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Global and Local Nuclear Mass Formulas *

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A new method is proposed to describe masses of nuclei belonging to single a major shell. It is based on a global formula for the macroscopic part of the nuclear mass while the remaining (shell + deformation) part is considered in the context of the interacting boson model. The framework enables a simultaneous calculation of spectra and binding energies.

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1. Introduction

Over the years many different approaches have been developed to calculate masses of atomic nuclei. These fall into two classes. The first comprises *global* approaches in the sense that a single formula or algorithm is used to reproduce as closely as possible all known nuclear masses. Once parameters have been fixed from known nuclei, it is then possible to attempt extrapolations to regions away from stability. There exist now three standard global procedures which are complementary since each starts from a different picture of the nucleus. The first is the finite-range droplet model (FRDM) [1] which can be viewed as a sophisticated liquid-drop formula. The second global mass formula is based on the mean-field *ansatz* of Hartree-Fock-Bogolyubov (HFB) in its different versions, the latest of which is reported in Ref. [2]. The third is a shell-model based mass formula developed by Duflo and Zuker (DZ) [3] which yields the most accurate results in terms of root-mean-square deviation from the measured nuclear masses.

Local formulas are based on a different philosophy by focussing on a particular region of the nuclear mass table or, alternatively, by ‘predicting’ the mass of a nucleus through the systematic use of the masses of its neighbours. Local mass formulas obviously have less predictive power but usually attain greater accuracy in a limited region of the nuclear chart. Over the

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years many local formulas have been proposed some of which are discussed in the review of Lunney *et al.* [4]. The Garvey–Kelson (GK) relations [5] constitute a particularly useful example of a local approach by proposing a linear combination of six nuclear masses which should vanish. As a result the GK relations can be used to ‘predict’ the mass of one nucleus from those of five of its neighbours. It is clear that this is not a theoretical prediction since much experimental input is needed to calculate one single nuclear mass. Nevertheless, by defining a suitable averaging procedure of several (up to twelve) GK relations [6], the deviation from it can be reduced down to less than 100 keV, much lower than what can be obtained with a global mass formula. This procedure has been used by Barea *et al.* [6] to show that a random component to the nuclear masses, if it exists at all, must be smaller than 100 keV on average—a result which came in handy in the discussion related to the presence (or not) of a chaotic component in nuclear masses [7, 8]. The GK relations can also be used to check the consistency of a global mass formula. It is in fact found that, while the three standard approaches are consistent with the GK relations (to the extent that the data are) in known regions of the nuclear chart, this is not the case for the extrapolated masses calculated with FRDM or HFB [9].

In this contribution the combination of global and local mass formulas is explored from a different angle. The essential idea is to use a global, macroscopic formula in order to ‘unfold’ the mass data, that is, to subtract a macroscopic part from the experimental binding energies, and to describe the remainder with a realistic nuclear model, namely the interacting boson model (IBM) [10]. The full hamiltonian of the IBM should be able to account for shell and deformation effects that remain after a global unfolding. A simultaneous description of the excitation spectra of all nuclei in the data set is sought. Because the IBM is a valence-nucleon model which assumes an inert core, the calculation is restricted to a single major shell and in that sense it is local.

An outline of the method as well as preliminary results of a first application are presented. Since the approach is based on a global unfolding of the mass data, let us begin with a brief reminder of the latter.

2. The liquid-drop nuclear mass formula

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

$$M(N, Z)c^2 = Nm_n c^2 + Zm_p c^2 - B(N, Z), \quad (1)$$

where $M(N, Z)$ is the mass of the nucleus and m_n (m_p) the mass of the neutron (proton). The binding energy $B(N, Z)$ thus represents the energy

Table 1. Summary of coefficients in the liquid-drop mass formula (in MeV).

Eq.	a_v	a_s	a_c	S_v	y_s	a_p	$-a_1$	a_2
(2)	15.706	18.060	0.704	33.661	2.91	5.962	—	—
(2+3)	15.757	17.728	0.712	34.588	2.94	5.496	0.853	0.0163

needed to pull a nucleus into its $N+Z$ separate nucleons. Note that $M(N, Z)$ here refers to the mass of the nucleus only and not to that of the atom; so the binding energy $B(N, Z)$ is that of the neutrons and the protons and does not include contributions from the electrons.

A simple, yet surprisingly accurate formula for the binding energy of an atomic nucleus is given by

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

where $A = N + Z$ is the total number of nucleons and $T = |N - Z|/2$. Equation (2) is known as the liquid-drop mass formula [11, 12]. The first three terms appearing in the formula are referred to as volume, surface and Coulomb, and have a macroscopic origin that can be understood intuitively by viewing the nucleus as a dense, charged liquid drop. The fourth so-called symmetry term is a consequence of the Pauli principle and its $(N - Z)$ -dependence can be understood from the analysis of a Fermi gas [13]. The formula (2) uses a somewhat sophisticated form of the symmetry energy where surface and so-called Wigner effects are considered via the inclusion of y_s and r , respectively. The last term represents a simple parametrization of the most important correlation in nuclei, pairing, by assuming $\Delta(N, Z) = +2, +1$ and 0 in even-even, odd-mass and odd-odd nuclei, respectively. In the convention of positive binding energies, the volume and pairing contributions are positive while others are negative; as a result all a coefficients in the formula (2) are positive.

In Fig. 1 are shown the differences between the formula (2) with $r = 1$ and parameters given in Table 1, and the measured nuclear binding energies taken from the 2003 atomic mass evaluation AME03 [14]. Immediately obvious from the figure are the large deviations that occur for doubly magic nuclei such as ^{100}Sn , ^{132}Sn or ^{208}Pb which have a diamond-like appearance. This suggests the use of a term linear in $n_\nu + n_\pi$ where n_ρ is the number of valence neutrons ($\rho = \nu$) or protons ($\rho = \pi$) which are taken particle- or hole-like and counted from the nearest closed shell. Furthermore, the ellipse-like deviations in mid-shell regions suggest another term which is quadratic

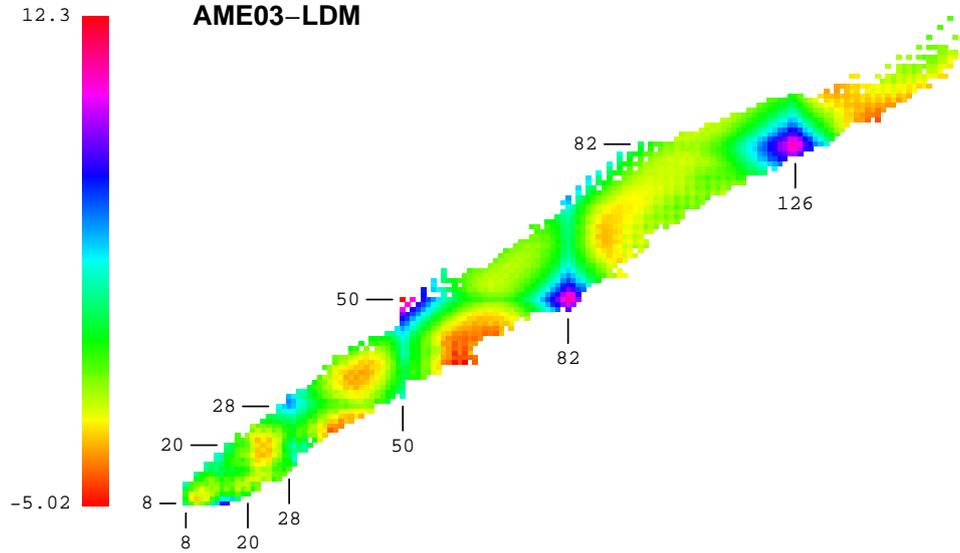


Fig. 1. Differences between measured and calculated binding energies for nuclei with $N, Z \geq 8$. The binding energies are calculated with the mass formula (2).

in $n_\nu + n_\pi$. This simple visual inspection of the deviations thus suggests to add to the liquid-drop mass formula (2) the two-parameter term [15]

$$B_{\text{shell}}(N, Z) = a_1(n_\nu + n_\pi) + a_2(n_\nu + n_\pi)^2. \quad (3)$$

The corrections (3) can be considered as a basic version of the successful DZ mass formula [3]. Several modifications can be considered such as, for example, a correction for the average value of $B_{\text{shell}}(N, Z)$ [16].

The prescription (3) requires pre-defined magic numbers in the nuclear shell model, for which the standard values are 8, 20, 28, 50, 82, 126 and 184. It turns out, in fact, that a lower root-mean-square (rms) deviation (1.201 instead of 1.397 MeV) is found if the shell closure at $N, Z = 20$ is replaced by $N, Z = 14$ [16]. Furthermore, several microscopic nuclear mass calculations (see, *e.g.* the review of Oganessian [17]) indicate a proton shell closure at $Z = 114$ and it is indeed found here that the currently known masses are better described if this magic number is considered, the rms deviation further reducing from 1.201 to 1.161 MeV. (If the magic number $Z = 114$ is included, results become independent of higher proton magic numbers since the compilation AME03 does not go beyond element $Z = 108$.) As yet no empirical evidence exists for a neutron shell closure at $N = 184$ which is taken here on the basis of microscopic mass calculations. There are very few nuclei in AME03 with more than 155 neutrons (mid-shell between 126

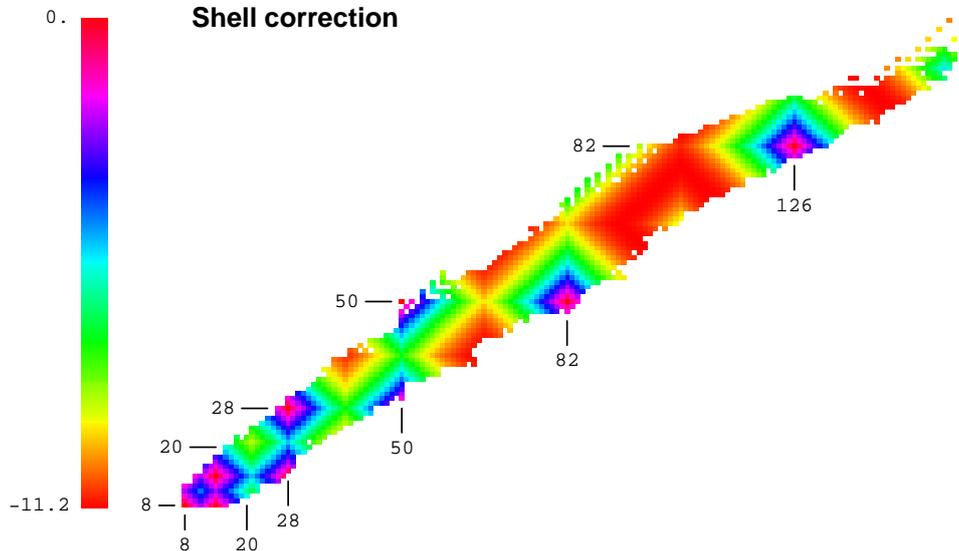


Fig. 2. The shell correction (3) for nuclei with $N, Z \geq 8$ calculated with $a_1 = -0.853408$ and $a_2 = 0.016283$ (in units of MeV).

and 184) and thus the existence of the magic number at $N = 184$ can at present not be probed on the basis of mass data.

The use of these two simple corrections with the appropriate magic numbers reduces the rms deviation for more than 2000 nuclear masses from 2.479 to 1.161 MeV with the coefficients as shown in Table 1. The shell corrections themselves are shown in Fig. 2 for the parameters a_1 and a_2 as obtained from the fit and they indeed reveal a pattern similar to that in Fig. 1. A large fraction of the remaining rms deviation of 1.161 MeV is due to nuclei lighter than ^{56}Ni which is also obvious from a comparison of the two figures.

3. Mass calculations with the interacting boson model

In the previous section it was shown that the deviations of the liquid-drop mass formula from the measured nuclear masses can be parametrized in a simple fashion in terms of the number of nucleons in the valence shell. The proposed shell correction (3) can, for even-even nuclei, be rewritten as

$$B_{\text{shell}}(N, Z) = a'_1(N_\nu + N_\pi) + a'_2(N_\nu + N_\pi)^2, \quad (4)$$

with $a'_1 = 2a_1$ and $a'_2 = 4a_2$. In Eq. (4) N_ρ is the number of neutron ($\rho = \nu$) or proton ($\rho = \pi$) bosons which are identified with pairs of valence nucleon particles or holes [10]. Note that $N_\nu + N_\pi$ coincides with the total number

of bosons of the IBM. The usual notation N for this number is not used here in order to avoid confusion with neutron number.

Given that the two terms (4) are part of the IBM hamiltonian, this suggests the possibility of using the latter model in a simultaneous calculation of nuclear masses and spectra, an idea that is explored in this section. To keep matters simple in this exploratory calculation, the simplest version of the IBM of even–even nuclei is used where no distinction is made between neutron and proton bosons, the so-called IBM-1. For an introduction to the IBM the reader is referred to the monograph of Iachello and Arima [10]. Suffice it to say here that the model aims at a description of low-lying collective states of even–even nuclei in terms of interactions between s and d bosons which can be thought of as approximated correlated fermion pairs coupled to angular momentum zero and two, respectively.

If one limits the hamiltonian of the IBM-1 to interactions that are at most of two-body nature between the bosons, the total number of parameters is ten. Six of the parameters determine the energy spectrum of individual nuclei while the four remaining ones exclusively contribute to the binding energy. The parameter systematics of the former is by now well established through phenomenological studies with input from microscopic theory (for references, see [10]). Surprisingly little has been done with IBM concerning absolute binding energies and in most cases only two-nucleon separation energies have been considered, such as in the recent detailed studies of García-Ramos *et al.* [18] and Fossion *et al.* [19]. The work reported here is most closely related to that of Davis *et al.* [20].

To make to above discussion more explicit, note that the most general IBM-1 hamiltonian up to second order in the interactions between the bosons can be written as

$$\hat{H} = E_0 + \hat{H}_1 + \hat{H}_2, \quad (5)$$

where the index refers to the order of the interaction. The first term E_0 is a constant. The second term is the one-body part

$$\hat{H}_1 = \epsilon_s [s^\dagger \times \tilde{s}]^{(0)} + \epsilon_d \sqrt{5} [d^\dagger \times \tilde{d}]^{(0)} \equiv \epsilon_s \hat{n}_s + \epsilon_d \hat{n}_d, \quad (6)$$

where \times refers to coupling in angular momentum (shown as an superscript in round brackets), $\tilde{b}_{\ell m} \equiv (-)^{\ell-m} b_{\ell, -m}$ and the coefficients ϵ_s and ϵ_d are the energies of the s and d bosons. The third term in the hamiltonian (5) represents the two-body interaction

$$\hat{H}_2 = \sum_{\ell_1 \leq \ell_2, \ell'_1 \leq \ell'_2, L} \tilde{v}_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L [[b_{\ell_1}^\dagger \times b_{\ell_2}^\dagger]^{(L)} \times [\tilde{b}_{\ell'_2} \times \tilde{b}_{\ell'_1}]^{(L)}]_0^{(0)}, \quad (7)$$

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

$$v_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L \equiv \langle \ell_1 \ell_2; LM | \hat{H}_2 | \ell'_1 \ell'_2; LM \rangle = \sqrt{\frac{(1 + \delta_{\ell_1 \ell_2})(1 + \delta_{\ell'_1 \ell'_2})}{2L + 1}} \tilde{v}_{\ell_1 \ell_2 \ell'_1 \ell'_2}^L. \quad (8)$$

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, together with the two boson energies ϵ_s and ϵ_d and the constant E_0 , leads to the ten parameters quoted above.

The hamiltonian (5) by itself cannot provide an adequate description of the *total* binding energy of the nucleus. 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. In summary, the hamiltonian

$$\hat{H}^{\text{full}} = -B(N, Z) + E_0 + \hat{H}_1 + \hat{H}_2, \quad (9)$$

contains all terms up to second order, including a contribution from the core inspired by the liquid-drop model. Note the minus sign in front of $B(N, Z)$ which is needed to convert from positive binding energies to negative absolute energies. All two-body interactions between the bosons are assumed constant throughout the entire shell; only three-body interactions can represent $(N_\nu + N_\pi)$ -dependent two-body interactions.

The hamiltonian (9) 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 are excluded because they are known to exhibit a seniority spectrum which does not allow an interpretation in terms of IBM. 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 the *sd* shell [21].

The hamiltonian (9) is first written in a simplified notation as

$$\hat{H} = \sum_{i=1}^P v_i \hat{O}_i, \quad (10)$$

where v_i are the P parameters that need to be determined and \hat{O}_i are the P operators in the hamiltonian (5). In the present application the

parameters a_i in $B(N, Z)$ have been determined first from a fit to all masses of nuclei with $N, Z \geq 8$. These parameters are kept fixed in the subsequent adjustment of the v_i to the data set in the shell with $82 < N < 126$ and $50 < Z < 82$. More sophisticated procedures can be envisaged involving iterative or even simultaneous adjustments of a_i and v_i . If both pieces of the hamiltonian are treated consistently, it will then probably be possible to absorb the constant E_0 into the liquid-drop expression for $B(N, Z)$.

The parameters v_i are fitted to a data set consisting of M experimental energies E_{expt}^k , $k = 1, \dots, M$. In the shell with $82 < N < 126$ and $50 < Z < 82$, the available data set comprises 128 ground-state and 1019 excited-state energies. One of the main difficulties in carrying out the analysis is the selection of relevant data. As the IBM is a model of collective behaviour of nuclei, only excited states of such character should be included, and this selection is far from obvious in many cases. Nevertheless, a selection of this kind has to be carried out and for each selected level a theoretical counterpart is proposed with an energy

$$\lambda_k \equiv \langle \Phi_k | \hat{H} | \Phi_k \rangle = \sum_{i=1}^P v_i \langle \Phi_k | \hat{C}_i | \Phi_k \rangle \equiv \sum_{i=1}^P v_i \beta_i^k. \quad (11)$$

The wave functions $|\Phi_k\rangle$ are obtained by diagonalizing \hat{H} for an initial choice of parameters $\{v_i^0\}$ and are iteratively improved in the manner explained below.

The optimal set of parameters is obtained by minimization of the rms deviation

$$\chi^2 = \sum_{k=1}^M \left(\frac{E_{\text{expt}}^k - \lambda_k}{\sigma_{\text{expt}}^k} \right)^2, \quad (12)$$

where σ_{expt}^k is the error on the experimental energy. Minimization with respect to $\{v_i\}$, under the assumption of v_i -independent matrix elements β_i^k , leads to a set of linear equations of the form

$$\sum_{i=1}^P G_{ij} v_i = e_j, \quad \text{or} \quad v_i = \sum_{j=1}^P (G^{-1})_{ji} e_j, \quad (13)$$

where \mathbf{G} and \mathbf{e} are $P \times P$ and $P \times 1$ matrices, respectively, defined as

$$G_{ij} = \sum_{k=1}^M \frac{\beta_i^k \beta_j^k}{(\sigma_{\text{expt}}^k)^2}, \quad e_i = \sum_{k=1}^M \frac{E_{\text{expt}}^k \beta_i^k}{(\sigma_{\text{expt}}^k)^2}. \quad (14)$$

The inverse matrix \mathbf{G}^{-1} is known as the error matrix and contains all information on correlations between parameters. In particular, diagonal-

ization of \mathbf{G} (or \mathbf{G}^{-1}) yields a hierarchy of parameters. The diagonalization of \mathbf{G} amounts to finding a unitary transformation \mathbf{A} such that $\mathbf{D} = \mathbf{A}\mathbf{G}\mathbf{A}^T$ is diagonal, $D_{ij} = D_i\delta_{ij}$, or, equivalently, $\mathbf{D}^{-1} = \mathbf{A}\mathbf{G}^{-1}\mathbf{A}^T$ with $(D^{-1})_{ij} = d_i\delta_{ij} = (1/D_i)\delta_{ij}$. The transformation \mathbf{A} defines a set of *uncorrelated* parameters $\nu_i = \sum_j A_{ij}v_j$ with associated errors given by d_i . Consequently, the parameter ν_i can be considered as well determined if the corresponding eigenvalue d_i is small; the ordering of d_i in increasing size thus provides a hierarchy of parameters ν_i . This enables one to use the full hamiltonian (9) with all P Casimir operators but to fit only $p \leq P$ parameter combinations ν_i . For a given number of parameters $p \leq P$ the following fitting procedure can therefore be defined [21]. From an initial choice of parameters $\{\nu_i^0\}$ a subsequent set is defined according to

$$\nu_i^1 = \begin{cases} \sum_{j=1}^P A_{ij}v_j = \sum_{j,j'=1}^P A_{ij}(G^{-1})_{j'j}e_{j'}, & \text{if } i \leq p, \\ \nu_i^0, & \text{if } i > p, \end{cases} \quad (15)$$

where it is assumed that \mathbf{A} is the unitary matrix which diagonalizes \mathbf{D}^{-1} into eigenvalues d_i that are ordered in increasing value. With this set of parameters $\{\nu_i^1\}$ new wave functions $|\Phi_k\rangle$, matrix elements β_i^k , and matrices \mathbf{G} and \mathbf{e} are obtained with which the next set of parameters $\{\nu_i^2\}$ can be calculated, and so on, until convergence is reached.

Two additional points should be mentioned. The first is that, although ultimately one would like to treat ground and excited states on the same footing, this is not done at present. The *absolute* energies of the 128 ground states are fitted while for excited states the fitted quantity is the excitation energy, that is, the energy *relative* to the ground state. The second point is that the use of the experimental error σ_{expt}^k on its own is unsatisfactory since in many cases (*e.g.*, most excitation energies) this error is negligible compared to the theoretical error. The proper way to deal with this issue is to consider instead for each experimental data point the error

$$\sqrt{(\sigma_{\text{expt}}^k)^2 + (\sigma_{\text{th}})^2}, \quad (16)$$

where σ_{th} is an intrinsic model error. An estimate of σ_{th} can be obtained via the maximum-likelihood method following the discussion in ref. [1] (which can be applied here with $\mu_{\text{th}} = 0$). It is clear that the consideration of the experimental error becomes important only when it is larger than or of the same order as σ_{th} . In the present calculation σ_{th} is still relatively large and hence close to but somewhat smaller (about 10 keV) than the rms deviation.

Figure 3 shows the rms deviation for masses and for excitation energies as a function of the number of parameters up to $p = 10$. In spite of the so-

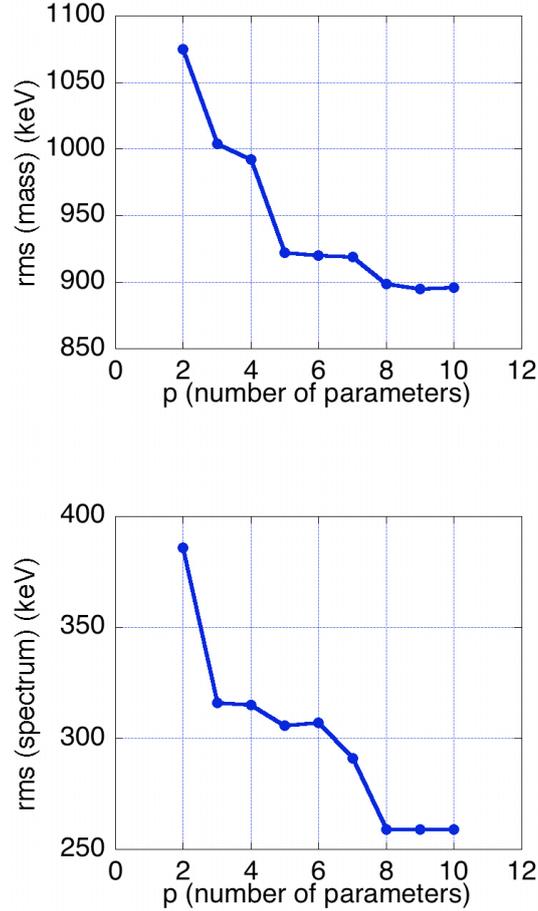


Fig. 3. The rms deviation in units of keV for masses (top) and for excitation energies (bottom) as a function of the number of parameters p .

phisticated fitting procedure explained in the preceding paragraphs, 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 $\{v_i^0\}$. The rms deviations shown in fig. 3, $\text{rms}(\text{masses}) = 896$ keV, $\text{rms}(\text{spectra}) = 259$ keV, $\text{rms}(\text{total}) = 386$ keV and $\sigma_{\text{th}} = 376$ keV are those found after a preliminary exploration of the parameter space. The corresponding boson parameters are shown in Table 2 in terms of the boson energies and boson–boson interactions defined in Eqs. (6)

Table 2. Parameters in the IBM-1 hamiltonian for rare-earth nuclei (in keV).

E_0	ϵ_s	ϵ_d	v_{ddd}^0	v_{ddd}^2	v_{ddd}^4	v_{dds}^2	v_{dds}^0	v_{dsds}^2	v_{ssss}^0
-6101	277	611	-233	-121	-60	29	-162	-11	-5

and (8). It should be emphasized once more that the corresponding rms deviation is not necessarily the lowest that can be obtained with the full one-plus two-body IBM-1 hamiltonian.

4. Conclusion

To summarize, a strategy has been outlined for merging the calculations of ground- and excited-state energies and preliminary results have been presented for even-even nuclei in the major shell with $82 < N < 126$ and $50 < Z < 82$. No definitive results for the one- and two-body parameters are available yet. 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 determined from known nuclei, it might be of use for the *prediction* of spectral properties of nuclei far from the line of stability.

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