Enhanced Sensitivity of Nuclear Binding Energies to Collective Structure

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We have studied calculated collective contributions to nuclear binding and separation energies and find that there is a deeper and much more sensitive link to nuclear structure than previously recognized or expected, especially near midshell in medium mass and heavy nuclei. As a consequence, measured masses may help understand the structure of well-deformed nuclei (e.g., intrinsic excitations). Conversely, future structure calculations must consider their implications for binding energies.

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Nuclear masses and binding energies reflect the sum of all nucleonic interactions. Those same interactions lead to shell structure and residual interactions and, hence, to nuclear structure in all its various forms. Therefore, it is obvious that masses and nuclear structure should be related. We will show in this Letter, however, a much more highly amplified interrelation than previously expected, especially in heavy deformed nuclei. A plot of two-neutron separation energies, as shown in Fig. 1 [1], illustrates aspects of the connection of masses and structure. These S_{2n} values are the energies required to remove the last two neutrons from the nucleus. One sees a sudden drop in S_{2n} after the $N = 82$ major shell closure, reflecting the much lower binding of neutrons entering the next shell. Near $N = 90$, the extra binding as deformation sets in results in a flattening of S_{2n}. Aside from exceptions such as this, however, the general trend in S_{2n} values is a series of parallel, more or less straight, lines. Careful inspection of Fig. 1, though, does show gentle curvatures to these S_{2n} lines whereas the Weizsäcker mass formula [2], and other approaches [3], suggest a linear behavior. Therefore, it is likely that these curvatures have their origin in certain collective effects [3].

There have been a few attempts to calculate these contributions to S_{2n} in collective models, most notably the early interacting boson approximation (IBA) [4] model calculations of Sm isotopes [5], and in recent detailed studies [3,6,7] of several isotopic sequences. In particular, Ref. [6] analyzed transitional sequences of nuclei and noted that different fits, in roughly comparable agreement with the known data, differ significantly in binding and separation energies, concluding that it is important to treat binding energies and excitation spectra on an equal footing in the study of long chains of isotopes.

It is the purpose of the present Letter to demonstrate a highly magnified, heretofore unexpected, sensitivity of binding energies to structure, to identify a large class of nuclei where this occurs, to understand why the effects are so large in these nuclei, and to demonstrate that the sensitivity is such that ground state binding energies (BEs) can even be used to assess their structure and intrinsic excitations. We will see, for example, that alternate calculations yielding collective states in deformed nuclei at excitation energies ~1.3 MeV that differ in energy by only 200 keV, can lead to calculated separation energy differences of ~4 MeV. This has wide implications for future calculations of structure and for future mass measurements, especially now that high-precision mass measurements even far from stability are possible with advanced Penning traps and storage ring techniques [8].

This work should also be of interest in a wider context. The binding of complex many-body systems is of fundamental interest in many areas of science. Moreover, there is

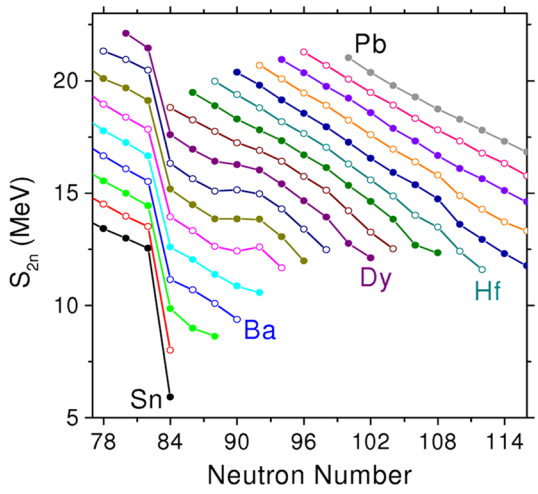

FIG. 1 (color online). Two-neutron separation energies showing the effects of shell closures, the sudden onset of deformation near $N = 90$, the general linear behavior of S_{2n} and curvatures resulting from collective effects near midshell.

an intimate relation in these systems between their stability and the emergence of coherence and collectivity. In quantum mechanical systems, binding often results primarily from interactions that mix eigenstates of some Hamiltonian, thereby lowering the energy of the collective configuration. It is precisely this kind of contribution to binding that we study here in a nuclear context. Finally, an understanding of the role of valence contributions to binding in nuclei is becoming of increasing importance in two key areas—the stability of the heaviest nuclei and of exotic nuclei far from stability.

The S_{2n} is given, in terms of BEs, by

$$S_{2n}(Z, N) = \mathrm{BE}(Z, N) - \mathrm{BE}(Z, N-2). \quad (1)$$

There are many factors affecting S_{2n}. It is convenient to split S_{2n} into two parts, one containing binding effects from the average nuclear potential and certain specific interactions, such as pairing, and another arising from collective correlations induced by residual interactions among (primarily) the valence nucleons. That is, we write

$$S_{2n}(Z, N) = S_{2n}(Z, N)_0 + S_{2n}(Z, N)_{\mathrm{coll}}, \quad (2)$$

where the collective component $S_{2n}(Z, N)_{\mathrm{coll}}$ is

$$S_{2n}(Z, N)_{\mathrm{coll}} = \mathrm{BE}(Z, N)_{\mathrm{coll}} - \mathrm{BE}(Z, N-2)_{\mathrm{coll}}. \quad (3)$$

We will calculate these collective contributions to the binding energies and to S_{2n} directly with the IBA model. The IBA model embodies a broad range of collective behavior arising from quadrupole correlations among the valence nucleons. This model is both a truncation of the shell model and a phenomenological collective model. It has a good track record as a phenomenological description of collective behavior and an inherent simplicity due to its economy of parameters. The main ansatz is to employ a basis space consisting only of pairs of nucleons coupled to angular momentum zero (s bosons) and two (d bosons), with simple interactions between them. We use the following common form of the IBA Hamiltonian [9–11]:

$$H = \epsilon \hat{n}_d - \kappa QQ = c\left[(1-\zeta)\hat{n}_d - \frac{\zeta}{4N_B} QQ\right], \quad (4)$$

where N_B is the boson number and

$$Q = (s^\dagger \tilde{d} + d^\dagger s) + \chi (d^\dagger \tilde{d})^{(2)}, \qquad \zeta = \frac{4N_B}{4N_B + (\epsilon/\kappa)}. \quad (5)$$

In the Hamiltonian in Eq. (4), the structure depends solely on two parameters, the ratio ϵ/κ and χ. The first term (with strength ϵ) is just the energy of the d bosons and, alone ($\kappa = 0$), drives the nucleus spherical, giving a vibrational spectrum typical of nuclei near closed shells, coinciding with the dynamical symmetry called $U(5)$. The second term (with strength κ) induces quadrupole collective effects. The quadrupole interaction, Q, acts between bosons and is expressed in terms of bilinear combinations of s and d boson operators that mix the pure s and d configuration basis states. For $\epsilon = 0$, one obtains deformed nuclei, whose structure is further specified by χ: $\chi = -\sqrt{7}/2 = -1.32$, gives the $SU(3)$ limit corresponding to a subset of axially symmetric nuclei, while $\chi = 0$ gives the $O(6)$ limit of a γ-soft rotor. Intermediate χ values give varying degrees of γ dependence. The symmetry triangle [12] showing these three limits is shown in Fig. 2. The shading will be explained below.

To avoid an infinite range of ϵ/κ, the second form is often used, where ζ ranges from 0 (vibrational nuclei) to 1 (deformed nuclei). In this form, a scale factor, c, has been factored out. In fitting actual nuclei, it is usually chosen to reproduce the observed energy of the first excited 2^+ state in order to put all calculated energies on the correct scale. In the triangle of Fig. 2, the parameter ζ corresponds to a radius vector from the $U(5)$ vertex and χ is the angle of this vector off the bottom leg.

The key point of this Letter focuses on the binding and separation energies calculated with the IBA. To illustrate the results, we study the Er isotopes and, in particular, will focus on the $N = 100$ isotope. We will make use of existing IBA parameter sets [7], scale ϵ and κ (equivalently, c) to reproduce the 2_1^+ energy and inspect the resulting binding energies. The results are shown in Fig. 3. The left panel shows some of the energy systematics in Er and the middle and right panels show the results for the collective components of the binding and separation energies.

For the nucleus ^{168}Er, there are two excited 0^+ states, at 1217 and 1422 keV, each of which could correspond to the lowest collective intrinsic 0^+ excitation in the IBA. Therefore, Ref. [7] carried out two separate fits, each reproducing the energy of one of these levels, and obtained alternate parameters sets. The differences stem both from

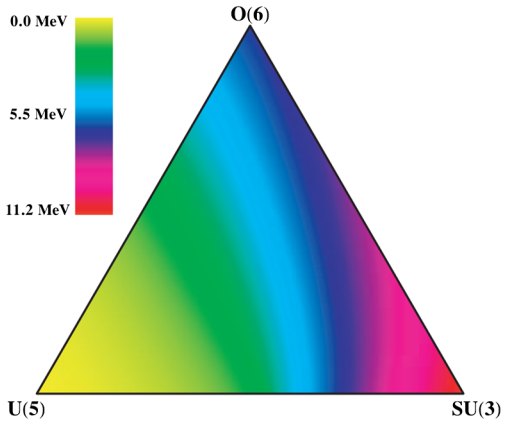

FIG. 2 (color online). The symmetry triangle of the IBA showing the three dynamical symmetries at the vertices. The IBA Hamiltonian of Eq. (4) spans all points in the triangle. The triangle shows the binding energies across the triangle calculated with Eq. (4) (with c constant) for $N_B = 16$ according to the legend at upper left.

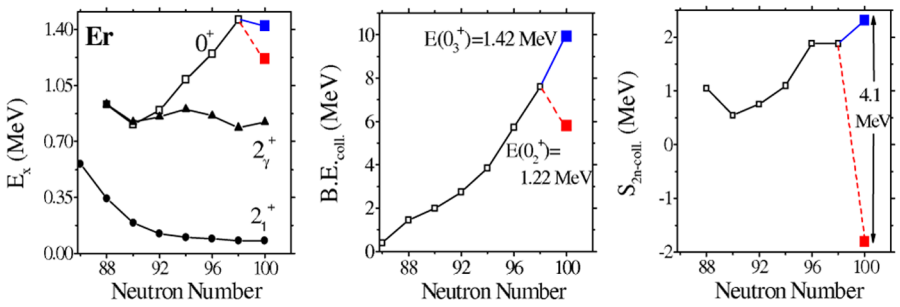

FIG. 3 (color online). (Left): Relevant energy systematics in Er isotopes. (Middle and Right): IBA calculations for collective components of the binding energies (taken as positive) and $S_{2n-\mathrm{coll}}$ values for Er. For $N = 100$, the two points (large solid squares) correspond to fits to two different 0^+ states.

the changes in ζ and χ and from the normalization factor c to reproduce the first 2^+ energy.

The results are startling. If one were to ask what effect changing the predicted energy of an excited 0^+ state by 200 keV in a collective model would have on the calculated binding energy, one would likely estimate at most a couple hundred keV. Instead, one sees a difference of over 4 MeV although the two parameter sets are very close in the triangle ($\zeta = 0.82$, $\chi = -0.36$ and $\zeta = 0.96$, $\chi = -0.25$).

The consequences of these results are significant. Away from closed shells and shape transitions, the S_{2n} trends are rather smooth: deviations from the trend lines for adjacent points are not more than a couple hundred keV or so. Hence a change in $S_{2n\text{-coll}}$ of 4 MeV is more than an order of magnitude outside of the normal systematic trends. Prior to these results, it would not have been thought possible to study the structure of intrinsic excitations a couple hundred keV apart by looking at ground state binding energies. Yet, Fig. 3 suggests that only the calculation corresponding to the higher 0^+ state (the higher $S_{2n\text{-coll}}$ value) gives a contribution to S_{2n} that could result in a smooth systematics like that in Fig. 1.

An obvious question is how such sensitivity arises and why it was not noticed before. Such an effect was hinted at in Ref. [6] by two different fits to ^{156}Gd but, in that case, the two parameter sets spanned nearly half the full range of allowed values in the symmetry triangle ($\zeta = 1$ and 0.54, and $\chi = -1.32$ and -0.6). In this Letter, we see larger effects for much smaller changes in parameters. Figure 4 analyzes this sensitivity. The left panel shows that the binding energy increases almost quadratically with N_B [3–5]. The middle and right panels show, for a given N_B, that the binding increases substantially as ζ approaches unity and as χ approaches -1.32, where one has the greatest mixing of $U(5)$ basis states and therefore the largest depression of the ground state energy. Thus, the effect we observe, centering on well-deformed nuclei with many valence nucleons, is nearly on the order of magnitude larger per change ζ and χ.

Figure 2 gives a broader perspective on the variation of collective binding effects in the IBA across the triangle. The maximum, and the rapid changes, in binding are evident near the $SU(3)$ corner. The sensitivity is much reduced for transitional nuclei, partly because their boson numbers are less (typically $\sim$10), and partly because their ζ values are nearer to 0.5 where Fig. 2 shows little variation in binding (and even less for $N_B \sim 10$).

We can ask if Er is an exceptional case. In some senses it is—it is the largest effect we have encountered. However, other isotopic sequences show similar effects. We show examples for Yb and Hf nuclei in Fig. 5. The Yb results

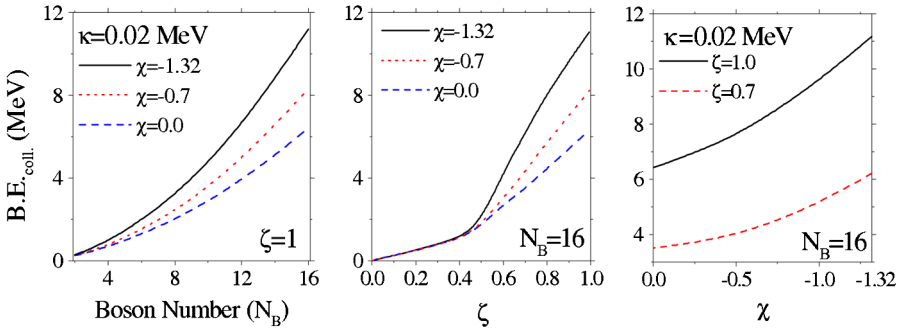

FIG. 4 (color online). Dependence of binding energies. (Left): IBA calculations of $\mathrm{BE}_{\mathrm{coll}}$ as a function of N_B, for $\zeta = 1$ (with $\kappa = 0.02$ MeV) and three χ values. (Middle): Similar except showing the dependence on ζ for constant $N_B = 16$ and for three choices of χ. (Right): Similar except as a function of χ for two ζ values in the deformed region.

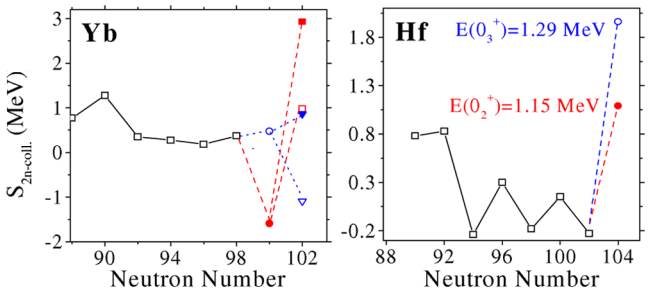

FIG. 5 (color online). Further examples of the effect shown in Fig. 3. (Left): IBA results for Yb using the ζ and χ values of Ref. [7] for $N = 100$ and 102 scaled to fit the experimental 2_1^+ energies. (Right): Similar for Hf isotopes.

show $S_{2n\text{-coll}}$ values for alternate fits [7] for $N = 100$ and 102 (giving four $S_{2n\text{-coll}}$ values for the latter). For Hf, only one fit was given [7] but, for illustration, we also fit the IBA to the next higher 0^+ state. In both cases, large differences in $S_{2n\text{-coll}}$ values occur—well beyond those allowed by the smooth behavior of Fig. 1.

Last, one needs to ask if these results are somehow an anomalous effect of having used a particular collective model, the IBA. We therefore also studied the geometric collective model (GCM) of Gneuss and Greiner [13]. Fits to an energy spectrum typical of well-deformed nuclei [$E(2_1^+) \sim 80$ keV, $E(2_\gamma^+) \sim 940$ keV, and 0^+ state energies of $E(0_2^+) = 1.21$ MeV and 1.40 MeV] give binding energies differing by over 2.3 MeV. Thus, a similar sensitivity characterizes the GCM for the same class of nuclei.

In summary, we have shown that calculated collective contributions to separation energies are far more sensitive to structure, especially in near-mid-shell deformed nuclei, than heretofore realized. This sensitivity is such that measured separation energies may even help understand the structure and intrinsic excitations in such nuclei. This perhaps suggests new strategies for modelling such nuclei. One might, for example, use the binding energy, $E(2_1^+)$ and, say, the γ-bandhead, to obtain the IBA parameters and then predict other intrinsic excitations (e.g., 0^+ states). It is premature to assess such approaches but they are currently being studied. In any case, it seems clear that collective model calculations should always consider the implications for separation energies—particular interpretations of excited modes might be supported or ruled out by such considerations—and, conversely, new measurements of masses may have consequences for structure not previously recognized.

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