Semi-empirical mass formula and its application to the nuclear reactions

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Part I
Basic Defintions, Notations and Units

1.1: Fundamental Constituents of Matter

a) Leptons: These are one of the two fundamental types of buliding blocks of all the matters. They are the elementary particles having spin$\frac{1}{2}$ hence follow Pauli exclusion principle. Some of the examples are electrons(e) and neutrinos (ν). Electrons are the one which govern the Atomic and Molecular chemistry.

b) Quarks: These are other elementary particles with spin $\frac{1}{2}$ and they carry a fractional electronic charge. Quarks combine to form a class of particles called "Hadrons". Some of the examples are protons and neutrons which are constituents of atomic nuclei.

All atoms are made up of electrons and nuclei. Nuclei are made of spin $\frac{1}{2}$ protons and neutrons which are made up of quarks.

1.2: Fundamental Interactions

After the immense efforts of lots of best minds over centuries all the physical phenomena known till today are explained as the consequences of four fundamental interactions which are "*Gravitation, Electromagnetic Interaction (EM), Strong Interaction and Weak Interaction.*" All three forces except Gravitation, can be today understood in terms of discrete quantum fields (part of Quantum Field Theory (QFT)).The QFT combines EM with Quantum mechanics (QM) in Quantum Electrodynamics (QED), which further was reduced along with weak interaction in Electroweak theory(EWT). The strong interaction was modeled as Quantum Chromodynamics (QCD), which further along with EWT and Higgs mechanism constitute the "Standard model of Particle physics." QFT predicts that all these interactions (except Gravitation about which we will not discuss further, which is assumed to be mediated by a hypothetical particle Graviton) are mediated by exchange of Intermediate Bosons(particles with spin 1). These bosons are *Photons* in EM interactions, *Gluons* in Strong interactions and the W^+, W^- and the Z^0 in Weak interactions. These particles have been experimentally confirmed today.

1.3: Properties of different Interactions

The well known Electromagnetic force is a long-range force as it does not become equal to zero within any finite distance, but the two Nuclear forces are short-ranged and they are considerable only till short distances. What is meant by mediating a force is that when two particles interact, they exchange an intermediate boson, i.e. an intermediate boson is created and moves from one of them to the other where it is absorbed.These properties can loosely be understood using Heisenberg's uncertainity principle which relates the energy ΔE of that intermediate boson with time Δt of its existence.

Mathematically, Uncertainity principle says-

$$\Delta E \cdot \Delta t \sim \frac{\hbar}{2} \tag{1}$$

Now since W and Z bosons are very heavy particles (rest masses are 80 GeV/c^{2}and 91 GeV/c^{2}respectively) they can only be produced a virtual, intermediate particles in scattering processes for extremely short time as can easily be seen from equation (1), therefore the weak interaction is short ranged. But as the rest mass of photon is zero the electromagentic interaction is infinite. But the gluons having rest mass zero but unlike electromagnetic interaction the strong force is short ranged, this is due to carrying a charge by gluons, which enables them to interact with each other.

1.4: Invariancy of Physical laws

Symmetries and invariance properties of fundamental interactions play a very important role in physics. Some lead to conservation laws that are universal. For example translational invariance leads to the conservation of linear momentum, similarly rotational invariance leads to the conservation of angular momentum. In fact conservation of angular momentum plays very important role in nuclear and particle physics as it leads to a scheme for the classification of states based, among other quantum numbers, on their spins. Like conservation laws Symmetries also play a very significant role in physics. In non-relativistic Quantum mechanics the concept of reflection symmetry is very important and depending on whether the sign of wave function changes under reflection or not, the system is said to have negative or positive $parity(P)$ respectively. The concept of $parity$ was first introduced in context of atomic physics by Wigner. It refers to the behaviour of a state under a spatial reflection, i.e. $\vec{r} \to \vec{-r}$. Mathematically the $parity$ operator is -

$$\hat{P}\psi(\vec{r},t) = P\psi(\vec{-r},t) \tag{2}$$

where $\psi(\vec{r},t)$ = non-relativistic wave function. The spatial wave function of a bound system with angular momentum $l\hbar$ has parity P = $(-1)^l$. The laws of nature which are invariant under a reflection in space, the parity P is conserved. Conservation of parity leads to the selection rules in electromagnetic transitions in atomic physics. The quest to verify theoretical predictions of particle physics lead to the development of particle detectors and accelerators. Some very known examples are particle detectors (LHC), spectrometers and scatterers.

1.5: Units in Particle Physics

Since the atomic size is of order *femtometer* (1 fm = 10^{-15} m or Fermi) and energy is of order *electron volt* (eV), they are the most useful units. 1eV is defined as the energy gained by one electron by traversing a potential difference of 1 V. Therefore mathematically,

$$1eV = 1.602 \cdot 10^{-19} J$$

Also the rest masses are expressed in terms of Einstein Mass-energy formula ($E=mc^2$) as MeV/c^2or GeV/c^2, length and energy are connected via uncertainity principle so Planck's constant is written in form-

$$h{\cdot}\mathrm{c} \approx 200 \;\; MeV{\cdot}fm$$

Also a frequently used quantity which is called coupling constant for electromagnetic interactions is defined by:

$$\alpha = \frac{e^2}{4\pi\varepsilon_o hc} \approx \frac{1}{137} \tag{3}$$

Usually both the SI system and CGS system are used in particle physics but we will only use SI unit to make our life simpler. But sometimes we will use eqn. (2) as a constant.

Part II
Global Properties of Nuclei

For a long time an atom was assumed to be indivisible (in fact Dalton's atomic theory supported it.), until the most revolutionary discoveries of "Electron" and "Radioactivity" were done in early 19th century which commenced the new era of investigation of matters. Similarly using these discoveries and theories Protons and Neutrons were discovered which finally constituted an atom. Also to study these particles new techniques and advancements were developed like particle accelerators, vacuum tubes and detectors. We will discuss some experiments in next sections.

2.1: Electrons, Protons and Neutrons

The year 1897 was very revolutionary for physics as the first fundamental particle was discovered by Thomson by producing cathode rays (of which electrons are constituents particles) in a discharge tube. He also estimated the famous charge-to-mass ($\frac{e}{m_e} = (1.7588{\pm}39){\times}10^{11}C/kg$) ratio to be independent to the cathode material, using trajectory of electron in external electric and magnetic fields.[1] After this very important discovery Thomson also proposed an atomic model, called *"Plum pudding model"*, in which atom was thought to be composed of electrons surrounded by a cloud of positive charge to make the atom neutral. In this model electrons were assumed to be positioned throughout the atom.

2.2: Nuclear reactions and discovery of Protons and Neutrons

Thomson model was correct till it was proven wrong by Rutherford. He experimentally studied the scattering of α- particle with gold sheet and concluded the fact that most of the space in an atom was empty,but they had extremely small, dense matter with positive charges which were tightly bound together.The positive charge was concluded because it repelled α- particle which was assumed to be doubly ionized Helium atom.. He named those extremely small dense matter, Nucleus. Now the baffling questions was that what were those positive charges. Rutherford again performed an experiment in which he bombarded the α- particles on nitrogen nucleus, which ejected a long-range particle which was one of the constituents of nucleus. He also discovered the fact that these particles were actually Hydrogen nuclei (protons). The reaction which he had indeed observed was-

$$^{14}N +^4 He \rightarrow^{17} O + p$$

[1] In 1910 Millikan calculated the electronic charge (e = $1.602{\cdot}10^{-19}$C), by performing oil-drop experiment and won 1923 Nobel Prize in Physics.

where p = proton. In this way Rutherford built the foundation of modern nuclear physics. He also proposed an atomic model in which he suggested that electrons should be moving around nucleus in circular orbits under the action of centrepetal force (consequence of Coulombic interaction). This was also proved to be wrong when quantum mechanical model of an atom was developed by Bohr. Although the charge of nucleus was exactly $Z \mid e \mid$, so there was no problem with charge of nucleus, but one question was still baffling the physicists that why nuclear mass was more than expected. The nuclear mass $M_{nucleus}$ was expected to be $M_{nucleus} = A \cdot M_p$ where M_p = mass of a proton, but the experimental values were even more than two times of the expected value. This was answered by Chadwick in 1932 with the discovery of neutral particle "Neutron",[2] which made nucleus heavier than expected. The mass of this particle was slightly more than the proton, and this established the fact that nucleus contained neutron and proton.

2.3: Nuclear force and binding

But after finding the building blocks of an atom the obvious question was to ask that what interactions were responsible for binding these nuclear particles (protons and neutrons), they couldn't be electromagnetic interaction because neutron was neutral, also size of nucleus and masses of these tiny particles did clearly rule out the possibility of this one. These forces were evidently much stronger than electromagnetic and also short ranged, and this question actually gave rise to the concept of Binding energy which is defined as differnce between the mass of system and the sum of the masses of its constituents. This phenomenon, historically was the first proof of $E = mc^2$

2.4: Nuclides

a)The atomic number: For an atom the total number of proton is the atomic number Z of that atom. Since the magnitude of protonic charge is same as electronic charge, therefore charge of nucleus can be expresses as, $Q = Ze$. In neutral atom the number of protons is exactly equal to number of electrons so the net charge on atom, $\sum Q \approx 0$ as $\mid e_p + e_e \mid \leq 10^{-18} e$. Classically the atomic number is calculated using charactersitc X-rays of the atom which is produced when atom is excited using elctrons, protons or synchrotron radiation. Moseley's law relates the energy of produced X-ray to the atomic number by following empirical formula-

$$hv = C{\cdot}(Z - 1)^2 \tag{4}$$

where ν=frequency of X-ray, Z = atomic number of atom, C = Moseley constant, which depends on characterstic of X-ray. This formula can easily be derived using Bohr's atomic model which relates energy of transition with the energy of emitted photon.

[2] This was the reaction ${}^{9}_{4}Be +^{4}_{2} He \rightarrow^{12}_{6} C +^{1}_{0} n$ which Chadwick performed.

b)The mass number: Since the nucleus contain Z protons and N neutrons, so a new quantity was defined as mass number, $A = Z+N$, and different combinations of these numbers are called *nuclides*. Using these concepts we define, Binding energy, $B(Z, A)$ as,

$$B(Z,\ A) = [ZM(^1H) + (A - Z)M_n - M(A, Z)]c^2 \tag{5}$$

Here, $M(^1H) = M_p + m_e$ is the mass of the hydrogen atom, M_n is the mass of the neutron and $M(A, Z)$ is the mass of an atom with atomic number Z and mass number A.

c)Determination of masses using mass spectrography: In an external electric field $\vec{E}$ and magnetic field $\vec{B}$ the Lorentz force on a charged particle having charge Q and velocity $\vec{v}$ is, $\vec{F_L} = Q(\vec{v} \times \vec{B}) + Q\vec{E}$. Due to this force the charged particle deflects which allows us to calculate its momentum $p = Mv$ and its kinetic energy $E_{kin} = \frac{1}{2}Mv^2$ simultaneously. Mathematically, Newton's second law says-

$$\sum \vec{F_{ext}} = M\vec{a} \tag{6}$$

, where M = mass of the particle, and $\vec{a}$ = acceleration of the particle. Using equation (5) we can solve the motion of charged particle for electric field and magnetic field seperately as follows,

In electric field the force is given by,

$$QE = \frac{Mv^2}{r_E} \tag{7}$$

where r_E = radius of curvature of the ionic path in elctric sector, which is clearly proportional to kinetic energy of the charged particle. Similarly in magnetic field the force is-

$$QvB = \frac{Mv^2}{r_B} \tag{8}$$

where r_B = radius of curvature of the ionic path in magnetic sector, which is clearly proportional to the momentum of the charged particle. In this way using eqn. (6), (7) and eliminating v we calculate $\frac{M}{Q}$ which gives us the atomic mass of the atom.

d) Determining masses from the nuclear reactions: The mass defect in a nuclear reaction is an indicator of binding energy of an atom, this can easily be understood by following example. Consider a nuclear reaction-

$$^1_0n +^1 H \rightarrow^2 H + \gamma$$

Now mathematically the energy released in this reaction can be calculated as the binding energy of deuterium ^2H which is-

$$B = (M_n + M_{^1H} - M_{^2H})c^2 = E_\gamma + \text{recoil energy of } {}^2H$$

where $E_{recoil} = \frac{p^2_{^2H}}{2M_{^2H}}$ and $p_{^2H} = \frac{E_\gamma}{c}$. This term is a consequence of momentum conservation.

2.5: Parametrisation of Binding Energies

Till 1930s binding energies per nucleon for most of the elements were experimentally calculated, apart from the lightest elements most of them were lying in between 8-9 MeV. Obviously it was dependent on mass number but after lots of efforts, $Weizsäcker$ in 1935 came up with *semi empirical mass formula* which is given as follows:

$$M(A,Z) = NM_n + ZM_p + Zm_e - a_vA + a_sA^{\frac{2}{3}} + a_c\frac{Z^2}{A^{\frac{1}{3}}} + a_a\frac{(N-Z)^2}{4A} + \frac{\delta}{A^{\frac{1}{2}}} \quad (9)$$

The parameters a_v, a_s, a_a, a_c *and* δ depend on the range of masses for which the formula is used. These extra terms do show the importance of binding energy, and can be physically understood using relation between nuclear radius R and mass number A, which is experimentally verified as

$$R \propto A^{\frac{1}{3}} \quad (10)$$

This phenomenological formula (eqn. (8)) is based on *"Liquid-Drop model"*, which treats nucleus as an incompressible liquid drop which is made up of nucleons (since the size of nucleus is very small therefore it should be considered as quantum liquid not the classical one). And the experimental values of binding energy for most of the stable nuclei were very close which led to the comparison of nucleus to the liquid of constant density independent of number of molecules, and the heat required to vaporize the liquid is proportional to the number of molecules analogous to the binding energy proprtional to mass number.The physical meaning of extra terms are explained as follows:

a) Volume coefficient: The nuclear volume is made up of nucleons which itself contribute to the binding energy of nucleus, and this roughly explains the short range nature of nuclear force, which is approximately proportional to the distance between two nucleons, and this term is proportional to the volume of nucleus (assuming nucleus to be sphere so $Volume \propto R^3$) which from eqn. (9) is proportional to mass number A.

b)Surface coefficient: Since the interior nucleons are surrounded by outer ones which effectively reduces the overall binding energy (due to surface tension type effects) and is proportional to $R^2 \propto A^{\frac{2}{3}}$.

c)Coulomb term: The average electrostatic energy beween two protons $(charge = +e = \rho\frac{4\pi r^3}{3})$ at nuclear distance R is given as-

$$U_o = 2\int V(r)\,\mathrm{d}q(r) = 2\int_0^R k_o \frac{q(r)}{r}\rho 4\pi r^2\,\mathrm{d}r = 2\int_0^R k_o \rho\frac{4\pi r^3}{3}\frac{1}{r}\rho 4\pi r^2\,\mathrm{d}r \quad (11)$$

Solving eqn. 10 in terms of charge e we get $U_o = \frac{6k_o e^2}{5R}$, where $k_o = \frac{1}{4\pi\epsilon_o}$. Now for nucleus having Z no. of protons there are $\frac{Z(Z-1)}{2}$ such pairs so final electrostatic potential energy we will get as-

$$E_{Coulomb} = \frac{3k_o Z(Z-1)e^2}{5R} \quad (12)$$

And this is approximately proportional to $\frac{Z^2}{A^{\frac{1}{3}}}$.

d)Asymmetry term: As the mass number is defined as, $A = Z + N$ for lighter elements the no. of protons Z and no. of neutrons N are almost same but as the mass number increases for heavier elements this does not happen and no. of neutrons increases in comparison to no. of protons leading to some asymmetry to nucleus, which is explained by *Fermi Gas model* and it turns out that this asymmetry is proportional to $\frac{(N-Z)^2}{4A}$ and it also affects the binding energy of nucleus.

e)Pairing term: The last term in eqn. (9) indicates the effect of pairing of protons and neutrons, and energy required in this process is dependent on mass number of atom and also the overlap of wave functions of thse nucleons due to this coupling is smaller for heavier nuclei. Consequently this has been onserved that nuclei with even number of protons and neutrons are more stable. The sign of δ depends on eveness or oddness of *N and Z.* From eqn. (9) it can easily be seen that energy contribution to binding energy per nucleons follows below order:

$$Volume\ energy > Surface\ energy > Coulomb\ energy > Asymmetry\ energy$$

Protons and neutrons have nearly same masses, and their interaction is almost similar as they both are made up of quarks (only difference is the combination of quarks in both of them), and this gives the concept of isospin, which explains the similar behaviour of different charged particles under the strong interaction. Rigorous mathematical treatment of this isospin can tell us about the stability of isobars and isotopes.

Part III
Nuclear Stability

Experiments have shown that binding energy is maximum for Fe- and Ne-isotopes, after that for heavier elements binding energy decreases as the repulsin between increases, this makes those nuclei unstable and due to which heavier elements tend to decay. And since spontaneous decay is only possible if energy is released after decay. So using Einstein's mass-energy equivalence we can say if-

$$M(A, Z) > M(A - A', Z - Z') + M(A', Z') \tag{13}$$

where *M(A,Z) = mass of parent nuclei* , *M(A-A',Z-Z') and M(A',Z') are masses of daughter nuclei.*

3.1: Decay Constants

The spontaneous nuclear decay (radioactive decay) is governed by first order kinetics, which can be expressed by a first order differential equation in following manner-

$$A = \frac{dN}{dt} = -\lambda \cdot N \tag{14}$$

where $A=$ activity (number of decays per unit time) $N=$ no. of radioactive nuclei in sample at time t, $\lambda=$ first order decay constant, which is probability per unit time for a radioactive nuclei to decay.

Solving equation (13) by integrating both side we finally get no. of radioactive nuclei in sample at time t as-

$$N(t) = N_o e^{-\lambda t} \tag{15}$$

where N_o = no. of radioactive nuclei at $t = 0$.

Now there is something called $half\ life\ t_{\frac{1}{2}}$, which is defined as the time when half of initial amount of nuclei have decayed, which can easily be calculated using eqn. (14) and it turns out to be

$$t_{\frac{1}{2}} = \frac{ln2}{\lambda} \tag{16}$$

. Then there is concept of *mean life,* τ which is defined as -

$$\tau = <t> = \frac{\int tN(t)\,dt}{\int N(t)\,dt} = \frac{1}{\lambda} \tag{17}$$

The unit of $Activity, A$ is defined to be *1 Bq (Bequerel) = 1 decay/s.*

3.2: β- Decay

Consider nuclei with equal mass numbers A (isobars), also equation (8) can be re-written in the following form-

$$M(A,Z) = a_1 \cdot A - a_2 \cdot Z + a_3 \cdot Z^2 + \frac{\delta}{A^{\frac{1}{2}}} \tag{18}$$

where, $a_1 = M_n - a_V + a_s A^{\frac{-1}{3}} + \frac{a_a}{4}$, $a_2 = a_a + (M_n - M_p - m_e)$, $a_3 = \frac{a_a}{A} + \frac{a_c}{A^{\frac{1}{3}}}$, $\delta =$ same as in eqn. (8)

This clearly shows that nuclear mass is the quadratic function in Z, so graph of nuclear mass (with constant A) yields a parabola. The structure of parabola depends on eveness and oddness of mass number A, like for odd A we'll get one parabola but for even mass numbe there can be two cases as even-even nuclei or odd-odd nuclei and due to that we get two vertically shifted parabolas. The minimum of parabola can be found using simple calculus by differentiating the quadratic function as-

$$\frac{d}{dZ}(M(A,Z)) = 0 \Rightarrow Z = \frac{a_2}{2a_3} \tag{19}$$

This clearly means that for a constant mass number A nuclei the most stable nucleus for β decay is the nucleus with lowest nuclear mass, so the heavier nuclei will tend to decay to this nucleus so that they can become stable. Now in case of nuclei with even mass number there often more than one β- stable nuclei so decay process is somewhat different from odd one.

3.3: Lifetimes

The lifetimes of β- unstable nuclei is strongly dependent on energy (E) released in the decay process as-

$$\frac{1}{\tau} \propto E^5 \tag{20}$$

So lower the energy released in decay higher the lifetime of the parent nuclei. For example, The decay of a free neutron into a proton, an electron and an antineutrino releases 0.78 MeV and this particle has a lifetime of $\tau = 886.7 \pm 1.9$ s.

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References

[1] Particles and Nuclei by- Povh, Rith, Scholz,Zetsche