Microscopic - Macroscopic Mass Calculations with Wigner - Kirkwood expansion

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Abstract. The systematic study and calculation of ground state nuclear masses continues to be one of the active and important areas of research in nuclear physics. The present work is an attempt to determine the ground state masses of nuclei spanning the entire periodic table, using the Microscopic - Macroscopic approach. The semi - classical Wigner - Kirkwood (WK) $\hbar$ expansion method is used to calculate shell corrections for spherical and deformed nuclei. The expansion is achieved up to the fourth order in $\hbar$. The shell corrections, along with the pairing energies obtained by using the Lipkin - Nogami scheme, constitute the microscopic part of the nuclear masses. The macroscopic part is obtained from a liquid drop formula with six adjustable parameters. It is shown that the Microscopic - Macroscopic mass calculation thus achieved, yields reliable description of ground state masses of nuclei across the periodic table. The present status of the WK mass calculations and the possible future perspectives are discussed.

1. Introduction

Theoretical determination of ground state nuclear masses has been an active research area from the very early days of nuclear structure physics. These activities have become even more relevant, since it is now possible to produce and study the neutron rich and deficient nuclei spanning the entire periodic table. Besides, reliable description of the processes like the astrophysical $r$-process requires accurate knowledge of the masses of the highly neutron rich nuclei. Even with the recent experimental developments, these nuclei are still inaccessible, and one is compelled to rely on theoretical models for the masses.

A large number of models with varying degree of sophistication for the determination of nuclear masses are available in the literature. Generically, they are known as the ‘mass formulas’. In this work, we report a mass formula, within the microscopic - macroscopic (often called ‘Mic - Mac’) framework. The Mic - Mac formulas are based on the Strutinsky’s theorem, according to which, the binding energy of a given nucleus can be written as sum of a smooth part, and an oscillatory part. Most of the Mic - Mac mass formulas available in the literature differ from...
each other only in the macro part, which is adopted from the Liquid Drop formula. The micro part, almost always is computed using the well-known Strutinsky smoothing scheme. The Strutinsky smoothing scheme, amounts to convolution of single particle spectrum over a given energy interval. The energy interval, in practice, is required to be wide enough, typically a few $\hbar \omega$, to ensure that the fluctuations are washed out. This implies, that for a practical Strutinsky calculation, one needs to include the continuum as well. The problem becomes more serious, particularly for the neutron rich or deficient nuclei, where, the Fermi state may lie close to the continuum itself. The smoothing based on Wigner Kirkwood averaging, on the other hand, is free from this difficulty, since there, one does not require a knowledge of single particle spectrum. This motivates us to explore the possibility of employing the Wigner-Kirkwood expansion technique to determine the smooth part of the energy, and hence the shell corrections.

We shall develop the essential formalism in the second section. The third section contains some of the representative results. The fourth section contains the summary and future outlook.

2. Formalism
As stated earlier, the Strutinsky theorem plays a central role in the Mic Mac models. According to the Strutinsky theorem, binding energy $E$ of a given nucleus with $N$ neutrons and $Z$ protons, can be written as sum of a smooth part ($E_{LDM}$) and an oscillatory part ($\delta E$). The liquid drop or droplet formulas constitute $E_{LDM}$. The second term, that is, the oscillatory part comprises of shell correction, and pairing energy. The shell correction is traditionally computed by subtracting the averaged energy for given Hamiltonian, from the corresponding quantum mechanical energy of the system. The semi-classical Wigner Kirkwood averaging scheme [1–8], achieves the smoothing through expansion of quantal partition function in the 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 $\beta_2, \beta_4$ and $\gamma$. The quantum mechanical partition function for such a system is given by:

$$Z(\beta) = \text{Tr} \left( \exp (-\beta \hat{H}) \right).$$

(1)

The variable $\beta$ appearing in this equation is a variable for the purpose of Laplace inversion; $\hat{H}$ is the Hamiltonian of the system, given by:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) + \hat{V}_{LS}(\vec{r}),$$

(2)

where $V(\vec{r})$ is the one-body central potential and $\hat{V}_{LS}(\vec{r})$ is the spin-orbit interaction, given by,

$$\hat{V}_{LS} = \frac{\kappa \hbar^2}{2m} \left( \vec{\nabla} f \times \vec{\nabla} \right) \cdot \hat{\sigma},$$

(3)

where $\hat{\sigma}$ is the unit Pauli matrix, $\kappa$ is the strength of spin-orbit interaction, and $f$ is the spin-orbit form factor.

The partition function can be readily expanded in powers of $\hbar$ as described in Ref. [3]. The expansion neatly separates into two parts:

$$Z_{WK}^{(4)}(\beta) = Z^{(4)}(\beta) + Z_{LS}^{(4)}(\beta).$$

(4)

where, the two term, respectively, correspond to the mean field and the spin-orbit interaction. The explicit forms of the two terms can be found in Refs. [3,9]. The level density $g_{WK}$, particle number $N$, and energy $E$ can be calculated directly from the WK partition function by Laplace inversion. For more details, see Ref. [9]. Detailed description of choice of potential can also
be found in the same reference. The quantum mechanical energy of the system is obtained by diagonalising the Hamiltonian in the axially symmetric deformed harmonic oscillator basis. In all, 15 oscillator shells are used for such an expansion. The pairing energy is obtained within the Lipkin - Nogami scheme [10–12].

Here, we use a simple liquid drop model, with six adjustable parameters [13]. Explicitly,

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

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 \( \chi^2 \) minimisation, with experimental binding energies taken from Audi - Wapstra evaluation [14].

3. Results and Discussions
In the present exploratory study, we consider a set of 367 spherical nuclei [15]. This set has been adopted from the Möller - Nix compilation [16], with a criterion that the quadrupole deformation parameter should be smaller than 0.005. 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: \( a_v = -15.828 \) (MeV), \( a_s = 19.134 \) (MeV), \( k_v = -1.951 \), \( k_s = -2.579 \), \( r_0 = 1.189 \) (fm) and \( C_4 = 1.247 \) (MeV). The \( \text{rms} \) deviation in the binding energies obtained here, turns out to be 634 keV. The corresponding deviation in the Möller - Nix framework is 741 keV [16, 17].

![Figure 1](image-url)  
**Figure 1.** The calculated (WK) and the corresponding experimental [14] single and two neutron separation energies for Y isotopes.

As representative cases, we here present the single and two neutron separation energies for the chain of Y isotopes (considered to be spherical) in Fig. 1. It is seen that the expected odd - even staggering in the single neutron separation energies is well reproduced in the present calculations. The two neutron separation energies, too, are well reproduced, indicating that the mass formula proposed in the present work, indeed, is reliable.

Finally, we note that the same set of liquid drop parameters, modified suitably to take the deformation effects into account, reproduce the binding energies of the deformed nuclei well. As an illustration, the difference between the calculated and the corresponding experimental [14]
binding energies for Gd and Ru isotopes is plotted in Fig. 2. It is seen that the calculations agree well with the experiment. The nuclei $^{102-110}$Ru turn out to have finite tri-axiality in the ground state, in agreement with the observations reported by Möller et al. [18].

4. Summary
The Wigner Kirkwood technique for obtaining averaged energy is developed up to fourth order in $\hbar$, for a system of nucleons with deformation parameters $\beta_2$, $\beta_4$ and $\gamma$. The shell corrections thus obtained, along with the pairing energies calculated by using the well known Lipkin Nogami scheme constitute the ‘micro’ part of the binding energy. The macro part is adopted from traditional liquid drop formula with six adjustable parameters. These parameters are determined so as to reproduce the experimental binding energy of spherical nuclei. It is found that the fit yields mean squared deviation of 634 keV, indicating that the present approach is reliable. Further investigations are in progress.

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