Valence pairing, core deformation and the development of two-neutron halos

F.M. Nunes\textsuperscript{a} *

\textsuperscript{a} NSCL and Department of Physics and Astronomy Michigan State University, East Lansing MI 48824 USA

We explore the evolution of the structure of the ground state of a nucleus with two valence nucleons as the system approaches the two particle threshold. We use a three-body model of core + n + n where the core is deformed and allowed to excite. We find that both NN correlations and correlations due to deformation/excitation of the core inhibit the formation of halos. Our results suggest that it is unlikely to find halo nuclei on the dripline of deformed nuclei.

1. Motivation

One of the most interesting results from experiments with Radioactive Beams was the discovery of the halo phenomenon \cite{halo_exp}. Nuclear Halos can develop when the system approaches a threshold and the relative motion is not constrained by a strong long range repulsive force. Then the tail of the wavefunction extends out well beyond the region of the nuclear interaction, generating an unusual outer region of low nuclear density. In the well known examples of $^6$He or $^{11}$Li the valence neutrons spend a large fraction of their time in an s- and/or p-wave motion relative to the core. In such systems, the neutrons are well decoupled from the core, which is often taken to be inert. Three body models \cite{three_body_models} have been very successful in describing a variety of properties of these Borromean systems. The decoupling of valence nucleons and core-nucleon degrees of freedom is not a good approximation when we move away from the dripline. In most cases, somewhere between the valley of stability and the dripline, the valence nucleons are somewhat correlated with the nucleons in the core\textsuperscript{2}. An effective way to take this correlation into account without solving the many body problem is providing the core with collective degrees of freedom. These could in principle be derived microscopically but can also be introduced phenomenologically. An extension of the three-body model (core+N+N) to include core excitation and deformation was performed and applied to $^{11}$Be, $^{12}$Be and $^{14}$Be \cite{extended_models}.

The observation of nuclear halos has been limited to light nuclei on the driplines (mainly the neutron dripline, although a couple of cases have been found on the proton dripline).

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\textsuperscript{2}If the valence neutron and the core are completely uncorrelated, the system’s wavefunction can be written as a single product of the core’s wavefunction and the valence particles’ wavefunction. In general this is not the case.
Toward heavier nuclei the neutron dripline is not well defined. One very interesting question is whether halos exist for heavier systems. This question has been partly addressed within Hartree-Fock-Bogolyubov (HFB) looking specifically into the issue of pairing [9]. Results show that, for a given isotope, by adding neutrons, pairing prevents the divergence of the rms radius and thus hinders the appearance of the halo state. More recently similar studies [10] show that, as the valence neutron binding energy artificially approaches zero, the contribution of the pair correlation is very low for single-particle s-waves, suggesting the appearance of the halo. Further work [11] shows explicitly that the halo phenomenon appears even in the presence of stronger many-body pair correlations. In any case, one should keep in mind that the single particle s-wave valence neutron is so decoupled from the mean field when approaching threshold that a HFB description may not adequate.

In heavier systems one often needs to consider deformation. The possibility of a deformed one-neutron halo [12] was studied within a Nilsson type model, but using a spheroidal basis. Results in [12] show that even with deformation, one-neutron halo states completely decoupled from the rest of the system can appear in the limit of low binding. Recent work [13] has looked into the effect of deformation within the single particle Nilsson model, without pairing. It is shown that the s-wave component becomes dominant as the binding energy of the system approaches zero, irrespective of deformation. In other words, deformation does not hinder the formation of halos. The p-wave orbitals were also studied in detail [14] although they are less likely to produce halo states. Note that in both [13,14] only the one-neutron halo case was considered. Here, we are interested in two-neutron halos.

The few-body models for halos [3] take into account the few body dynamics between the valence-halo nucleons and the core exactly, whilst oversimplifying the interaction with the core. The decoupling approximation of core and halo degrees of freedom is valid for low binding energy, consequently one can expect that the few-body models with core excitation are the adequate tool to explore the possibility of existence of halos in intermediate mass nuclei. The effect of deformation can be studied in a natural way, within the deformed core model developed in Ref. [6]. Pairing in the sense discussed in [10] does not have an easy translation into the few-body nomenclature. Some microscopic pairing is already included effectively through the phenomenological core-n interaction. The only pairing explicitly taken into account is that of the valence NN correlation through the S-wave component of the NN interaction. We will come back to this point at a later stage.

With the aim of exploring the possibility of two-neutron halo states in heavier nuclei, we look at the effects of pairing and deformation on the formation of halo states, using a three-body model with core deformation/excitation. In section 2, we briefly introduce the model, definitions, and some technical details. In section 3. the results are shown and compared with previous findings. Finally conclusions are drawn in section 4.

2. Technical considerations and some definitions

It is clear that a one-neutron halo state is most likely to appear if the occupancy of s-wave components is large, given that the centrifugal barrier will hinder the appearance of the tail. Thus a large occupancy of the $l = 0$ orbit, or at most $l = 1$, as the binding energy tends to zero, is a necessary condition for the appearance of the halo phenomenon.
dependence (see [6] for more details). If the coordinate set, in terms of known polynomials containing the angular and hyper-angular coordinates can be transformed into the hyperspherical coordinates: the hyper-radius \( \rho \) related to the size of the three-body system, and the hyper-angle \( \theta \) related to the correlations between the two Jacobi variables. The hyperspherical expansion represents the three-body wavefunction in a particular \( i \) Jacobi coordinate set, in terms of known polynomials containing the angular and hyper-angular dependence (see [4] for more details). If \( \psi_{i,J}(x_i, y_i) \) is the three-body wavefunction written in the \( i \) Jacobi coordinates, and \( (l_i, l_j) \) are the associated orbital angular momenta, then:

\[
\psi_{i,J}(x_i, y_i) = \rho_i \sum_{K_i}^{\frac{i}{2}} \chi_{\alpha_i K_i}^i J(\rho) \varphi_{K_i}^{l_i l_j}(\theta_i) ,
\]

with

\[
\varphi_{K_i}^{l_i l_j}(\theta_i) = N_{K_i}^{l_i l_j}(\sin \theta)^{l_i} (\cos \theta)^{l_j} P_{n_i}^{l_i + 1/2, l_j + 1/2}(\cos 2\theta_i) .
\]

The Jacobi polynomial \( P_{n_i}^{l_i + 1/2, l_j + 1/2} \), normalized by \( T_{n_i}^{l_i l_j} \), depends on a new quantum number, \( K_i \), the hyper-momentum. \( K_i \) is directly related to the order of the corresponding Jacobi polynomial \( K_i = l_i + l_j + 2n_i \) \((n_i=0,1,2,...)\). All other quantum numbers are represented by \( \alpha_i \), including internal spins and relative orbital angular momenta.

The introduction of the hyperspherical coordinates and the hyperspherical expansion mentioned above is extremely useful, since it reduces the three-body problem to coupled hyper-radial equations of the form [16]:

\[
(\frac{-\hbar^2}{2m} \frac{d^2}{d\rho^2} + \frac{\hbar^2(K_i + 3/2)(K_i + 5/2)}{(2m \rho^2)} - E)\chi_{\alpha_i K_i}^i (\rho) + \sum_{j=K_i} V_{\alpha_i K_i, \alpha_j K_j}^{ij} (\rho) \chi_{\alpha_j K_j}^j (\rho) = 0 ,
\]

where \( m \) is an arbitrary mass unit. For a detailed definition of the coupling potential \( V_{\alpha_i K_i, \alpha_j K_j}^{ij} (\rho) \) see [16]. Eq. 3 shows that the centrifugal barrier for two valence neutrons depends on the hyper-momentum, which in turn relates to the sum of the relative angular momenta between the three bodies. For two-neutron halos to occur this centrifugal barrier needs to be minimal, i.e. the occupancy of the K=0 component needs to be large. In [4], it is stated that only the K=0 or K=1 components can give rise to a halo structure. For the

![Figure 1. Jacobi coordinates for the three-body problem.](image)
ground state of this system, there are no $K=1$ components. Thus, for our test case, the necessary condition for the appearance of a two-neutron halo is that the $K=0$ component should be larger than 50%. This will be the criterion followed in our work. Some are more familiar with the use of a divergent radius as a halo signature. It should be stressed that in the three-body case, $K=0$ is the only component that produces a divergent rms radius. Thus, the two conditions are closely related.

The hyperspherical transformation can be performed for any number $N_v$ of valence neutrons, and the resulting coupled hyper-radial equation will contain a centrifugal barrier similar to the one in Eq. 3 but incremented. For this reason it has been remarked before that one does not expect to find halos with $N_v > 2$. The conclusions to be drawn from our work are thus an upper limit to any system with a larger number of valence neutrons.

In the model derived in [6], excitation appears through the assumption of a rotational model for the core, with a deformation $\beta$. The effective interaction between the core-n is not central and contains higher multipoles which couple different core states. The strength of those couplings obviously depends on the deformation parameter $\beta$ which can be estimated from electric transition data between the core’s ground state and the relevant excited state. The particular example studied in [6] takes into account the strong E2 transition between the core $0^+$ ground state and the $2^+$ excited state, through a quadrupole deformation $\beta_2$. Calculations can be easily generalized to include any other transition within a collective model (for example in [17] the model for $^{16}$O core also included octupole deformation $\beta_3$ based on the large E3 connecting the ground state $0^+$ with the first excited $3^-$ state).

In the three-body core+n+n model one can define several relative orbital angular momenta. To avoid confusion, we will always use lower case $s$, $p$, $d$, etc for the core-nucleon relative angular momentum and capital letters $S$, $P$, $D$ for the NN partial waves.

As mentioned before, pairing is partly embedded in the effective core-n interaction. Relating mean field pairing with the NN correlations seen in few-body problems is by no means trivial. In some sense, the mean field pairing has more than the few-body NN correlations we include. While in mean field pairing, all pairs contribute, including those within the core, in the few-body case, only the valence pair contributes explicitly, and any other pairing contribution appears effectively in the fitted core-N interaction. On the other hand, pairing in BCS is by definition the correlation energy associated with the existence of the bound cooper pair in the medium. In HFB it is clearly separated from the total mean field. It is standard practice to parameterize it as a delta function in the S-wave NN channel, and only very recently have finite range effects been included [18]. In few-body models, the free NN interaction is included explicitly: it is finite range, L-dependent, with a tensor part, such that it reproduces the low energy NN phase shifts. What we can try to assess within the three-body model, is the importance of the correlation between the two valence neutrons, by switching off different parts of the NN interaction. It is clear that we need to go beyond the few-body formalism to make accurate predictions for heavy dripline nuclei, but we are still learning how to generate halo phenomena in a microscopic mean field type model. It is thus important to try to make the link between the mean field and the few-body languages.
3. Results

3.1. Fixed deformation

Starting with the three-body model for $^{12}$Be [6] we performed a series of calculations to explore the possible development of the two-neutron halo when the system is forced artificially to approach threshold. We allow the core to exist in its ground state and its first $2^+$ excited state at $E_x = 3.368$ MeV. In [6] the effective n-core interaction corresponding to $\beta_2 = 0.67$ is modeled with a Woods-Saxon plus spin-orbit term:

$$V_{n-core}^b(r) = V_{ws}(r) + (\vec{l} \cdot \vec{s}) V_{so}(r). \tag{4}$$

The Woods-Saxon term depends on the orientation/excitation of the core, and has the standard form:

$$V_{ws}(r, \theta, \phi) = V_{ws} \left[ 1 + e^{(r-R_{ws}(\theta, \phi)) / a_{ws}} \right], \quad R(\theta, \phi) = R_{ws}(1 + \beta Y_{20}(\theta, \phi)). \tag{5}$$

The spin-orbit term is undeformed and defined as

$$(\vec{l} \cdot \vec{s}) V_{so}(r) = -\left( \frac{\hbar}{m\pi c} \right)^2 (2\vec{l} \cdot \vec{s}) \frac{V_{so}}{r} \frac{d}{dr} \left[ 1 + e^{(r-R_{so}) / a_{so}} \right]^{-1}. \tag{6}$$

The Woods-Saxon depth is parity dependent $V_{ws}(l = 0, 2) = -54.239$ MeV and $V_{ws}(l = 1) = -49.672$ MeV, the radius is $R_{ws} = 2.4883$ fm and the diffuseness is $a_{ws} = 0.65$ fm. The spin-orbit has the same radius and diffuseness as the Woods-Saxon part, and its strength is $V_{so} = -34.0$ MeV.

In this work, we force the system to move toward threshold by artificially decreasing the strength of the interaction $V_{n-core}^b(r) = \lambda V_{n-core}^{12}$. Smaller values of $\lambda$ will force $^{11}$Be to cross threshold, which in turn will provide smaller binding energies for the $^{12}$Be three-body system. We explore the behaviour of the ground state wavefunction of $^{12}$Be as its binding energy tends to zero. Note that, in our procedure, the spin-orbit force is scaled too. Throughout this work, we take the NN interaction between the two valence neutrons to be the GPT interaction [19] (the same as in [6]). This interaction, built from the sum of three gaussians, contains central S-, P- and D-terms, as well as a spin-orbit and a tensor force.

Calculations for the ground state $0^+$ were performed in a truncated subspace and checked for convergence. The main concern had to do with $K_{max}$, the maximum value of hyper-momentum included in expansion [6]. The smaller the two-neutron binding energy of the $^{12}$Be system, the larger the required $K_{max}$. As seen before [6], the probabilities associated with the most significant parts of the wavefunctions converge faster than the binding energy. Due to computational limitations, we could only obtain convergence for states with $S_{2n} \geq 0.08$ MeV, where $S_{2n}$ is the two-neutron binding energy.

Fig. 2 shows the fraction of the ground state three-body wavefunction that exists in the K=0 state. We consider four distinct situations: a) the realistic case where both the deformation and the NN interaction are included (solid line); b) considering core deformation but switching off the NN interaction (dotted line); c) including the NN interaction but keeping $\beta_2 = 0$ (dashed line); and d) the most simple case, where there is no NN interaction and no core excitation/reorientation (dot-dashed line). For the $\beta_2 = 0$
results, the starting point for the core-n interaction was refitted to obtain realistic $1/2^+$ and $1/2^-$ energies for the $^{11}$Be system.

Expectedly, in d), as the system approaches threshold, it favours the K=0 component such that the probability of finding K=0 tends to $\lim_{S_{2n} \to 0} P(K = 0) \approx 0.8$. Introducing the correlation between the two valence neutrons reduces this to $\lim_{S_{2n} \to 0} P(K = 0) \approx 0.6$. According to the criterion in [1], in both cases the K=0 component is larger than 50% and thus the system would be considered a halo in the low binding limit. However, when core excitation comes into the picture, the K=0 component saturates at much lower values $\lim_{S_{2n} \to 0} P(K = 0) \approx 0.4$ suggesting that in this situation no halo would develop. When we take both NN GPT interaction and deformation, $\lim_{S_{2n} \to 0} P(K = 0) \approx 0.3$. When introducing deformation, the excitation (or reorientation) coupling mixes in higher angular momentum components (in this case mainly d-waves) reducing the probability of generating long halo tails in the wavefunction. When the two neutrons are strongly bound to the core, the core+N+N model is not a good approximation, consequently we do not discuss the results for $S_{2n}$ larger than $\approx 4$ MeV. We looked explicitly at the sum of all core excited components as the binding approaches zero and found that these remain finite ($> 20\%$).

All four curves in Fig. 2 have a similar dependence on the binding energy. We find that the K=0 occupancy near threshold can be parameterized by the three parameter polynomial expression

$$\text{Prob}(K = 0) = \frac{P_1}{(P_2 + \log(S_{2n}))^{P_3}}.$$ (7)
We also checked the separate contributions of the NN interaction. As mentioned before, the GPT interaction [19] contains a central term for S-, P- and D-waves, a spin-orbit term and a tensor part. Compared to results where the NN interaction was switched off, it is mainly the tensor part that produces the reduction from $d \to c$ observed in Fig. 2.

We now come back to the issue of translating these results into the pairing language used in HFB [10,11], and other mean field approaches. Since we found that the tensor part of the NN interaction is the main contributor to the hindrance of the halo, the mean field pairing force, which contains S-waves only, would not be able to reproduce the same effect. This issue needs to be carefully addressed in future work.

Often, the dineutron model is used to describe reactions of systems with two loosely bound neutrons. If there is a strong correlation between the two valence neutrons, such that a dineutron could be formed, then a halo in the two body sense (i.e. $l_{y2} = 0$ from Fig. 1) could appear: the dineutron halo (this is most likely the case of $^6$He where $\approx 85\%$ of the wavefunction is in the $l_{y2} = 0$). We have compared the $l_{y2} = 0$ components of the ground state wavefunction when including the GPT NN interaction with that resulting from switching off the NN interaction. The GPT interaction enhances the $l_{y2} = 0$ component by $\approx 3\%$ and does not change the energy behaviour significantly. We conclude that, in our simulation of the dripline, the realistic NN correlation is not enough to generate a dineutron halo.

Information identical to Fig. 2 could be expressed through the evolution of the occupation of the $s_{1/2}$ orbital near threshold (where both $l_x = 0$ and $l_y = 0$). Here again, we find that the NN interaction reduces somewhat the occupancy of the orbital, and this reduc-
tion is accentuated when including the core deformation. Essentially, core deformation mixes in many other components of higher angular momentum, reducing the occupation of the s-wave orbitals.

In [1] a sufficient condition for a halo is given in terms of the rms of the hyper-radius. One needs to define a typical hyper-radius scale associated with the two body forbidden regions, \( \rho_0 \) as in Eq. (7) of [1]. In the \(^{12}\)Be example, the relevant quantities are the radius for the \(^{10}\)Be-n interaction and the scattering length for the nn interaction. Then the scale becomes \( \rho_0^2 = 53 \) fm\(^2\). The condition for a halo is now \( \langle \rho^2 \rangle > \rho_0^2 > 2 \). In Fig. 3 we plot this ratio as a function of binding energy for the four cases presented above. A typical halo develops naturally when there are no core-n or nn correlations. It is clearly seen that both core excitation/deformation and the NN interaction hinder the development of the halo.

3.2. Other ways of reaching the dripline

There are several issues associated with this simplified prescription of reaching the dripline. Probably, nature is not kind enough to preserve the same parameters in Eq. (4), when moving away from the valley of stability. For instance, one expects the deformation of the core to vary throughout the nuclear chart, when adding neutrons to reach the corresponding dripline nucleus. For this reason, we have repeated the above calculations, starting with the same n-core interaction, but varying the binding energy now through the deformation parameter \( \beta_2 = 0.05 \rightarrow 1 \) and found that the qualitative features discussed in the previous section remained unchanged.

Moreover, we have explored a combination of possible initial compositions of the subsystem \(^{11}\)Be=\(^{10}\)Be+n’. We have tried other geometries for the n-core interactions (\( R_{ws} \) and \( a_{ws} \)) which produce a starting \(^{12}\)Be’ with different ground state dominant components, within the same model space. We also tried variations on the deformation parameter. Nowhere in the explored parameter space did we find the possibility of a two-neutron halo developing with the inclusion of NN and n-core correlations.

3.3. Heavier systems

In the deformed nuclear region of intermediate mass, the competing shells are no longer \( 2s_{1/2}, 1d_{5/2} \) and \( 1p_{1/2} \). One possibility among many is the example explored in [10] where \( 3s_{1/2}, 1g_{7/2} \) and \( 2d_{5/2} \) play a role. Ideally we would have repeated the calculations for the \( 3s_{1/2} \) and neighboring shells. The number of forbidden states as well as the number of channels in our model space would drastically increase. Then, the calculations with core excitation would no longer be feasible. Nevertheless, the larger partial waves, if anything, will only enhance the findings for the case discussed above. It is the recoil of the heavy core that will be smaller than for \( A=10 \), which may reduce the impact of the core couplings. Also the typical deformation parameter is smaller than \( \beta_2 = 0.67 \). We have thus repeated the calculations by artificially increasing the mass of the core to \( A=100 \) whilst keeping the same shell structure. We take this estimate to be an upper limit for the existence of a halo in this region.

We refit the n-core interaction to produce a ground state at around \( S_{2n} = 4 \) MeV, the \( 1/2^+ \) and \( 1/2^- \) level ordering for the n-core subsystem, using \( \beta_2 = 0.3 \), more adequate for heavier systems. The resulting ground state wavefunction has a configuration similar to \(^{12}\)Be; mainly an admixture of \( 2s_{1/2}, 1d_{5/2} \) and \( 1p_{1/2} \) with a significant amount of
core excitation. We then reduce the overall strength of the n-core interaction to simulate the proximity of the dripline. The separate effects of the NN interaction and core deformation are shown in Fig. 4. Expectedly the role of deformation is reduced compared to section 3.1. The effect of the NN interaction alone is now larger than the effect of deformation. Interestingly, the calculation including both, the NN interaction and core deformation/excitation, is at the border line \( \lim_{S_{2n}\to 0} P(K = 0) \approx 0.5 \).

We also checked whether the NN interaction is sufficient to form a 'dineutron'+core system as then one may obtain a halo system in the two body sense. The dineutron component with s-motion relative to the core, does increase to 68\% but throughout the simulated path toward the dripline the average distance between the two valence neutrons is increasing and is always larger than the average distance between the neutrons and the core. Consequently a dineutron picture does not make sense.

4. Conclusions

We have explored the configuration of the ground state wavefunction of the three-body nuclear system when approaching threshold. The aim of the work was to determine whether core deformation and/or pairing of the valence nucleons would hinder the appearance of the two-neutron halo phenomenon. The three-body model with core excitation is most adequate to explore these physical aspects explicitly. A variety of three-body calculations based on the \(^{12}\text{Be}\) model with core excitation were performed. Our results show that both the NN tensor interaction, which goes beyond the usual pairing in HFB,
and the couplings due to core deformation can significantly reduce the probability of a three body halo developing when approaching the neutron dripline.

For this work, the rotor core model includes a \(0^+\) core g.s. and its first excited state \(2^+\). The addition of the \(2^+\) excited state has brought into the picture couplings to higher angular momentum: namely, the core-n system in its ground state contains not only the s-wave with the core in the g.s. but also a d-wave with the core in the \(2^+\) state. This is an essential feature for the disappearance of the halo phenomenon. Of course there may be situations where coupling to higher angular momentum is obtained just with reorientation effects or, on the other end, there may be particular cases where no additional angular momentum is added to the system even including the most important excited states of the core. However, in the general case, the core-n single particle s-state, which would develop into a halo state at threshold, will couple to higher angular momentum when including collective degrees of freedom of the core, hindering the appearance of the halo.

Our conclusions are based on the assumption of the three-body model with core deformation/excitation. This model, while of interest for qualitative features, is certainly not appropriate for quantitative predictions. Improvements on the description of the core can be obtained within AMD [20]. In order to predict the existence or non-existence of a heavy halo, one needs a step further: a fully antisymmetric self-consistent mean field model that includes both pairing and deformation to all orders [21]. In the near future there is a plan to explore the dripline around the deformed mass region, using the fully self-consistent microscopic mean field which includes both static pairing and quadrupole deformation (e.g. [22]).

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