}_{aa},$$

$$\langle A|\mathcal{H}|B\rangle = \langle B|\mathcal{H}|A\rangle = \mathcal{H}_{ab},$$

$$\langle A|B\rangle = \langle B|A\rangle = \mathcal{O}. \quad (4)$$

The wavefunctions are normalized so that

$$\langle A|A\rangle = \langle B|B\rangle = 1. \quad (5)$$

We find

$$\mathcal{H}_{aa} = S_{2n} + 2\langle A|V_b(r_{1b})|A\rangle = S_{2n} + 2I,$$

$$\mathcal{H}_{ab} = S_{2n}\mathcal{O}^2 + 2\langle A|V_b(r_{1b})|B\rangle\mathcal{O} = S_{2n}\mathcal{O}^2 + 2\mathcal{O}J,$$

$$\langle\Psi|\Psi\rangle = 2 + 2\mathcal{O}^2, \quad (6)$$

where $S_{2n} = 0.3$ MeV is the binding energy of the two valence neutrons in ^{11}Li.

The expectation value of the energy of the valence neutrons in the presence of the ^{9}Li cores is

$$E = \frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{S_{2n}(1+\mathcal{O}^2) + 2\mathcal{O}J + 2I}{1+\mathcal{O}^2}, \quad (7)$$

where I and J are the integrals defined in eq. (6). They are determined by using the single-particle wavefunctions for the neutrons in the $0p_{1/2}$ orbital. These integrals are most easily calculated using parabolic coordinates for the two-center problem. They are functions of the distance R between the ^{9}Li nuclei. The energy given by the above equation minus the separation energy of the neutrons from ^{11}Li, i.e. $\mathcal{E}(R) = E - S_{2n}$, corresponds to the attractive extra-energy, or molecular bond energy, caused by the exchange of the two neutrons between the ^{9}Li cores.

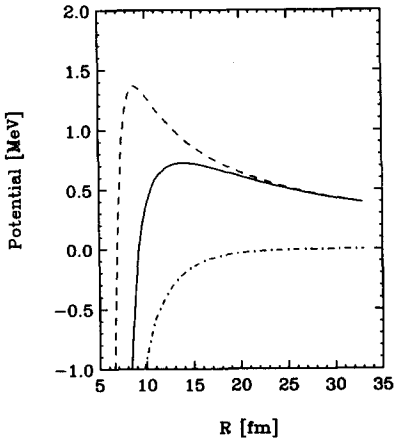

Fig. 1. Coulomb plus nuclear potential energy (dashed line) for the system ^{9}Li + ^{11}Li as a function of their relative position. The solid line corresponds to the addition of molecular bond effects in these potentials. The molecular bond potential is also shown separately (dash-dotted curve).

The potential energy function for the ^{11}Li + ^{9}Li system is obtained by adding the nuclear potential, the Coulomb potential and molecular bond energy, i.e.,

$$V(R) = V_N(R) + \frac{Z^2e^2}{R} + \mathcal{E}(R). \tag{8}$$

In fig. 1 we show the the potential energy for the ^{11}Li + ^{9}Li system at positions around the Coulomb barrier. We choose a Woods–Saxon form for the nuclear potential with range $R_0 = 6$ fm, depth $V_0 = -50$ MeV, and diffuseness $a_0 = 0.65$ fm. The dashed curve corresponds to the nuclear plus Coulomb potential only. The solid curve includes the molecular bond energy. In this figure, we also show the molecular bond energy separately (dash-dotted curve). We see that the height of the Coulomb barrier is reduced substantially by the inclusion of this effect. One should point out that, due to the large extension of the neutron halo in ^{11}Li, our value for the diffuseness is perhaps to conservative. It is plausible that there is a large tail of the nuclear potential which could be mocked up by using a bigger diffuseness.

The fusion cross section for the system ^{9}Li + ^{11}Li is calculated as usual by using

$$\sigma(\epsilon) = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1)\, T_l(\epsilon), \tag{9}$$

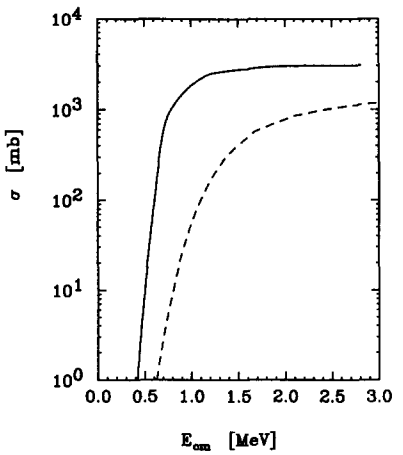

Fig. 2. Fusion cross section for ^{9}Li + ^{11}Li as a function of their relative kinetic energies. The solid curve includes the effect of the molecular bonding in the entrance channel.

where ϵ (k) is the relative energy (momentum). T_l is the barrier penetrability for a partial wave l which we calculate by means of the WKB approximation (see, e.g., ref. [10]),

$$T_l(\epsilon) = \left\{1 + \exp\left[\sqrt{\frac{2\mu}{\hbar^2}} \int_{R_1}^{R_2} \mathrm{d}R \times \left(V(R) + \frac{l(l+1)}{2\mu R^2} - \epsilon\right)^{1/2}\right]\right\}^{-1}, \tag{10}$$

where R_1 and R_2 are the classical turning points (which are complex for $\epsilon > V_B$).

In fig. 2 we show the fusion cross sections as a a function of the relative energy for ^{9}Li + ^{11}Li. The dashed (solid) curve corresponds to the use of the Coulomb plus nuclear potential without (with) the molecular bond energy included. We observe that the inclusion of the molecular bond effect increases dramatically the magnitude of the fusion cross section. The enhancement is about a factor 1000 for relative energies on the order of 0.1 MeV. Note that if we had used a bigger diffuseness to take the large tail of the nuclear potential into account, this enhancement effect would have been even larger, since this increases the molecular bonding energy (eq. (7)).

One should investigate further if the ^{10}Li resonance plays an important role in the reaction we studied. Although we ignored the effects of this resonance for

the sake of simplicity, it is in principle possible to incorporate its effects in a manner similar to the studies of molecular orbitals of nucleons in heavy ion collisions [11]. Such an analysis is beyond the scope of the current letter and will be carried out in forthcoming publications.

The next question one should discuss is if this effect applies to only the ^{9}Li + ^{11}Li (or ^{4}He + ^{6}He) system or if it it of a more universal character. Studies of fusion reactions between non-halo nuclei (for example ^{16}O + ^{17,18}O [12]) taking nucleon transfer fully into account does not exhibit such an effect. As we pointed out in our introduction, this effect is not only due to the neutron transfer mechanisms, but also relies strongly on the fact that the separation energies of the valence neutrons are very small and consequently that these neutrons may reach distances far away from the core. As a result we do not expect this effect to play a role in the fusion of non-halo nuclei. We used the example of ^{11}Li + ^{9}Li since ^{11}Li is by now the best studied among the halo nuclei. In the theory of inhomogeneous big-bang an appreciable amount of halo nuclei could conceivably be formed in neutron-rich regions [13]. In the presence of neutrons the molecular bond effect which we have studied could be of extreme relevance for the fusion to halo heavier nuclei. It would be of interest if the molecular bond effect studied here could be measured experimentally.

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