Binding Energies of Isoscalar and Isovector Ground States of $N = Z$ Nuclei in the Interacting Boson Model

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An algebraic model is developed to calculate the $T = 0$ and $T = 1$ ground-state binding energies of $N = Z$ nuclei in the 28-50 shell which is currently the object of many experimental studies.

I Introduction

Nuclei at the proton (neutron) driplines constitute nowadays the most active research area of nuclear structure physics. With the advent of new radioactive beam facilities it is now possible to produce exotic nuclei that may have occurred naturally in the interior of exploding supernovas [1].

There are several theoretical approaches that reproduce the systematics of masses of nuclei and it is worthwhile to mention here two of them. The Extended Thomas-Fermi plus Strutinsky Integral [3] (ETFSI) is a high-speed approximation to the Hartree-Fock (HF) method with pairing correlations taken into account through BCS theory. In earlier versions a Wigner term was not included and this has been claimed to be the reason for the systematic calculated underbinding by about 2 MeV for even-even $N = Z$ nuclei [4]. This effect persists for $N = Z$ odd-odd systems and for $N = Z \pm 1$ odd-mass nuclei but with less prominence. The mass formula based on the Finite Range Droplet Model (FRDM) [5] starts from a sophisticated liquid drop mass formula to which microscopic corrections due to shell effects are added. Both approaches have comparable numbers of parameters (about 15) and make reliable predictions with impressive success. In the FRDM and also in a recent ETFSI calculation [6] a Wigner (correction) term is included that specifically deals with the peculiar behavior of binding energies of $N \approx Z$ nuclei and has a cusp-like behavior for $N = Z$. This treatment is effective for known masses but, as the correction is *ad hoc*, it has the drawback that an extrapolation to unknown nuclei can be dangerous. It is therefore of interest to develop models based on simple physical principles that can account for the behavior of nuclear masses at the $N \approx Z$ line.

Many models have been used over the past years to investigate the structure of heavier $N \approx Z$. We mention in particular recent applications of the Hartee-Fock-Bogolyubov (HFB) method that includes proton-neutron pairing correlations [7]. This approach is tailor-made for the treatment of $N \approx Z$ nuclei but has the drawback of the lack of particle-number projection. Shell-model calculations [8] are generally extremely successful in reproducing spectroscopic nuclear data but require large configuration space diagonalizations. This makes the shell model less appropriate when a calculation of many masses is required. An algebraic approach [9], which has affinities with the one presented here, utilizes the concept of dynamical supersymmetry for the calculation of the binding energies in the sd shell but does not go beyond it.

In this paper the Interacting Boson Model (IBM) [10] in its isospin invariant version is applied to proton-rich $N \approx Z$ nuclei. Reliable estimates are obtained of binding energies of $T = 0$ and $T = 1$ ground states in self-conjugate ($N = Z$) nuclei based on the concept of dynamical symmetry. The Hamiltonian proposed is relatively simple and con-

tains terms with an intuitively understandable significance. A particular ingredient is its treatment of the competition between isoscalar and isovector pairing.

II An IBM-4 "mass formula"

The Interacting Boson Model in its original version (IBM-1) [11] successfully describes collective aspects of nuclei through the use of s and d bosons which are thought to approximate pairs of valence nucleons coupled to angular momentum 0 and 2. No distinction is made between neutron and proton bosons. Whenever the difference between the neutron and proton fluids plays a role, one is forced to use more elaborate versions of the IBM. The neutron-proton interacting boson model, or IBM-2, was introduced mainly to provide a microscopic foundation to the model [12]. It uses as building blocks s and d bosons constructed from neutron-neutron (nn) and proton-proton (pp) pairs solely. In the third and fourth versions of IBM, IBM-3 and IBM-4, the isospin quantum number is introduced in a natural way. In IBM-3 the entire isospin triplet $T = 1$ is included, leading to nn, np, and pp pairs with $T_z = +1, 0, -1$ [13]. The IBM-4 considers both $T = 0$ and $T = 1$ pairs; the $T = 1$ bosons are assigned an intrinsic spin $S = 0$ while $T = 0$ bosons carry an intrinsic spin $S = 1$ [14]. A justification of this choice is that the two-particle isospin-spin combinations $(TS) = (10)$ and $(TS) = (01)$ are lowest in energy and that they give rise to an SU(4) algebra which is the boson equivalent of Wigner's supermultiplet algebra [15].

Recently, the IBM-4 was applied to the spectroscopy of exotic $N \approx Z$ nuclei in the $pf_{5/2}g_{9/2}$ shell [16]. In this approach the IBM-4 Hamiltonian is derived from a realistic shell-model Hamiltonian through a mapping carried out for $A = 58$ and 60 nuclei. The boson energies and the boson-boson interactions are thus derived microscopically and no parameter enters the calculation (since the shell-model interaction is considered as an input). This microscopically derived Hamiltonian gives good results in ^{62}Ga (when compared to the shell model) and predicts the energy spectra of heavier $N = Z$ nuclei (such ^{66}As and ^{70}Br). The approach is reasonably successful in obtaining a spectroscopy of low-spin states in $N \approx Z$ nuclei. It makes use, however, of a complicated Hamiltonian and, moreover, calculations beyond ^{70}Br seem difficult.

Prompted by these considerations, in particular the need for reliable binding energy predictions at the $N = Z$ line and the existence of a microscopically derived IBM-4 Hamiltonian, we propose here a simple calculation of these binding energies in the context of IBM-4. The calculation requires the diagonalization of matrices of very low dimension (of the order of half the number of bosons). Although it is not a mass formula as such (it is not a closed formula), the calculation can be readily carried out for any nucleus.

In previous work [17] one of us introduced an algebraic Hamiltonian (which can be regarded as the s-boson channel of the general IBM-4 Hamiltonian of Ref. [16]) with the specific aim to study the competition between the isovector and isoscalar pairing modes in self-conjugate nuclei. The model is formulated in terms of bosons which do not have an orbital structure but carry spin-isospin $(ts) = (01)$ or (10) and which will be denoted as $s^\dagger_{ts}$. They give rise to the symmetric representation of the spin-isopin algebra U(6). As an approximation to the full IBM-4 which includes s and d bosons, this can be justified for even-even and odd-odd $N = Z$ nuclei (the only ones considered here) where the favored U(6) representation is indeed symmetric [14]. It is also justifiable in $N \neq Z$ nuclei when they are even-even but not when they are odd-odd since in that case the favored U(6) representation of the full IBM-4 is non-symmetric [14].

The previous studies [16, 17] suggest that the relevant terms in a simple IBM-4 Hamiltonian must be taken from two different symmetry classifications:

$$\mathrm{U}(6) \supset \left\{ \begin{array}{c} \mathrm{SU}(4) \\ \mathrm{U}_T(3) \otimes \mathrm{U}_S(3) \end{array} \right\} \supset \mathrm{SO}_T(3) \otimes \mathrm{SO}_S(3). \quad (1)$$

A detailed analysis of the chains (1) is given in Ref. [18] where the definition of all Casimir operators can be found. The ones of interest for the calculation of binding energies of $N = Z$ nuclei are the following. First, the linear and quadratic Casimir operators of U(6) are included. The symmetric representations of U(6) is labeled by the total number of bosons, N; as a result, the U(6) Casimir operators take account of the bulk properties of the nucleus and lead to a smooth variation of the mass with particle number. The next two terms to be included are the quadratic Casimir operator of SU(4) and the linear Casimir operator of $\mathrm{U}_S(3)$. They are defined in Ref. [18]

$$\begin{aligned} \hat{C}_2[\mathrm{SU}(4)] &= 3(\hat{Y} \times \hat{Y})^{(00)} + \hat{S}^2 + \hat{T}^2, \\ \hat{C}_1[\mathrm{U}_S(3)] &= \hat{n}_{01}, \end{aligned} \quad (2)$$

with

$$\begin{aligned} \hat{Y}_{\mu\nu} &= (s^\dagger_{01} \times \tilde{s}_{10} + s^\dagger_{10} \times \tilde{s}_{01})^{(11)}_{\mu\nu}, \\ \hat{T}_\mu &= \sqrt{2}(s^\dagger_{10} \times \tilde{s}_{10})^{(10)}_{\mu 0}, \\ \hat{S}_\mu &= \sqrt{2}(s^\dagger_{01} \times \tilde{s}_{01})^{(01)}_{0\mu}, \\ \hat{n}_{10} &= (s^\dagger_{10} \times \tilde{s}_{10})^{(00)}_{00}, \\ \hat{n}_{01} &= (s^\dagger_{01} \times \tilde{s}_{01})^{(00)}_{00}, \end{aligned} \quad (3)$$

where the coupling is in spin and isospin, $\hat{Y}_{\mu\nu}$ is a Gamow-Teller-like operator which is a vector in spin and isospin, $\hat{T}_\mu$ and $\hat{S}_\mu$ are the total isospin and spin operators, and $\hat{n}_{01}$ and $\hat{n}_{10}$ are the number operators that count the isoscalar and isovector $(st) = (10)$ and (01) bosons. The operator $\hat{C}_2[\mathrm{SU}(4)]$ implies equal $T = 0$ and $T = 1$ interaction strengths while $\hat{C}_1[\mathrm{U}_S(3)]$ splits states with different spin S. In Ref. [17] the *quadratic* Casimir operator of $\mathrm{SU}_S(3)$ is considered while here the *linear* Casimir operator of $\mathrm{U}_S(3)$ is preferred. This choice is guided by a mapping argument: In Ref. [19] it is shown that the one-body spin-orbit term $v_{\mathrm{so}}\bar{l} \cdot \bar{s}$ of the nuclear mean-field potential is converted via a Dyson boson mapping into a combination of $\hat{n}_{01}$ and

$\hat{n}_{10} = \hat{N} - \hat{n}_{01}$ with coefficients that depend on $v_{\rm so}^2$. Also, an eventual asymmetry between the $T = 0$ and $T = 1$ pairing interaction can be represented in this way [19]. These important structural effects, i.e., the spin-orbit term and the difference between the isoscalar and isovector pairing interactions, can thus be represented algebraically. The final term to be included is the quadratic Casimir operator $\hat{C}_2[{\rm SO}_T(3)] = \hat{T}^2$ which is known to represent the nuclear symmetry and Wigner energies.

In summary, the following Hamiltonian is taken:

$$\begin{aligned}\hat{H} &= BE_0 + \alpha\hat{C}_1[{\rm U}(6)] + \beta\hat{C}_2[{\rm U}(6)] + \gamma\hat{C}_2[{\rm SU}(4)] \\ &\quad +\xi\hat{C}_1[{\rm U}_S(3)] + \eta\hat{C}_2[{\rm SO}_T(3)], \qquad (4)\end{aligned}$$

where BE_0 is the binding energy of the doubly magic core, specific for a given mass region. Note the absence from (4) of operators associated with ${\rm U}_T(3)$ and ${\rm SO}_S(3)$; these are not needed because, in the context of the simple model discussed here, their effect is equivalent to the corresponding operators of ${\rm U}_S(3)$ and ${\rm SO}_T(3)$.

All operators in (4) mutually commute, except for $\hat{C}_2[{\rm SU}(4)]$ and $\hat{C}_1[{\rm U}_S(3)]$ and hence the solution of $\hat{H}$ involves a numerical diagonalization which is most conveniently done in the second basis in (1), labeled as $|[N]\lambda_T T\times \lambda_S S\rangle$. These states are simultaneous eigenstates of $\hat{n}_{10}$ and $\hat{n}_{01}$ with eigenvalues λ_T and λ_S, respectively, which are the numbers of isovector and isoscalar bosons. The allowed values of λ_T and λ_S follow from the ${\rm U}(6) \supset {\rm U}_T(3) \times {\rm U}_S(3)$ branching rule. For a symmetric U(6) representation $[N]$ the allowed values are all those that satisfy $\lambda_T + \lambda_S = N$. Finally, the allowed values of T and S follow from the ${\rm SU}(3) \supset {\rm SO}(3)$ branching rule [20]: $T = \lambda_T, \lambda_T-2, \ldots, 1$ or 0 and $S = \lambda_S, \lambda_S - 2, \ldots, 1$ or 0.

The matrix elements of $\hat{C}_2[{\rm SU}(4)]$ in this basis can be calculated analytically [17] and closed expressions for the eigenvalues of the Hamiltonian (4) can be found in Ref. [22].

Summarizing our procedure for finding the binding energyof the lowest $T = 0$ and $T = 1$ states in an $N = Z$ nucleus:

1. Determine the number of bosons N outside the closed shell.

2. Construct the Hamiltonian matrix in the basis $|[N]\lambda_T T\times\lambda_S S\rangle$ with $\lambda_T = T, T+2, \ldots, (N-S-1)$ or $(N-S)$ and $\lambda_S = N - \lambda_T$. for different values of S. The dimension of this matrix is $\lfloor (N-S-T)/2 \rfloor + 1$ where $\lfloor x \rfloor$ is the largest integer smaller than or equal to x.

3. Diagonalize the Hamiltonian matrix. The largest eigenvalue gives the binding energy.

We have found that for $T = 0, 1$ states in $N = Z$ nuclei the largest binding energy is obtained for $S = T$ in even-even and for $S = T - 1$ in odd-odd nuclei.

III Results

A first application concerned to $N = Z$ nuclei in the sd shell, from ^{16}O to ^{40}Ca, where the experimental masses are well known [21], and can be found in Ref. [22]. Since reliable results were obtained we present here the calculations to the $28 - 50$ shell which is currently under experimental focus since there are few experimental data available up to now. Before carry on the calculations in the $28 - -50$ shell we sould remark that the fitting procedure is essentially the same as in the sd shell. Two fits for each half of the shell are need in order to avoid mid-shell effects and a Coulomb correction calculation is performed according to the prescription of Ref. [5].

We begin with a discussion of the first half of the 28–50 shell, for nuclei ranging from ^{58}Cu to ^{78}Y. The ground state of all these self-conjugate nuclei has $J^\pi = 0^+$, with either $T = 0$ in even-even or $T = 1$ in odd-odd nuclei, with the exception of ^{58}Cu which has a $(J^\pi, T) = (1^+, 0)$ ground state. Up to ^{64}Ge the masses are well known and can be taken from the compilation of Audi and Wapstra [21]. Of the heavier $N = Z$ nuclei, also the masses of ^{72}Kr and ^{74}Rb are listed by Audi and Wapstra. The masses of ^{66}As and ^{68}Se are available from a recent measurement [24] and that of ^{76}Sr from Ref. [25]. The latter experiment also gives a mass for ^{68}Se but since it is far off the systematics of Audi and Wapstra, the result from [24] is used. The mass of ^{70}Br is not known experimentally but as it is in the middle of a region of nuclei with measured masses close to the extrapolations of Audi and Wapstra, we have adopted their extrapolated value for ^{70}Br. The mass of ^{78}Y is not known and not included in the fit. The binding energies of the lowest $T = 1$ states in even-even $N = Z$ nuclei are derived from those of the isobaric analogues (also taken from Ref. [21]) after an appropriate Coulomb correction. The evolution of the splitting between $(J^\pi, T) = (0^+, 1)$ and $(J^\pi, T) = (1^+, 0)$ states in odd-odd nuclei is of particular interest as regards the question of $T = 0$ and $T = 1$ pairing and is currently the object of several experimental studies. The $(0^+, 1)$ state in ^{58}Cu lies 0.202 MeV above the $(1^+, 0)$ ground state [26]. This order is reversed in ^{62}Ga where the $(1^+, 0)$ state is 0.571 MeV above the $(0^+, 1)$ ground state [27]. The $BE(0^+, 1) - BE(1^+, 0)$ splitting then continues to rise to 0.837 MeV in ^{66}As [28]. A very recent experiment on ^{70}Br [29] has not observed a $(1^+, 0)$ level; the lowest observed $T = 0$ level (with $J^\pi = 3^+$) is at an excitation energy of 1.337 MeV. Similarly, the lowest $T = 0$ state in ^{74}Rb measured by Rudolph *et al.* [30] at an excitation energy of 1.006 MeV has $J = 3$ and the energy of the $J^\pi = 1^+$ state is unknown. With these data as input, the parameters in (4) can be adjusted through a fit procedure that minimizes the rms deviation in the binding energies of two states per nucleus (if known). The resulting parameters are shown in the line labeled '^{56}Ni to ^{78}Y' of Table and lead to an rms deviation of 0.396 MeV. In Fig. 1 the differences in energy between the $T = 1$ and $T = 0$ states are compared to the observed ones. One notes the good agreement that is

obtained which gives confidence in the energy splittings of 0.847, 1.037, and 1.214 MeV predicted in ^{70}Br, ^{74}Rb, and ^{78}Y, respectively. As already mentioned, the energy difference $BE(0^+,1) - BE(1^+,0)$ is not known experimentally in these isotopes. In the former two, ^{70}Br and ^{74}Rb, the energy difference with the lowest (known) $T = 0$ state is shown in Fig. 1.

Table 1. Core binding energies and parameters (in MeV) for the 28–50 shell.

Shell	BE_0	α	β	γ	ξ	η
^{56}Ni to ^{78}Y	607.2890	22.8140	0.1175	−0.0672	−1.9584	−0.9020
^{78}Y to ^{100}Sn	1172.9697	−28.4637	0.1183	−0.1877	−1.0450	−1.0248

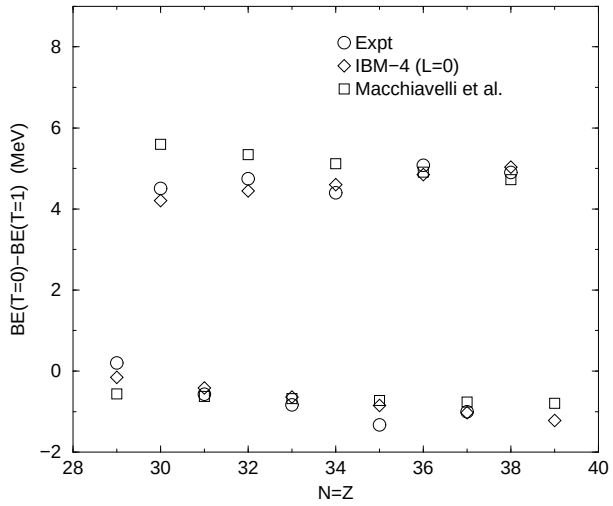

Figure 1. Calculated binding energy differences $BE(T = 0) - BE(T = 1)$ in $N = Z$ nuclei between ^{58}Cu to ^{78}Y for the parameters given in Table , compared with the experimental differences and those of Macchiavelli *et al.* [23].

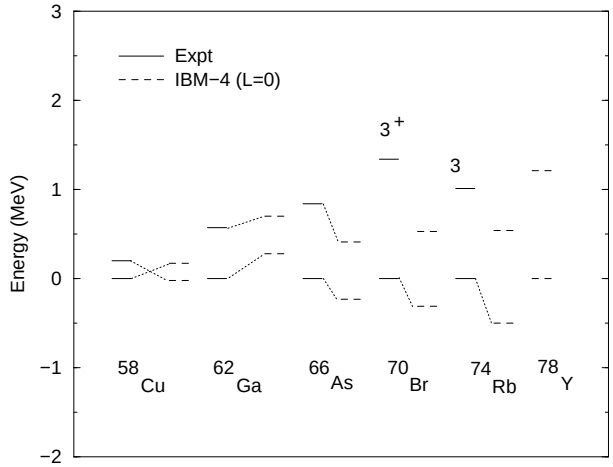

Figure 2. Experimental and calculated energies of $(1^+, T = 0)$ and $(0^+, T = 1)$ levels in odd-odd $N = Z$ from ^{58}Cu to ^{78}Y. In ^{70}Br, ^{74}Rb, and ^{78}Y the $(1^+, T = 0)$ levels are not known experimentally and in the former two nuclei the angular momentum of the lowest (known) $T = 0$ state is indicated.

To emphasize the point that these energy splittings result from a calculation of total binding energies, the odd-odd results are represented in a different way in Fig. 2. Note that this plot implies a comparison of *absolute* binding energies: for representation purposes the measured binding energy of the ground state of a particular nucleus is drawn at zero and other levels of that nucleus are given relative to that ground-state energy.

For the second half of the 28–50 shell the situation is more complicated since there are no data available. The core is ^{100}Sn with a ground-state mass measured in Ref. [31]. Since so little is known experimentally, we use the extrapolations from Audi and Wapstra [21] for the masses of even-even and odd-odd nuclei, complemented with the results for ^{78}Y from the fit to the first half of the 28–50 shell. The resulting parameters are shown in the line labeled '^{78}Y to ^{100}Sn' of Table . The predictions for the splitting between $T = 1$ and $T = 0$ states for the entire 28–50 shell are shown in Fig. 3. One notes a satisfactory agreement with the data, when available. The use of extrapolated data, however, should weaken the confidence in the predictions for the $BE(0^+,1) - BE(1^+,0)$ splitting in odd-odd nuclei.

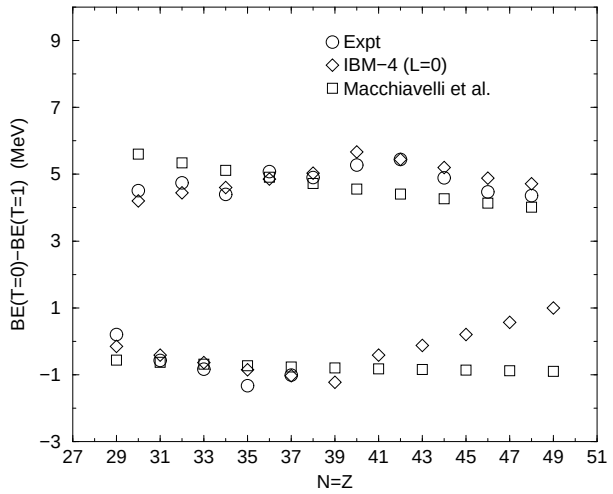

Figure 3. Binding energy differences $BE(T = 0) - BE(T = 1)$ for the entire 28–50 shell with parameters fitted separately for each half (see text for details). In the first half (up to ^{78}Y) 'Expt' refers to measured masses while in the second half it refers to the extrapolations of [21]. Also the results of Ref. [23] are shown.

IV Conclusions

A simple approach based on IBM-4 has been proposed to calculate the binding energies of the lowest $T = 0$ and $T = 1$ states of self-conjugate nuclei. It has linear and quadratic terms in the boson number that account for the smooth variation of the mass with particle number, supplemented with three contributions that have a clear physical meaning: an SU(4), a spin-orbit and a $\hat{T}^2$ term. It can be considered as a local "mass formula" that gives predictions of a specific interest to current experiments at the $N = Z$ line. As an application we considered nuclei from ^{56}Ni to ^{78}Y where predictions could be made for some of the heavier isotopes currently under study. Also the second half of the 28–50 shell was considered although there predictions are more questionable due to the lack of reliable data. The advantage with respect to previous IBM-4 work [16] is that the Hamiltonian used is much simpler and that only the $L = 0$ channel is considered. The numerical diagonalization then becomes trivial and the calculations can be performed, without much effort, for arbitrary numbers of bosons. This is much harder to achieve with the full version of IBM-4. On the down side it should be noted that, for odd-odd nuclei, this approach is restricted to $N = Z$ since odd-odd nuclei with $N \neq Z$ have a dominant non-symmetric U(6) representation which cannot be constructed from s bosons only. Also, deformation effects which are present with s *and* d bosons and which must be included through orbital operators are outside the scope of the simple approach presented here.

Acknowledgments

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