Simple nuclear mass formula

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(Received 13 July 2013; revised manuscript received 19 October 2014; published 4 December 2014)

A simple formula for ground state nuclear masses based on the microscopic-macroscopic approach is proposed. Considering a set of 2353 nuclei with $Z \geqslant 8$ and $N \geqslant 8$, the formula yields an rms deviation of just 266 keV. A few applications, including the loosely bound proton rich nuclei, superheavy nuclei, and cluster emitters, are presented and discussed, establishing the reliability of the proposed formula. The present investigation has a major advantage: it allows one to reliably parametrize the fluctuating part of the ground state energy. This result is very interesting and important, since the fluctuating part of the energy is related directly to the trace formula, which in turn encodes the interaction itself.

DOI: 10.1103/PhysRevC.90.064306 PACS number(s): 21.10.Dr, 21.60.−n

I. INTRODUCTION

Systematization of the ground state nuclear masses has been a subject of interest for many decades. Models with different levels of sophistication and different flavors have been developed so far that yield excellent descriptions of the masses of nuclei spanning the entire periodic table [1–11]. Such investigations are crucial, since understanding of a number of physical phenomena such as the astrophysical r-processes depends on the ground state masses of the nuclei involved in them, which includes highly neutron rich species [12,13]. The recent advances in mass measurements (see, for example, [13–17]) have made it possible to determine masses of neutron rich as well as neutron deficient nuclei with high degree of precision. However, experimentally determining masses of all the nuclei of astrophysical interest may not be feasible in the near future. Therefore, one needs to rely on theoretical models for nuclear masses.

The nuclear mass models belong to two distinct categories, namely, (a) the microscopic models (see, for example, [7–9]) and (b) the microscopic-macroscopic (mic-mac) models [1–6,10,11]. In the present work, a simple mass formula, based on the ideas of the mic-mac approach, has been proposed. The mic-mac approach is developed in the next section. Applications of the proposed model are presented and discussed in the third section. The last section contains summary and conclusions.

II. FORMALISM AND DETERMINATION OF MODEL PARAMETERS

Consider a system of N neutrons and Z protons at zero temperature. Let A be the total number of particles in the system, that is, $A = N + Z$. According to Strutinsky's theorem [18], the ground state energy of a system of A particles can be written as sum of a "smooth" energy and an oscillatory term. This result has its roots in the fact that the quantal level density can be broken up into a smooth term that originates from the orbits of measure zero and an oscillatory term that originates from classical periodic orbits [18]. The smooth part is obtained, for instance, from the Thomas Fermi model or its extensions, whereas the determination of the oscillatory part falls in the domain of the semi-classical periodic orbit theory, leading to what are known as the trace formulas. There are a few Hamiltonians for which the trace formulas are known analytically [18]. A close examination of these reveal that the trace formulas (at zero temperature) are functions of the Fermi momentum (or the Fermi energy, as the case may be). In the case of nuclei, the situation is rather complicated for two reasons. The nucleon-nucleon interaction itself is enormously complex, and second, the nucleus is a very complex many-body self-bound system. Even if the interactions were known as precisely as one wishes, if would have been a formidable task to determine the corresponding trace formula.

The purpose of the present work is twofold: (a) to obtain an accurate and reliable mass formula within the mic-mac scheme and (b) to obtain information about the trace formula through reliable parametrization of the fluctuating part of the ground state energy, which in turn could be useful in deducing information about the interaction itself.

In the light of the Strutinsky's theorem stated above, the binding energy of a nucleus with N neutrons and Z proton can be expressed as

$$-E(N,Z) = E_{\mathrm{LDM}} + \delta E. \tag{1}$$

Note that by convention, the binding energy $E(N,Z)$ is a positive quantity. Here, E_{LDM} is the macroscopic part and the δE is the fluctuating part of the binding energy. The above expression does not include the extra binding energy due to electrons.

The calculation proceeds in two steps. In the first step, the smooth part of the total binding energy has been separated out. This is done within the framework of the liquid drop model. Following the literature [11,19], it is taken to be the sum of a volume term (with an isospin dependence), a surface term, a Coulomb term, the term representing correction to Coulomb energy due to surface diffuseness, and finally the pairing energy. Thus, the liquid drop formula assumed in the

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present work reads

$$E_{\rm LDM} = a_v\left[1+\frac{4k_v}{A^2}T_z(T_z+1)\right]A + a_s\left[1+\frac{4k_s}{A^2}T_z(T_z+1)\right]A^{2/3} + \frac{3Z^2e^2}{5r_0A^{1/3}} + \frac{C_4Z^2}{A} + E_p. \quad (2)$$

Here, T_z is the third component of isospin and e is the electronic charge. The coefficients a_v (volume energy), k_v (isospin dependence of volume energy), a_s (surface energy), k_s (isospin dependence of surface energy), r_0 (Coulomb radius), and C_4 (correction to Coulomb energy due to surface diffuseness) are treated as free parameters. Explicitly, the (smooth) pairing energy is given by [20]

$$\begin{aligned} E_p &= \frac{d_n}{N^{1/3}}, \quad \text{for} \quad N \text{ odd and } Z \text{ even},\\ &= \frac{d_p}{Z^{1/3}}, \quad \text{for} \quad Z \text{ odd and } N \text{ even},\\ &= \frac{d_n}{N^{1/3}} + \frac{d_p}{Z^{1/3}} + \frac{d_{np}}{A^{2/3}}, \quad \text{for} \quad Z \text{ and } N \text{ odd},\\ &= 0, \quad \text{for} \quad Z \text{ and } N \text{ even}. \end{aligned} \quad (3)$$

The constants d_n, d_p, and d_{np} are treated as free parameters. The free parameters of the liquid drop formula are obtained by χ^2 minimization of nuclear binding energies, considering a set of 2353 nuclei with $Z \geqslant 8$ and $N \geqslant 8$:

$$\chi^2 = \sum_{j=1}^{N}\left[\frac{E^{(j)}_{\rm expt} - E(N_j,Z_j)}{\Delta E^{(j)}_{\rm expt}}\right]^2, \quad (4)$$

where $E(N_j,Z_j)$ is the calculated total binding energy for the given nucleus and $E^{(j)}_{\rm expt}$ is the corresponding experimental value [21]. The experimental uncertainty $\Delta E^{(j)}_{\rm expt}$, for the sake of simplicity, is assumed to be 0.007 MeV for all the nuclei [see the discussion following Eq. (8)]. The values of the coefficients thus obtained are $a_v = -15.505$ MeV; $a_s = 17.830$ MeV; $k_v = -1.825$; $k_s = -2.265$; $r_0 = 1.215$ fm; $C_4 = 1.297$ MeV; $d_n = 4.687$ MeV; $d_p = 4.717$ MeV; and $d_{np} = -6.495$ MeV. The rms deviation obtained for the fit, as expected [1], is 2.456 MeV. The difference ΔE between the experimental and the corresponding calculated binding energies is plotted in Fig. 1. It is clearly seen that the difference is large and negative for doubly closed shell nuclei. In the present work, it is this difference that is identified with the fluctuating part of the binding energy, δE. The values of the fluctuations are seen to be dependent on the proximity of a given particle number to the shell closures.

As argued earlier, the fluctuations are linked to the trace formulas and hence should be functions of the Fermi momentum. Thus, in addition to the proximity to shell closures, δE is also expected to be a function of $N^{1/3}$ and $Z^{1/3}$. Based on these arguments, the following ansatz for δE is proposed:

$$\delta E(\vec{x}) = \sum_{\vec{k}=\vec{0}}^{\vec{M}}\left\{a_{\vec{k}}\cos\left(2\pi\frac{\vec{x}\cdot\vec{k}}{M}\right) + b_{\vec{k}}\sin\left(2\pi\frac{\vec{x}\cdot\vec{k}}{M}\right)\right\}, \quad (5)$$

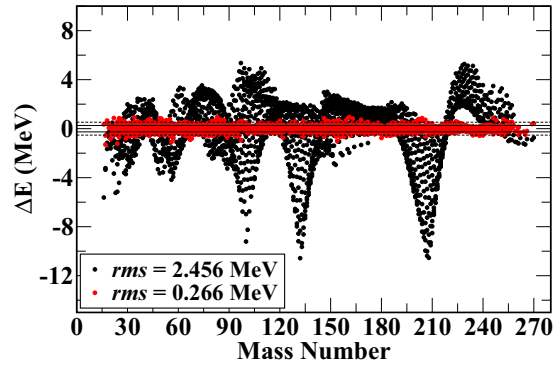

FIG. 1. (Color online) Difference between the calculated and the experimental [21] binding energies.

where $\vec{k} \equiv (k_1,k_2,k_3,k_4)$, with $0 \leqslant k_i \leqslant M$ for $i = 1, 2, 3, 4$. The vector $\vec{x} \equiv (x_1,x_2,x_3,x_4)$ stands for

$$x_1 = \beta_1\left|\frac{N-N_o}{N}\right|, \quad x_2 = \beta_2\left|\frac{Z-Z_o}{Z}\right|, \quad x_3 = \beta_3 N^{1/3}, \quad x_4 = \beta_4 Z^{1/3}. \quad (6)$$

Here, N_o and Z_o are suitable magic numbers, assumed to be (a) 8, 20, 50, 82 and 126 for protons and (b) 8, 20, 50, 82, 126 and 184 for neutrons. The magic number N_o (Z_o) is determined by demanding it to be the closest to the given N (Z). The factors β_1, β_2, β_3, and β_4 are constants. Thus, the first two variables describe the proximity of a given N or Z to a shell closure. The variables x_3 and x_4 are proportional to the Fermi momenta. In the language of Fourier transforms, the expression above can be viewed as

$$\delta E(\vec{x}) = {\rm Re}\sum_{\vec{k}} \alpha_{\vec{k}} e^{-2i\pi\vec{x}\cdot\vec{k}/M}. \quad (7)$$

The coefficients $a_{\vec{k}}$ and $b_{\vec{k}}$, at least in principle, should be determined from the knowledge of nuclear interaction. The nucleon-nucleon interaction, though well parametrized (see, for example, [22]), is not yet known exactly. Even if the interaction was known exactly, due to the complex many-body nature of the nucleus, it would have been a formidable task to determine these coefficients. Here, an "inverse" problem is attempted, in which these coefficients are treated as free parameters. These are then determined from the known values of δE for the set of 2353 nuclei. The number of parameters in such cases becomes quite large ($2M^4 + 4$). However, in practice, this number can be reduced dramatically by realizing that it is not necessary to extend the summations over all k_i to M. Explicitly, Eq. (5) is expressed as

$$\delta E(\vec{x}) = \sum_{k_1=0}^{M}\sum_{k_2=0}^{M-k_1}\sum_{k_3=0}^{M-k_1-k_2}\sum_{k_4=0}^{M-k_1-k_2-k_3}\left\{a_{\vec{k}}\cos\left(2\pi\frac{\vec{x}\cdot\vec{k}}{M}\right) + b_{\vec{k}}\sin\left(2\pi\frac{\vec{x}\cdot\vec{k}}{M}\right)\right\}, \quad (8)$$

which reduces the number of parameters to $2(M+1)(M+2)(M+3)(M+4)/4! + 4$. Finally, since the average of δE is almost zero, in the above summation, the term with

$\vec{k} \equiv (0,0,0,0)$ is dropped, thereby reducing the number of parameters by 2. Here, the value of M is taken to be 4. With this choice, the total number of free parameters becomes 142, which is still large, but considering the complexity of the problem and the number of data points to be fitted to (2353), the number is still quite reasonable, 6% of the total number of data points.

Least squares minimization is carried out using the well-known Levenberg-Marquardt (LM) algorithm [23,24] to determine these parameters. The LM algorithm is a Newton-type algorithm, which carries out linearization in a neighborhood of the current approximation. This neighborhood is known as the "trust region." The LM procedure is known to be quite robust, and has also been extended to the "ill posed" problems [25]. The NETLIB implementation [26] of the LM algorithm has been employed here, which has a lot better control over the so-called LM parameter [24] used in it. This makes the program more stable and dependable. It should be noted that the present ansatz is linear in 138 parameters, whereas the four parameters appearing within the sinusoids make the problem somewhat nonlinear. However, it turns out that these four parameters are fairly robust and have numerical values around 4 for β_1 and between 1.5 and 2.5 for the rest. The initial guess values of β have been chosen to be $\sim$2. For the remaining parameters, initial values around 0.01 seem to be satisfactory. The fit thus obtained yields the mean squared deviation of just 266 keV, which is indeed encouraging. As a comparison, the Möller-Nix mass formula [5] has a reported mean squared deviation of 676 keV, Duflo-Zuker mass formula [3,4] has a mean squared deviation of 373 keV, whereas the recently reported formula due to Liu *et al.* [10] has rms deviation of merely 336 keV.

The values of parameters and a routine to generate the δE have been provided in the Supplemental Material [27]. The fit has been tested by slightly changing the initial guess values of these parameters, leading to results of similar qualities. The fitted and the corresponding binding energies have also been listed in the Supplemental Material [27].

In principle the analysis should be carried out with the experimental error bars included. However, the individual masses and hence the binding energies have widely varying error bars associated with them. These range from $\sim$eV to several tens of keV or even more. A χ^2 minimization with error bars with such variations is very difficult to carry out. In the present analysis, for the sake of simplicity, a constant error of 0.007 MeV has been assumed for all the nuclei, which corresponds to the median of the errors for all the measured masses. In order to make the error estimation, the variance-covariance matrix has been worked out by inverting the Hessian matrix by employing suitable NETLIB routines [26]. The positive definiteness of the resulting variance-covariance matrix has been explicitly verified by determining all the eigenvalues of the same. The square root of the diagonal elements of the matrix yields errors on the individual parameters, which turn out to be small for most of the parameters in the present case (refer to [27] for the detailed error bars on the parameters). This observation implies that the parameters are indeed well determined. The statistical error bars on the calculated masses have been estimated again from the variance-covariance matrix. The resulting statistical uncertainties turn out to be of the order of a few keV in most of the cases, indicating that the fit indeed is dependable. Further, it has been verified that the statistical uncertainty remains at a few keV level for entire isotopic chains throughout the periodic table.

In a model where the parameters have been fitted by using χ^2 minimization, goodness of fit is usually judged from the explicit value of the χ^2 per degree of freedom. As seen from Eq. (4) above, a small value of $\Delta E^j_{\rm expt}$ even for a single j case may produce a huge χ^2. The χ^2 per degree of freedom in the present context (assuming that the "experimental" errors are 0.007 MeV for all the nuclei), turns out to be $\sim$1540, indeed a large number. Ideally, for a model to be good, the χ^2 per degree of freedom is expected to be of the order of 1. Interestingly, the Möller-Nix mass model, for the same set of 2353 nuclei considered here and with the experimental errors assumed to be 0.007 MeV, yields a χ^2 per degree of freedom of the order of 8000. This is about 5 times larger than that obtained for the present model. However, the Möller-Nix model is known for its excellent ability to extrapolate and hence considered to be a reliable mass model. This apparently paradoxical situation can be understood easily if one realizes that the experimental error bars on the measured masses are usually very small (could be as small as 1 eV) [21], and the models do not predict the masses with that small an rms deviation. Therefore, it is best to judge reliability of a mass model by its ability to extrapolate as well as the statistical errors on the calculated binding energies.

As indicated above, one of the aims of this work is to obtain information about the trace formula. As is well known (see, for example, [18]), the level density for a system is related to energy through an inverse Laplace transform. In the present case, the variables involved are essentially discrete, and at least in principle, the level density can be obtained from δE through a multi-dimensional Z transform [28]. Given that the fit that has been obtained is reliable and accurate, the proposed analysis is expected to be dependable. Uniqueness of such an inversion is guaranteed by Lerch's theorem, according to which if two functions have the same integral transforms, then they could differ at the most by a null function (see, for example, [29]). This ensures that the resulting level density will be reliable. A detailed investigation along these lines is underway and will be reported in due course.

The expansion in Eq. (8) has been tested for convergence, and it is found that the choice $M = 4$ is optimal. The liquid drop energy and δE together define the ground state binding energy of a nucleus with N neutrons and Z protons completely. The difference between the experimental [21] and the corresponding calculated binding energies is shown in Fig. 1 as red stars. An important feature of this figure is that there are practically no fluctuations remaining in ΔE. This has been substantiated by working out the running averages of the ΔE values, and it turns out that the running averages become zero quickly with the subset size. A closer inspection of the parameters obtained reveals that some of them do have rather small numerical values, and therefore, one may think of dropping them from the analysis. However, one needs to be cautious, since this might lead to the introduction of uncontrollable correlations among the remaining parameters.

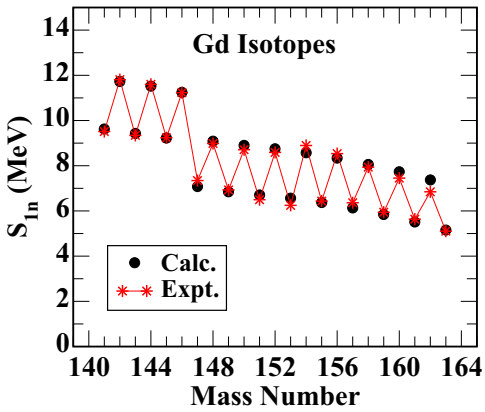

FIG. 2. (Color online) Calculated and experimental S_{1n} values [21] for Gd isotopes.

III. RESULTS AND DISCUSSION

A number of tests have been carried out to examine the validity of the proposed model. In particular, here, the investigations of (a) single and two neutron separation energies, (b) α-decay Q values for nuclei in the Sn region as well as superheavy nuclei, and (c) cluster decay Q values of heavy nuclei have been reported. All these observables are obtained by taking differences between the suitable binding energies, and hence they impose a stringent test of the validity of the proposed model.

The one and two neutron separation energies (S_{1n} and S_{2n}) are calculated for all the 2353 nuclei and are compared with the experimental values (where available). The calculations are found to be in excellent agreement with the experiment. It is found that the rms deviation in S_{1n} (S_{2n}) with respect to the experiment is merely 277 keV (269 keV), which is in tune with the rms deviation of the mass formula. As an example, the calculated and experimental one and two neutron separation energies for Gd isotopes have been plotted in Figs. 2 and 3. The excellent agreement between the two is amply clear from the figures.

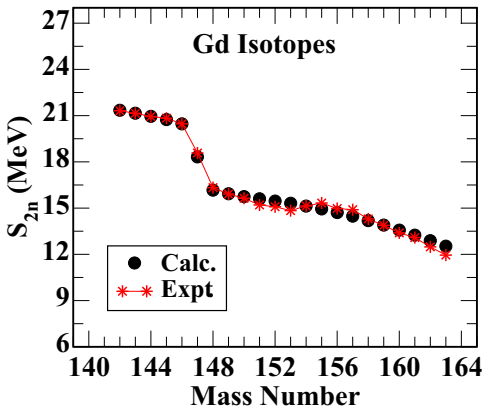

FIG. 3. (Color online) Calculated and experimental S_{2n} values [21] for Gd isotopes.

TABLE I. Calculated and experimental S_{1p} for proton rich nuclei. The uncertainties in the calculated and the experimental separation energies have also been indicated in parentheses. Throughout this paper, error bars have been represented in parentheses. For example, 2.561 (3) stands for 2.561±0.003.

	S_p (MeV)			S_p (MeV)	
	Calc.	Expt.		Calc.	Expt.
^{63}Ge	2.561 (3)	2.210 (46)	^{67}Se	2.354 (4)	1.852 (74)
^{65}As	−0.179 (3)	−0.090 (85)	^{71}Kr	1.876 (6)	2.184 (142)

Similar remarks hold even for proton separation energies. As an example, the calculated and the corresponding experimental one proton separation energies S_p for the recently measured highly neutron deficient nuclei [30] are presented in Table I. It is found that the model predicts the separation energies to a good degree of accuracy. In particular, the proton drip line at ^{65}As is reproduced by the model, indicating that the model seems to be working well even for the exotic nuclei.

Investigations of the structure and decay properties of neutron deficient nuclei in the Sn region is of current interest. Here, the α-decay properties of a few Xe isotopes have been presented as illustrative examples. The calculated and corresponding experimental [31] α-decay Q values for Xe isotopes are presented in Table II. It is found that the calculations are very close to the experimental values. Even the small Q values are reproduced accurately, indicating the reliability of the model in that region. In particular, the model predicts ^{134}Xe to be only very slightly bound against α decay (with a Q value of 9 keV) which is well within the limits obtained experimentally (-20 ± 40 keV).

Next, the α-decay Q values of the superheavy nuclei are investigated. The experimental as well as theoretical investigations of superheavy nuclei is of current interest and is important in a number of respects. For instance, it attempts to answer a crucial question: is there an upper bound on the periodic table. In addition, description of superheavy nuclei is a challenge to the nuclear models, since comparatively little is known about the superheavy region. Here, the calculated α-decay Q values of the decay chains of two of the superheavy nuclei, ^{294}118 and ^{293}116, and also for the nucleus ^{288}115 are presented. The calculated Q values

TABLE II. Calculated and experimental Q values for α decay of a few Xe isotopes. The uncertainties in the calculated and experimental Q values have also been indicated.

Parent	Q_{calc}	Q_{expt}
^{110}Xe	3.995 (3)	3.885 (14)
^{112}Xe	3.376 (2)	3.330 (6)
^{114}Xe	2.802 (2)	2.770 (50)
^{116}Xe	2.152 (2)	1.830 (170)
^{118}Xe	1.482 (2)	1.380 (30)
^{120}Xe	0.933 (2)	0.670 (30)
^{138}Xe	0.009 (2)	−0.020 (40)

TABLE III. Calculated and experimental Q values for α decay of some of the heaviest superheavy nuclei. The uncertainties in the calculated Q values have also been indicated.

Z	A	Q_{calc}	Q_{expt}	Z	A	Q_{calc}	Q_{expt}
118	294	11.714 (34)	11.81	115	288	10.629 (21)	10.61
116	290	10.988 (25)	10.80	113	284	9.971 (15)	10.15
114	286	10.299 (18)	10.33	111	280	9.399 (10)	9.87
112	282	9.681 (12)	<10.69	109	276	8.940 (7)	9.85
116	293	10.683 (29)	10.69	107	272	8.611 (8)	9.15
114	289	9.969 (20)	9.96	105	268	8.256 (8)	<7.83
112	285	9.311 (14)	9.28				
110	281	8.736 (9)	<9.00				

are listed in Table III along with the experimental data [32]. The agreement between the two is found to be quite satisfactory, indicating that the proposed mass formula has good extrapolatability.

Finally, the Q values for cluster radioactivity are presented and discussed. The existence of cluster radioactivity (heavier than ^{4}He) was predicted by Sandulescu, Poenaru, and Greiner [33], which was confirmed later experimentally by Rose and Jones [34]. So far, the lightest cluster emitter is known to be ^{114}Ba, which decays by emitting ^{12}C to ^{102}Sn, and the heaviest cluster emitter is ^{242}Cm, which decays to ^{208}Pb by emitting ^{34}Si. It has recently been pointed out [35] that the cluster emission mode could be appreciable (with probabilities larger than that of the α-decay mode by several orders of magnitude) in certain regions of the yet undetected superheavy nuclei, thereby making the cluster emission mode an important tool for identifying and studying the superheavy nuclei. These predictions depend crucially on the reliability of the Q values involved. As in the case of α decay of superheavy nuclei, accurate prediction of cluster decay Q values poses a challenge to the theoretical models, since the Q values are obtained by taking the difference between the relevant binding energies. The calculated and the experimental [36] Q values of a few cluster emission processes are presented in Table IV. The calculated Q values are found to be very close to the experimental data, underlining the reliability of the proposed mass formula.

In addition, binding energies for all 8979 nuclei listed in the Möller-Nix tables [6] have been computed. These, along with the corresponding Möller-Nix values can be found in the Supplemental Material [27]. It can be seen that the two agree with each other closely. However, particularly in the case of extremely neutron rich regions, there are differences. Furthermore the drip lines predicted by the present model seem to be reasonable and are similar to those predicted by the Möller-Nix model.

TABLE IV. Calculated and corresponding experimental [36] cluster decay Q values. The uncertainties on the calculated Q values have also been indicated.

Parent	Daughter	Cluster	Q values (MeV)	
			Calc.	Expt.
^{114}Ba	^{102}Sn	^{12}C	19.195 (4)	18.3–20.5
^{223}Ra	^{209}Pb	^{14}C	32.299 (2)	31.85
^{228}Th	^{208}Pb	^{20}O	45.154 (5)	44.72
^{231}Pa	^{208}Pb	^{23}F	51.898 (5)	51.84
^{230}U	^{208}Pb	^{22}Ne	61.724 (4)	61.40
^{230}Th	^{206}Hg	^{24}Ne	58.011 (4)	57.78
^{233}U	^{208}Pb	^{25}Ne	61.424 (4)	60.75
^{232}U	^{204}Hg	^{28}Mg	74.055 (3)	74.32
^{235}U	^{206}Hg	^{29}Mg	72.523 (4)	72.61
^{236}U	^{206}Hg	^{30}Mg	72.471 (3)	72.51
^{238}Pu	^{206}Hg	^{32}Si	91.424 (4)	91.21
^{242}Cm	^{208}Pb	^{34}Si	96.469 (5)	96.53

IV. SUMMARY AND CONCLUSIONS

In summary, a simple mass formula based on the ideas of trace formulas is proposed. The formula yields an rms deviation of just 266 keV, which, as far as the author knows, is one of the smallest deviations reported in the literature. The reliability of the formula is demonstrated through a number of illustrative examples, spanning the entire periodic table. The ability of the formula of reliable extrapolation is also indicated. The analysis of the variance-covariance matrix establishes that the results are dependable within a few keV. The present work, in addition to the accurate description of nuclear masses, indicates that the fluctuating part of the total ground state energy of a nucleus can be accurately parametrized. The implications of this simple result could be significant, since the fluctuating part of the energy is ultimately related to the trace formulas and hence the nuclear interaction itself. Further investigations along these lines are in progress. The formalism presented here is very simple, and so is the corresponding FORTRAN code, which can be found in the Supplemental Material [27].

ACKNOWLEDGMENTS

The author is thankful to Roberto Liotta and Y. K. Gambhir for a number of very fruitful discussions, encouragement, and support. The author thanks X. Viñas, M. Centelles, P. Schuck, and R. Wyss for their interest in this work. Partial financial support from the Department of Science and Technology, Government of India (Grant No. SR/S2/HEP-34/2009) and the Swedish National Research Council (VR) is gratefully acknowledged. The author thanks the KTH Nuclear Physics group for their kind hospitality.

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