

Global Mass Formula with Shell Corrections Based on Wigner-Kirkwood Method: an Overview

A. Bhagwat^{1,*}, X. Viñas², M. Centelles², P. Schuck^{3,4}, and R. Wyss⁵

¹*Dept. of Physics, IIT Gandhinagar, 382424 Ahmedabad, INDIA*

²*Departament d'Estructura i Constituents de la Matèria and Institut de Ciències del Cosmos,
Facultat de Física, Universitat de Barcelona,
Diagonal 647, E-08028 Barcelona, SPAIN*

³*Institut de Physique Nucléaire, IN2P3-CNRS,*

Université Paris-Sud, F-91406 Orsay-Cédex, FRANCE

⁴*Laboratoire de Physique et Modélisation des Milieux Condensés,
CNRS and Université Joseph Fourier, 25 Avenue des Martyrs,
Boîte Postale 166, F-38042 Grenoble Cedex 9, FRANCE and*

⁵*KTH (Royal Institute of Technology), Alba Nova University Center,
Department of Nuclear Physics, S-10691 Stockholm, SWEDEN*

Study of nuclear masses and their systematics is of great importance. Accurate knowledge of the nuclear masses plays a decisive role in the reliable description of processes like the astrophysical r-process. Considerable progress has already been achieved in the accurate prediction of the masses, and it is still being pursued vigorously by a number of groups around the globe. There are primarily two distinct approaches to calculate nuclear masses: the microscopic nuclear models based on density functional theory, like Skyrme Hartree Fock Bogoliubov or Relativistic Mean Field models, and the macroscopic - microscopic (Mic - Mac) models. Here, we report the mass calculation based on the Mic - Mac approach. According to the Mic - Mac approach, mass of a nucleus is written as sum of Macroscopic part (liquid drop) and a microscopic part, which comprises of shell correction and pairing energies. Here, the semi-classical Wigner - Kirkwood (WK) \hbar expansion method is used to calculate shell corrections for spherical and deformed nuclei. The expansion is achieved upto the fourth order in \hbar . The pairing energies are obtained by using the Lipkin - Nogami scheme. The macroscopic part is obtained from a liquid drop formula, with six adjustable parameters. These parameters are adjusted to reproduce experimental masses of 367 spherical nuclei, which yields a *rms* deviation of 630 keV. It is shown that the approach based on WK expansion can be reliably used for accurate prediction of nuclear masses.

1. Introduction

With the advent of mass spectrometry, it is now a days possible to measure masses of short lives nuclei with great precision [1, 2]. For example, the ISOL based mass analyser for superheavy atoms (MASHA) [3, 4] developed at JINR-Dubna is expected to measure masses of the separated atoms in the range $112 \leq 120$, the shortest measurable half life being ~ 1 s [3]. The JYFLTRAP [5] developed at University of Jyväskylä, enables measurement of highly neutron deficient nuclei upto mass

numbers ~ 120 , with high precision.

On the theoretical front as well, a number of groups around the world are actively involved in developing nuclear mass formulas. Primarily, two distinct approaches are adopted for this purpose, namely, the microscopic approach, based on density functional theory, like the Skyrme Hartree - Fock - Bogoliubov [6] or Relativistic Mean field models [7] and the microscopic - macroscopic (Mic - Mac) approach [8–12]. These different models agree with each other, and with the experimental binding energies [13], however, differ widely in the regions where, the mass measurements are not available yet, implying that the extrapolation of nuclear masses is still a chal-

*Electronic address: ameeya@kth.se

lenge. Particularly, for proper understanding of the astrophysical r - processes, one needs to know masses of all the nuclei, containing 30 or so neutrons more than the heaviest measured isotope of the same element. Thus, in such cases, one has to rely on theoretical mass formulas. Therefore, the development of dependable mass formulas is relevant, and important.

In the present work, we shall be discussing the Mic - Mac approach with shell corrections obtained by using the semi - classical Wigner - Kirkwood expansion [16–23].

2. Formulation

The microscopic - macroscopic models are based on the well - known Strutinsky theorem, according to which, the nuclear binding energy (E) can be written as sum of a smooth part (E_{LDM}), and an oscillatory part (δE).

$$E = E_{LDM} + \delta E \quad (1)$$

The smooth part is adopted from the traditional liquid drop or droplet formulas. The oscillatory part is made of pairing energy and shell correction. The shell correction is calculated by taking difference between quantum mechanical energy of the system and the corresponding averaged energy. The latter is usually obtained within the framework of the Strutinsky smoothing scheme [14, 15]. The Strutinsky smoothing scheme runs into practical difficulties, particularly for finite potentials, since, in this smoothing scheme, one needs to incorporate single particle spectrum with cut off well above ($\sim 3\hbar\omega$) the Fermi energy. For realistic potentials, the continuum may begin within $\hbar\omega$ of Fermi energy. This problem is tackled in practice, by discretising the continuum by diagonalising the Hamiltonian in a basis of suitable dimension. The problem becomes more serious, particularly for neutron rich and neutron deficient nuclei, since the Fermi level in these cases may lay close to continuum.

The semi classical Wigner Kirkwood averaging scheme [16–23], on the other hand, does not use the single particle spectrum at all. Instead, the smoothing is achieved by expanding the quantal partition function, in powers

of Planck's constant, \hbar . In the present work, we employ the Wigner - Kirkwood expansion, upto the fourth order in \hbar , for a system of nucleons at zero temperature, with deformation parameters β_2 , β_4 and γ . For further details, see Ref. [12].

As stated earlier, the microscopic part of the binding energy is made of the shell correction and the pairing energy. In the present work, the shell corrections are obtained by taking difference between the quantum mechanical energy of the system and the corresponding Wigner - Kirkwood energy. The quantum mechanical energy is obtained by diagonalising the Hamiltonian in the harmonic oscillator basis, with 15 shells. The potential required here, is chosen to be of Woods - Saxon type, with parameters determined by reproducing experimental single particle energies of some of the doubly magic nuclei [12]. The Coulomb potential is obtained by folding the nuclear charge density with Coulomb interaction. The charge density, for simplicity, is assumed to be of Woods - Saxon form, with the radius and diffuseness parameters taken to be the same as that for the corresponding nuclear potential for protons [12]. The pairing energy is calculated by using the well - established Lipkin - Nogami scheme [24–26].

Here, we use a simple liquid drop model, with six adjustable parameters. Explicitly,

$$\begin{aligned} E_{LDM} = & a_v \left[1 + \frac{4k_v}{A^2} T_z (T_z + 1) \right] A \\ & + a_s \left[1 + \frac{4k_s}{A^2} T_z (T_z + 1) \right] A^{2/3} \\ & + \frac{3Z^2 e^2}{5r_0 A^{1/3}} + \frac{C_4 Z^2}{A}, \end{aligned} \quad (2)$$

where the terms respectively represent: volume energy, surface energy, Coulomb energy and correction to Coulomb energy due to surface diffuseness of charge distribution. The coefficients a_v , a_s , k_v , k_s , r_0 and C_4 are free parameters; T_z is the third component of isospin, and e is the electronic charge. The free parameters are obtained by χ^2 minimisation, with experimental binding energies taken from Audi - Wapstra evaluation [13].

3. Results and Discussions

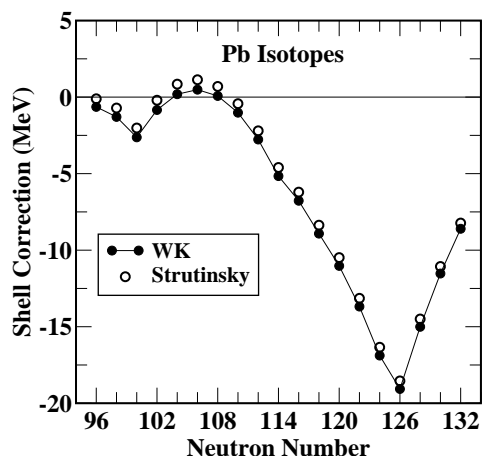


FIG. 1: The WK and Strutinsky shell corrections for Pb isotopes.

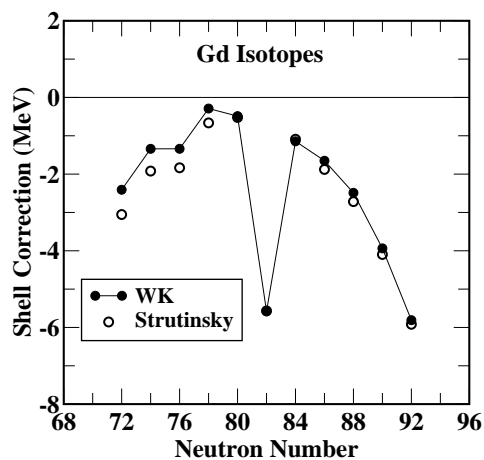


FIG. 2: The WK and Strutinsky shell corrections for Gd isotopes.

First, we compare the shell corrections obtained for chain of lead isotopes (spherical) and Gadolinium isotopes (deformed) with those obtained from the conventional Strutinsky smoothing scheme (see [12] for details).

The calculated and the corresponding Strutinsky values of shell corrections for Pb and Gd isotopes are presented in in Figs. (1) and (2). It is seen that the shell corrections

reach a minimum at neutron numbers 126 and 82, as expected. The WK values of shell corrections are similar to those of the Strutinsky method. At a finer level, however, they do differ from each other. The differences change as a function of neutron excess or deficiency.

In the present study, we have considered a set of 367 nuclei, expected to be spherical [27]. The 6 liquid drop parameters described above are fitted to reproduce the experimental binding energies of these nuclei. The liquid drop parameters thus obtained, are: $a_v = -15.841$ (MeV), $a_s = 19.173$ (MeV), $k_v = -1.951$, $k_S = -2.577$, $r_0 = 1.187$ (fm) and $C_4 = 1.247$ (MeV). The *rms* deviation in the binding energies obtained here, turns out to be 630 keV. The corresponding deviation in the Möller - Nix framework is 741 keV [8, 9].

As representative cases, we next plot the difference between the calculated and the corresponding experimental values of binding energies for Ca, Ti and Pb isotopes in Figs. (3) and (4) respectively.

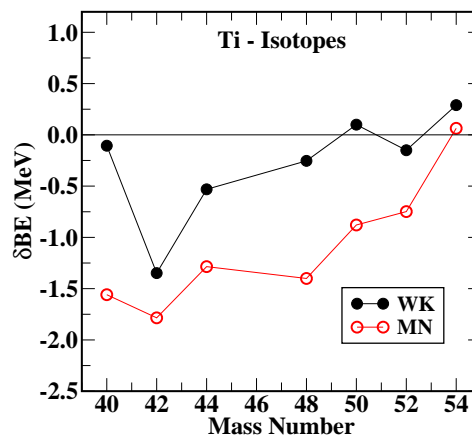


FIG. 3: The difference between the calculated and the corresponding experimental binding energies for Ti isotopes (denoted by WK). The corresponding differences for Möller - Nix mass formula (MN) are also presented for comparison.

It is amply clear from these figures that the present calculations agree very well with the experimental binding energies. The differences between the calculated and the experimental values vary smoothly as a function of

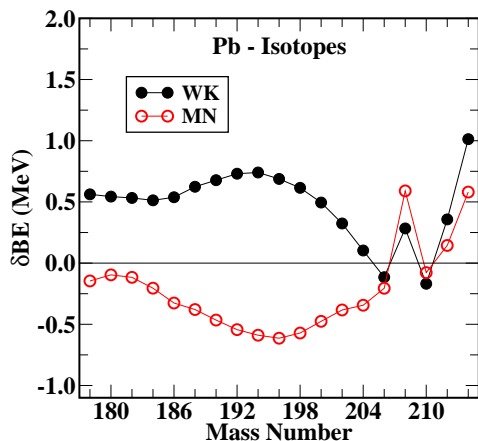


FIG. 4: Same as Fig. (3), but for Pb isotopes.

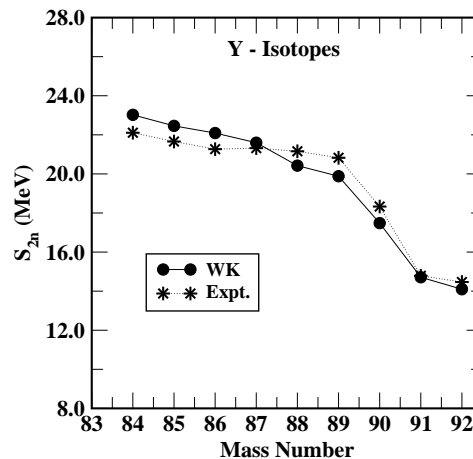


FIG. 6: The calculated (WK) and the corresponding experimental [13] two neutron separation energies for Y isotopes.

mass number.

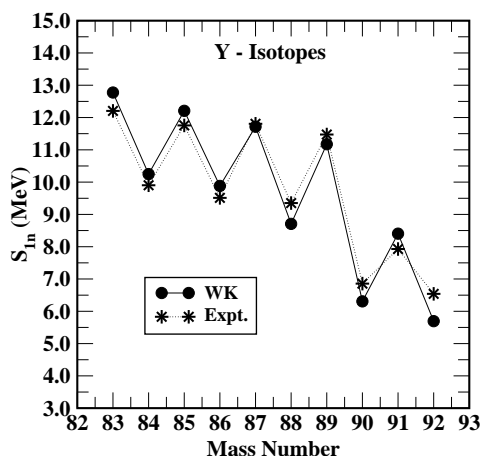


FIG. 5: The calculated (WK) and the corresponding experimental [13] single neutron separation energies for Y isotopes.

The single and two neutron separation energies are next investigated. As representative cases, we here present the results for chains of Y and Tl isotopes in Figs. (5-8). It is seen that the expected odd - even staggering in the single neutron separation energies is well reproduced in the present calculations, both for Y and Tl isotopes. The two neutron separation energies, too, are well reproduced, indicating that the mass formula proposed in the

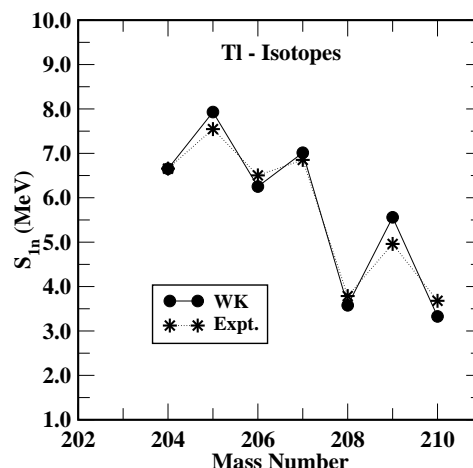


FIG. 7: The calculated (WK) and the corresponding experimental [13] single neutron separation energies for Tl isotopes.

present work, indeed, is reliable.

4. Summary

In the present work, the mass calculations based on the Mic - Mac approach are reported. The shell corrections are obtained by using the semi - classical Wigner - Kirkwood averaging technique. The expansion is achieved upto the fourth order in \hbar , for a system of nucleons at

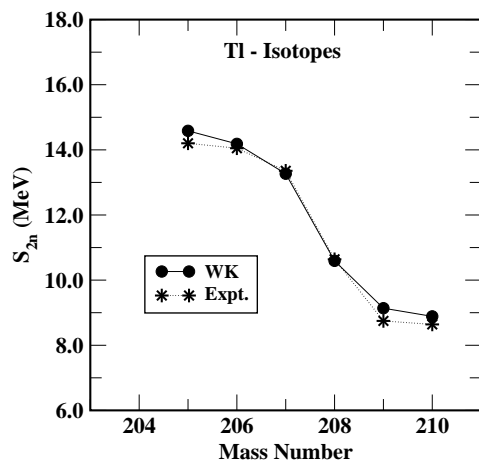


FIG. 8: The calculated (WK) and the corresponding experimental [13] two neutron separation energies for Tl isotopes.

zero temperature, with deformation parameters β_2 , β_4 and γ . The pairing energies, essential for reliable description of the open shell nuclei, are obtained within the framework of the Lipkin - Nogami scheme. The liquid drop formula with six adjustable parameters is employed. These six parameters are obtained by chi square fit to the experimental binding energies of the 367 spherical nuclei. It is found that the present mass formula yields *rms* deviation of just 630 keV, indicating its reliability.

Acknowledgments

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