



Revista Mexicana de Física

ISSN: 0035-001X

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Sociedad Mexicana de Física A.C.

México

Van Isacker, P.

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Revista Mexicana de Física, vol. 55, núm. 2, 2009, pp. 66-70

Sociedad Mexicana de Física A.C.

Distrito Federal, México

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# Global calculations with the interacting Boson model

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Recibido el 3 de febrero de 2009; aceptado el 6 de marzo de 2009

The use of the interacting boson model is proposed for systematic calculations of nuclear properties for large regions of the nuclear chart, including exotic nuclei. In the simplest approach a constant hamiltonian is adopted for all nuclei and nuclear shape transitions are governed solely by total boson number or, equivalently, by total valence particle number. More sophisticated methods require a dependence of hamiltonian parameters on the fractional filling of the valence shell. It is also shown how to include in this framework the nuclear binding energy. The method is illustrated with the example of even–even nuclei in the rare-earth region with neutron number  $82 < N < 126$  and proton number  $50 < Z < 82$ .

*Keywords:* Nuclear masses; collective levels; interacting boson model.

Se propone el uso del modelo de bosones interactuantes para el cálculo sistemático de propiedades nucleares en un rango amplio de la mapa de los núcleos. En el procedimiento más simple se propone un Hamiltoniano constante para todos núcleos y las transiciones de forma de los núcleos es gobernada solo por el número total de bosones o, equivalentemente, por el número total de partículas. Métodos más sofisticados requieren un llenamiento fraccional de la capa de valencia. También se muestra como incluir en este marco la energía de amarre nuclear. El método se ilumina con un ejemplo de núcleos par-par en la región de las tierras raras con el número de neutrones de  $82 < N < 126$  y el número de protones de  $50 < Z < 82$ .

*Descriptores:* Masas nucleares; niveles colectivos; modelo de bosones interactuantes.

PACS: 21.10.Dr; 21.10.Re; 21.60.Ev

## 1. Introduction

Over the years many different approaches have been developed to calculate masses of atomic nuclei [1]. In particular, global approaches have been attempted in which a single formula or algorithm is used to reproduce as closely as possible all known nuclear masses. There exist now three standard global procedures which are complementary since each starts from a different *ansatz*: either the liquid-drop model [2], the mean-field approach [3] or the shell model [4]. The main goal of these attempts is to make mass extrapolations to regions away from stability, once parameters have been fixed from known nuclei.

These mass formula are limited to nuclear ground-state properties and have little to say about excited nuclear states. The latter is the realm of the interacting boson model (IBM) proposed by Arima and Iachello in 1975 [5]. Over the years many systematic calculations of nuclear spectral properties have been performed with this model [6]. Again, one of the purposes of these studies was the prediction of properties of nuclei away from stability based on parameter systematics established in stable ones. Surprisingly little, however, has been done with the IBM concerning binding energies. In one study Davis *et al.* [9] constructed a mass formula based on the concept of  $F$  spin in the IBM. In most cases only two-nucleon separation energies have been considered, such as in the more recent studies of García–Ramos *et al.* [7] and Fission *et al.* [8].

In this contribution a method is proposed to calculate simultaneously the absolute energies of the ground states and the excitation energies of the collective levels of all even–

even nuclei in a single major shell. It is based on a global formula for the macroscopic part of the nuclear binding energy while the remaining (shell + deformation) part is calculated with the IBM.

## 2. The interacting boson model

Let us begin with a brief reminder of some of the properties of the IBM. A full account of the model can be found in the monograph by Iachello and Arima [6]. The building blocks of the IBM are  $s$  and  $d$  bosons with angular momenta  $\ell = 0$  and  $\ell = 2$ . A nucleus is characterized by a constant total number of bosons  $N_b$  which equals half the number of valence nucleons (particles or holes, whichever is smaller). No distinction is made here between neutron and proton bosons, an approximation which is known as IBM-1.

Since the hamiltonian of IBM-1 conserves the total number of bosons, it can be written in terms of the 36 operators  $b_{\ell m}^\dagger b_{\ell' m'}$  where  $b_{\ell m}^\dagger$  ( $b_{\ell m}$ ) creates (annihilates) a boson with angular momentum  $\ell$  and  $z$  projection  $m$ . This set of 36 operators generates the Lie algebra  $U(6)$ . A hamiltonian that conserves the total number of bosons is of the generic form

$$\hat{H}_{\text{IBM}} = E_0 + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \dots, \quad (1)$$

where the index refers to the order of the interaction in the generators of  $U(6)$ . The first term  $E_0$  is a constant which represents the binding energy of the core. The second term is the one-body part

$$\hat{H}_1 = \epsilon_s [s^\dagger \times \tilde{s}]^{(0)} + \epsilon_d \sqrt{5} [d^\dagger \times \tilde{d}]^{(0)} \equiv \epsilon_s \hat{n}_s + \epsilon_d \hat{n}_d, \quad (2)$$

where  $\times$  refers to coupling in angular momentum (shown as an upperscript in round brackets),  $\tilde{b}_{\ell m} \equiv (-)^{\ell-m} b_{\ell, -m}$  and the coefficients  $\epsilon_s$  and  $\epsilon_d$  are the energies of the  $s$  and  $d$  bosons. The third term in the hamiltonian (1) represents the two-body interaction

$$\hat{H}_2 = \sum_{\ell_1 \leq \ell_2, \ell'_1 \leq \ell'_2, L} \tilde{v}_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L [[b_{\ell_1}^\dagger \times b_{\ell_2}^\dagger]^{(L)} \times [\tilde{b}_{\ell'_2} \times \tilde{b}_{\ell'_1}]^{(L)}]_0^{(0)}, \quad (3)$$

where the coefficients  $\tilde{v}$  are related to the interaction matrix elements between normalized two-boson states,

$$\begin{aligned} & \langle \ell_1 \ell_2; L | \hat{H}_2 | \ell'_1 \ell'_2; L \rangle \\ &= \sqrt{\frac{(1 + \delta_{\ell_1 \ell_2})(1 + \delta_{\ell'_1 \ell'_2})}{2L + 1}} \tilde{v}_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L \equiv v_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L. \end{aligned} \quad (4)$$

Since the bosons are necessarily symmetrically coupled, allowed two-boson states are  $s^2$  ( $L = 0$ ),  $sd$  ( $L = 2$ ) and  $d^2$  ( $L = 0, 2, 4$ ). Since for  $n$  states with a given angular momentum one has  $n(n+1)/2$  interactions, seven independent two-body interactions  $v$  are found: three for  $L = 0$ , three for  $L = 2$  and one for  $L = 4$ . This analysis can be extended to higher-order interactions. One may consider, for example, the three-body interactions  $\langle \ell_1 \ell_2 \ell_3; LM | \hat{H}_3 | \ell'_1 \ell'_2 \ell'_3; LM \rangle$ . The allowed three-boson states are  $s^3$  ( $L = 0$ ),  $s^2d$  ( $L = 2$ ),  $sd^2$  ( $L = 0, 2, 4$ ) and  $d^3$  ( $L = 0, 2, 3, 4, 6$ ), leading to  $6 + 6 + 1 + 3 + 1 = 17$  independent three-body interactions for  $L = 0, 2, 3, 4, 6$ , respectively.

At each order the interaction can be of two types depending on whether it contributes an equal amount to all states of a single nucleus (a ‘constant’ type I interaction) or not (a ‘variable’ type II interaction). It can be shown [10] that for fits of an excitation spectrum of a single nucleus there is a single one-boson energy of relevance, as well as five two-body and ten three-body interactions. If also binding energies are included in the analysis, an additional one-boson energy can be considered as well as two two-body and seven three-body interactions.

### 3. Spectra calculations with IBM

Energy spectra of many even–even nuclei have been calculated with the IBM-1. A commonly used parametrization of the hamiltonian in such calculations is limited to two-body interactions and is of the form

$$\hat{H}_{1+2} = \epsilon \hat{n}_d + \kappa \hat{Q} \cdot \hat{Q} + \kappa' \hat{L} \cdot \hat{L} + \kappa'' \hat{P}_+ \cdot \hat{P}_- + \lambda \hat{n}_d^2, \quad (5)$$

where  $\hat{n}_d$ ,  $\hat{P}_+$ ,  $\hat{L}$  and  $\hat{Q}$  are the  $d$ -boson number, boson pairing, angular momentum and quadrupole operators, as defined in Ref. 6. In the quadrupole operator

$$\hat{Q}_\mu \equiv [d^\dagger \times \tilde{s} + s^\dagger \times \tilde{d}]_\mu^{(2)} + \chi [d^\dagger \times \tilde{d}]_\mu^{(2)}, \quad (6)$$

appears  $\chi$  which together with  $\epsilon$ ,  $\kappa$ ,  $\kappa'$ ,  $\kappa''$  and  $\lambda$  constitutes the full set of six parameters needed to determine the spectrum of a single nucleus with a hamiltonian with up to two-body interactions. The dependence of excitation spectra on the parameter  $\chi$  is very weak however and in the following  $\chi$  is fixed to its SU(3) value,  $\chi = -\sqrt{7}/2$ .

Although reasonable results are obtained with a constant hamiltonian, they are considerably improved if parameters are allowed to vary with the number of nucleons in the valence shell, as suggested by the shell-model interpretation of IBM-1. Two possible types of dependence are proposed here:

$$x = \sum_{ij} x_{ij} (F_\nu)^i (F_\pi)^j, \quad (7)$$

or

$$x = \sum_i x_i (P)^i, \quad (8)$$

where  $x$  is a parameter of the hamiltonian (*i.e.*,  $x$  should be identified with  $\epsilon$ ,  $\kappa$ , ...) and the expansion is taken up to a given order. In Eq. (7) appear the ‘fractional fillings’  $F_\rho \equiv N_\rho / \Omega_\rho$ , with  $N_\rho$  the number of valence neutron ( $\rho = \nu$ ) or proton ( $\rho = \pi$ ) bosons and  $\Omega_\rho$  the size of the corresponding valence shell. In Eq. (8) occurs the so-called ‘promiscuity factor’ [11] defined as  $P = N_\nu N_\pi / (N_\nu + N_\pi)$ . The original parameter  $x$  is thus replaced by a set of parameters  $\{x_{ij}\}$  or  $\{x_i\}$  which will be adjusted to the available data.

The parametrizations (7) and (8), in conjunction with the hamiltonian (5), constitute a possible strategy for describing excitation spectra of nuclei in an entire major shell. It should be noted, however, that Eq. (5) does not represent the full IBM-1 hamiltonian since the terms that give a constant contribution in energy to all states of a given nucleus are lacking. One therefore cannot expect this hamiltonian to give a proper description of binding energies. How this can be achieved in the context of the IBM is explained in the next section.

### 4. Mass calculations with IBM

We begin by recalling that the binding energy  $B(N, Z)$  of a nucleus with  $N$  neutrons and  $Z$  protons is defined through

$$M(N, Z)c^2 = Nm_n c^2 + Zm_p c^2 - B(N, Z), \quad (9)$$

where  $M(N, Z)$  is the mass of the nucleus and  $m_n$  ( $m_p$ ) the mass of the neutron (proton). A simple, yet surprisingly accurate formula for this binding energy is

$$\begin{aligned} B_{\text{LDM}}(N, Z) &= a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} \\ &- \frac{S_v}{1 + y_s A^{-1/3}} \frac{4T(T+1)}{A} + a_p \frac{\Delta(N, Z)}{A^{1/3}}, \end{aligned} \quad (10)$$

where  $A = N + Z$  is the total number of nucleons,  $T = |N - Z|/2$  and  $\Delta(N, Z) = +2, +1$  and  $0$  for even-even, odd-mass and odd-odd nuclei, respectively. Equation (10) is

known as the liquid-drop mass (LDM) formula [12, 13], containing the usual volume, surface, Coulomb, symmetry and pairing terms.

A visual inspection of the differences between measured binding energies and those obtained with the LDM formula (10) suggests the addition of the two-parameter term [14]

$$B_{\text{shell}}(N, Z) = a_1(N_\nu + N_\pi) + a_2(N_\nu + N_\pi)^2, \quad (11)$$

where  $N_\rho$  is half the number of valence neutron ( $\rho = \nu$ ) or proton ( $\rho = \pi$ ) nucleons (particles or holes, whichever is smaller). Although of a very simple and naive nature, the addition of the linear and quadratic terms in  $N_\nu + N_\pi$ , leads to a remarkable decrease in the root-mean-square (rms) deviation of the mass formula, from 2.5 to 1.4 MeV [14]. These ‘shell’ corrections are reminiscent of some of the elementary terms in the successful mass formula of Duflou and Zuker [4], which is also based on a counting of valence nucleons. Several modifications of Eq. (11) can be considered such as, for example, a correction for the average value of  $B_{\text{shell}}(N, Z)$  [15].

Since the sum  $N_\nu + N_\pi$  can be identified with the total number of bosons  $N_b$ , the two terms (11) are part of the IBM-1 hamiltonian. This suggests the possibility of using this model in a simultaneous calculation of nuclear masses and spectra. The method proposed here consists of subtracting a global liquid-drop contribution (*without* shell or deformation effects) from the nuclear binding energy and modelling the remainder with the IBM-1 hamiltonian. The total binding energy of the nucleus then becomes

$$B(N, Z) = B_{\text{LDM}}(N, Z) - \langle 0_1^+ | \hat{H}_{\text{IBM}} | 0_1^+ \rangle, \quad (12)$$

where  $\hat{H}_{\text{IBM}}$  is the *full* IBM-1 hamiltonian up to a certain order in the interactions and  $0_1^+$  is the lowest-energy eigenstate of that hamiltonian. Note the minus sign in front of  $\langle 0_1^+ | \hat{H}_{\text{IBM}} | 0_1^+ \rangle$  which is needed to convert from negative energies to positive binding energies. It should be emphasized again that a hamiltonian as used in standard IBM-1 calculations [as, for example, in Eq. (5)] is not appropriate for the mass formula (12) because it is essential that  $\hat{H}_{\text{IBM}}$  contains interactions of the two types discussed in Sec. 2.

## 5. Applications

The hamiltonians (1) or (5) can be applied to a set of nuclei belonging to a single major shell which, by way of example, is chosen here to be all even–even nuclei with  $82 < N < 126$  and  $50 < Z < 82$ . Semi-magic nuclei should be excluded because they are known to exhibit a seniority spectrum which does not allow an interpretation in terms of IBM. Whether more nuclei in the neighbourhood of shell closures should be omitted from the fit is less clear. In this first application of a global IBM-1 calculation also tellurium ( $Z = 52$ ) and mercury ( $Z = 80$ ) isotopes as well as  $N = 84$  and  $N = 124$  isotones are excluded from the fit. This still leaves a large

data set which comprises 1280 excited levels in 123 nuclei, together with their ground-state binding energies.

Two different approaches are discussed in this section which differ in the choice of the hamiltonian. In the first, the hamiltonian is taken to be constant while in the second its interaction parameters are varied according to Eqs. (7) or (8).

### 5.1. A constant hamiltonian

The approach summarized in this subsection consists of taking a constant IBM-1 hamiltonian for the 123 nuclei considered in the fit. This might seem a hopeless undertaking unless one is aware of what is implied with the ‘constancy’ of the most general IBM-1 hamiltonian, taken up to a certain order in the interaction. This feature can be illustrated with the example hamiltonian

$$\hat{H}_{\text{ex}} = \epsilon_0 \hat{n}_d + \epsilon_1 \hat{n}_d (\hat{n}_s + \hat{n}_d), \quad (13)$$

which is part of a general one- plus two-body IBM-1 hamiltonian, that is, it corresponds to a particular choice of boson energies and of boson–boson interactions  $v_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L$  that appear in the  $\hat{H}_1 + \hat{H}_2$  part of the hamiltonian (1). Since the total number of bosons is conserved for the calculation of a single nucleus, the hamiltonian (13) can be rewritten as

$$\hat{H}_{\text{ex}} = \epsilon_d \hat{n}_d, \quad \epsilon_d = \epsilon_0 + N_b \epsilon_1. \quad (14)$$

This shows that the *constant* one- plus two-body hamiltonian (13) effectively corresponds to a one-body hamiltonian  $\epsilon_d \hat{n}_d$  of which the single-boson energy  $\epsilon_d$  varies linearly with the total boson number  $N_b$ .

This mechanism of separating the hamiltonian into parts that are genuinely constant and those that vary with boson number can be generalized to all orders. Formally, a  $k$ -body interaction can be divided into  $k + 1$  parts,

$$\hat{H}_k = \hat{H}_k^{(k)} + \hat{H}_k^{(k-1)} + \hat{H}_k^{(k-2)} + \cdots + \hat{H}_k^{(0)}, \quad (15)$$

where the first term  $\hat{H}_k^{(k)}$  is a constant  $k$ -body interaction while each of the remaining  $k$  terms can be considered as a  $k'$ -body interaction ( $k' < k$ ) according to the decomposition

$$\hat{H}_k^{(k')} = (\hat{N}_b)^{k-k'} \hat{H}_{k'}^{(k')}, \quad (16)$$

that is, its strength depends on the boson number as  $(N_b)^{k-k'}$ .

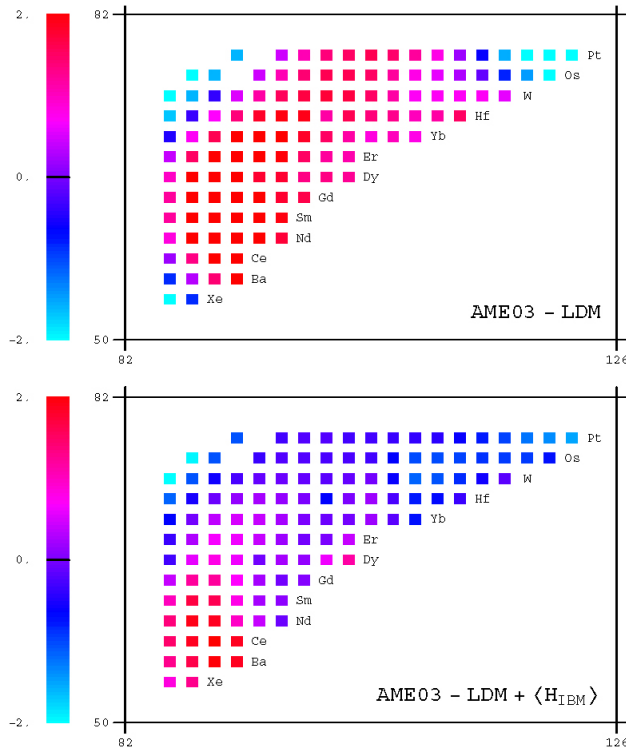
A first calculation of this type has been carried out using all ten parameters of the IBM-1 hamiltonian up to second order in the interactions. Since a simultaneous fit of many nuclei is attempted with spectra that vary from vibrational to rotational, there exists no obvious *ansatz* for the correct parameter set and an efficient fitting procedure is needed. The method followed here is based on the diagonalization of the error matrix which establishes a hierarchy of the most relevant parameter combinations. The approach is identical to that of the determination of shell-model matrix elements in

TABLE I. Parameters in the IBM-1 hamiltonian (1) and rms deviations  $\sigma$  (in keV) for even–even rare-earth nuclei with  $86 \leq N \leq 124$  and  $54 \leq Z \leq 78$ .

| $E_0$   | $\epsilon_s$ | $\epsilon_d$ | $v_{ddd}^0$ | $v_{ddd}^2$ | $v_{ddd}^4$ | $v_{ddd}^2$ | $v_{dds}^0$ | $v_{dds}^2$ | $v_{sss}^0$ | $\sigma_{\text{masses}}$ | $\sigma_{\text{spectra}}$ |
|---------|--------------|--------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|--------------------------|---------------------------|
| -6101.2 | 277.5        | 610.9        | -233.0      | -121.1      | -60.5       | 28.7        | -161.7      | -11.1       | -5.0        | 896                      | 259                       |

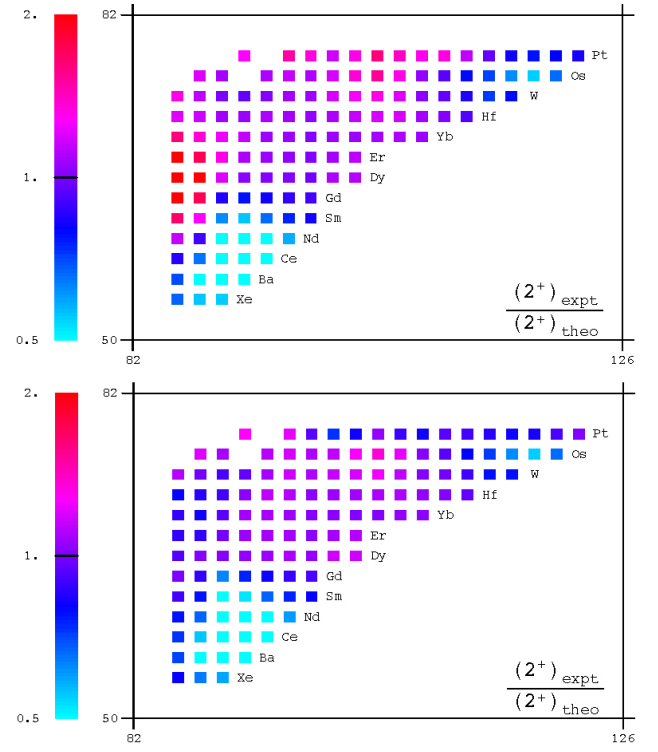
 TABLE II. Parameters in the IBM-1 hamiltonian (5) and rms deviation  $\sigma$  (in keV) for even–even rare-earth nuclei with  $86 \leq N \leq 124$  and  $54 \leq Z \leq 78$ .

| $\epsilon_{00}$ | $\epsilon_{10}$ | $\epsilon_{01}$ | $\kappa_0$ | $\kappa_1$ | $\kappa_2$ | $\kappa'_0$ | $\kappa'_1$ | $\kappa'_2$ | $\kappa''_0$ | $\kappa''_1$ | $\kappa''_2$ | $\lambda_{00}$ | $\lambda_{10}$ | $\lambda_{01}$ | $\sigma_{\text{spectra}}$ |
|-----------------|-----------------|-----------------|------------|------------|------------|-------------|-------------|-------------|--------------|--------------|--------------|----------------|----------------|----------------|---------------------------|
| 675.2           | —               | —               | 6.5        | —          | —          | 8.1         | —           | —           | -5.8         | —            | —            | -24.9          | —              | —              | 232                       |
| 232.5           | 622.8           | 1518.9          | -33.0      | 67.7       | -9.7       | 12.6        | -1.8        | 0.3         | 4.9          | -7.1         | 1.1          | -25.4          | 8.7            | -94.2          | 178                       |


 FIGURE 1. The differences between the measured nuclear binding energies and those obtained with the LDM formula (10) (left) and with the IBM-corrected LDM formula (12) (right) for even–even rare-earth nuclei with  $86 \leq N \leq 124$  and  $54 \leq Z \leq 78$ .

the  $sd$  shell [16] where the number  $p$  of parameter combinations is gradually increased until no further significant improvement is found. In spite of this sophisticated fitting procedure, convergence towards the optimal parameter set is not guaranteed. In fact, the final parameters, obtained by gradually increasing  $p$  starting from  $p = 2$ , may depend on the choice of the initial set.

After a preliminary exploration of the parameter space the rms deviation for the full one- plus two-body IBM-1 hamiltonian ( $p = 10$ ) is  $\sigma_{\text{rms}} = 896$  keV for the masses and  $\sigma_{\text{rms}} = 259$  keV for the spectra. The corresponding final boson parameters are shown in Table I in terms of the boson


 FIGURE 2. The ratios of the experimental and calculated energies of the first-excited  $2^+$  level in the approximation of constant (left) and variable (right) hamiltonian parameters for even–even rare-earth nuclei with  $86 \leq N \leq 124$  and  $54 \leq Z \leq 78$ .

energies and boson–boson interactions defined in Eqs. (2) and (3).

As an illustration of the results obtained in this way, the differences between the measured nuclear binding energies [17] and those obtained with the LDM formula (10) and with the IBM-corrected LDM formula (12), respectively, are shown in Fig. 1.

A significantly lower rms deviation is obtained in the latter calculation. This is not surprising since the IBM-1 hamiltonian includes the valence-nucleon terms (11) which proved so successful as a shell correction to the LDM formula. In principle, the IBM-1 hamiltonian contains additional corre-

lations (e.g., deformation) but it remains to be seen whether these lead to a systematic improvement in the description of nuclear masses.

An improvement of these one- plus two-body results may be attempted by increasing the order of the interactions in the hamiltonian. The increase up to third-order interactions introduces 17 new parameters, bringing its total to 27, still manageable given the large available data set. A first exploration of this parameter space did not lead to a significant lowering of the rms deviation. Further studies are needed to explore this idea in combination with the separation of the IBM-1 hamiltonian according to Eq. (15).

## 5.2. A variable hamiltonian

In this subsection the hamiltonian (5) is used to describe the spectra of the 123 nuclei included in the fit. As argued before, this hamiltonian is inappropriate for a binding-energy calculation and masses are left out of the fit as a consequence. The dependence on fractional fillings is chosen as follows:

$$\begin{aligned}\epsilon &= \epsilon_{00} + \epsilon_{10}F_\nu + \epsilon_{01}F_\pi, \\ \kappa &= \kappa_0 + \kappa_1P + \kappa_2P^2, \\ \kappa' &= \kappa'_0 + \kappa'_1P + \kappa'_2P^2, \\ \kappa'' &= \kappa''_0 + \kappa''_1P + \kappa''_2P^2, \\ \lambda &= \lambda_{00} + \lambda_{10}F_\nu + \lambda_{01}F_\pi.\end{aligned}\quad (17)$$

With the parameters as given in Table II an rms deviation of  $\sigma = 232$  keV is obtained for constant parameters whereas this deviation decreases to 178 keV if the fractional-filling dependence (17) is adopted.

In Fig. 2 are shown the ratios of the experimental [18] and calculated energies of the first-excited  $2^+$  level in the 123 nuclei in the approximation of constant and variable parameters, respectively.

## 6. Conclusion

To summarize, a strategy has been outlined for merging the calculations of ground- and excited-state energies in the framework of the interacting boson model. Preliminary results have been presented for even-even nuclei in the major shell with  $82 < N < 126$  and  $50 < Z < 82$  with a hamiltonian that includes up to two-body interactions. A further possible improvement is to include three-body interactions between the bosons which would allow for boson-number-dependent two-body interactions.

The overall purpose of the present approach is that once a reliable parameter set can be established from known nuclei, it might be of use for the *prediction* of spectral properties of nuclei far from the line of stability. Given that the IBM-1 is a valence-nucleon model, such extrapolations will crucially depend on the definition of neighbouring closed-shell configurations and on the assumption of the persistence of magic numbers.

## Acknowledgments

I would like to thank my collaborators Alejandro Frank, Lex Dieperink, Jorge Hirsch, José Barea and Irving Morales with whom I developed the ideas related to nuclear masses.

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