OPTIMISATION OF COEFFICIENTS IN SEMI EMPIRICAL MASS FORMULA USING LIQUID DROP MODEL

SUBMITTED BY

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PREFACE

The goal of the project is optimisation of coefficients in semi empirical formula using liquid drop model. Optimisation is done by least square method using python programming by fitting experimental data on liquid drop model.

The dissertation is divided into 4 chapters:

- Chapter 1 : Nuclear structure and properties
- Chapter 2 : Binding energy and nuclear models
- Chapter 3 : Liquid drop model and semi empirical formula
- Chapter 4 : Methods and results

CHAPTER 1 : NUCLEAR STRUCTURE AND PROPERTIES

Atom

- Basic unit of matter
- Consists of nucleus surrounded by electrons
- Electrons are bound to the nucleus by the electromagnetic force
- Electrically neutral. Otherwise exists as an ion
- Represented by $_{Z}X^{A}$

  Z : atomic number

  A : mass number

  A = Z + N (N : no.of neutrons)

Nucleus

- Tiny central core of the atom
- Consists of protons and neutrons known as nucleons
- Almost entire mass of the atom is concentrated in it
- Size : 10^{-15} m

Nuclide

- Any atomic nucleus with a specific no.of atom Z and mass number A
- Isotopes & isobars

Isotopes : Nuclei with same no.of protons but different no.of neutrons

$_{14}Si^{28}$, $_{14}Si^{29}$, $_{14}Si^{30}$

Isobars : Nuclides with mass number but different atomic number

$_{8}O^{16}$, $_{7}N^{16}$

Properties of nuclei

- Nuclear size
- Nuclear mass
- Nuclear density
- Nuclear charge
- Nuclear forces
- Nuclear stability

CHAPTER 2 : BINDING ENERGY AND NUCLEAR MODELS

Mass defect

- Difference between actual atomic mass and sum of the masses of the nucleons

  $\Delta m = [(Zm_p + Nm_n) - M]$

  $(Zm_p + Nm_n)$: sum of the masses of the nucleons

  M : actual mass of the nucleus

- This mass defect can be converted into energy using the mass-energy equivalence formula

  $E = mc^2$

  $E = \Delta mc^2$

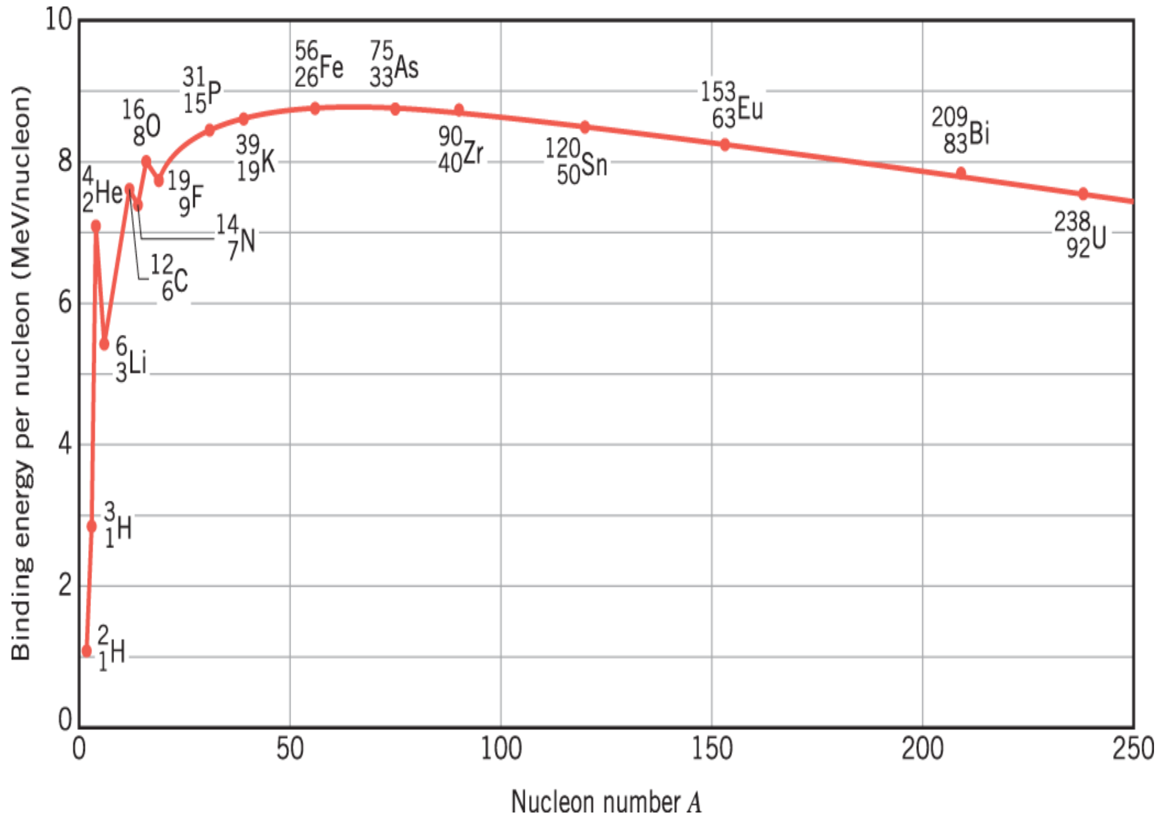
Binding energy

- The energy equivalent to the mass defect of a nucleus is called binding energy.
- $BE = \Delta mc^2 = \{(Zm_p + Nm_n) - M\}\, c^2$
- It is the energy required to separate an atomic nucleus completely into its constituent protons or neutrons, or, the energy liberated by combining individual protons and neutrons into a single nucleus.
- If $BE > 0$: nucleus is stable and energy must be supplied from outside to split it into constituents

  If $BE < 0$: nucleus is unstable and it will disintegrate by itself
- BE per nucleon = total BE of a nucleus / number of nucleons.

  It is plotted as a function of mass number A.

Binding energy per nucleon curve



- The curve increases steeply and teaches a maximum of 8.8 MeV at A = 56 (for Fe), then drops slowly to about 7.6 MeV at the highest mass numbers.
- Large amount of energy will be liberated if heavier nuclei split into lighter ones (nuclear fission) or if light nuclei joined to form heavier ones (nuclear fusion).

Nuclear models

- To explain the behaviour and properties of nuclei
- The nuclear models proposed so far can be classified into two broad types

1. strong interaction model - liquid drop model
2. independent particle model - shell model

CHAPTER 3 : LIQUID DROP MODEL AND SEMI EMPIRICAL MASS FORMULA

Liquid drop model

- Proposed by Niels Bohr and Fritz Kalckar, it is widely used to explain the binding energy of the nucleus.
- Based on the striking similarities between liquid drop and nucleus
  - shape
  - balance between two forces
  - density is independent of its volume

Semi empirical mass formula

- Used to calculate the mass and various other properties of an atomic nucleus.
- Theory is based on liquid drop model
- The formula has five terms which represents the five types of energies, named as :

1. Volume energy
2. Surface energy
3. Coulomb energy
4. Asymmetry energy
5. Pairing energy

Volume energy

- When an assembly of nucleons of the same size is packed together into the smallest volume, each interior nucleon has a certain number of other nucleons in contact with it. So, this nuclear energy is proportional to the volume.
- $E_v = a_v.A$ MeV

  where A is mass number, A_v is constant. Its value is 16.11

Surface energy

- A nucleon at the surface of a nucleus interacts with fewer other nucleons than one in the interior nucleus and hence its binding energy is less. This surface energy term takes that into account and is therefore negative and is proportional to the surface area.
- $E_s = a_s. A^{2/3}$ Mev

  where A is mass number, a_s is constant. Its value is 20.21

Coulomb energy

- The electrostatic repulsion between each pair of protons in a nucleus contributes toward decreasing its binding energy.
- $E_c = a_c Z^2 A^{-1/3}$ Mev

  where A is mass number, Z is atomic number, a_c is constant. Its value is 0.583

Asymmetry energy

- An energy associated with the Pauli exclusion principle. If it wasn't for the coulomb energy, the most stable form of nuclear matter would have the same number of neutrons as protons, since unequal numbers of neutrons and protons imply filling higher energylevels for one type of particle, while leaving lower energy levels vacant for the other type.
- $E_a = a_a ((A-2Z)^2/A)$ MeV

  where A is mass number, Z is atomic number, a_a is constant. Its value is 20.65

Pairing energy

- An energy which is a correction term that arises from the tendency of proton pairs and neutron pairs to occur. An even number of particles is more stable than an odd number.
- $E_p = \pm \delta/A^{3/4}$ MeV

  where A is mass number, Δ is constant. Its value is 33.

BE - SEMF

- $E_B = [\ m_p - (A\text{-}Z)\ m_n + E_v - E_s - E_c - E_a \pm E_p]$ MeV

  m_p - mass of proton : 1.0072766u

  m_n - mass of neutron : 1.0086654u

CHAPTER 4 : METHODS AND DISCUSSION

Least square method

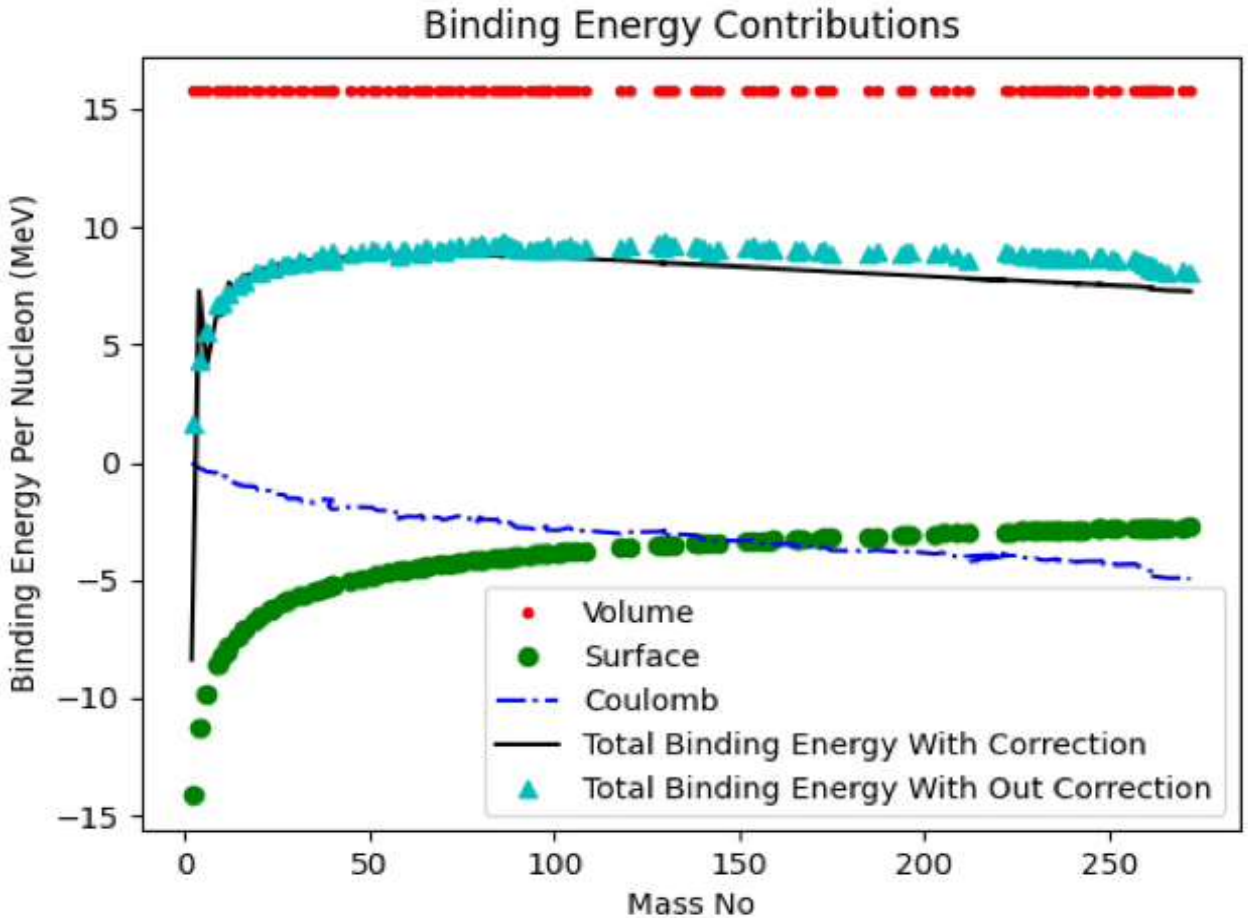
- It is a standard approach in regression analysis to the approximate solution of over dominated systems, that is, sets of equations in which there are more equations than unknowns.
- Least squares mean that the overall solution minimises the sum of the squares of the errors made in the results of every single equation.
- The least square fit method is a technique used to estimate the values of the parameters in a mathematical model that best fits a set of data. In the case of the liquid drop model, the parameters are the coefficients a_v, a_s, a_c, a_a, and a_p.
- To use the least square fit method to determine the values of these coefficients, we start by collecting experimental data on the binding energies of a set of nuclei with different mass numbers.

Nuclear binding energy contributions

We plotted contribution terms in semi empirical formula and total binding energy per nucleon with correction factors (asymmetric and pairing terms) and without correction factors using python code.

```
import matplotlib.pyplot as plt
import numpy as np

Z, A, BA, t = np.loadtxt("Be sorted.txt").T
    return y
def liquid_drop2(Z, A, t):
    y = 15.753 - 17.80*(A)**(-0.333333) - 0.713*Z*(Z-1)*(A)**(-1.33333333)
    return y

def vol(Z, A):
    y1 = np.full_like(A, 15.753)
    return y1

def sur(Z, A):
    y2 = -17.80*(A)**(-0.333333)
    return y2

def colm(Z, A):
    y3 = -0.713*Z*(Z-1)*(A)**(-1.33333333)
    return y3

BA_L1 = liquid_drop1(Z, A, t)
BA_L2 = liquid_drop2(Z, A, t)
volume = vol(Z, A)
surface = sur(Z, A)
coloumb = colm(Z, A)

# Plot all energy contributions on the same graph
plt.plot(A, volume, 'r.', label='Volume',  lw=0.5)
plt.plot(A, surface, 'go', label='Surface', lw=0.5)
plt.plot(A, coloumb, 'b-.', label='Coulomb', lw=1.5)
plt.plot(A, BA_L1, 'k-', label='Total Binding Energy With Correction', lw=1.5)
plt.plot(A, BA_L2, 'c^', label='Total Binding Energy With Out Correction', lw=0.1)


plt.xlabel("Mass No")
plt.ylabel("Binding Energy Per Nucleon (MeV)")
plt.title("Binding Energy Contributions")
plt.savefig('BE curve contribution.tif',dpi=300)

plt.legend()
plt.show()
```

Output:-



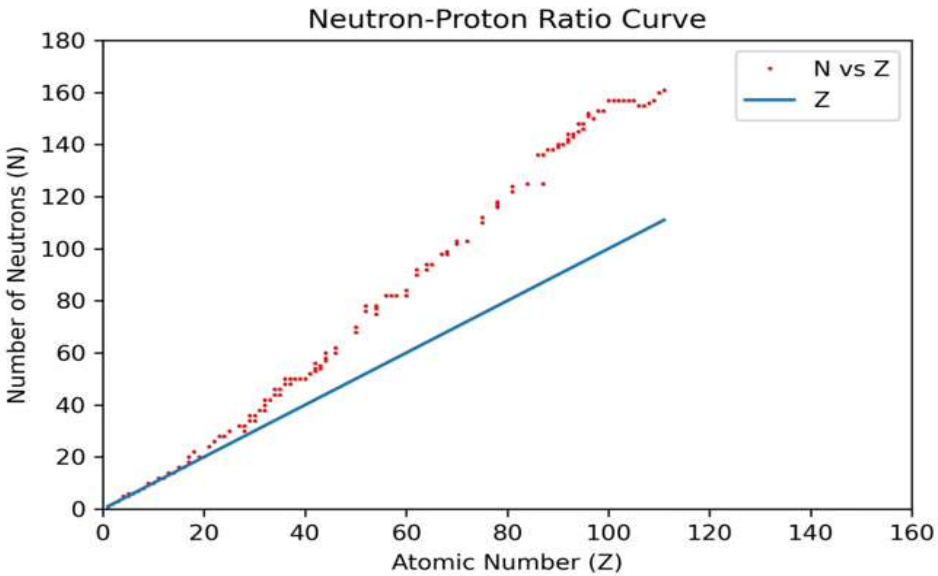
Contribution terms : volume energy, surface energy, coulomb energy

Correction terms : asymmetry energy, pairing energy

Analysis of correction terms

1. Asymmetry energy
    - Due to the difference in no.of protons and neutrons. Determines the stability and properties of atomic nuclei.
    - lighter nuclei : almost equal no.of protons and neutrons : stable
    - heavier nuclei : more protons than neutrons : unstable

      additional neutrons require to stabilize the nucleus
    - It can be explained on the basis of neutron-proton ratio curve



Python code for the plot:-

```
import numpy as np
import matplotlib.pyplot as plt

# load data from file
Z, A = np.loadtxt("Neutron-Proton Ratio Curve Data.txt").T

# plot data
plt.plot(Z, A-Z, 'r.', markersize=1.5, label="N vs Z")
plt.plot(Z, Z, label="Z")

# set axis limits and labels
plt.ylim(0, 180)
plt.xlim(0, 160)
plt.xlabel("Atomic Number (Z)")
plt.ylabel("Number of Neutrons (N)")
plt.title('Neutron-Proton Ratio Curve')

# add legend
plt.legend()

plt.savefig('Neutron-Proton Ratio Curve.tif',dpi=300)

# show plot
plt.show()
```

- As proton number increases, nucleus becomes unstable. In order to solve this naturally, no.of neutrons found to be higher than the proton number with increase in atomic number.

Pairing energy

- Even no.of particles is more stable than odd number.
- $E_p = \pm \delta/A^{3/4}$ MeV

even-even nuclei : +ve

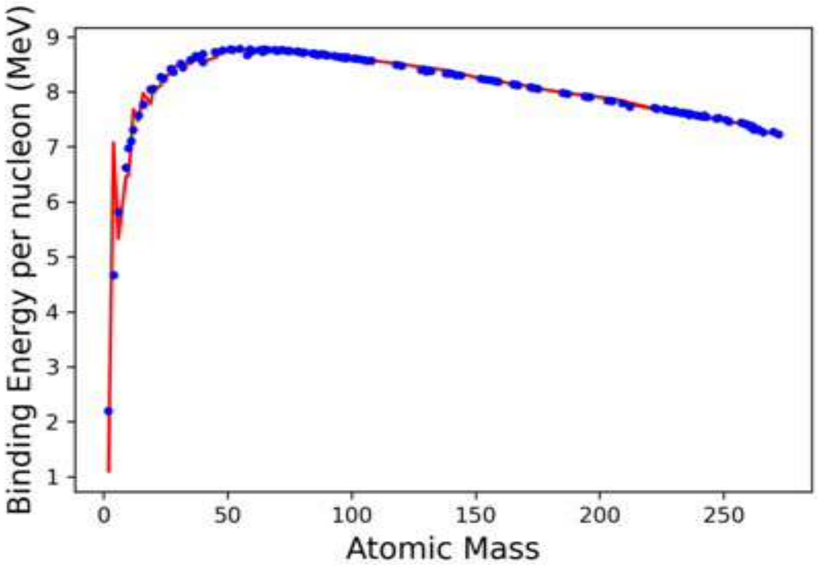
odd-odd : -ve

even-odd/odd-even : 0

Optimisation of coefficients in semi empirical mass formula using liquid drop model

```
from scipy.optimize import leastsq
import numpy as np
import matplotlib.pyplot as plt


# load the mass data from text file
Z, A, B, t = np.loadtxt("Be sorted.txt").T

# define the liquid drop model function to fit
def liquid(Z,A,a,t):
    # note: there was a typo in the function definition (missing parenthesis)
    y = a[0] - a[1] * A**(-1/3) - a[2] * Z * (Z-1) / (A**(4/3)) -a[3] * ((A-2*Z)**2 )/ (A**2) +(t * a[4] )/ (A**(-7/4))
    return y

# define the residuals function for least-squares optimization
def residuals(a, A, t, y):
    error = y - liquid(Z,A, a,t)
    return error

# initial guess for the fit parameters
a = [0, 0, 0, 0, 0]

# perform the least-squares optimization to obtain the fit parameters
#a_opt, ier = leastsq(residuals, a, args=(A, t, B), full_output=1)
a_opt, cov_x, infodict, mesg, ier = leastsq(residuals, a, args=(A, t, B), full_output=1)

# check if the optimization converged successfully
#if ier not in [1, 2, 3, 4]:
    #print("Optimization failed with error code", ier)

# obtain the fit curve with the optimized parameters
fit = liquid(Z,A, a_opt,t)

# plot the results
plt.plot(A, B, 'r-', markersize=2+.5)
plt.plot(A, fit, 'b.', lw=0.75)
plt.xlabel('Atomic Mass', fontsize=14)
plt.ylabel('Binding Energy per nucleon (MeV)', fontsize=14)
plt.savefig('BE curve final.tif',dpi=300)
plt.show()

# print the fit parameters
print("The coefficients are", a_opt)
```

Output:-




```
The coefficients are [1.52284804e+01 1.64202306e+01 6.79750509e-01 2.20228365e+01
7.64368586e-07]
```

Python code we described above gave output for optimized values of coefficients in semi empirical mass formula along with plot of binding energy fit

The coefficients are: -

a_v =15.2284804 MeV

a_s=16.4202306 MeV

a_c=0.679750509 MeV

a_s=22.0228365 MeV

a_p=7.64368586×10-7 MeV

CONCLUSION

In this study, with our focus on the topics semi empirical mass formula and liquid drop model, we explored the complex world of nuclear physics. The least square method allowed us to optimise the coefficients in semi empirical mass formula to best fit experimental data on atomic masses. From this study, we were able to understand the nuclear binding energies and nuclear stability.

THANKYOU

ADDITIONAL DATA

Atomic mass data :

https://www-nds.iaea.org/amdc/ame2003/mass.mas03