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Self-consistent calculations of Be isotopes

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The properties of the Be isotopes are studied by the deformed Hartree-Fock method with Skyrme interactions. It is shown for ^{11}Be that the configuration where the last neutron occupies a $K^{\pi}=1/2^{+}$ orbital is not the ground state but has a matter density distribution with a tail typical of a halo nucleus. Correlations are introduced in deformed mean-field wave functions by a restoration of rotational invariance. These correlations bring the amount of energy necessary to correct the deficiencies of pure mean-field wave functions. [S0556-2813(96)01710-4]

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I. INTRODUCTION

Halo nuclei were initially observed ten years ago in high-energy nuclear reactions [1]. The large-matter radii deduced from reaction cross sections were rapidly related to the very low binding energies of a few valence neutrons. In ^{11}Li [2], the last two neutrons are bound by only 0.30 MeV; in ^{11}Be [3], a one-neutron halo system, the separation energy of the last neutron is 0.50 MeV. Other Be isotopes exhibit a similar structure where the last neutrons are loosely bound to the rest of the system. The properties of halo nuclei are mainly determined by these neutrons [4].

The theoretical description of halo nuclei has met several difficulties. It is indeed hard to reproduce with sufficient accuracy all their properties: particularly, the low binding energies of the last neutrons, which require a good reproduction of the relative energies of chains of isotopes and the extended tails of the halo particles. Moreover, the large excess of neutrons with respect to protons tests effective nuclear interactions far from the isospin values for which they have been adjusted. Another difficulty is that the ground state of ^{11}Be is not a $1/2^{-}$, as one should expect, but a $1/2^{+}$ state. That such an inversion should occur in ^{11}Be was already suggested at the beginning of the 1960s on the basis of a simple shell model analysis [5]. However, models starting directly from an effective two-body interaction have failed to reproduce it without an *ad hoc* renormalization.

In particular, mean-field calculations based on Skyrme-like interactions have been unsuccessful in reproducing the properties of ^{11}Li and ^{11}Be. Shell model calculations based on Hartree-Fock (HF) single-particle wave functions have been more successful provided that the single-particle energies are renormalized [6–8]. Bertsch and Esbensen [9] have shown that the description of ^{11}Li is significantly improved by introducing a residual interaction between the two valence neutrons in the form of a density-dependent pairing interaction. For ^{11}Be, the inclusion of correlations beyond a mean-field method by the variational shell model has been necessary to obtain the correct parity for the ground state [10]. Even Be isotopes have also been rather well described by a relativistic density-dependent mean-field calculation [11] and by different variants of the cluster model [12,13]. However, this last model fails in reproducing correctly the order of the ^{11}Be levels [13].

From this intensive theoretical activity, one can conclude that the description of halo nuclei, in particular ^{11}Li and ^{11}Be, requires the introduction of correlations beyond the mean-field approximation. In this work, we will focus on the description of the Be isotopes. We are motivated by the results of Otsuka *et al.* [10], whose starting point is a Skyrme interaction widely used in mean-field calculations. Here we shall examine simple correlations introduced on top of deformed mean-field calculations using Skyrme-like interactions that may be responsible for the parity inversion found in ^{11}Be. Our aim is rather similar to the recent work of Vinh Mau [14], but for a different kind of collective correlations.

Our starting point is the formalism developed in the past few years to study deformed nuclei by the Hartree-Fock method and to introduce correlations beyond the Hartree-Fock method [15–17]. In the next section we present results of deformed HF calculations for Be isotopes. In Sec. III, we discuss the results obtained with different parametrizations of the Skyrme interaction. In Sec. IV, we show that the restoration of angular momentum of deformed configurations provides the number of correlations that are necessary to reproduce the experimental data.

II. HARTREE-FOCK RESULTS

The Hartree-Fock equations are solved on a three-dimensional Cartesian mesh [15]. Our calculation is therefore free of the problems encountered in describing the tail of the single-particle wave functions when they are expanded on an oscillator basis. Since the number of individual wave functions is very small, the dimensions of the box can easily be chosen large enough to represent correctly this tail far away from the nuclear surface. For all the calculations of ^{11}Be, the nucleus has been explicitly treated as an odd one thanks to the formalism presented in Ref. [17]. No pairing correlations have been introduced.

The energies of ^{10}Be and of two configurations of ^{11}Be are plotted on Fig. 1 as a function of the axial mass quadrupole moment. The Skm* parametrization of the Skyrme force has been used. In the lowest configuration of ^{11}Be,

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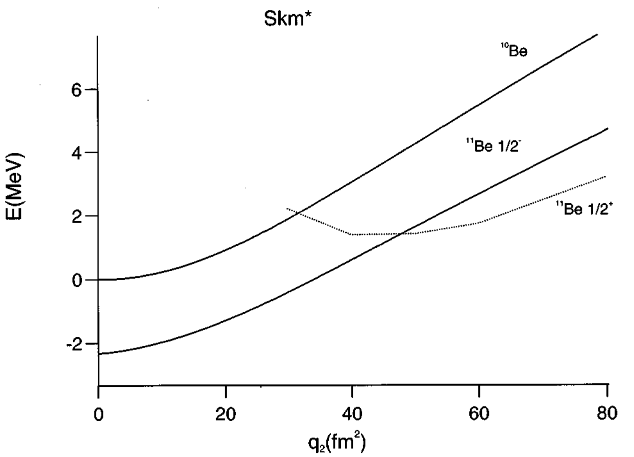

FIG. 1. Energies of ^{10}Be and ^{11}Be as a function of the axial quadrupole moment. For ^{11}Be configurations are plotted in which the last neutron occupies either a $K^{\pi}=1/2^{+}$ or $1/2^{-}$ orbital.

labeled ^{11}Be^{-}, the last neutron occupies a $p1/2$ orbital and in the excited configuration a positive-parity orbital with a projection of the angular momentum along the symmetry axis equal to 1/2.

The energy minimum for both ^{10}Be and ^{11}Be^{-} is obtained for the spherical configuration. The energy gain due to the extra neutron in ^{11}Be^{-} is of the order of 2 MeV and is nearly independent of deformation. The ^{11}Be^{+} configuration does not exist for small quadrupole moment: the single-particle state of positive parity with a projection 1/2 is unbound for a quadrupole moment lower than 30 fm^2. For larger deformations, the meaning of the quadrupole moment as a collective variable is questionable [18]: the contribution of an $l=0$ state to the quadrupole moment diverges as its energy tends to zero. The quadrupole constraint is used here as a tool to locate the energy minimum for this configuration. It is obtained for a quadrupole moment around 50 fm^2 and a single-particle energy of the $K=1/2$ state around -1.3 MeV. The configuration is slightly unbound with respect to ^{10}Be and has an excitation energy of 2.5 MeV with respect to ^{11}Be^{-}. The energy gain due to deformation is thus not sufficient to obtain the correct parity for the ^{11}Be ground state. This negative result confirms an old Nilsson model calculation of Ragnarsson *et al.* [19].

However, although it does not have the right energy, the $1/2^{+}$ configuration has the right shape. On Fig. 2 the neutron densities obtained for both Be isotopes are compared. The density of the ^{11}Be^{+} configuration has a much larger extension, exclusively due to the last neutron orbital. The value of the density around 8 fm is 0.5×10^{-4}, in qualitative agreement with the experimental density [20] and with Ref. [10]. It is at least two orders of magnitude larger than the density of ^{10}Be.

That the deformed configurations obtained with Skyrme interactions have the right geometrical properties is confirmed by a determination of the variation of the rms radii of Be isotopes from $N=6$ to 10. They are compared to the experimental data for mass radii on Fig. 3. The large increase observed at ^{11}Be is present in the mean-field calculation. Although the mean-field variations underestimate the experimental ones, the general trends are correctly reproduced, pro-

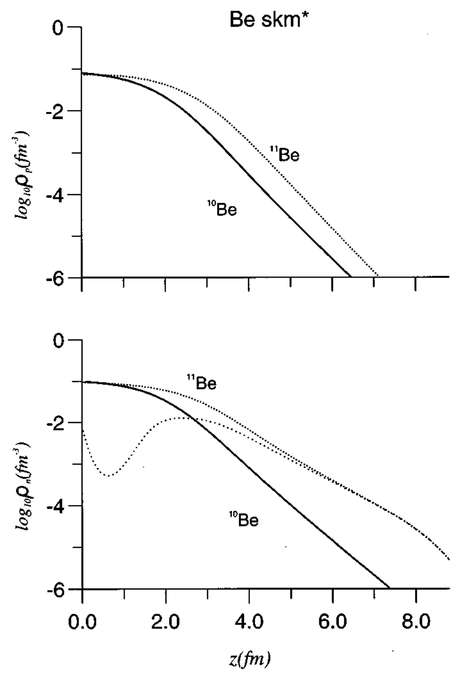

FIG. 2. Upper part: proton density distributions of ^{10}Be (solid line) and of the halo configuration of ^{11}Be (dashed line) in the z direction. Lower part: same as the upper part, but for the neutrons. Also plotted is the square modulus of the last neutron wave function $|\psi|^2$ (long-dashed line).

vided that one considers for ^{11}Be and ^{12}Be the configurations where the neutrons occupy the $K^{\pi}=1/2^{+}$ orbits.

The quadrupole moment of the ^{11}Be^{+} minimum is mainly due to the extra neutron. However, this neutron polarizes the other nucleons leading to a deformed ^{10}Be core with a quadrupole moment of about 20 fm^2. This result supports the coupled channel treatment of a valence neutron coupled to a deformed core made by Esbensen *et al.* [21].

III. THE SKYRME PARAMETRIZATION

The binding energies of Be isotopes obtained with four different Skyrme parametrizations are compared to the experimental data on Fig. 4. For ^{11}Be the values corresponding to the configuration where the extra neutron occupies a positive-parity state are given; the other configuration is systematically 2–2.5 MeV more bound. For ^{12}Be the results obtained for the configurations where the last two neutrons

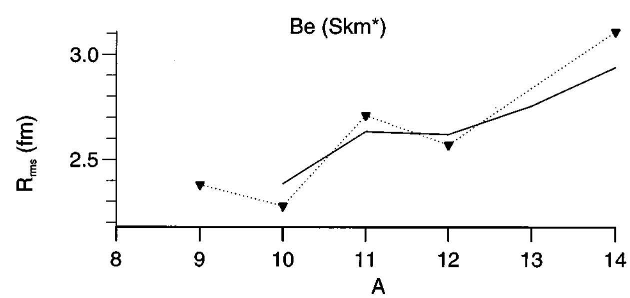

FIG. 3. Comparison between experimental (triangles connected by the dashed line) and theoretical (solid line) rms matter radii of Be isotopes.

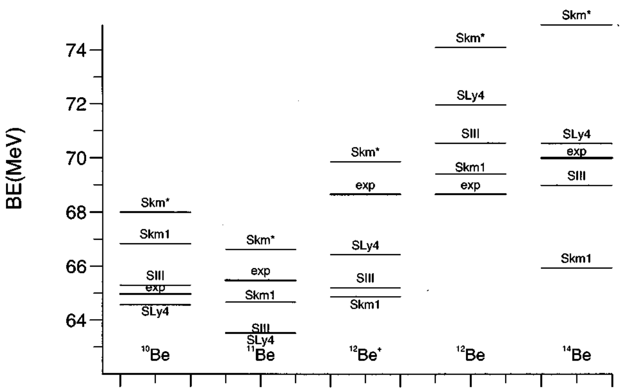

FIG. 4. Binding energies of Be isotopes calculated with four different Skyrme parametrizations (thin solid lines) compared to the experimental data (heavy solid line). For ^{11}Be and ^{12}Be$^+$, the last neutrons occupy single-particle states with $J^\pi = 1/2^+$.

occupy either negative- or positive-parity orbitals are shown.

We have used two parametrizations, SIII and Skm*, which have been extensively tested on binding energies and collective properties of many nuclei in different regions of the nuclear chart. As quoted in Ref. [22], binding energies obtained with Skyrme interactions are usually in rather good agreement with the data, even for light nuclei: the error on the ^{4}He energy is of the order of 1.0 MeV for both SIII and Skm* and is still lower for ^{12}C and ^{16}O. The results obtained for the neutron-rich Be isotopes are not as satisfactory. The Skm* parametrization overbinds all the isotopes. The discrepancy is the largest for ^{12}Be, leading to large errors on the one- and two-neutron separation energies. The SIII parametrization has a smoother behavior, leading to errors of at most 2 MeV. However, ^{14}Be is predicted by SIII to be unstable for two-neutron emission. Gomez and Casas have suggested to slightly modify the Skm* parametrization in order to lower the symmetry energy. The parameters of this new interaction, Skm1, are the same as Skm* except for $x_0 = 1.3$ and $x_3 = 1.734$, leading to a symmetry energy of 25.2 MeV. This modified force shows clear improvments. However, it also predicts an unbound ^{14}Be. The parametrization Sly4 [23] has been adjusted with special care for the properties of the symmetric infinite nuclear matter and the low- and high-density neutron matter equation of state. It has also been fitted to the binding energies and rms radii of spherical stable nuclei. Its predictions for the Be isotopes are rather similar to those of SIII, with a slight improvment in the case of ^{14}Be. None of the interactions predicts a stable $1/2^+$ state for ^{11}Be, which has always a $1/2^-$ ground state.

IV. CORRELATIONS BEYOND THE MEAN FIELD

For nuclei close to the stability lines, correlations beyond a mean-field approach may be naturally introduced by the coupling to excitations with respect to a collective variable. The generator coordinate method (GCM) has been extensively used to study the dynamics of the nucleus with respect to deformation modes defined by multipole operators [16]. The situation is more complicated in the case of nuclei far from stability. It may be shown that the single-particle matrix element of an operator of multipolarity n diverges for a state of angular momentum l whose energy is going to zero provided $n \geqslant 2l+1$ [18]. The difficulties related to such a divergence have been recently encountered in a study of ^{11}Li by the GCM using Hartree-Fock-Bogoliubov wave functions generated by a monopole contraint [24]. It seems therefore inadequate to generate a collective path with a quadrupole constraint, which would lead to even more dramatic divergences. A sign of this instability is given by the very close to 1 overlap between ^{12}Be wave functions with quadrupole moments differing by 20 fm^2. It shows that large modifications of the quadrupole moment require very small changes in the total wave functions.

TABLE I. Energies and BE2(2-0) values obtained for the 2^+ and 4^+ states of even Be isotopes by projecting on the angular momentum the intrinsic configurations corresponding to the quadrupole moments indicated on the second line. Energies are in MeV and BE2 values in e^2 fm^4. Experimental data are given in parentheses.

Isotope	q (fm^2)	2^+	4^+	BE2(2-0)
^{10}Be	20	2.7 (3.4)	8.5	5.6 (10.5)
^{10}Be	30	4.6	8.5	8.3
^{12}Be	60	2.5 (2.1)	6.0 (5.8)	8.9
^{14}Be	80	1.9	5.4	11.6

To restore a broken symmetry is another way of introducing correlations in a mean-field wave function. In particular, the correlations brought by angular momentum projection will modify the energy difference between a spherical and a deformed configuration. On the basis of their variational shell model calculation, Otsuka *et al.* [10] have also suggested that such a symmetry restoration may improve the description of ^{11}Be. We have therefore constructed a code for the projection of wave functions discretized on a three-dimensional mesh. This code uses the same techniques as a previous one written for a schematic Skyrme interaction [25], but is limited to the projection of axially deformed time-reversal invariant configurations. These restrictions preserve the reality of the densities entering the Skyrme functional. The exactness of the code and the accuracy of the projection have been tested by reconstructing the overlap and the Hamiltonian matrix element between two nonprojected wave functions from their projection on angular momentum. Spins up to $J=6$ have to be included for a ^{12}Be wave function with a quadrupole moment equal to 60 fm^2. This $J=6$ component still represents 7% of the total wave function. Quadrupole transition matrix elements have been calculated using standard formulas [26,27]

To restore a symmetry, in principle, one requires to vary the mean-field wave functions after projection [28]. However, a variation after projection method necessitates new developments, which are beyond the scope of this work. Therefore we have tried only to estimate the gain of energies that a restoration of angular momentum would bring in ^{11}Be by projecting the ^{10}Be and ^{12}Be wave functions corresponding to various quadrupole moments. For the configurations of ^{12}Be and ^{14}Be with two neutrons in positive-parity orbitals, due to the limited meaning of the quadrupole moment, we have projected only the wave function corresponding to the energy minimum. Results are given in Table I.

For ^{10}Be, the minimum of the projected energy is obtained for a deformed configuration. The energy of the $J=0$ state is lower than the corresponding intrinsic state by 0.8 MeV at 20 fm^2 and 4.6 MeV at 30 fm^2. These gains bring the 30-fm^2 state below the spherical minimum by around 500 keV. The excitation energy of the 2^+ state varies from 2.7 MeV at 20 fm^2 to 4.6 MeV at 30 fm^2, to be compared with the experimental value of 3.4 MeV. This confirms that ^{10}Be is deformed in its ground state, with a deformation between 20 and 30 fm^2. The BE2 value between the 2^+ and the ground state varies between 5.6 and 8.3 e^2 fm^4 between 20 and 30 fm^2, close to the experimental value of 10.5 e^2 fm^4. For all deformations, the excitation energy of the 4^+ is above 8.0 MeV.

In the ^{12}Be configuration with neutrons in p states, the rotational energy gain is never large enough to compensate the loss of energy due to deformation. On the other hand, for all the interactions that we have tested, the 0^+ state of the configuration with neutrons in positive-parity states is lowered approximately by 3.5 MeV with respect to the intrinsic state, for a deformation of 60 fm^2. This decreases the excitation energy of the deformed configuration to around 1.0 MeV (see Fig. 4). The 2^+ state has an excitation energy of approximately 1.5 MeV with respect to the deformed configuration and 2.5 MeV with respect to the spherical configuration, to be compared with an experimental value of 2.1 MeV [29]. The BE2 value for this state is 8.9 e^2 fm^4. The 4^+ state is situated around 6.0 MeV, close to the energy at which such a state has been suggested experimentally [29]. For ^{14}Be, the projection of the configuration with a deformation of 80 fm^2 leads to a 2^+ state at 1.9 MeV with a BE2 value of 11.6 e^2 fm^4 and a 4^+ state at 5.4 MeV.

From these results, one can give an estimate of how relative energies will be affected by the projection of the ^{11}Be$^+$ deformed configuration. This gain of energy should be at least 50% of the gain of the ^{12}Be configuration and thus of the order of 2 MeV, depending of the nuclear interaction. Looking to the modification of the energy of ^{10}Be, one sees that the ^{11}Be$^+$ configuration will now be slightly bound. Although this modification of energy is not sufficient to bring the $1/2^+$ state below the $1/2^-$ state with the interactions that we have tested, it will account for a large fraction of the difference.

V. CONCLUSION

In this paper we have applied the deformed Hartree-Fock method with Skyrme interactions to the study of ^{11}Be. We have shown that a configuration with the last neutron occupying a positive-parity spin-1/2 state exists for a quadrupole moment around 50 fm^2. However, this configuration is unstable with respect to one-neutron emission and is less bound than the negative-parity state. This result does not depend qualitatively on the parametrization of the Skyrme interaction. Except for its energy, this positive-parity state has geometrical properties that agree with the experimental data. We have also shown that the correlations brought by the restoration of rotational invariance bring an amount of correlations of the right order of magnitude. Since our treatment of angular momentum projection is not fully variational, one cannot make definitive conclusions. However, the projection of the deformed minima of ^{10}Be and ^{12}Be has permitted us to reproduce qualitatively the excitation energies of the experimental 2^+ and 4^+ states when they are known. The BE2 value obtained for the 2^+ to 0^+ transition in ^{10}Be is also close to the experimental data. These results give some confidence in the ability of the projected HF method to describe the properties of light halo nuclei.

This work opens a new range of applications for the extensions of mean-field methods that we have developed in the recent years. In particular, the code that we have constructed to project mean-field wave functions on angular momentum and to calculate transition matrix elements will have applications in nuclei for which there is a coexistence between a spherical and a deformed configuration. To go beyond qualitative results, this will require one to set up an algorithm of variation after projection. Another development that is suggested by this work is a definition of a collective path by variables that are not related to the shape of the nucleus. This will be necessary for the study of nuclei close to the drip line when pairing correlations couple single-particle states of positive and negative energies [30].

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