# GOGNY-FORCE INSPIRED MASS FORMULA WITHIN THE WIGNER–KIRKWOOD AVERAGING SCHEME*

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A comprehensive calculation of ground state properties of a large number of even–even nuclei has been carried out using the Gogny D1S force within the extended Thomas–Fermi scheme. It is found that the calculated self consistent potentials and densities can be parametrised as Fermi distributions. As the next step, the parametrised potentials and densities are used to calculate the smooth part of energy and the shell corrections within the Wigner–Kirkwood semi-classical averaging scheme. The shell corrections thus obtained, along with a simple liquid drop prescription, is found to yield a reasonably good description of ground state masses for nuclei spanning the entire periodic table.

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## 1. Introduction

The determination of the one-body density matrix is an important step in the calculation of ground and excited state properties of the nuclear many-body systems. In the case of a finite nucleus, obtaining the one-body density matrix is a computationally demanding task, and hence several approximation schemes of varying degree of sophistication have been developed in the

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past. Some of the notable approaches are the Negele–Vautherin approach [1], the Campi–Bouyssy approach [2] and the semi-classical Extended Thomas–Fermi (ETF) approach of Soubbotin and Viñas [3, 4].

The ETF approach is based on the semi-classical Wigner–Kirkwood $\hbar$ expansion of the distribution function. It has a number of advantages. Firstly, it gives a very intuitive picture of the physical process, since the ETF is deeply rooted in the classical periodic orbit theory [6]. Secondly, it is very systematic and yields the density functionals order by order. The ETF approach with the Skyrme interaction has been applied very successfully to a range of nuclear problems [5]. The ETF approach has been extended to the non-local single particle Hamiltonians [3], and hence can be employed in the case of finite range forces, like the Gogny force. It has been shown that the ETF density functional obtained for the Gogny force yields the ground state properties almost coincident with the Hartree–Fock calculations [3, 4].

On the other hand, alternative approaches to ground state properties like the microscopic–macroscopic (mic–mac) scheme using the semi-classical Wigner–Kirkwood averaging [6–10] has been shown to be quite successful in describing the ground state masses of the nuclei belonging to all the parts of the periodic table [11, 12]. In the present work, we attempt to explore an interesting possibility: use of self consistent potentials and densities obtained within the ETF framework to calculate nuclear masses in the Wigner–Kirkwood based mic–mac approach.

We begin with a very brief overview of the ETF formalism, followed by the essentials of the mic–mac approach using Wigner–Kirkwood averaging scheme. The results will be presented and discussed in the third section. The summary and conclusions are contained in the last section.

## 2. Formalism and details of calculations

### *2.1. ETF calculations*

The ETF expansions are usually derived from the Wigner–Kirkwood distribution [6]. The latter is known to have an apparent divergence problem at the classical turning points: in principle, this does not matter since, ultimately, the integrated quantities, such as particle numbers, energies, *etc.* are relevant. However, the divergence can also be eliminated, for instance, from the kinetic energy distribution, by expressing the latter as a functional of the local density. Effectively, this is achieved by elimination of the chemical potential, the potential energy $V$ and its derivatives, in favour of local density and its derivatives. This is often called the Extended Thomas–Fermi expansion. The ETF expansion, therefore, automatically leads to a density functional. The ETF functional can be employed within the framework of the well-known Kohn–Sham scheme, and the resulting energy as a functional

of the local density can be expressed as [3]

$$\epsilon\left[\rho\right] = \frac{\hbar^2}{2m}\tau\left[\rho\right] + \frac{1}{2}V_{\mathrm{D}}\rho + \epsilon_{\mathrm{ex}}^{\mathrm{KS}}\left[\rho\right] . \tag{1}$$

Here, $\tau$ is kinetic energy functional, $V_{\mathrm{D}}$ is direct potential and $\epsilon_{\mathrm{ex}}^{\mathrm{KS}}$ represents exchange correlation energy (see Ref. [3] for details). The energy of the system of fermions can be obtained either by solving the Kohn–Sham equation explicitly or equivalently by minimisation of the energy functional directly.

In the present work, we employ the well-known finite range Gogny D1S interaction. The ground state energy is obtained through minimisation, and for the analysis reported here, we have chosen a set of 818 even–even nuclei from $^{12}$O to $^{282}$Ds. Assuming spherical symmetry, the ETF calculations are carried out for each of these nuclei resulting in self-consistent potentials and densities. It is found that the self-consistent potentials and densities follow the standard Woods–Saxon form to an excellent degree of approximation. Our principal goal of this work is to explore the possibility of using these potentials and densities. Therefore, it is desirable if the parameters appearing in the Woods–Saxon form factor could be written as simple functions of certain relevant quantities. It turns out that such a parametrisation is indeed possible, and the general form that is used here, can be written as:

$$\mathcal{Q} = P_0\left(1 + P_1\, I + P_2\, I^2\right) + P_3\left(1 + P_4\, I + P_5\, I^2\right) A^{1/3} . \tag{2}$$

Here, $I = (N - Z)/A$. The quantity $\mathcal{Q}$ could be half density radius or diffusivity or strength of potential, and $P_j$ are free parameters. Depending on the quantity, one or more of these parameters are set to zero.

It turns out that the above Ansatz gives an excellent description of the Woods–Saxon parameters for the entire mass range considered here. As an example, we now present and discuss the half density radii and diffusivities appearing in the neutronic mean field. The half density radius and diffusivity have been parametrised as:

$$R_{1/2}^{(n)} = 0.438\left(1 - 2.207\, I\right) + 1.184\left(1 + 0.067\, I - 0.045\, I^2\right) A^{1/3} , \tag{3}$$

$$a_n = 0.346\left(1 + 0.379\, I + 2.724\, I^2\right) + 0.023\left(1 - 2.097\, I\right) A^{1/3} . \tag{4}$$

Differences between the exact and the fitted values of these parameters have been plotted in Fig. 1. Clearly, the proposed parametrisation is satisfactory. Quantitatively, the respective r.m.s. deviations are 0.02 fm and 0.01 fm respectively for half density radius and diffusivity, indicating high degree of accuracy of these parametrisations.

Having determined the potentials and densities, we now present and discuss elements of the mic–mac approach, particularly, with the Wigner–Kirkwood semi-classical expansion.

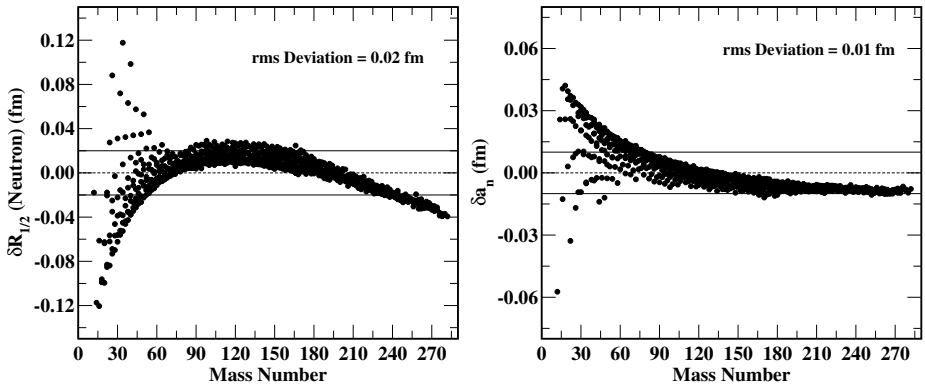


Fig. 1. Difference between exact and fitted values of half density radius and diffusivity for neutronic mean field.

### *2.2. Mic–mac model with Wigner–Kirkwood expansion*

The starting point for the WK expansion is the quantal partition function,

$$Z(\beta) = \mathrm{Tr}\left(\exp\left(-\beta\hat{H}\right)\right), \tag{5}$$

where $\hat{H}$ is the Hamiltonian of the system [11, 12]. The WK semi-classical expansion amounts to an expansion of the partition function in the powers of Planck's constant $\hbar$, that yields systematic corrections to the Thomas–Fermi energy and particle number [6–8, 10]. Here, we expand the partition function up to the fourth order in $\hbar$. The level density, energy and particle number can be obtained through suitable Laplace inversions of the partition function. The details of this procedure and the corresponding formulas for various quantities can be found in Refs. [11, 12].

The Wigner–Kirkwood averaged energy along with the quantal energy yield the shell corrections. The shell corrections, along with pairing energies define fully the 'mic' energy ($\delta E$) of the mic–mac model, in which, the total ground state energy of a system of $N$ neutrons and $Z$ protons can be expressed as $E(N,Z) = E_{\mathrm{mac}} + \delta E$.

The 'mac' part of the energy is determined using the liquid drop model. Here, we use [11–13]

$$\begin{aligned} E_{\mathrm{mac}} &= a_v\left[1+\frac{4k_v}{A^2}T_z\left(T_z+1\right)\right]A + a_s\left[1+\frac{4k_s}{A^2}T_z\left(T_z+1\right)\right]A^{2/3} \\ &\quad + a_{\mathrm{cur}}\left[1+\frac{4k_{\mathrm{cur}}}{A^2}T_z\left(T_z+1\right)\right]A^{1/3} + \frac{3Z^2e^2}{5r_0A^{1/3}} + \frac{C_4Z^2}{A} + E_{\mathrm{W}}\,, \end{aligned} \tag{6}$$

where, $a_v$, $a_s$, $a_{\rm cur}$, $k_v$, $k_s$, $k_{\rm cur}$, $r_0$ and $C_4$ are free parameters, $T_z$ is the third component of isospin, $e$ is electronic charge and $E_{\rm W}$ is the Wigner energy, given by

$$E_{\rm W} = w_1 \exp\left\{-w_2 \left|\frac{N-Z}{A}\right|\right\} \Theta\,(20-Z)\,\Theta\,(40-A) \tag{7}$$

with $w_1$, $w_2$ as free parameters. Most of the nuclei considered in the investigation are deformed. The liquid drop quantities defined above, in particular, surface, curvature and Coulomb energies, therefore become deformation dependent. Details can be found in [12].

## 3. Results and discussions

For the mic–mac study, we consider the same set of 561 even–even nuclei as we had considered in Ref. [12]. The calculations proceed in two steps. In the first step, the Wigner–Kirkwood calculations are carried out using the mean fields, spin-orbit potentials and densities obtained from ETF–Gogny calculations. The shell corrections are deduced from these and the single-particle spectrum obtained by diagonalisation of the Hamiltonian. The pairing energies are then obtained within the well-known Lipkin–Nogami scheme. The two together define the 'mic' part of the binding energy. In the next step, the liquid drop parameters are fitted by demanding that the liquid drop part of the binding energy must coincide with the difference between the experimental binding energy and the 'mic' part of the binding energy. The deformation parameters have been assumed to be the same as those reported in Ref. [12]. The fit turns out to be a reasonable one, with r.m.s. deviation of 953 keV. The resulting liquid drop parameters are: $a_v = -15.871(-15.435)$, $k_v = -1.827(-1.874)$, $a_s = 20.203(16.673)$, $k_s = -2.060(-2.430)$, $r_0 = 1.195(1.219)$, $C_4 = 1.329(0.963)$, $a_{\rm cur} = -3.767(3.161)$, $w_1 = -1.632(-2.762)$ and $w_2 = 13.444(3.725)$. The values presented in parentheses are those reported in Ref. [12]. It is clear that the volume and Coulomb terms obtained in the present calculation are similar to those reported in Ref. [12]. However, it is seen that the terms linked with structure of the surface are strongly affected.

The differences between the calculated and the experimental [14] binding energies for the chains of Fe, Sn, W and Pb isotopes have been presented in Fig. 2. The calculated binding energies are found to be in a reasonably good agreement with the experiment. Notice that near the shell closure, our calculations tend to deviate strongly from the experiment, and elsewhere the agreement is more reasonable. This behaviour is peculiar and needs to

be investigated further. As the first step, we compare our calculations with the results quoted at [15], particularly for Pb isotopes. The comparison is tabulated in Table I.

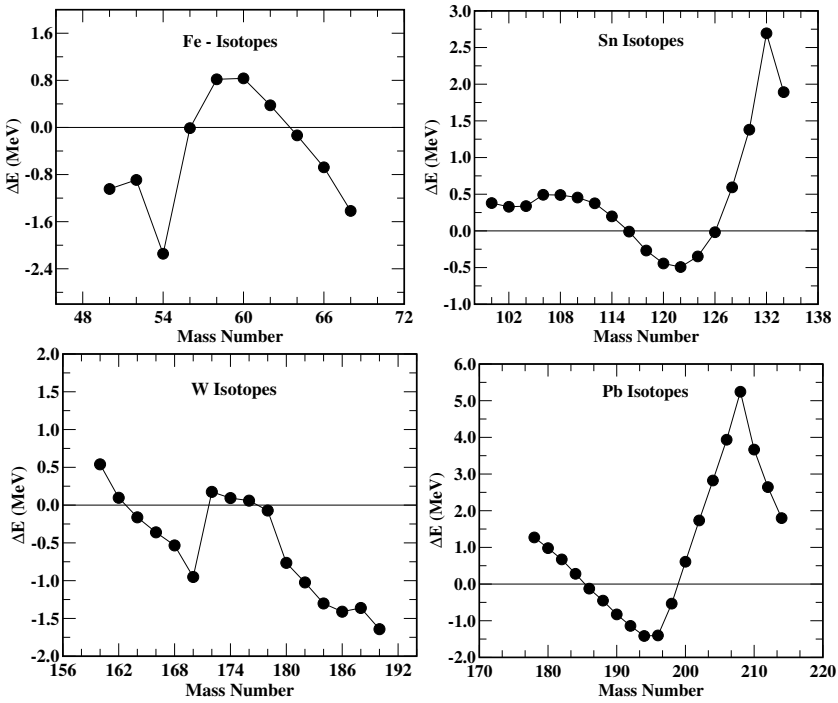


Fig. 2. Difference between calculated and the experimental [14] binding energies for chains of Fe, Sn, W and Pb isotopes.

TABLE I

Binding energies for Pb isotopes. Those reported at [15] and the experimental values are also quoted for comparison.

| $A$ | Present | Ref. [15] | Expt. | $A$ | Present | Ref. [15] | Expt. |
|---|---|---|---|---|---|---|---|
| 178 | −1367.16 | −1368.43 | −1368.52 | 198 | −1560.01 | −1559.48 | −1557.78 |
| 180 | −1389.10 | −1390.08 | −1389.32 | 200 | −1575.20 | −1575.81 | −1574.52 |
| 182 | −1410.44 | −1411.11 | −1409.57 | 202 | −1589.91 | −1591.65 | −1590.88 |
| 184 | −1431.19 | −1431.47 | −1429.32 | 204 | −1604.14 | −1606.96 | −1606.88 |
| 186 | −1451.38 | −1451.25 | −1448.59 | 206 | −1617.85 | −1621.78 | −1622.38 |
| 188 | −1470.98 | −1470.53 | −1467.42 | 208 | −1630.64 | −1635.89 | −1637.27 |
| 190 | −1490.10 | −1489.27 | −1485.85 | 210 | −1641.34 | −1645.01 | −1651.65 |
| 194 | −1526.76 | −1525.35 | −1521.85 | 214 | −1660.95 | −1662.75 | −1658.39 |
| 196 | −1544.05 | −1542.64 | −1540.72 | | | | |

It is seen that the HFB–Gogny results [15] for Pb exhibit a systematic behaviour with respect to the present calculations. In particular, for neutron deficient Pb isotopes, both agree well with the experiment. With increasing neutron number, the two deviate from each other. The WK results remain close to the experiment, but the HFB–Gogny results deviate strongly from it. As the shell closure approaches, the WK calculations start deviating from experiment, whereas the HFB–Gogny results go on improving. Away from the shell closure, the WK calculations again improve, whereas the HFB–Gogny starts deviating from experiment ($^{214}$Pb). It is to be noted that the shell closure and spin-orbit interaction are closely related, hinting towards a possible requirement of improvement in the spin-orbit potential as deduced from the ETF–Gogny. If this is so, it should manifest in shell corrections. It is well-known that the shell corrections have a dominant contribution from the spin-orbit potential [11, 12]. In particular, the fourth order spin-orbit contribution is found to be most significant. With this motivation, we plot in Fig. (3) a comparison between the shell corrections obtained in this work and those reported in Refs. [11, 12]. The present shell corrections are indeed found to differ in structure from the ones reported in Refs. [11, 12]. In particular, deviations near the shell closure are striking, hinting towards the possibility of necessary improvements in the spin-orbit sector, as deduced earlier.

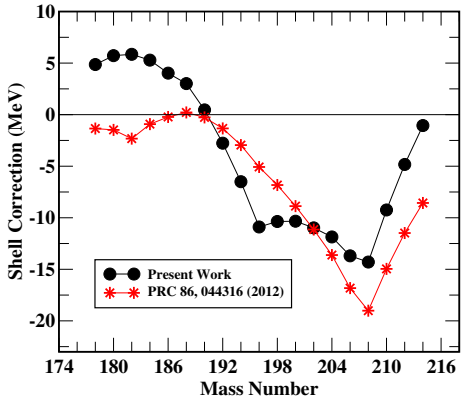


Fig. 3. Comparison between shell corrections for Pb isotopes.

## 4. Summary and conclusions

In summary, the mic–mac calculations with the ETF–Gogny inspired potentials are found to yield a reasonably good description of ground state binding energies for the nuclei spanning the entire periodic table. The results are somewhat similar to HFB–Gogny calculations, but systematic differences

between the two have been observed. The present calculations tend to perform well in the regions away from shell closures, whereas the HFB–Gogny results are found to be better near the shell closures. It has been conjectured that the spin-orbit potential may be responsible for this behaviour. Further investigations along these lines are in progress.

## REFERENCES

[1] J.W. Negele, D. Vautherin, *Phys. Rev. C* **5**, 1472 (1972); **11**, 1031 (1975).
[2] X. Campi, A. Bouyssy, *Phys. Lett. B* **73**, 263 (1978).
[3] V.B. Soubbotin, X. Viñas, *Nucl. Phys. A* **665**, 291 (2000).
[4] V.B. Soubbotin, V.I. Tselyaev, X. Viñas, *Phys. Rev. C* **67**, 014324 (2003).
[5] M. Brack, C. Guet, H.-B. Håkanson, *Phys. Rep.* **123**, 275 (1985).
[6] M. Brack, R.K. Bhaduri, *Semi Classical Physics*, Addison-Wesley, 1997.
[7] B.K. Jennings, R.K. Bhaduri, M. Brack, *Nucl. Phys. A* **253**, 29 (1975).
[8] P. Ring, P. Schuck, *The Nuclear Many-body Problem*, Springer-Verlag, Berlin 1980.
[9] M. Centelles *et al.*, *Ann. Phys. (N.Y.)* **266**, 207 (1998).
[10] M. Centelles, P. Schuck, X. Viñas, *Ann. Phys. (N.Y.)* **322**, 363 (2007).
[11] A. Bhagwat *et al.*, *Phys. Rev. C* **81**, 044321 (2010).
[12] A. Bhagwat *et al.*, *Phys. Rev. C* **86**, 044316 (2012).
[13] K. Pomorski, J. Dudek, *Phys. Rev. C* **67**, 044316 (2003).
[14] M. Wang *et al.*, *Chin. Phys. C* **36**, 1287 (2012); **36**, 1603 (2012).
[15] `http://www-phynu.cea.fr`