

The master term in Duflo-Zuker inspired mass formulas

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Abstract. We present a detailed analysis of the term containing the information about monopolar interaction in Duflo-Zuker inspired mass formulas, usually known as the 'master term'. We discuss the physics involved in this master term and carefully study its asymptotic behavior with the aim of properly describe shell effects. We explore different dependence of the master terms with shell degeneracies. Ideas to improve the fits of experimental data in the future are shared

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INTRODUCTION

Nuclear mass is the most fundamental property of nuclei. From deuteron to uranium, there are almost 1700 species that occur naturally on earth. In addition, large numbers of others are created in the laboratory and in the interior of stars. Any course of nuclear physics starts with the understanding of nuclear properties, like the saturation of the nuclear force, the existence of pairing and shell effects, the distribution of stable and long-lived nuclei as a function of neutron and proton numbers, the existence of the 'valley of stability', and the description of fission and fusion processes. This is usually made easy through the description of nuclear masses in terms of a phenomenological Liquid Drop Mass (LDM) formula [1]. On the other side, nuclear masses are very important for astrophysics, mainly because the Q -values of different nuclear reactions, obtained from mass differences, must be accurately known to allow the astrophysical origin of the elements [2].

Nuclear mass is directly related with the binding energy, $BE(N, Z)$, which measures the energy to remove all Z protons and N neutrons from the nucleus:

$$BE(N, Z) = [Zm_H + Nm_n - M(N, Z)]c^2,$$

where $M(N, Z)$ is the mass of the neutral atom, m_H is the mass of the hydrogen atom, and m_n is the mass of a free neutron. Thus, to know binding energies means to know nuclear masses. A very important victory of nuclear physicists would be to describe the nuclear masses of the measured 2149 species (with $N \geq 8$, $Z \geq 8$) reported in the more recent Atomic Mass Evaluation performed in the year 2003 (AME03) [3], mainly because it will allow to predict nuclear masses of species not yet measured. Accurate theoretical predictions of nuclear masses remain a challenge [4], sharing the difficulties with other

quantum many-body calculations, and complicated by the absence of a full theory of the nuclear interaction.

Decades of work have produced several microscopic and macroscopic mass formulas [5]. They allow for the calculation of masses, charge radii, deformations, and in some cases also fission barriers. They all contain a macroscopic sector which resembles the LDM formula, and include deformation effects. Between them, we mention:

1. The pioneering mass formula from Bethe-Weizsäcker (BW) [6] which has spherical symmetry, known as the Liquid Drop Model, which reproduces the bulk properties of the binding energies and allows to explain the nuclear saturation.
2. The Droplet Model from Myers-Swiatecki [7], which is basically a modification of the drop model which allows for departures from spherical symmetry implied in BW model.
3. The microscopic-macroscopic models, like the Finite Range Droplet Model (FRDM) [8] and its improvements [9]. In the macroscopic sector, the original drop model was generalized in three distinct stages: the first of these consisted of the replacement of the 'drop model' by the 'droplet model', the second, the introduction of finite-range surface effects originated by the N-N interaction [10], while the third stage consisted of the addition of a purely phenomenological exponential compressibility term [11]. Additionally, in the microscopic sector, shell corrections are included consistently with the Strutinsky theorem [12].
4. The Skyrme and Gogny Hartree Fock Bogolyubov (HFB) [13, 14] which are mean-field models based in the HFB method in which a Skyrme force, with correlations represented by a δ pairing force, is assumed. The energy is determined from a variational method.
5. The microscopic-macroscopic realistic Thomas-Fermi (TF) models [15, 16], which offers a much closer approximation to the Hartree-Fock method than does the FRDM or any of the other drop model based methods. It is based entirely on a Skyrme force, and calculates the energy of any given nucleus in the fourth-order extended Thomas-Fermi approximation instead of a variational method.
6. The Duflo-Zuker (DZ) mass formula [17, 18, 19], where the starting point is the assumption that there exist effective interactions ('pseudopotentials') smooth enough for Hartree-Fock calculations to be possible. The corresponding Hamiltonian can be separated into monopole and multipole terms. The monopole term is entirely responsible for saturation and single-particle properties, serving in principle as a platform for Hartree-Fock calculations, while the multipole term acts as a residual interaction that permits the method to be pushed beyond pure Hartree-Fock by admitting a very general configuration mixing that includes, but is not confined to, pairing and Wigner correlations. The term of the DZ mass formula which contains the information of the monopole interaction is called the 'master term'.

At present, the most successful approaches seem to be the microscopic-macroscopic models, like the FRDM or TF model. HFB calculations are now able to fit known nuclear masses with deviations competitive with the microscopic-macroscopic calculations, while the most precise and robust nuclear mass predictions are given by the DZ model [5], with an RMS of 373 keV. The DZ formula contains 33 terms, built by Jean

Duflo and Andres Zuker combining a deep knowledge of the nuclear interactions and the shell model with some kind of 'magic' and 'intuition'. Being the model with smaller RMS and the more predictive one to our disposal, it would be very useful and instructive to extend the model, inspired in its ideas, in a way that could be understood, shared and improved on by the nuclear physics community.

Some efforts in this direction were performed in the recent works from Refs. [20, 21, 22], where the interplay between deformations and shell effects was discussed.

Motivated by our previous arguments, we analyze here the master term in DZ mass formulas and discuss the physics involved in it. A summary of our mass model adopted to perform our analysis is presented in Sect. 2. In Sect. 3 we describe the master term and carefully study its asymptotic behavior. Conclusions and future improvements are outlined in Sect. 4.

OUR MASS MODEL

Analyzing the ability of the LDM formulas to describe nuclear masses for nuclei in various deformation regions, it has been recently shown that different LDM formulas exhibit a similar behavior [21, 22]: the masses of prolate deformed nuclei are better described than those of spherical ones. In fact, the prolate deformed nuclei are fitted with an RMS smaller than 750 keV, while for spherical and semi-magic species the RMS is always larger than 2000 keV. These results are found to be independent of pairing. Based in it we select here an improved version of the LDM formula with modified symmetry and Coulomb terms, built following a consistent treatment of nuclear bulk and surface effects [23]. The negative nuclear binding energy is given by:

$$E_{LDM} = -a_v A + a_s A^{2/3} + S_v \frac{4T(T+1)}{A(1+yA^{-1/3})} + a_c \frac{Z(Z-1)}{(1-\Lambda)A^{1/3}} - a_p \frac{\Delta}{A^{1/3}}, \quad (1)$$

where: i) the pairing interaction is given by $\Delta = 2, 1$, and 0 for even-even, odd-mass and odd-odd nuclei, respectively; ii) a correction to the radius of the nucleus is included through a modification Λ in the Coulomb term, $\Lambda = \frac{N-Z}{6Z(1+y^{-1}A^{1/3})}$; iii) the symmetry term employs $4T(T+1)$, with $T = |N-Z|/2$, instead of $(N-Z)^2$ to account for the Wigner energy; and iv) the Coulomb interaction is proportional to $Z(Z-1)$ to avoid the Coulomb interaction of a proton with itself.

We know that the major challenge in the construction of an algebraic microscopic mass formula is the proper description of shell effects. In Ref. [22] we have compared the ability of different models to describe masses of nuclei in spherical, prolate and semi-magic groups. We find out that models based in the LDM plus algebraic corrections are not as good in introducing the shell effects as DZ, which erases any trace of shell closure effects. How DZ model works? The original model from Refs. [17, 18, 19] includes the monopole part ($J = 0$) of the many body interaction in a master term based on the

harmonic-oscillator (HO) degeneracies:

$$M^{HO} = \frac{1}{\rho} \left[\left(\sum_p \frac{n_v}{\sqrt{D_p^{HO}}} \right)^2 + \left(\sum_p \frac{n_\pi}{\sqrt{D_p^{HO}}} \right)^2 \right], \quad (2)$$

where the sums run over all occupied proton and neutron orbitals up to the Fermi level, $D_p^{HO} = (p+1)(p+2)$ is the degeneracy of the major HO shell of principal quantum number p , and n_v, n_π are number operators for neutrons and protons, respectively, and $\rho = A^{1/3} \left[1 - \left(\frac{T}{A} \right)^2 \right]^2$ is the scaling factor. When this master term is used, the closures are obtained at $N, Z = 8, 20, 40, 70, \dots$ consistently with the fact that we are using HO degeneracies [20]. In order to change into the observed extruder-intruder (EI) closures at $N, Z = 14, 28, 50, 82$ and 126, Duflo has proposed, with very much intuition, to add an S operator, given in Eq. (18) of Ref. [20]. Alternatively, Mendoza-Temis et al have proposed a modified master term M_a , which directly includes the EI shell closures using an expression similar to (2), but with the index p now referring to the EI major shell with degeneracies $D_p \rightarrow D_p^{HO} + 2$:

$$M_a = \frac{1}{\rho} (e_{1v}^2 + e_{1\pi}^2), \quad e_{1v} = \sum_{p_v} \frac{n_v}{\sqrt{D_{p_v}}}, \quad e_{1\pi} = \sum_{p_\pi} \frac{n_\pi}{\sqrt{D_{p_\pi}}}, \quad (3)$$

where $D_{p_{v,\pi}} = (p_{v,\pi} + 1)(p_{v,\pi} + 2) + 2$ contains the $HO \rightarrow EI$ information. When the asymptotic behavior of this master term is removed, shell effects emerge, with well-defined peaks at shell closures. This allows to reproduce the observed closures without adding any S term.

Based on these arguments, we have proposed in Ref. [22] a mass formula which combines the ability of LDM formulas to describe deformations and that of DZ models to reproduce shell effects:

$$E_{LDM+DZ} = E_{LDM} + a_{vol}(M_a - M_{a,asym}) + a_{surf}(M_a - M_{a,asym})/\rho. \quad (4)$$

In fact, the shell effects are introduced by ‘‘volume’’ and ‘‘surface’’ shell corrections (which resemble the shell effects not included in the LDM) defined as $M_a - M_{a,asym}$ and $(M_a - M_{a,asym})/\rho$, respectively, where

$$M_{asym} = \frac{1}{\rho} (e_{1v,asym}^2 + e_{1\pi,asym}^2), \quad (5)$$

with the asymptotic form

$$e_{1v,asym} = -0.90892 + 0.54259N^{1/3} + 0.98851N^{2/3} + 0.0018N. \quad (6)$$

THE MASTER TERM

We know that there exists some uncertainty in the parametrization of the monopole part of the nuclear Hamiltonian [20]. Particularly, we can understand the dependence of

the form $D_p^{-1/2}$ in Eq. (2) looking at the unitary transformation which diagonalize the monopole Hamiltonian, and keeping only the eigenvector with the largest eigenvalue. In fact, numerical studies of realistic interactions (chiral N3LO interaction) show that, when the major shell is full, the dominant isoscalar master eigenvector U_p behaves as $U_p \propto D_p^{-1/2}$. However, an important point needs to be remarked here: a variant $U_p \propto D_p^{-1/2} - (2/15)D_p^{-1}$ behavior has been seen to be almost indistinguishable from the first one!

Thus, it would be interesting to analyze how the description of shell effects changes when we replace the dependence of the master term with the shell degeneracy. For example, we could analyze a polynomial replacement of the form

$$D_p^{-1/2} \rightarrow A_0 + A_1 D_p^{-1/2} + A_2 (D_p^{-1/2})^2 + \dots + A_n (D_p^{-1/2})^n, \quad (7)$$

with A_i , $i = 0, \dots, n$ being constant coefficients to be determined. To start with, we propose to explore here if changes in the denominator of the master term lead to a better description of shell effects, still conserving the analogy with the origin associated to the monopolar term of the nuclear interaction. Specifically, we propose a new master term of the form

$$\tilde{M}_a(A_2) = \frac{1}{\rho} [e_{1\nu}^2(A_2) + e_{1\pi}^2(A_2)], \quad (8)$$

where

$$e_{1\nu}(A_2) = \sum_{p\nu} \frac{n_\nu}{D_{p\nu}^{-1/2} + A_2 D_{p\nu}^{-1}}, \quad e_{1\pi}(A_2) = \sum_{p\pi} \frac{n_\pi}{D_{p\pi}^{-1/2} + A_2 D_{p\pi}^{-1}}, \quad (9)$$

with A_2 being a free parameter. Note that we work with the EI closures previously defined, below Eq. (3). Next, our procedure will be the following: we need firstly to select some values for the parameter A_2 and then, to construct our mass model and properly describe shell effects, we need to find the asymptotic term for each one of the masters defined in (8).

We separate our analysis in two parts: i) in the first one, we work with all the 2149 measured species; ii) in the second, we will work with a reduced number of semimagic nuclei: those belonging to the tin chain with $Z = 50$, which contains only 33 nuclei with $50 \leq N \leq 84$.

- All 2149 measured nuclei

With the main purpose of analyzing the effects of a change in the denominator in the master term, we have selected three values for the parameter: $A_2 = -2/15$, $A_2 = 0$, $A_2 = +2/15$. The asymptotic behaviors determined by including terms with different powers of $N^{1/3}$ were

$$\begin{aligned} e_{1\nu,asy}(A_2 = -2/15) &= -0.73646 + 0.28689N^{1/3} + 0.99847N^{2/3} + 0.00123N, \\ e_{1\nu,asy}(A_2 = 0) &= -0.90892 + 0.54259N^{1/3} + 0.98851N^{2/3} + 0.0018N, \\ e_{1\nu,asy}(A_2 = +2/15) &= -1.11605 + 0.82695N^{1/3} + 0.97095N^{2/3} + 0.00301N. \end{aligned} \quad (10)$$

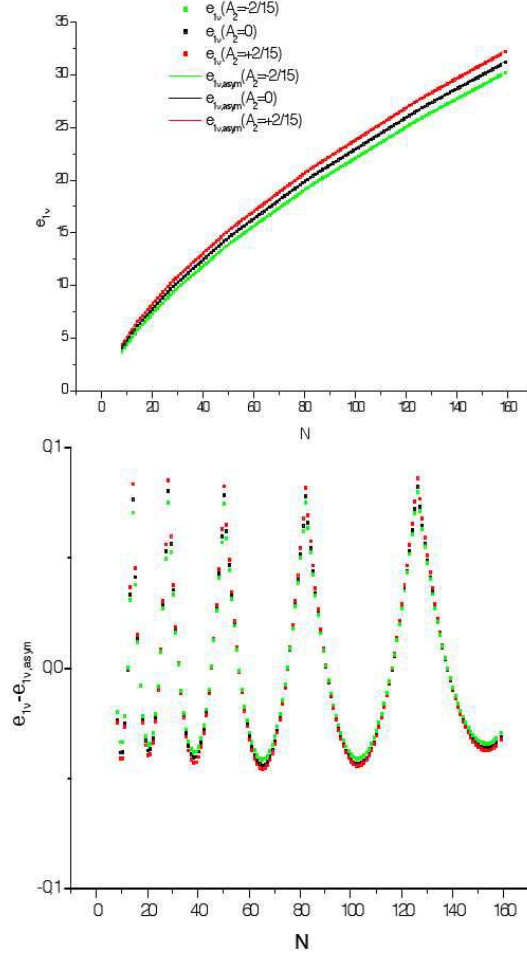


FIGURE 1. $e_{1\nu,asym}$ and $e_{1\nu} - e_{1\nu,asym}$ for three different values of the parameter A_2 , for the 2149 measured nuclei.

We show in Figure 1 the plots for $e_{1\nu}$, its asymptotic term $e_{1\nu,asym}$ and the difference $e_{1\nu} - e_{1\nu,asym}$ as a function of the neutron number N , for the three values of A_2 . From these results we can observe that shell effects are satisfactory reproduced with three models, and a general tendency needs to be remarked: when we move A_2 from $-2/15$ to $+2/15$, the smaller differences between $e_{1\nu}$ and its asymptotic behavior are obtained for the negative value of the parameter, in agreement with

the fit found in [20].

• 33 nuclei from $Z = 50$ Tin chain

Because the bigger differences in Figure 1 are obtained for the magic numbers, we would like to learn here how to improve the description of the shell effects contained in semimagic nuclei. Thus, we will work with the species from the Tin chain with $Z = 50$. For the parameter A_2 we will choose a little more wide range than for the 2149 nuclei: $A_2 = -0.25, -2/15, -0.05, 0, +0.05, +2/15, +0.25$. The asymptotic behavior found in each case is:

$$\begin{aligned}
 e_{1v,asy}(A_2 = -0.25) &= 41.43924 - 27.54929N^{1/3} + 6.92967N^{2/3} - 0.41134N, \\
 e_{1v,asy}(A_2 = -2/15) &= 43.36571 - 28.7017N^{1/3} + 7.21951N^{2/3} - 0.43196N, \\
 e_{1v,asy}(A_2 = -0.05) &= 44.72744 - 29.51423N^{1/3} + 7.42392N^{2/3} - 0.44648N, \\
 e_{1v,asy}(A_2 = 0) &= 45.55337 - 30.00831N^{1/3} + 7.54818N^{2/3} - 0.45532N, \\
 e_{1v,asy}(A_2 = +0.05) &= 46.37475 - 30.4991N^{1/3} + 7.67164N^{2/3} - 0.46409N, \\
 e_{1v,asy}(A_2 = +2/15) &= 47.74986 - 31.32151N^{1/3} + 7.87848N^{2/3} - 0.47881N, \\
 e_{1v,asy}(A_2 = +0.25) &= 49.66295 - 32.46404N^{1/3} + 8.1659N^{2/3} - 0.49923N \quad (11)
 \end{aligned}$$

Figure 2 shows the differences $e_{1v} - e_{1v,asy}$ and $\tilde{M}_a - \tilde{M}_{a,asy}$ as a function of N for the different values of A_2 . Here $\tilde{M}_{a,asy}$ is constructed as in Eq. (5) with the asymptotic term corresponding to each value of A_2 .

These plots indicate that now the peaks at the magic numbers ($N = 50$ and $N = 82$) are less pronounced than in Figure 1. This shows that the asymptotic behavior we are subtracting to construct our master term adjust much better the values of e_{1v} when we consider only 33 species in the interpolation than when we include all the 2149 nuclei. However, if we extrapolate the asymptotic behaviors given in Eq. (11) to other nuclei outside of the $Z = 50$ chain, we can observe large discrepancies between e_{1v} and its asymptotic behavior, as can be seen from Figure 3. There we compare the results for $e_{1v}(A_2 = -2/15) - e_{1v,asy}(A_2 = -2/15)$ in the complete interval of N .

CONCLUDING REMARKS

We have performed a detailed analysis of the master term in Duflo-Zuker inspired mass formulas. We have explored a polynomial dependence of the master term with shell degeneracies of the type $D_p^{-1/2} + A_2 D_p^{-1}$. We have compared the description of shell effects through the subtraction of the asymptotic behavior in the complete region of measured nuclei, with the corresponding one obtained for the species belonging to the chain with $Z = 50$. We have shown that, in spite of giving a better fit of the master term along the chain, the second behavior exhibit to much large departures for species outside that chain.

Our results set out an interesting point: which is the more convenient asymptotic form to properly describe shell effects? To answer this question, we remember that in our model we estimate the asymptotic master term for all the nuclei, in order that the

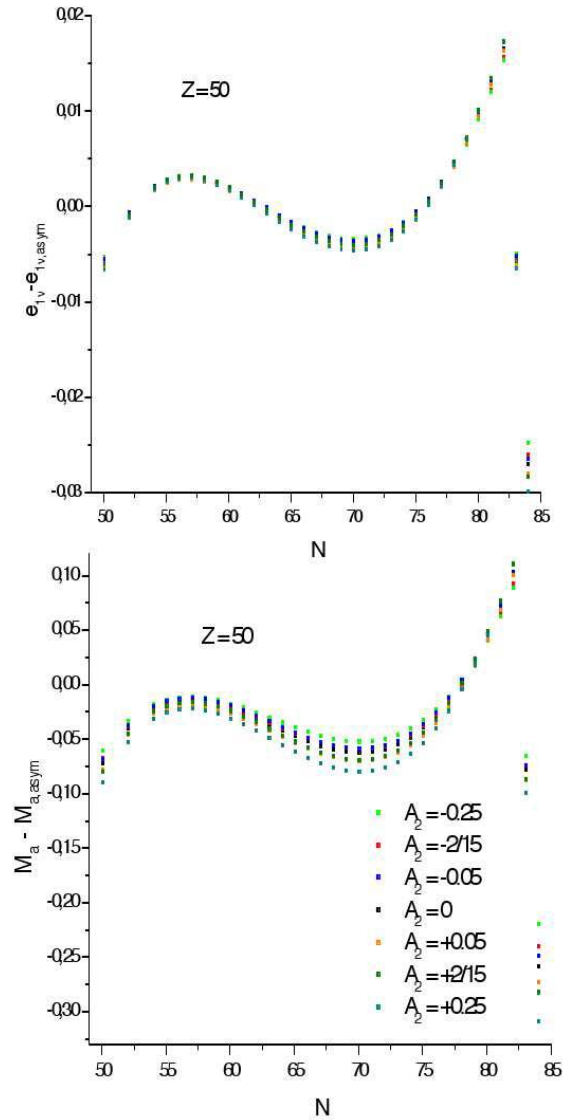


FIGURE 2. $e_{1V} - e_{1V,asym}$ and $\tilde{M}_a - \tilde{M}_{a,asym}$ for different values of the parameter A_2 , for the nuclei belonging to the $Z = 50$ tin chain (see text for explanation).

difference between the master and its asymptotic behavior give us the shell effects. By this reason, we do not prefer adjustments by smaller regions in N and Z . In fact, if we imagine an ideal scenario in which we can arrive to an asymptotic behavior which leads to a null difference between e_{1V} and $e_{1V,asym}$, all the shell effects will be erased from our model! This is not exactly our aim.

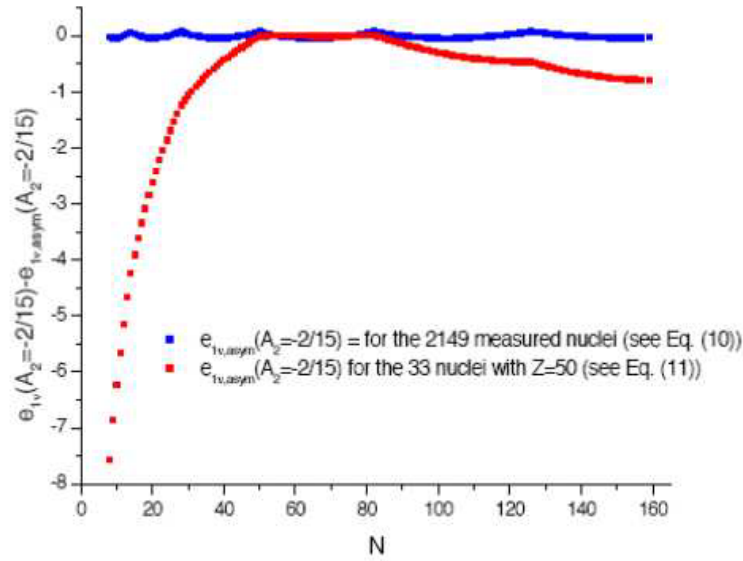


FIGURE 3. Comparison of $e_{1\nu}(A_2 = -2/15) - e_{1\nu,asym}(A_2 = -2/15)$ for two different asymptotic behaviors in the complete interval of N .

Anyway, from the present analysis we can conclude that futures efforts to improve the physics described by the master term should be performed.

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