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To cite this article: S Pittel *et al* 2013 *J. Phys.: Conf. Ser.* **445** 012031

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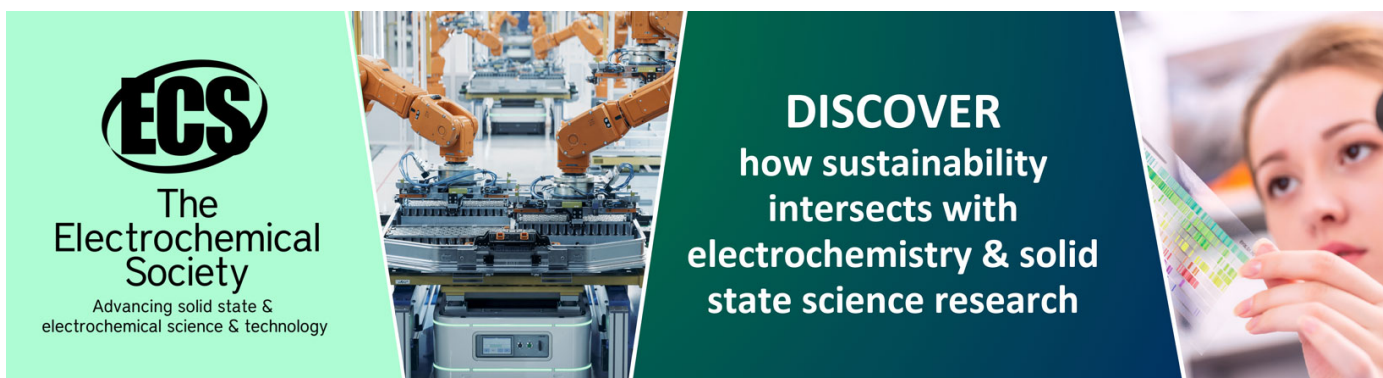
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Spherical to deformed shape transitions in the nucleon pair shell model

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Abstract. A study of the shape transition from spherical to axially deformed nuclei in the even *Ce* isotopes using the nucleon-pair approximation of the shell model is reported. As long as the structure of the dominant collective pairs is defined in a framework appropriate to deformed nuclei, the model is able to produce a shape transition. The resulting transition is too rapid, however, with nuclei that should be transitional being fairly well deformed. The possibility of using several pairs with each angular momentum to improve the description of the transitional region is discussed as is the possibility of using a larger single-particle space to better describe the moments of inertia in the deformed regime.

1. Introduction

A major goal of nuclear structure theory is to obtain a unified microscopic description of the variety of collective structures exhibited by atomic nuclei and the phase transitions linking them. A major advance was realized recently with the development of a unified microscopic theory of the Interacting Boson Model (IBM) [1], through the use of a procedure that maps the physics of density functionals onto the parameters of the model in the various collective domains [2].

We are interested in seeing whether these competing collective modes can be described using the Nucleon Pair Approximation (NPA) to the shell model [3, 4], a model that like the IBM is based on the introduction of collective pairs, but in which the collective pairs are not bosonized. In this work, we focus on nuclei that are known to undergo a shape transition from vibrational to rotational character, to see whether the NPA can describe such a shape transition and if so under what circumstances.

2. The Nucleon Pair Approximation

The NPA involves a truncation of the nuclear shell model in terms of collective pairs of alike nucleons. Originating in the Generalized Seniority (GS) and Broken Pair (BPA) approximations, it became a practical approach for the study of systems with a large number of pairs through the work of Chen [3], who obtained a set of recursive formulae that enabled the calculation of matrix elements for states involving many non-*S* pairs.

As a truncation of the shell model, the NPA inputs a single-particle space and an effective hamiltonian. It also inputs a set of collective pairs in terms of which the model space is defined.



This typically includes an $L = 0$ (S) pair and an $L = 2$ (D) pair, both for neutrons and protons, but can include additional pairs as well, either other S and D pairs or non- $S - D$ pairs.

The collective pairs have typically been chosen using the GS or BPA approach, with the S pairs obtained by a variational treatment in the GS=0 space and non- S pairs from a variational treatment in the GS=2 space. This approach is appropriate for semi-magic or near semi-magic nuclei, but not for nuclei with sufficiently large numbers of neutrons and protons where pn correlations need to be taken into account in defining the dominant pairs.

We have thus considered an alternative method for defining the dominant collective pairs for the NPA, based on the Hartree Fock Bogolyubov (HFB) approach, which dynamically incorporates the physics of the pn interaction.

For well-deformed nuclei, the dominant pairs can be obtained from an HFB treatment [5, 6]. For axially-symmetric nuclei, the HFB wave function in the canonical basis is given by

$$|\Phi\rangle = c \exp\left(\sum_{\tau=\nu,\pi} \Gamma_{\tau}^{\dagger}\right) |\tilde{0}\rangle, \quad (1)$$

where

$$\Gamma_{\tau}^{\dagger} = d_{\tau} \sum_{\alpha m > 0} \frac{v_{\alpha m}^{(\tau)}}{u_{\alpha m}^{(\tau)}} \tau_{\alpha m}^{\dagger} \tau_{\alpha - m}^{\dagger} \quad (2)$$

creates a coherent pair for particles of type τ , $|\tilde{0}\rangle$ denotes the doubly-magic core, and the v and u amplitudes are related to the eigenvalues of the density matrix in the canonical basis.

The pair creation operators $\Gamma_{\tau}^{\dagger}$ contain components with all allowed even angular momenta,

$$\Gamma_{\tau}^{\dagger} = \sum_L a_L^{(\tau)} \Gamma_{\tau}^{(L)\dagger}, \quad (3)$$

where the square of the amplitude $a_L^{(\tau)}$ indicates the importance of the correlated pair of type τ and angular momentum L in the ground band intrinsic state and the operator $\Gamma_{\tau}^{(L)\dagger}$ gives the structure of that correlated pair.

3. Calculations and Results

3.1. Computational ingredients

The calculations we report here are for the even-mass Ce isotopes from ^{142}Ce through ^{148}Ce . We assume a ^{132}Sn doubly-magic core and distribute the 8 valence protons over the orbits in the 50 – 82 shell and the 2 – 8 valence neutrons over those in the 82 – 126 shell.

Our hamiltonian is of the form

$$H = \sum_{\tau=\nu,\pi} \left(\sum_j \epsilon_{\tau j} \tau_j^{\dagger} \tau_j - \sum_{L=0,2} G_{\tau L} A_{\tau L}^{\dagger} \cdot \tilde{A}_{\tau L} \right) - \kappa Q_{\pi} \cdot Q_{\nu}. \quad (4)$$

It contains a single-particle energy term, multipole pairing interactions in the nn and pp channels and a separable quadrupole-quadrupole interaction in the pn channel.

The single-particle energies, extracted from the spectra of ^{133}Sb and ^{133}Sn , are listed in Table 1. The two-proton interaction parameters, extracted from the binding energy (BE) and 2_1^+ energy of ^{134}Te , are given by $G_{\pi 0} = -0.18$ MeV and $G_{\pi 2} = 0$. Those for the two-neutron interaction, extracted from the BE and 2_1^+ energy of ^{134}Sn , are given by $G_{\nu 0} = -0.13$ MeV and $G_{\nu 2} = -0.012$ MeV. Finally, the strength of the pn quadrupole interaction, chosen to optimally describe the 0_1^+ and 2_1^+ states of ^{136}Te , is given by $\kappa = -0.20$ MeV.

Table 1. Single-particle energies (in MeV) used in the calculations for the Ce isotopes described in the text, as obtained from the low-lying levels of ^{133}Sb and ^{133}Sn .

$l_{j\pi}$	$s_{1/2}$	$d_{3/2}$	$d_{5/2}$	$g_{7/2}$	$h_{11/2}$	
ϵ_{π}	2.990	2.708	0.962	0.000	2.793	
$l_{j\nu}$	$p_{1/2}$	$p_{3/2}$	$f_{5/2}$	$f_{7/2}$	$h_{9/2}$	$i_{13/2}$
ϵ_{ν}	1.656	0.854	2.005	0.000	1.561	1.800

Table 2. Ratios of experimental excitation energies of the Ce isotopes. $R_{4/2}$ gives the 4_1^+ to 2_1^+ ratio, and $R_{6/2}$ the 6_1^+ to 2_1^+ ratio. The last column gives the results in the rotational limit.

	^{142}Ce	^{144}Ce	^{146}Ce	^{148}Ce	$SU(3)$
$R_{4/2}$	1.90	2.36	2.58	2.87	3.33
$R_{6/2}$	2.72	4.15	4.52	5.32	7.00

3.2. Results and discussion

We first ask whether the chain of Ce isotopes indeed exhibits a transition from vibrational to rotational character. Table 2 shows the ratios of experimental excitation energies in the even Ce isotopes. $R_{4/2}$ gives the 4_1^+ to 2_1^+ ratio, $R_{6/2}$ the 6_1^+ to 2_1^+ ratio and the last column gives the $SU(3)$ results. ^{142}Ce , with 2 valence neutrons, has a vibrational character, with a $R_{4/2}$ ratio of 1.90, while ^{148}Ce with 8 valence neutrons has a fairly rotational character with $R_{4/2} = 2.87$. The transition from vibrational to rotational is fairly smooth. We should emphasize, however, that we are only considering the properties of the ground band in this discussion.

In Fig. 1, we show the deformation energies ($E_{\text{deformed}} - E_{\text{spherical}}$) from our HFB calculations of these nuclei. As expected, the deformation energy grows with increasing neutron number, with the energy gain reaching 1.27 MeV in ^{148}Ce . This is a bit small for a well-deformed nucleus, perhaps reflecting the fact that our model space does not include all the orbits that could contribute meaningfully. Nevertheless, the results suggest that the HFB calculations are producing the observed shape transition in the ground band.

Next we turn to our NPA results. In all calculations we included the lowest S pair, the lowest D pair and the lowest G pair (with $J^{\pi} = 4^+$), for neutrons and protons, allowing however only a single G pair for each type of particle. Fig. 2 compares several sets of NPA results with the experimental data. The spectra denoted BPA make use of the broken pair prescription for the S , D and G pairs. The spectra denoted HFB make use of the axially-symmetric HFB prescription. The spectra denoted COM include the S and D pairs from the two prescriptions in the same calculation, with their nonorthogonality taken into account. We explain later why we have included the latter results.

There are several points to note. First, the traditional broken pair (BPA) results are unable to describe the vibrational to rotational shape transition as we proceed through the chain. The HFB results, in contrast, give rise to a clear shape transition. While ^{142}Ce does not exhibit a rotational pattern, adding just two neutrons leads to a rotational spectrum, which becomes even more pronounced with the addition of further neutrons.

We can get a clearer understanding as to why it is important to use dynamically-determined collective pairs by looking at the ground state binding energies that emerged relative to ^{132}Sn . These results are shown in Fig. 3. When we use the BPA prescription for the collective pairs of the model we obtain much less binding than with the HFB pairs, which include crucial pn

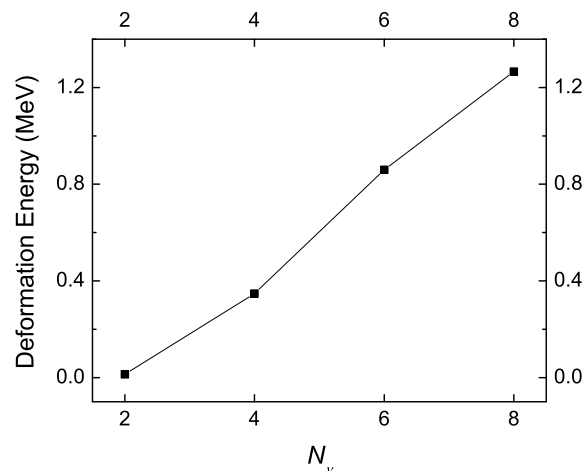


Figure 1. Deformation energies ($E_{\text{deformed}} - E_{\text{spherical}}$) from axially-symmetric HFB calculations for the even-mass *Ce* isotopes as a function of the number of valence neutrons N_v

correlation effects in their structure.

While the method with HFB pairs does produce a shape transition from vibrational to rotational nuclei, it produces it too rapidly. As is evident from Fig. 2, it yields a well-deformed spectrum for ^{144}Ce , which from Table 2 should be transitional. It is not surprising that we are unable to adequately describe transitional nuclei, since an axially-symmetric HFB treatment should not be very meaningful for such nuclei as it is unstable against zero-point fluctuations. A possible thought is to include more than one pair for each angular momentum in this regime. As a first step in this direction, we have carried out calculations in which we include both the HFB pairs and the BPA pairs, properly orthogonalized. Those are the results denoted COM in Fig. 2. The inclusion of a second *S* and *D* pair for each type of nucleon improves the description substantially, giving a better reproduction of the properties of *all* nuclei considered. However, the shape transition it produces is still too rapid. Nevertheless, we believe that including more than one pair with each angular momentum is a possible approach for future consideration, as it can be readily included in the analysis, but further thought as to which pairs to include is needed.

It is also worth noting that even in the most deformed nucleus considered, ^{148}Ce , the moment of inertia from our best NPA calculation, that denoted COM, is still too small and the spectrum is thus too spread-out. Interestingly the same result emerged in the first efforts to microscopically derive the IBM in deformed nuclei through a mapping of the fermionic density functional onto a corresponding one in the boson space. Recently it was shown that it is necessary to add a further term to the IBM hamiltonian of the form $\alpha J(J+1)$ to better reproduce the moment of inertia of the rotational systems that were studied [7]. The NPA seems to also have need for an additional contribution to the rotational moment of inertia, with perhaps a similar origin. It is not clear at this time, however, how to incorporate it in the NPA formalism. Minimally, we should probably first increase the size of our model space to include other orbitals thought to be important in this region, as this might already improve the moments of inertia.

4. Summary and closing remarks

In this paper, we have addressed the issue of whether the NPA is able to describe the transition from vibrational to rotational nuclei in real nuclear systems. We focused on the even-mass *Ce*

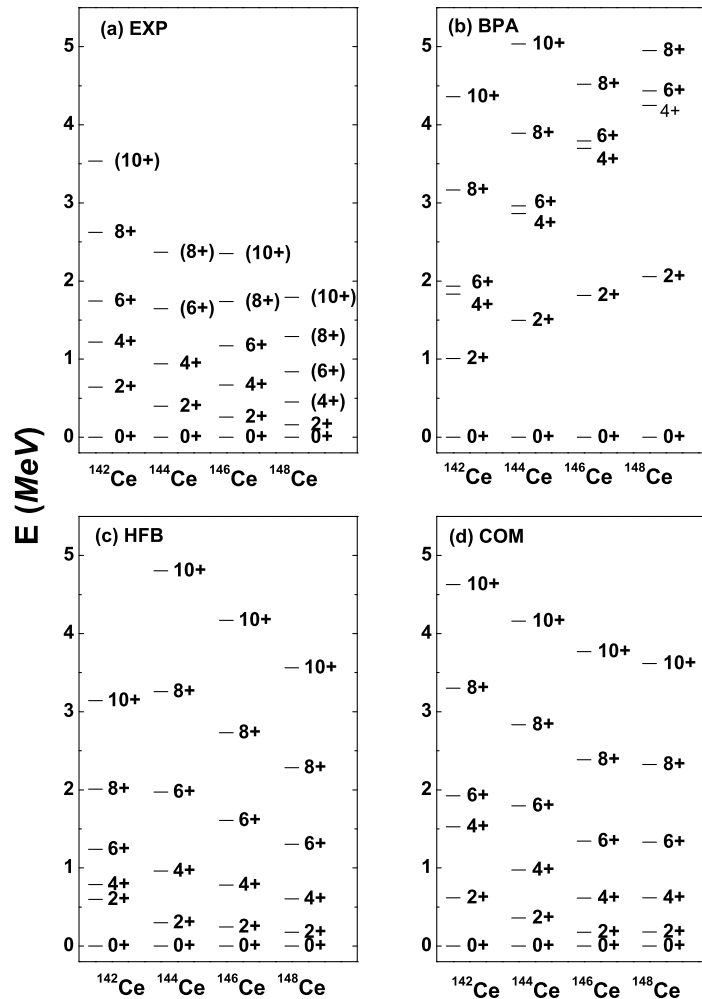


Figure 2. Comparison of the spectra calculated using the NPA for the even *Ce* isotopes (panels b-d) with the corresponding experimental spectra (panel a, denoted EXP). Panel (b) uses a model space based on BPA pairs, panel (c) uses a model space based on HFB pairs, and panel (d) (denoted COM) uses a direct sum of those used in panels (b) and (c).

isotopes, where such a shape transition seems to occur experimentally in the ground band. We see that when we use the traditional collective pairs derived from the broken pair approach, the model cannot describe the shape transition. In contrast, a description that uses collective pairs from the HFB approximation, which includes crucial *pn* correlation effects, is able to produce the observed shape transition. The shape transition produced is a bit too sharp, however, reflecting the fact that the correlated pairs produced in the HFB calculations are not adequate for the transitional region. Furthermore, the moments of inertia it produces are too small.

The difficulty in obtaining appropriate collective pairs to use in the NPA in the various nuclear regimes is reminiscent of the difficulty that arose in early efforts to microscopically derive the

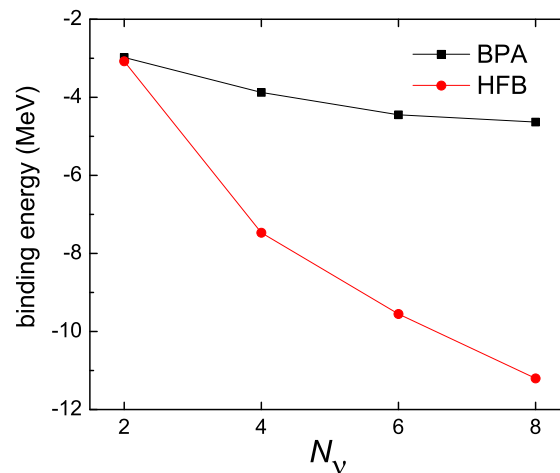


Figure 3. Comparison of the binding energies arising from the NPA calculations for the *Ce* isotopes described in the text, based on the use of BPA collective pairs and HFB collective pairs.

IBM for these different regimes. It is only recently with the advent of methods that map the fermionic collective surface onto an associated bosonic collective surface that it has been possible to obtain a unified microscopic derivation of the IBM. Since there is no analogous procedure for the NPA, we have suggested the possibility of using several collective pairs in those regimes in which a single HFB pair for each angular momentum is not sufficient. Further work to identify how to optimally obtain those pairs in transitional regimes is still needed, as is further thought on how to increase the moments of inertia that emerge within the NPA method for traditional shell-model spaces.

Acknowledgments

The work of S. P., Y. L. and G. F. was supported in part by the National Science Foundation under Grant No. PHY-0854873, and that of Y. M. Z., Y. L., and G. J. F. by the National Science Foundation of China under Grants No. 10975096 and 11145005, and by the Science & Technology Committee of Shanghai city under Grant No. 11DZ2260700.

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