$E2$ collectivity in shell-model calculations for odd-mass nuclei near ^{132}Sn

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Abstract. Shell-model calculations for ^{127,129}In and ^{129,131}Sb are presented, and interpreted in the context of the particle-core coupling scheme, wherein proton $g_{9/2}$ holes or $g_{7/2}$ particles are added to semimagic ^{128,130}Sn cores. These results indicate that the particle-core coupling scheme is appropriate for the Sb isotopes, whilst less so for the In isotopes. $B(E2)$ excitation strengths are also calculated, and show evidence of enhanced collectivity in both Sb isotopes, especially ^{131}Sb. This observation suggests that ^{131}Sb would be an excellent case for an experimental study seeking to investigate the early onset of collectivity near ^{132}Sn.

1 Introduction

The emergence of nuclear collectivity from the underlying nucleonic motion is a leading inquiry in nuclear structure research. The excited states of nuclei near double-magic shell closures are well described by the nuclear shell model. However, in regions away from shell closures, collective phenomena such as vibrations or rotations dominate the low-excitation behaviour of the nucleus. Understanding how and why the collective phenomena emerge from the underlying nucleon-nucleon interactions remains an open question. Typically, studies of emerging collectivity examine chains of even-even nuclei that transition from the single-particle toward collective limits. In this work, we present systematic shell-model calculations of odd-mass nuclei around ^{132}Sn and their semimagic even-even Sn cores, with a view to aiding experimental investigation into the question of emerging collectivity when a single proton (or hole) is added to a notional core.

The particle-core coupling scheme proposed by de-Shalit [1], provides a conceptual framework to relate odd-mass nuclei to their even-even neighbours. Several results follow from the assumption that the even-even core is largely unperturbed by the addition of a single extra nucleon. First, the odd-mass nucleus will have a "multiplet" of low-lying states corresponding to the allowed angular momentum couplings of the 2^+ "core" excitation with the single extra nucleon occupying the lowest allowed orbit. These states should be nearly degenerate in energy, and, even when the degeneracy is broken, the $(2I + 1)$ spin-weighted average of their energies should be equal to the energy of the first-excited 2^+ state of the core nucleus. Second, the sum of the $B(E2)$ excitation strengths from the ground- to multiplet-states should be equal to the $B(E2)$ value between the ground-state and first-excited 2^+ state in the core nucleus:

$$\sum B(E2\uparrow)_{\text{multiplet}} = B(E2; 0^+ \to 2^+)_{\text{core}}. \tag{1}$$

These predictions have proved remarkably reliable in many experimentally accessible nuclei adjacent to single shell-closures [2]; however in the vast majority of cases studied, the open shell of the semimagic core is near mid-shell. The sum rule is relatively untested near double shell closures. In recent work [3], the particle-core coupling scheme has been found to provide a useful framework to investigate the early indications of emerging collectivity.

The region around double-magic ^{132}Sn is well suited for investigations of emerging collectivity using the particle-core coupling scheme. ^{132}Sn has been shown to have a robust double shell closure, and the region is accessible at radioactive ion beam facilities. Moreover, the low-excitation proton shell-model orbitals are widely spaced, meaning that the low-excitation states of single-particle character in odd-Z nuclei can be well separated and relatively unmixed. Thus the particle-core multiplet members can potentially be rather pure, and the simple particle-core coupling model could be a valid approximation.

Recent experimental results on ^{129}Sb report enhanced $E2$ collectivity in comparison to a ^{128}Sn core [3]. The present work examines the particle-core coupling scenario from the shell-model perspective in greater detail in order to, first, scrutinize the applicability of the $E2$ sum

Table 1. Effective charges used in NuShellX calculations. $B(E2)$ strengths are for the $0^+_1 \to 2^+_1$ transition.

N	e_n	Experimental datum	Reference
78	0.80	$B(E2;^{128}\text{Sn}) = 0.080(5)$ e^{2}b^2	[4]
80	0.62	$B(E2;^{130}\text{Sn}) = 0.023(5)$ e^{2}b^2	[5]
Z	e_p	Experimental datum	Reference
51	1.7	$B(E2;^{134}\text{Te}) = 0.114(13)$ e^{2}b^2	[6, 7]
49	1.34	$T_{1/2}(8^+;^{130}\text{Cd}) = 239(17)$ ns	[8, 9]

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rule; and, second, identify cases where further experimenal studies are warranted. We present shell-model calculations of ^{129,131}Sb, and ^{127,129}In, which couple $g_{7/2}$ protons and $g_{9/2}$ proton holes to semimagic ^{128,130}Sn cores. Initially, we seek to establish whether the particle-core scheme is a good approximation by examining the $(2I+1)$ spin-weighted energy sums and dominant wavefunction components of the shell-model states, before turning to the $B(E2)$ predictions of the shell-model calculations.

2 Method

The shell-model program NuShellX [10] was used to run calculations for the nuclei studied. In the case of the Sb isotopes, the sn100pn interaction was used in the jj55pn model space. The model space has a ^{100}Sn core, with protons and neutrons in the $1g_{7/2}, 2d_{5/2}, 2d_{3/2}, 3s_{1/2}$, and $1h_{11/2}$ orbits. For the In isotopes, the jj45pna interaction was used in the jj45pn model space. The model space has a ^{78}Ni core, with neutrons in the $1g_{7/2}, 2d_{5/2}, 2d_{3/2}, 3s_{1/2}$, and $1h_{11/2}$ orbits, and protons in the $2p_{1/2}, 2p_{3/2}, 2f_{5/2}$, and $1g_{9/2}$ orbits. Both interactions are based on the CD-Bonn renormalised G matrix [11, 12].

Effective charges were chosen to reproduce experimental $B(E2)$ or lifetime data in the nearest singly-closed nucleus. Details of the effective charges adopted and relevant experimental data are shown in Table 1. Literature choices for the effective proton charge for the In isotopes range between $e_{\mathrm{p}} = 1.35$ [13] to $e_{\mathrm{p}} = 1.7$ [14–16]. A value of $e_{\mathrm{p}} = 1.34$ has been chosen for the present work based on the known lifetime of the $I^{\pi} = 8^{+}$, $E_x = 2130$ keV isomer in ^{130}Cd. However, the following discussion is not sensitive to the exact value of this effective charge.

3 Results and Discussion

Initially we seek to understand whether a multiplet of states that correspond to the 2^+_1 core excitation in the particle-core coupling scheme are predicted by the shell model. This is done in two ways: (i) comparing the spin-weighted energy sum of the multiplet candidates to the 2^+ energy of the Sn core, and (ii) examining the shell-model wavefunctions to establish if they are dominated by the $|\nu 2^+ \otimes \pi j\rangle$ configuration which corresponds to the particle-core multiplet excitation.

3.1 Identification of multiplet members

3.1.1 In isotopes

For the In isotopes, the single-proton hole occupies predominantly the $1g_{9/2}$ orbital. Hence the ground-states have spin $I^{\pi} = 9/2^+$ and there is a multiplet of $I^{\pi} = 5/2^+, 7/2^+, 9/2^+, 11/2^+$, and $13/2^+$ states at $\approx$ 1200 keV. The spin-weighted sum of energies for ^{127}In is 1298 keV and 1521 keV for ^{129}In, which compare with experimental (theoretical) core 2^+ energies of 1168 keV (1197 keV) for ^{128}Sn and 1221 keV (1381 keV) for ^{130}Sn. In both cases, the $7/2^+$ and $9/2^+$ states are $\sim$ 300 keV higher than the other multiplet states.

Table 2. Dominant wavefunctions components for In isotopes.

I^{π}_i	|Amplitude|^2 ^{127}In	|Amplitude|^2 ^{129}In	composition
$9/2^+_1$	0.46	0.56	$\|\nu 0^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_1$	0.34	0.26	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$5/2^+_1$	0.67	0.84	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$5/2^+_1$	0.12		$\|\nu 3^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$5/2^+_1$	0.12	0.08	$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_1$	0.32		$\|\nu 3^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_1$		0.42	$\|\nu 4^- \otimes \pi(p_{1/2})^{-1}\rangle$
$7/2^+_1$	0.28	0.22	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_1$	0.2		$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_1$		0.17	$\|\nu 1^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_2$	0.36	0.45	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_2$	0.18	0.41	$\|\nu 0^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_2$	0.11		$\|\nu 5^- \otimes \pi(p_{1/2})^{-1}\rangle$
$9/2^+_2$	0.1	0.09	$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$11/2^+_1$	0.51	0.53	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$11/2^+_1$	0.28	0.27	$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$13/2^+_1$	0.52	0.45	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$13/2^+_1$	0.18	0.18	$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$13/2^+_1$	0.08		$\|\nu 3^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$13/2^+_1$		0.13	$\|\nu 7^- \otimes \pi(p_{1/2})^{-1}\rangle$
$7/2^+_2$	0.24	0.4	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_2$	0.25		$\|\nu 1^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_2$		0.18	$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_2$	0.13		$\|\nu 4^- \otimes \pi(p_{1/2})^{-1}\rangle$
$7/2^+_2$	0.12		$\|\nu 3^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$7/2^+_2$		0.14	$\|\nu 5^- \otimes \pi(p_{3/2})^{-1}\rangle$
$7/2^+_2$		0.09	$\|\nu 3^- \otimes \pi(p_{1/2})^{-1}\rangle$
$7/2^+_2$		0.08	$\|\nu 6^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_3$	0.31	0.27	$\|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_3$	0.13		$\|\nu 4^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_3$	0.09		$\|\nu 5^- \otimes \pi(p_{1/2})^{-1}\rangle$
$9/2^+_3$	0.09		$\|\nu 3^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_3$	0.08	0.19	$\|\nu 0^+ \otimes \pi(g_{9/2})^{-1}\rangle$
$9/2^+_3$		0.33	$\|\nu 5^- \otimes \pi(p_{1/2})^{-1}\rangle$

An analysis of the dominant wavefunctions components present in the low lying states is shown in Table 2. Note that the ground-states are almost entirely mixed between $|\nu 0^+ \otimes \pi(g_{9/2})^{-1}\rangle$ and $|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$ configurations: i.e. what would be the "ground-state" and "multiplet" $g^{-1}_{9/2}$ states in the particle-core model. Moreover, the excited states cannot be characterized as pure multiplet configurations. Whilst the $|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$ configuration is often one of the leading components, there is also significant mixing with other dominant components. These other components consist of a variety of configurations, most having often other "core" excitations ($\nu 1^+, \nu 3^+, \nu 4^+$, etc.). This suggests that the applicability of the simple particle-core model to these isotopes will be limited.

Furthermore, the $|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$ configuration is strongly mixed beyond the multiplet. Both the $7/2^+_1$ and $7/2^+_2$ states have dominant $|\nu 2^+ \otimes \pi(g_{9/2})^{-1}\rangle$ contributions. The core $B(E2)$ strength must be fragmented over such states, making it more difficult to gather complete experimental information on the $B(E2)$ sum.

Table 3. Dominant wavefunction components for Sb isotopes.

I^π	$\lvert$Amplitude$\rvert^2$		composition
	^{129}Sb	^{131}Sb	
$7/2^+_1$	0.81	0.91	$\lvert\nu0^+ \otimes \pi g_{7/2}\rangle$
$7/2^+_1$	0.17	0.09	$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$5/2^+_1$	0.77	0.91	$\lvert\nu0^+ \otimes \pi d_{5/2}\rangle$
$5/2^+_1$	0.1		$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$3/2^+_1$	0.85	0.87	$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$3/2^+_1$	0.11	0.12	$\lvert\nu0^+ \otimes \pi d_{3/2}\rangle$
$9/2^+_1$	0.85	0.95	$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$9/2^+_1$	0.13		$\lvert\nu4^+ \otimes \pi g_{7/2}\rangle$
$11/2^+_1$	0.82	0.9	$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$11/2^+_1$	0.15	0.08	$\lvert\nu4^+ \otimes \pi g_{7/2}\rangle$
$5/2^+_2$	0.79	0.93	$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$7/2^+_2$	0.58	0.71	$\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$
$7/2^+_2$	0.25		$\lvert\nu4^+ \otimes \pi g_{7/2}\rangle$
$7/2^+_2$	0.12	0.21	$\lvert\nu0^+ \otimes \pi g_{7/2}\rangle$

3.1.2 Sb isotopes

For the Sb isotopes, the proton occupies the $1g_{7/2}$ orbital, and the ground-states are of spin $I^\pi = 7/2^+$. In this case, however, the $2d_{5/2}$ orbital is at reasonably low energy (< 1 MeV), and consequently a predominantly single-particle $d_{5/2}$ state with $I^\pi = 5/2^+$ is predicted at 937 keV and 954 keV in ^{129}Sb and ^{131}Sb, respectively. Above this state, a multiplet of states with $I^\pi = 3/2^+, 5/2^+, 7/2^+, 9/2^+$, and $11/2^+$ is predicted. The spin-weighted energy sums of these states are 1207 keV and 1369 keV, respectively. These spin-weighted energies are closer to those of the ^{128,130}Sn cores than the In isotopes.

Turning to the wavefunctions, Table 3 shows the dominant components for the Sb isotopes. It is clear that the particle-core scheme is much more applicable in this case. The ground states are almost pure $\lvert\nu0^+ \otimes \pi g_{7/2}\rangle$ configurations, and whilst the first-excited $5/2^+$ is dominated by the low-lying $\pi d_{5/2}$ orbital, it does not mix strongly with the "multiplet" $5/2^+_2$ state. Similarly, each multiplet state is dominated by the $\lvert\nu2^+ \otimes \pi g_{7/2}\rangle$ configuration, with no other strong contributions. Thus the particle-core model appears to be a good approximation for these nuclei, and the core $B(E2)$ strength can be expected to be fragmented almost exclusively amongst the multiplet members; the wavefunctions therefore suggest that the $E2$ sum rule should be valid. Experimental information on the total electric quadrupole excitation strength can test for any enhanced collectivity beyond the particle-core coupling scheme as a result of the extra proton.

Table 3 also shows that the multiplet assignments are more appropriate for ^{131}Sb than ^{129}Sb. The two $5/2^+$ configurations mix less, and the $\lvert\nu4^+ \otimes \pi g_{7/2}\rangle$ component which appears in the $9/2^+$, $11/2^+$, $7/2^+_2$ states, is less significant in ^{131}Sb than in ^{129}Sb. This outcome was surprising in that we expected the particle-core coupling scheme more likely to break down in proximity to the double shell closure.

Table 4. Calculated $B(E2)$ values for In isotopes. Core $B(E2)$ values are from Refs. [4, 5].

I^π_i	^{127}In E_x (keV)	^{127}In $B(E2\uparrow)$ (W.u.)	^{129}In E_x (MeV)	^{129}In $B(E2\uparrow)$ (W.u)
$5/2^+_1$	943	3.8	1470	1.1
$13/2^+_1$	1129	7.2	1325	2.1
$11/2^+_1$	1178	7.1	1295	2.4
$7/2^+_1$	1584	0.34	1974	0.000045
$9/2^+_2$	1663	0.20	1736	0.0061
$\sum B(E2\uparrow)$		18.6		5.6
$B(E2\uparrow)_{\rm core}$		20.9(13)		5.9(13)

Table 5. Calculated $B(E2)$ values for Sb isotopes. Core $B(E2)$ values are from Refs. [4, 5].

I^π_i	^{129}Sb E_x (keV)	^{129}Sb $B(E2\uparrow)$ (W.u.)	^{131}Sb E_x (MeV)	^{131}Sb $B(E2\uparrow)$ (W.u)
$5/2^+_1$	937	1.0	954	0.55
$3/2^+_1$	1079	9.1	1466	1.8
$11/2^+_1$	1091	4.0	1432	2.1
$9/2^+_1$	1173	6.9	1221	3.0
$5/2^+_2$	1245	0.64	1346	2.9
$7/2^+_2$	1449	1.7	1429	0.47
$\sum B(E2\uparrow)$		23.4		9.9
$B(E2\uparrow)_{\rm core}$		20.9(13)		5.9(13)

3.2 $B(E2)$ values

The calculated $B(E2)$ values for each of the isotopes are shown in Tables 4 and 5. In both Sb isotopes, enhancement of the $B(E2)$ strength is predicted relative to the sum rule (Eq. 1); ≈ 12% in ^{129}Sb, and ≈ 65% in ^{131}Sb. For the In isotopes it may superficially look like the sum rule is obeyed. However the above discussion of the wavefunctions shows that the states do not have the structure of a particle-core 2^+_1-coupled multiplet. Why this fragmentation of the odd-A wavefunctions occurs for the $\pi g_{9/2}$ hole whereas the $\pi g_{7/2}$ particle gives a structure closely resembling the $2^+ \otimes j$ multiplet is yet to be explored. It is reasonable to interpret the fragmentation of strength among many wavefunction components in the In isotopes as a step towards the development of collectivity, however the signal is less clear than in the Sb isotopes.

Returning to the case of the Sb isotopes, the enhancement of $B(E2)$ strength can be further understood by expressing the $B(E2)$ value as:

$$B(E2) = \frac{\langle J_f||E2||J_i\rangle^2}{2J_i+1} = \frac{(e_{\rm p}A_{\rm p} + e_{\rm n}A_{\rm n})^2}{2J_i+1}, \qquad (2)$$

where $A_{\rm p}$ ($A_{\rm n}$) is the reduced E2 matrix element for the protons (neutrons), divided by the effective charge. Hence the total $B(E2)$ strength comes from three components – a pure proton component ($B(E2)_{\rm p} = e_{\rm p}^2A_{\rm p}^2/(2J_i+1)$), a pure neutron component ($B(E2)_{\rm n} = e_{\rm n}^2A_{\rm n}^2/(2J_i+1)$), and a cross-term ($B(E2)_{\rm pn} = 2e_{\rm n}e_{\rm p}A_{\rm n}A_{\rm p}/(2J_i+1)$). Critically, when $e_{\rm n}A_{\rm n}$ and $e_{\rm p}A_{\rm p}$ have the same sign, this cross term is positive and can increase the total $B(E2)$ strength significantly. The proton, neutron, and cross-terms for each of the nuclei

Table 6. Proton and neutron components of $E2$ strength.

Isotope	$\sum B(E2)_{\mathrm{p}}$ (W.u.)	$\sum B(E2)_{\mathrm{n}}$ (W.u.)	$\sum B(E2)_{\mathrm{pn}}$ (W.u.)
^{127}In	0.53	14.1	4.0
^{129}Sb	1.7	18.2	3.4
^{129}In	0.57	2.9	2.1
^{131}Sb	1.3	5.5	3.1

studied are shown in Table 6. In both Sb isotopes, the neutron part is slightly smaller than that of the Sn core, and in the In cases this deficit is much more pronounced. This clearly shows that the excess strength (where present) is coming from the cross-term, i.e. the proton-neutron term. Notably the cross-term is positive for all isotopes studied.

The combination of $B(E2)$ predictions and wavefunction analysis shows that the simple particle-core model is not applicable for ^{127,129}In isotopes near doubly magic ^{132}Sn, though it is for mid-shell ^{113,115}In isotopes [2]. However, it seems to be a useful framework for ^{129,131}Sb. The microscopic origin of the difference of behaviour between the Sb and In isotopes is not yet clear. For future experimental studies, ^{131}Sb seems a promising candidate.

4 Conclusion

Shell-model calculations for the isotopes ^{127}In, ^{129}In, ^{129}Sb, and ^{131}Sb, have been interpreted in the framework of the particle-core coupling scheme with a view to investigate $E2$ collectivity. The calculated wavefunctions suggest that the particle-core coupling scheme is applicable to both Sb isotopes, more so to ^{131}Sb than ^{129}Sb. Moreover, ^{131}Sb also shows a more pronounced $E2$ enhancement over the partice-core sum rule, likely as a result of its proximity to the double-magic ^{132}Sn core. However, results indicate that in contrast, for the In isotopes, the particle-core "multiplet" configurations are highly fragmented over several excited states, so that the simplicity of the $E2$ sum rule is lost. ^{131}Sb looks to be a promising candidate for experimental Coulomb excitation studies that could help elucidate the emergence of quadrupole collectivity as protons and neutrons are added to doubly magic ^{132}Sn.

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