Positive parity states in $^{11}$Be

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(Received 29 August 1994)

The low-lying positive parity states of $^{11}$Be are calculated in a coupled channels treatment of a valence neutron interacting with a deformed core. The loosely bound nature of the valence neutron is taken into account by using a Woods-Saxon potential. Comparisons are made to shell-model predictions and to data. The model reproduces the measured spectrum quite well for realistic parameters of the neutron-core interaction.

PACS number(s): 21.10.–k, 27.20.+n

I. INTRODUCTION

The development in radioactive beam experiments has made it possible to study the properties of nuclei far from stability. An example is $^{11}$Be which has already been studied in several fragmentation experiments [1–3] and more detailed measurements of the two-body breakup $^{11}$Be$\rightarrow^{10}$Be$+n$ have recently been performed [4]. The analyses commonly employ a simple $s$ wave for the valence neutron in its ground state, and we shall in particular investigate the validity of this approximation.

The nucleus $^{11}$Be is of particular theoretical interest because of the parity inversion near the ground state, i.e., the ground state is a $1/2^+$ state, and not a $1/2^-$ state as one naively would expect from a spherical shell-model.

We have recently discussed this parity inversion [5] on the basis of shell-model wave functions and pointed out three competitive effects, viz. the quadrupole excitation of the core, the Pauli blocking of the pairing correlations, and the narrowing of the shell gap due to the proton-neutron monopole interaction. Thus we found that the $1/2^+$ ground has a large overlap with the $0^+$ ground state of the $^{10}$Be core coupled to an $s_{1/2}$ single-particle state. A loosely bound $s_{1/2}$ state has a large root mean square (rms) radius and a large dipole strength at low excitation energies, and both of these two features are clearly needed in order to explain the recent fragmentation measurements [1–4].

In the present study we focus on a realistic description of positive parity states in $^{11}$Be. Our approach is to solve coupled equations for a neutron interacting with a deformed core, including the effect of the quadrupole excitation of the core. This approach, also known as the weak coupling limit of the particle-rotor model, has previously been applied by many authors, for example to $A=13$ nuclei. An early application [6] made use of harmonic oscillator wave functions. It was found that this approach provides a reasonable picture of $A=13$ nuclei, whereas the strong coupling limit, implied by the Nilsson model, contradicts measurements. Later applications made use of a Wood-Saxon plus spin-orbit single-particle Hamiltonian, see, e.g., Refs. [7,8]. We shall use a similar parametrization since it provides a more realistic description of weakly bound orbitals; this was clearly demonstrated in the study of the strong dipole transitions in $^{11}$Be and $^{13}$C [9].

The main purpose of our study is to see how well one can predict the positive parity spectrum of $^{11}$Be from the knowledge of the structure of the $^{10}$Be core. The low-lying negative parity states, on the other hand, have a complicated structure because of the importance of pairing correlations, and they cannot be described reliably in the weak coupling limit.

The structure of $^{11}$Be has also been studied in a variational shell-model approach [10], and the physical picture that emerged from this study has a strong resemblance with our simpler model. We make comparisons to the predictions of this model, to shell-model calculations, which we have performed using the effective interactions constructed in Ref. [11], and to measurements. As an additional test, we also calculate the well-known spectrum of $^{12}$C. The model we use is described in the next section. The calibration of the neutron-core interaction is discussed in Sec. III, together with the results of our calculations.

II. COUPLED CHANNELS FORMULATION

We consider a valence neutron interacting with an axially symmetric, deformed core. We formulate the problem in terms of a coupled channels treatment and include the effect of the $2^+$ rotational excitation of the core. An example of this approach is the particle-rotor model, which is described in Chapter 5-A-1 of Ref. [12] for nucleon scattering on a deformed nucleus.

The single-particle potential for a neutron interacting with a spherical nucleus is parametrized the following way,

$$ V(r) = V_0 \left[ 1 - F_{s.o.} (1 \cdot S) \frac{r_0}{r} \frac{d}{dr} \right] f(r), $$

with
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\[ f(r) = \frac{1}{1 + \exp[(r - R_c)/a]} , \]

where \( R_c = r_0 A_c^{1/3} \) is the nuclear radius of the core with mass number \( A_c \) and \( a = 0.67 \) fm is the diffuseness we have chosen. The choice of the remaining parameters is discussed in the next section.

The shape of an axially symmetric deformed core is parametrized as

\[ R_c(\theta') = r_0 \left( \frac{A_c}{F_{\text{vol}}} \right)^{1/3} [1 + \beta_1 Y_{10}(\theta')] , \]

where

\[ F_{\text{vol}} = \int d\Omega [1 + \beta_1 Y_{10}(\theta')]^3 . \]

The angle \( \theta' \) is the polar angle of the particle with respect to the symmetry axis. The denominator \( F_{\text{vol}} \) in Eq. (3) is included in order to preserve the volume for different choices of the deformation. Inserting this parametrization into Eq. (2) we next perform a multipole expansion

\[ \left( - \frac{\hbar^2}{2\mu_n} \frac{d^2}{dr^2} + \frac{\hbar^2(l + 1)}{2\mu_n r^2} + V_0 \left[ 1 - F_{\text{s.o.}}(l \cdot s) \right] \frac{r_0}{r} \frac{d}{dr} \right) f_0(r) + E_{\text{rot}}(R) - E \right) \phi_{ijRI}(r) 

= -V_0 f_2(r) \sum_{ij'j''R'} \langle \ell(jR)|\ell'(j'R')\rangle |IM\rangle |P_2(|\ell|'j|R')\rangle \phi_{ij'j''R'R'I}(r) , \]

where \( \mu_n = m_n A_c/(A_c + 1) \) is the reduced mass of the valence neutron and \( E_{\text{rot}} \) is the rotational energy of the core. The coupling matrix has diagonal as well as off-diagonal matrix elements, and it is given by Eq. (5A-5) of Ref. [12].

The radial wave function for \( R = 0 \), \( \phi_{i0j} \), has \( j = I \), and it is associated with the elastic scattering channel. It is instructive to consider a few examples. A \( 1/2^+ \) state involves three channels: the elastic \( s_{1/2} \) single-particle state coupled to the \( 0^+ \) ground state of the core and a \( d_{5/2} \) and \( d_{3/2} \) state both coupled to the \( 2^+ \) excited state of the core. A \( 5/2^+ \) state, on the other hand, will involve six channels, namely the \( d_{5/2} \) elastic channel, and the five \( s, d, g \) single-particle states coupled to the \( 2^+ \) state of the core.

It is sufficient to solve the coupled equations (6) inside a certain interaction region, where couplings are significant. Outside that region, one can express the solutions in terms of spherical Bessel or Hankel functions, which are the exact solutions to the homogeneous equations for positive and negative channel energies, respectively. The coupled equations are solved with the usual boundary conditions for scattering states, c.f. Appendix 5A of Ref. [12]. Resonances in the continuum are then identified as the energy for which the elastic scattering phase shift is 90°. We do not show the \( 1/2^+ \) continuum states obtained in this way since they are very broad.

The boundary conditions for a bound state are obviously that the radial wave functions are exponentially decreasing in all channels at large distances from the core. The search for a bound state can be performed the following way. If there are \( N \) coupled equations then there are \( N \) independent sets of solutions. For each set of solutions, \( \phi_{iR}^{(n)}(r) \), one can determine the amplitudes for the exponentially decreasing and increasing components of the channel wave functions,

\[ \phi_{ijRI}(r) \rightarrow a_{ijRI}^{(n)} \exp(-kr) + b_{ijRI}^{(n)} \exp(kr), \quad r \rightarrow \infty, \]

where \( k = \sqrt{2\mu_n(E - E_{\text{rot}}(R))/\hbar} \). These amplitudes form two \( N \times N \) matrices. The condition for a bound state can be expressed in terms of a vanishing determinant,

\[ \det(b_{ijRI}^{(n)}) = 0 , \]

since it is then possible to find a nontrivial solution which decays exponentially in all channels. The numerical search for this condition is very simple, and one can also easily determine the associated bound state wave function.

III. CALCULATIONS FOR $^{11}$Be AND $^{13}$C

Our approach is to see how well one can predict the positive parity spectra of $^{11}$Be and $^{13}$C from known prop-
erties of the cores. The 2\(^+\) excitation of the core is characterized by the excitation energy and the \(\beta_2\) value which we determine from the measured \(B(E2)\) value [14]. The excitation energy for \(^{16}\)Be and \(^{12}\)C are 3.368 and 4.4389 MeV, respectively, and the associated \(\beta_2\) values are 1.13 and \(-0.592\). The negative \(\beta_2\) for \(^{12}\)C, i.e., an oblate deformation, is consistent with the measured electric quadrupole moment, \(Q_{2+} = +6 \pm 3 \text{ e fm}^2\), of the \(2^+\) state [15]. Before we can proceed with the calculations it is important to make a realistic calibration of the neutron-core interaction.

A. Calibration of interactions

The overall strength \(V_0\) of the interaction (1) is adjusted for each nucleus so that the energy of the lowest positive parity state reproduces the measured value. The two remaining parameters of the interaction are the radius and the strength of the spin-orbit interaction. We estimate their values by fitting the lowest \(5/2^+, 1/2^+,\) and \(3/2^+\) states of \(^{17}\)O [16], since excitations of the spherical \(^{16}\)O core are not expected to have a significant impact. The optimum fit for \(^{17}\)O is obtained for \(r_0 = 1.2233 \text{ fm}, F_{x.o.} = 0.38 \text{ fm, and } V_0 = -54.675 \text{ MeV.}\)

It is necessary to calibrate the radius more accurately since nuclear radii do not follow an \(A^{1/3}\) scaling in \(p\)-shell nuclei. The ratio of the measured rms charge radii of \(^{12}\)C and \(^{16}\)O is 0.916 [16,17], and the ratio of the rms matter radii of \(^{10}\)Be and \(^{12}\)C extracted from fragmentation measurements [1] is 0.98. We therefore adjust the parameter \(r_0\) for each nucleus so that the mean square radius associated with the neutron-core potential,

\[
\langle R^2 \rangle = \frac{3}{5} \int d\Omega R_0^2(\theta) = r_0^2 \frac{3}{5} \frac{A_c^{2/3}}{F_{x.o.}^{1/3}} \int d\Omega [1 + \beta_2 Y_2(\theta')]^2,
\]

follows the scaling predicted by these measurements. With \(r_0 = 1.2233 \text{ fm for the spherical } ^{16}\text{O core we obtain } r_0 = 1.064 \text{ fm for } ^{10}\text{Be and } r_0 = 1.1733 \text{ for } ^{12}\text{C, using the deformation parameters mentioned earlier.}\)

The calibrations made above can only provide a qualitative guidance for the interactions between a loosely bound or unbound neutron and a more tightly bound, deformed core. To really test the validity of the weak coupling limit would require an accurate knowledge of all the interactions involved. From Hartree-Fock calculations one might get a more realistic estimate of the interaction with the \(0^+\) ground state of the core. However, there would still be uncertainties in the off-diagonal \(0^+ - 2^+\) and the diagonal \(2^+ - 2^+\) interactions. Instead of addressing these difficulties, we have chosen to use the calibration made above as a first estimate and then discuss the sensitivity of the calculated spectra to the value of \(r_0\), and also to the quadrupole moment of the \(2^+\) state in \(^{10}\)Be.

B. Comparisons of positive parity spectra

We show in Fig. 1 the positive parity spectra for \(^{13}\)C (up to 9 MeV). Column (A) is the result we obtain as described in the previous sections. Column (B) is the result obtained by minimizing the deviation from the measured spectrum [18] (column EXP) with respect to both the radius and the spin-orbit strength. This leads the values \(r_0 = 1.085 \text{ fm and } F_{x.o.} = 0.375 \text{ fm.}\) The spin-orbit strength is almost identical to the value obtained by fitting the \(^{17}\)O spectrum, but the radius is 8% smaller. This is somewhat unsatisfactory, but the smaller radius is clearly needed if one wants to increase the separation between the lowest \(1/2^+\) and \(5/2^+\) levels. The spectrum of \(^{13}\)C has been studied in other weak-coupling models [7,8] and similar fits to the measured spectrum have been obtained by adjusting many parameters, for example by using different well-depths for \(s\) and \(d\) waves in order to reproduce the observed binding energies of the lowest \(1/2^+\) and \(5/2^+\) states. The last column (SM) in Fig. 1 shows the levels obtained from shell-model calculations [11]. There is also a \(7/2^+\) level in the measured spectrum. We have not tried to construct this state in our model; the shell-model predicts that it is essentially a \(d_{5/2}\) state coupled to the \(2^+\) excited state of the core.

Our calculations of the spectrum shown in column (B) of Fig. 1 predict an rms neutron-core distance of 4.7 fm in the lowest \(1/2^+\) state of \(^{13}\)C. About 95% of this state consists of an \(s_{1/2}\) single-particle state coupled to the \(0^+\) ground state of the core, whereas only 4% comes from a \(d_{5/2}\) state coupled to the \(2^+\) excited state of the core. Our model also predicts an rms neutron-core distance of 3.6 fm for the lowest (bound) \(5/2^+\) state, with 80% in a \(d_{5/2}\) state coupled to the \(0^+\) ground state of the core and 18% in a \(d_{5/2}\) state coupled to the \(2^+\) excited state of

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Calculated and measured positive parity states for \(^{13}\)C. Column (A) and (B) are results of calculations described in the text. The third column (EXP) are the measured levels [18], and the last column (SM) are the results of shell-model calculations [11].}
\end{figure}
the core. The decomposition of the two bound, positive parity states are in reasonable agreement with the shell-model predictions made by Millener et al. [19]. The measured $S$ factors [18] for the lowest $1/2^+$ and $5/2^+$ states (of 0.65 and 0.58, respectively) are about 30% smaller than our model predictions.

It is instructive to study the positive parity spectrum as a function of deformation. This is illustrated in Fig. 2 for $^{11}$Be. The parameters for the neutron-core interaction are those obtained from the $^{17}$O calibration except the overall strength which arbitrarily has been set to $V_0 = -65$ MeV, so that the lowest $1/2^+$ and $5/2^+$ states are bound for all deformations. In the spherical limit ($\beta_2 = 0$), we show only two states in the continuum; they consist of the $2^+$ excited state of the core coupled to the bound $s_{1/2}$ and $d_{5/2}$ single-particle states, respectively, and they are therefore simply displaced by the $2^+$ excitation energy with respect to the two bound single-particle states. For nonzero deformation, the two continuum states split into $3/2^+$ and $5/2^+$ states. There should also be a $1/2^+$ when one couples the $d_{5/2}$ state to the $2^+$ core state, but this is not shown. There is also a $d_{5/2}$ resonance at 4.9 MeV in the spherical limit, but we have chosen not to show it and its associated levels at nonzero deformation, since they are located at high excitation energies.

There are several interesting features to be noticed in Fig. 2. First of all, the spectrum is not symmetric when we change the sign of $\beta_2$, i.e., the spectra of prolate and oblate nuclei are qualitatively very different. The lowest two states are the $1/2^+$ and $5/2^+$ states. The next level for a large prolate deformation is a $3/2^+$ state followed by a gap to the much higher $3/2^+$ and $5/2^+$ levels. For oblate deformations, on the other hand, this gap disappears, and the upper $5/2^+$ and the two $3/2^+$ levels are close together. These characteristic features of prolate and oblate deformations are clearly seen in the spectra of $^{11}$Be and $^{13}$C, respectively; cf. Figs. 1 and 3.

The energy levels of $^{11}$Be are shown in Fig. 3 (up to 5 MeV). Column (A) is the positive parity states we obtain from the coupled channels calculations using the parameters determined in the previous section. The third column is the shell-model prediction which we have obtained using the effective interactions that were constructed in Ref. [11]. Although the spin and parity of the measured spectrum has not been uniquely identified for all levels, we indicate by the dashed lines the possible assignment and relation to the shell-model predictions and to our coupled channels calculations. The second $5/2^+$ state, which the shell-model predicts at 4.64 MeV, is located at a much higher excitation in our model, c.f., the discussion of Fig. 2.

The $1/2^+$ ground state of $^{11}$Be has an rms neutron-core distance of 6.70 fm in our model, and 87% of this state consists of an $s_{1/2}$ single-particle state coupled to the ground state of the core, whereas 10% is in a $d_{5/2}$ state coupled to the $2^+$ excited state of the core. The full shell-model calculation, which is based on the effective interactions of Ref. [11], predicts that about 80% of the ground is in an $s_{1/2}$ single-particle state. These results can be compared to an $S$ factor of 0.77 measured in $(d, p)$ reactions on a $^{10}$Be target [17]. The variational shell model [10], on the other hand, predicts an even smaller $s_{1/2}$ component of 55%, and a much larger $d_{5/2}$ component of 40%.

The density distribution of the valence neutron with respect to the center of mass of $^{11}$Be is very similar to that
obtained by Sagawa [20] from a Hartree-Fock model, using shell-model occupation probabilities. There are some differences inside the core but the tails are almost identical, and the rms distances from the center of mass are also very close (our value is 6.70 \times 10/11 = 6.09 fm, and from Ref. [20] one obtains 6.05 fm). Both calculations are consistent with the nuclear density that has been extracted from fragmentation measurements [2], at least for \( r \geq 6 \) fm, where the core density becomes insignificant. In fact, with a spectroscopic factor close to one, the tail of this distribution is primarily determined by the binding energy, and it can as well, within the uncertainties, be reproduced by a 2\( s_{1/2} \) single-particle wave function.

Shell-model calculations [21] indicate that \(^{10}\text{Be}\) is not a perfect rotor: the calculated quadrupole moment of the lowest 2\(^+\) state is only 34\% of the value predicted from the \( \beta_2 \) value, assuming a static deformation. We have therefore repeated our coupled channels calculations, reducing the 2\(^-\)-2\(^+\) coupling strength to 34\% of the value we used previously. The resulting spectrum is shown in column (B) of Fig. 3. The agreement with the measured spectrum is greatly improved by this adjustment. The s wave content of the ground state is now 91\% and the rms neutron-core distance is 6.87 fm. It would clearly be very important to have experimental information about the quadrupole moment of the 2\(^+\) state in \(^{10}\text{Be}\), in order to assess the validity of the weak-coupling model.

Finally, in addition to adjusting the quadrupole moment of the 2\(^+\) core state, one can also adjust the radius of the core and obtain an even better agreement with the observed states in \(^{11}\text{Be}\). From our discussion of the \(^{12}\text{C}\) spectrum it is obvious that one would have to increase this radius in order to lower the 5/2\(^+\) state. Thus one can obtain an almost perfect fit for \( r_0 = 1.1535 \) fm; only the 3/2\(^+\) level deviates by 60 keV. It is, however, somewhat disturbing that the best fit requires an 8\% increase in the core radius, whereas the best fit to the \(^{12}\text{C}\) spectrum was achieved by an 8\% reduction in the core radius. Anyway, the properties of the ground state do not change much by this adjustment: the s-wave content is 90\%, and the rms distance from the core is 6.93 fm. From the coupled channels calculations we can also extract the widths of continuum resonances. The result for the 5/2\(^+\) state is a width of 157 keV, which is somewhat larger than the measured width of 100 \pm 20 keV [17]. This can be compared to a single-particle width of 230 keV for a \( d_{5/2} \) neutron scattered off an equivalent spherical core, with \( r_0 = 1.392 \) fm and a potential depth adjusted to reproduce the observed resonance energy. The reduction of the width due to coupled channels effects is a factor of 0.68 for this state, which is close to the spectroscopic factor of 0.668 predicted by shell model calculations [22].

IV. CONCLUSIONS

We have studied the low-lying positive parity states in \(^{11}\text{Be}\) and \(^{13}\text{C}\) by solving the coupled channels equations for a neutron interacting with a deformed core. Critical quantities for the neutron-core interaction include the strength of the spin-orbit interaction and the radius parameter. They have been determined from a calibration to the observed spectrum of \(^{17}\text{O}\) and to measured rms radii. The deformation of the cores has been determined from measured \( B(E2) \) values.

Our model calculations show that the characteristic and qualitatively different features of the positive parity spectra for \(^{11}\text{Be}\) and \(^{13}\text{C}\) are closely related to a prolate deformation of the \(^{10}\text{Be}\) core and an oblate deformation of \(^{12}\text{C}\). The quantitative agreement with measured energy levels is similar to that obtained from shell-model calculations, and the decomposition of wave functions for specific states into single-particle s and d waves is also fairly consistent with shell-model predictions. The observed separation between the two lowest positive states in \(^{13}\text{C}\) is much better reproduced by using a slightly smaller core radius. Moreover, reducing the quadrupole moment of the 2\(^+\) state of \(^{10}\text{Be}\), as suggested by shell-model predictions, clearly improves the agreement with the measured \(^{11}\text{Be}\) spectrum.

Models, such as the one we have been using here, may also be very useful in studies of the structure of other nuclei which contain a single loosely bound or unbound valence nucleon. Examples of immediate interest to radioactive nuclei are \(^{10}\text{Li}\) and \(^{13}\text{Be}\). The (presently uncertain) structure of these nuclei is very important for a theoretical description of \(^{11}\text{Li}\) and \(^{14}\text{Be}\) in terms of a three-body model.

ACKNOWLEDGMENTS

Two of the authors (H.E. and H.S.) thank the staff at the Cyclotron Laboratory at Michigan State University for kind hospitality. We are grateful to Dieter Kurath for discussions and suggestions. This work was supported by the U.S. Department of Energy under Contract No. W-31-109-ENG-38, and in part by the National Science Foundation under Grant No. PHY-90-17077.

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