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Hartree–Fock shell model structure of Li and Be isotopes

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A shell model calculation for $^{6-11}$Li and $^{7-14}$Be isotopes is performed using a density dependent Skyrme interaction and Hartree–Fock single-particle wave functions. Without any parameter fit, quite good agreement with the experimental binding energies and matter radii is obtained. Only ^{10}Li and ^{13}Be are found to be unstable with respect to neutron emission. The calculated radius of ^{11}Li is too small and possible causes of this exception are discussed.

The structure of light neutron rich radioactive nuclei has attracted considerable attention in the last few years. Since the first measurements of interaction cross sections by Tanihata et al. [1,2], the technique of using exotic nuclear beams has made possible the discovery of interesting properties of unstable nuclei, like the neutron halos in ^{11}Li, ^{11}Be, ^{14}Be and ^{17}B, and the soft giant dipole resonances [3–6].

A large number of nuclear structure calculations have been performed trying to reproduce the peculiar properties of ^{11}Li and other exotic light nuclei. The fact that ^{10}Li is unbound with respect to neutron emission and that in ^{11}Li the two-neutron binding energy is only 0.2 MeV, seems to suggest that the interaction of the last two neutrons is responsible for the binding of ^{11}Li and cannot be treated in the mean field approximation. This is the basic idea behind the dineutron cluster models [7–10] for ^{11}Li, which is treated as a ^{9}Li core plus a dineutron structure. The loosely bound dineutron gives a long tail for the neutron density.

On the other hand, several calculations for these light nuclei have been performed in the framework of the shell model. Self-consistent calculations based on the density functional method [11] and Hartree–Fock theory [3,12] roughly reproduce the mass and isospin dependence of most of the experimental nuclear mass radii, although the exceptionally large experimental sizes of nuclei like ^{11}Li and ^{11}Be are not obtained in the calculations. A considerable improvement in the calculated mass radii was achieved by Bertsch et al. [13] by renormalizing the single-particle Hartree–Fock potential by a numerical factor depending on the orbital, in such a way that the single-particle energy fits the empirical one-neutron separation energy, or one half of the two-neutron separation energy. For a loosely bound nucleon the radial extent of the single-particle wave function increases, and consequently the calculated matter radii of nuclei with weakly bound neutrons become appreciably larger, in better agreement with experimental values.

Hoshino et al. [14] have performed a large scale shell model calculation to study the Li and Be isotopes, using the $(0+2)\hbar\omega$ configuration space of the p and sd shells. They use the Cohen–Kurath interaction for the p shell and the Millener–Kurath interaction for the other two-body matrix elements. For the description of $^{9-11}$Li and $^{9-12}$Be isotopes they use HF single-particle wave functions calculated in ^{12}C with the SIII force. They find that the influence of sd shell mixing on the radii is small. The calculated ^{11}Li matter radius becomes 2.48 fm, while the experimental value is 3.12+0.16 fm [3]. If the HF potential for the orbits near the Fermi surface is multiplied by an adjusted factor, following the procedure of Bertsch et al. [13], the radius increases to 2.84 fm, which is the same value obtained in the HF approximation by the same procedure. The shell model description of binding energies is of course more accurate than the HF approximation. The calculations of Hoshino et al. are, however, unable to reproduce, even qualitatively, the behaviour of very neutron rich nuclei. They obtain ^{11}Li less bound than ^{9}Li and ^{11}Be less bound than ^{10}Be, in disagreement with experiment. Similar difficulties have been found by other authors [15]. Thus the theoretical description of binding energies and matter radii of light unstable nuclei at present is needing improvements.

In this paper we present HF plus shell model calculations for Li and Be isotopes with a simple Skyrme density dependent interaction. In spite of its simplicity, this calculation gives a fairly good description of the trends in binding energies and matter radii of the stable and unstable isotopes, although perfect quantitative agreement is of course not achieved. In a recent paper [16] it has been shown that the excitation energies, charge radii, electric and magnetic moments ant other properties of the stable p shell nuclei are quite well predicted by shell model calculations using as input only the density dependent Ska force [17], without any additional parameter involved. Here we follow the same basic idea for the description of ground states. We start by a HF calculation for each nucleus using the uniform filling approximation and the Ska force. This gives the single-particle wave functions and kinetic energies for each nucleus. For the unbound single-particle states we follow the method of ref. [14] and treat them as bound states in a large spherical box with a radius of 12 fm. The next step is a conventional shell model calculation in a space defined by the $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$ and $2s_{1/2}$ active orbits. The $1s_{1/2}$ is treated as a closed shell. The two-body matrix elements are calculated with the same Ska interaction, using the HF single-particle wave functions. Because of the density dependence of the force and the self-consistency of the single-particle wave functions, the two-body matrix elements and the single-particle kinetic energies are different for every nucleus.

One of the diffculties of this approach is that, although we switch off the Coulomb interaction, for $N \neq Z$ the HF single-particle wave functions violate isospin invariance. This gives spurious contributions to the energy [18] and here it can be very important, since we are dealing with some nuclei with N/Z close to 3. On the other hand, the $N=Z$ wave functions of stable nuclei are just missing the pecularities of nearly unbound systems with respect to neutron emission. We have adopted the simple approach of using in every nucleus its HF neutron wave functions as the single-particle basis of states for all the nucleons in the shell model calculations. For the single-nucleon kinetic energies we adopt a weighted average of the proton and neutron HF kinetic energies.

Fig. 1 shows the binding energies of Li and Be isotopes obtained in the $(0+2)\hbar\omega$. calculation and the experimental values. For ^{11}Be we plot the values for the $\frac{1}{2}^-$ state, which experimentally is 0.3 MeV above the $\frac{1}{2}^+$ ground state. The calculated $\frac{1}{2}^+$ state is well above the $\frac{1}{2}^-$. This also happens with the Millener–Kurath interaction [14]. It can be brought down using a much smaller single-particle energy for the $2s_{1/2}$ state, but this is against the spirit of the present parameter free calculation. This property is simply not predicted by the Ska force. The ^{10,11}Li isotopes are overbound. Otherwise the general trends are quite well predicted by the calculation. We believe that the relative behaviour of binding energies as neutrons are added is more significant than the absolute values,

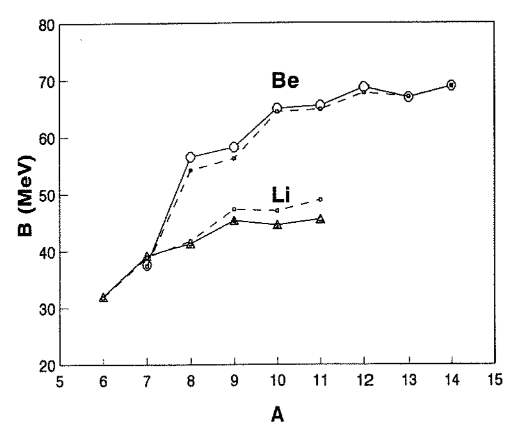

Fig. 1. Binding energy of Li and Be isotopes. The dashed line shows the calculated values. Full circles and triangles correspond, respectively, to experimental Be and Li values.

because it is much less dependent on details of the calculations. A nice feature of the results is that the only unbound nuclei with respect to neutron emission are ^{10}Li and ^{13}Be, in agreement with experiment.

Fig. 2 shows the one-neutron separation energies of Li and Be isotopes. The experimental odd–even staggering is very well described by the calculations. Note for example the spectacular decrease from about 19 MeV in ^{8}Be to about 2 MeV in ^{9}Be. It should be noted that the theoretical separation energies are defined by $S_n(Z,N)=\mathrm{BE}(Z,N)-\mathrm{BE}(Z,N-1)$, and not by the HF single-particle energy of the last occupied orbit. This is an important point, because these two quantities may be quite different in open shell nuclei. Especially for a density dependent force and very light nuclei, the addition of one nucleon produces important rearrangements in the orbits of the other nucleons.

Fig. 3 shows the two-neutron separation energies of Li and Be isotopes. The calculated values are systematically larger than the experimental ones, but the mass dependence is well reproduced.

The mixing of $2\hbar\omega$ components of the present calculation is small, never exceeding 10%. A feature of this mixing is that it increases with increasing neutron excess. The actual amount of mixing in very neutron rich nuclei is not at present well understood.

The RMS matter radii have been calculated defining the nucleon radius of an orbit as the average of the proton and neutron radii weighted with the occupation numbers in the HF calculation. The shell model calculation takes later into account the fractional occupation of the orbits. In fig. 4 results for point nucleons are compared with the experimental data of Tanihata et al. [3]. The experimental radii are inferred from the total reaction cross section using Glauber calculations. The uncertainties of the method may thus be larger than the estimated error bars. However, the trends are roughly confirmed by other measurements [4]. The most outstanding feature of the experimental data are the large radii of

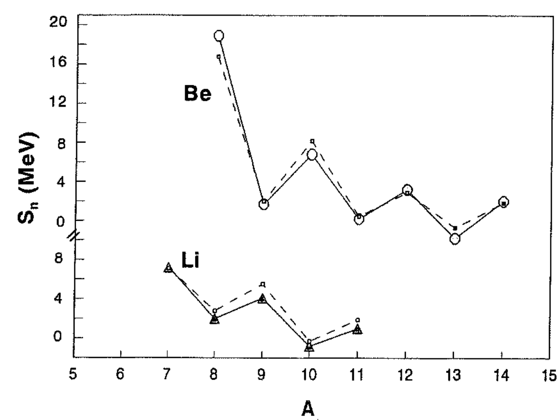

Fig. 2. Neutron separation energy of Li and Be isotopes. The dashed line shows the calculated values. Experimental values are represented by full triangles for Li isotopes and by full circles for Be isotopes.

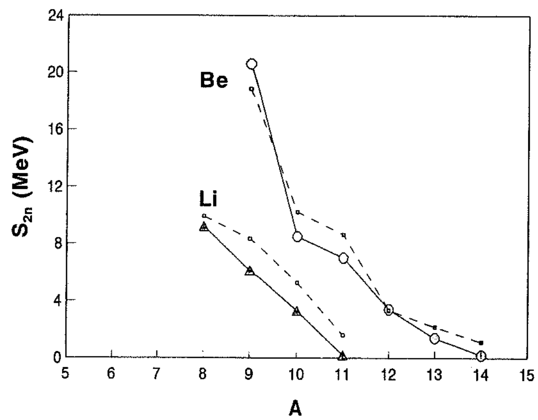

Fig. 3. Two-neutron separation energy of Li and Be isotopes. Symbols are the same as in figs. 1 and 2.

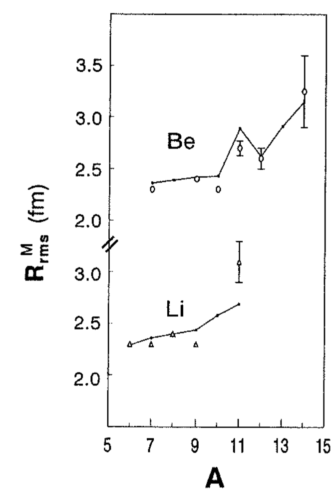

Fig. 4. The RMS matter radii of Li and Be isotopes. The solid line shows the calculated values. Full triangles and circles are the experimental data taken from ref. [3].

^{11}Li, ^{11}Be and ^{14}Be. Our calculations predict large radii for ^{11}Be and ^{14}Be. This is mainly a consequence of the occupation of the $2s_{1/2}$ neutron orbit. For example in ^{14}Be this orbit is slightly bound and has a very long tail, giving $\langle r^2 \rangle = 49.2$ fm, what is the kind of size needed to understand the peculiar behaviour of radii approaching the drip line. Furthermore, it agrees with the halo size deduced from the recent GANIL experiments [19]. In ^{11}Li, however, the shell model calculation gives a negligible occupation probability for the $2s_{1/2}$ orbit. The largest occupied orbit is the $1p_{1/2}$, with $\langle r^2 \rangle = 11.2$ fm. The needed enhancement of the theoretical matter radius could come in two ways. The first one is via a mean field which binds much less the $1p_{1/2}$ orbit. This was achieved by Bertsch et al. [13] multiplying the HF potential by an orbit dependent factor. In the framework of self-consistent calculations a similar effect can be obtained pushing the neutron density away from the center of the nucleus by modifying the symmetry energy of the force within reasonable limits compatible with experimental bulk properties, as was done in ref. [20]. Pushing this possibility to the limit we obtain a force Ska* with the same parameters as Ska except $x_0 = 1.70$ and $x_3 = 3.819$. The $1p_{1/2}$ orbit is then almost unbound, with $\langle r^2 \rangle = 24$ fm, and the ^{11}Li matter radius becomes 3.06 fm,in agreement with the experimental value. Nevertheless this approach will not explain the results of Anne et al. [19] on the radius of the two last neutrons. ($\langle r \rangle_{exp} \simeq 8$ fm versus $\langle r \rangle_{th} \simeq 5$ fm.) The second way to enhance the radius could be to increase the amplitude of the components with two neutrons in the $2s_{1/2}$ orbit in the ground state of ^{11}Li. It is not clear by the action of which mechanism this will be so, but there is a precedent of large intruder mixing in the ground states of nuclei very far from stability near a neutron shell closure, provided by ^{31}Na and ^{32}Mg [21]. If one assumes a 50% mixing of $(2s_{1/2})^2$ neutron configurations in the ground state and a $2s_{1/2}$ orbit identical to that of ^{14}Be, the matter radius of ^{11}Li would be 3.22 fm while the two outer neutrons will sit with a 50% probability in an orbit with $r \simeq 7$ fm. Both properties are now compatible with the experimental findings.

In conclusion, using a simple and well known force, that gives a good description of the nuclear bulk properties through the whole mass table, and also of excited states of nuclei in the p shell [16], we have been able to reproduce the main trends of the binding energies of Li and Be isotopes from the stable to the neutron drip line isotopes. It should be emphasized that the present calculations involve no parameters fitted to properties of these light nuclei. While agreement is also found for the radial properties of Be isotopes, we fail in the prediction of the large radius of ^{11}Li. Nevertheless we can soundly propose a cure to that by invoking the presence of a large amount of $(2s_{1/2})^2$ neutron configurations in the ground state of ^{11}Li.

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