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The Coulomb Energy of Finite Size Nucleus from the Study of Classical Electrodynamics Theory

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Abstract

The Coulomb energy for different nuclear model with small computing effort and high accuracy is a great challenge in physics as well as in quantum chemistry research. In this work we applied a classical electrodynamics theory and derived a simple procedure and expression for calculating the Coulomb energy for atomic nuclei taking into consideration the finite size of protons. The corresponding results are compared with the direct Coulomb energy obtained from two-parameter Fermi distributions. The formula obtained, which varies directly to the proton number and varies inversely to the cube root of mass number, was applied and calculated numerically the values of Coulomb energy for light, medium and heavy nuclei. To examine the effect of finite size of proton on Coulomb energy, a graph of Coulomb energy as a function of proton number was presented. The results obtained showed that due to the finite size of proton, the values of the previously calculated values of the Coulomb energy are reduced by less than 2%. This is because the proton – proton distance increased due to finite size effect of the proton and thus affects the magnitude of the Coulomb energy. This showed that calculation of Coulomb energy by taking into consideration, the finite size of proton leads to agreement with the experimental values. Thus, in studying the nuclear structure, it is very natural to assume the protons to be extended rather than point charges.

1. Introduction

The calculation of the Coulomb energy for nuclei or atoms with small computing effort and high accuracy is a great challenge in physics and quantum chemistry research [1-3]. It is very interesting and useful to accurately estimate the Coulomb energy acting in the nuclear interior using methods more quantitative and convenient for numerical calculation. This allows us to understand some phenomena, such as nuclear fission, in more detail. The Coulomb energy can be calculated in the framework of the liquid drop model, in which atomic nuclei have reorganized as charge drops of Van der Waal like fluid [4,5]. The Liquid Drop Model proposed by Von and Weizsäcker (1935) and Bohr and Wheeler, (1939) is found very successful in explaining collective nuclear excitations and fission [6-10]. A separate investigation was devoted to the calculation of the Coulomb energy of fission fragments at the scission point during nuclear fission using the assumption of their arbitrary shape and nuclear density distributions. In the liquid-drop model, the Coulomb energy is roughly

calculated under a uniform charge distribution approximation. Later, investigations of the dependence of Coulomb energy upon the shape and the density distributions of the nucleus have been made. Based on these investigations, some terms which depend on the shape and density distributions (including constant distribution, Gaussian distribution, diffuse surface distributions, two-parameter Fermi distribution and Wood Saxon distribution) are added to the expression of the Coulomb energy [11-14].

It has been established that the net contribution of all these correction terms in Ref. [1,10-14] are not consistent with experimental data. It was first pointed out by Ohmura, (2018) that contrary to earlier estimates, the Coulomb energy corrections due to the effect of finite size of proton is not negligible [15]. Ohmura based on his findings on Coulomb energy of Helium – 3, suggested that if an extended (finite-size) charge distribution is assumed for the proton, the Coulomb energy arising from the small inter-proton distance in the atomic nucleus would be reduced. Thus, more accurate results will be obtained.

In this work, we derive an analytical expression for calculating the Coulomb energy of atomic nuclei due to the effect of finite-size of the proton using classical electrodynamics theory.

2. Theoretical Background

In the framework of liquid drop model, Coulomb energy can be calculated by considering the nucleus as positively charged sphere with total charge $+Ze$ where Z is the proton number and e the electron charge. The charge density can be defined as:

$$\rho = \frac{\text{charge}}{\text{volume}} = \frac{3Ze}{4\pi R^3} \tag{1}$$

where $R = r_0 A^{1/3}$, is the outer radius of nucleus, A is the mass number of the nucleus**,** $r_0 = 1.2 \times 10^{-15} m$, is the radius parameter.

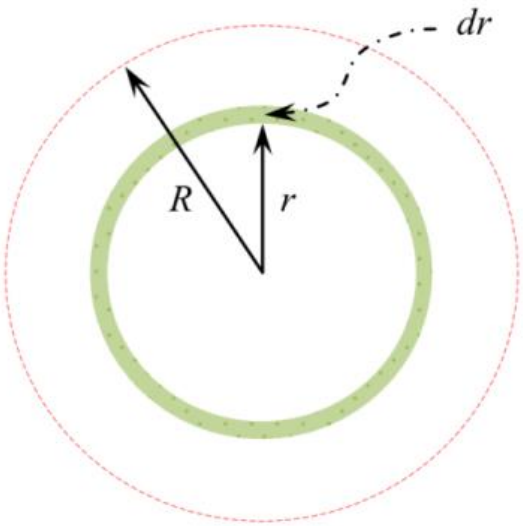

Figure 1: A charge drops of Van der Waal like fluid with a relatively thin surface layer dr

From Figure 1, the electrostatic potential at the surface of a sphere of radius $r < R$ is given by

$$V(r) = \frac{kq}{r} = \frac{k}{r}\frac{4\pi r^3 \rho}{3} = \frac{Zke}{R}\left(\frac{r}{R}\right)^2 \quad (2)$$

And the next layer of nuclear matter has a charge equal to $dq = 4\pi r^2 dr\rho$ and potential energy:

$$V(r)dq = \frac{Zke}{R}\left(\frac{r}{R}\right)^2 4\pi r^2 dr\rho$$

$$= k(Ze)^2 \frac{3r^4}{R^6} dr \quad (3)$$

Hence the total Coulomb energy,

$$E_C = \frac{3}{5}\frac{ke^2}{r_0}\frac{Z^2}{A^{1/3}} \quad (4)$$

is required to assemble a spherical nucleus, with uniform charge distribution. Equation (4) gives a classical Coulomb energy. Thus, it needs some corrections due to the Coulomb self-energy, nuclear surface diffuseness, nuclear deformation, finite-size effect of the proton and so on. Using a *constant distribution* of charge Bjornholm and Lynn (1980) give the expression for the Coulomb energy which depends on the shape of the nucleus as:

$$E_C = \frac{3}{5}\frac{e^2}{r_0}\frac{Z^2}{A^{1/3}}\mathrm{g}(shape) \quad (5)$$

where g(*shape*) is a factor, expressing the dependence of Coulomb energy on the shape parameters [12]. Hasse and Myers (1988) use the *Gaussian charge distribution* and expressed the Coulomb energy as

$$E_C^G = \frac{Z^2 e^2}{2\sqrt{\pi}\sigma} \quad (6)$$

where σ is the width (standard deviation) of the Gaussian distribution [1]. By introducing a factor (1 – l/*Z*) to remove the classical Coulomb self-energy in equation (1), Janecke (1972) use *the two-parameter Fermi distributions* and calculate the Coulomb energy as:

$$E_{dir} = \frac{3}{5}\frac{Z(Z-1)e^2}{R}\left[1 + b_1\left(\frac{a}{R}\right)^3 + b_2\left(\frac{a}{R}\right)^4\right] \quad (7)$$

where $e = 1.6 \times 10^{-19}C$, $a = 0.531\ fm$, $R = 1.2A^{1/3}fm$, $b_1 = 18.0295$ and $b_2 = -85.2330$. Yu *et. al*. (2010) found that the Coulomb energies of spherical nuclei with Woods-Saxon charge distributions can be well described with an analytical expression based on the leptodermous expansion as follows

$$E_C^{WS} = E_C\left[1 - \frac{5}{2}\omega^2 + c_3\omega^3 + \omega^4 + c_5\omega^5 + c_6\omega^6 \ldots\right] \quad (8)$$

where, $\omega = \frac{\pi}{\sqrt{3}}\frac{a}{R}$ and $R = \left[Z/\left(\frac{4\pi}{3}\rho_0\right)\right]^{1/3}$ is the corresponding radius of a spherical nucleus with uniform charge distribution and the coefficients $c_3 = 3.005$, $c_5 = -4.822$, $c_6 = 2.934$. With the same approach, Wang *et, al.* (2010) also investigate the Coulomb energies of nucleus with both the nuclear surface diffuseness, *a*, and nuclear deformation being taken into account and found the Coulomb energy of a nucleus with β_2 deformation as

$$E_C^{ND} = E_C\left[1 - \frac{1}{4\pi}\beta_2^2 + b_1\omega\beta_2^2 + b_2\omega^2\beta_2^2 + b_3\beta_2^3 + \cdots\right] \quad (9)$$

These results showed that the Coulomb energy of a nucleus gradually decreases with increase of the nuclear surface diffuseness and of the nuclear deformation.

3. Methodology

To calculate the Coulomb energy due to finite size of proton, we start by writing the most general expression for the classical Coulomb energy of an arbitrary nuclear system with charge density distribution $\rho(r)$ which can be represented as

$$E_C = \frac{1}{2}e\int \rho(r)V_C(r)dV = \frac{1}{2}\int_{\text{all space}} \rho(r)\phi(r)dV$$

where $\phi(r) = eV_C(r)$ is the scalar electrostatic potential. Using the differential form of Gauss's law for electrostatic field in states;

$$\nabla\cdot\vec{E} = \frac{\rho}{\varepsilon_0} \quad (10)$$

we have

$$E_C = \frac{\varepsilon_0}{2}\int_{\text{all space}} \left(\nabla\cdot\vec{E}\right)\phi dV \quad (11)$$

where the use of (10) has been made, $\vec{E}$ is the electric field vector, and ε_0 is the permittivity of free space. This equation can be evaluated using the divergence vector identity,

$$\nabla\cdot\left(\vec{A}B\right) = \left(\nabla\cdot\vec{A}\right)B + \vec{A}\cdot(\nabla B) \quad (12)$$

Therefore,

$$E_C = \frac{4\pi\varepsilon_0}{2}\left[\int_{\text{all space}} \nabla\cdot\left(\vec{E}\phi\right)r^2dr - \int_{\text{all space}} \vec{E}\cdot(\nabla\phi)r^2dr\right]$$

$$= \frac{1}{2k}\left[\int_{\substack{\text{boundary}\\ \text{of space}}} \phi r^2\vec{E}\cdot dA - \int_{\text{all space}} -(\nabla\phi)^2r^2dr\right]$$

Using the divergence theorem, $\int_{\text{All space}}\vec{E}\cdot dA = 0$ and taking the area to be at infinity where $\phi(\infty) = 0$, we obtain:

$$E_C = \frac{1}{2k}\int_{\text{all space}} (\nabla\phi)^2r^2dr \quad (13)$$

where $k = (4\pi\varepsilon_0)^{-1} = 9 \times 10^9 Nm^2C^{-2}$.

After the investigations of Coulomb energy based on liquid drop model of nucleus and taking into account corrections due to nuclear surface diffuseness and deformation, the concept of extended charge (finite-size) of proton was introduced to calculate the Coulomb energy. To do this, a new nuclear potential which describes the interior of the proton can be applied to calculate the electrostatic potential for a proton of charge $+e$ as a uniformly charged sphere of radius R and a spherical Gauss surface of radius r as shown in Figure 2. From this figure, for $r < R$, the total charge inside a sphere of radius r is

$$q_{\text{inside}} = +Ze\left(\frac{r}{R}\right)^3 \tag{14}$$

We can find the internal and external electric fields and hence the electrostatic potential, ϕ, by applying Gauss' law which states:

$$\iint \vec{E} \cdot d\vec{s} = \frac{q_{inside}}{\varepsilon_0} \tag{15}$$

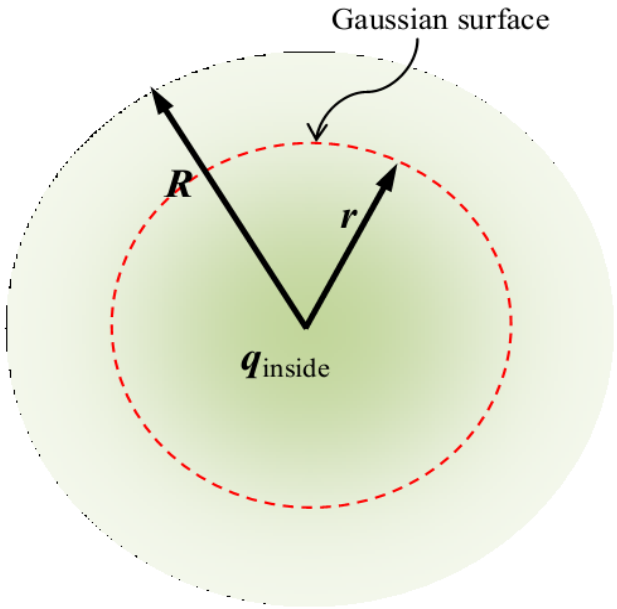

Figure 2: The Gaussian surface inside the charge distribution

By symmetry, the electric field, E is purely radial and so the flux through the Gaussian surface is $E \times 4\pi r^2$. Since E is constant, then

$$4\pi r^2 E = \frac{q_{inside}}{\varepsilon_0} = \frac{+Ze}{\varepsilon_0}\left(\frac{r}{R}\right)^3$$

and therefore,

$$E = \frac{Zer}{4\pi\varepsilon_0 R^3} = -\frac{d\phi}{dr}$$

Or

$$\phi = -\frac{Ze}{4\pi\varepsilon_0 R^3}\int r\,dr = -\frac{Zke}{R^3}\frac{r^2}{2} + C \tag{16}$$

where *C* is a constant of integration.

In a region $r > R$, the electric potential from Coulomb's law states:

$$\phi = \frac{+Zke}{r} \tag{17}$$

The electric field inside a sphere of radius *r* (Figure 3) is the same as for a point charge *e*, located at the origin.

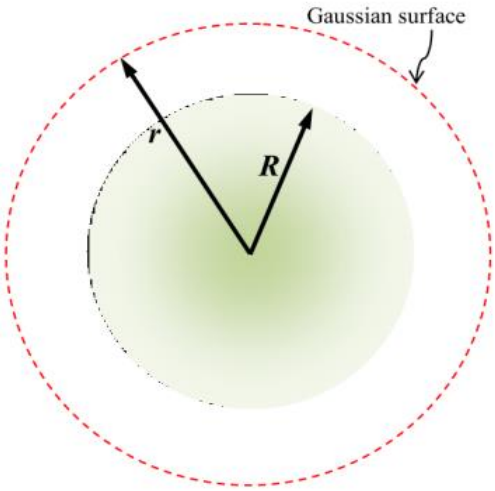

Figure 3: The Gaussian surface outside the charge distribution

By matching the interior (16) and exterior (17) solutions for ϕ at the surface of the nucleus, $r = R$ we find:

$$C = \frac{3Zke}{2R}$$

Thus, for $r \leq R$ we have from (13) that:

$$\phi = \frac{Zke}{2R}\left[3 - \left(\frac{r}{R}\right)^2\right] \tag{18}$$

This is the electrostatic potential for protons of charges +*Ze*.

4. Results and Discussion

Differentiating (18) with respect to *r*, we obtain:

$$\nabla\phi = -\frac{Zke}{2R}\left(\frac{2r}{R^2}\right)$$

By taking the scalar electrostatic potential of a finite-size proton (18) of uniform charge distribution, we can determine the Coulomb energy from (13) in a region $r \leq R$ as

$$E_{FN} = \frac{1}{2k}\int_0^{\infty} (\nabla\phi)^2 r^2 dr$$

Therefore,

$$E_{FN} = \frac{1}{2k}\left(\frac{Z^2k^2e^2}{R^6}\right)\int_0^{R} r^4\, dr = \frac{3}{5}\frac{ke^2}{r_0}\frac{Z^2}{A^{1/3}}\frac{1}{6} \tag{19}$$

Equations (3), (4), (5), (6), (7) and (19) say even one proton, *i.e.* $Z = 1$, could have a Coulomb energy, even though there is nothing to repel it.

To obtain the Coulomb energy that vanishes at $Z - 1$, we use the idea that each proton in the nucleus will repel the other $Z - 1$ proton in the nucleus. Based on this arrangement, the term Z^2 in (19) can be replaced with,

$$\frac{Z!}{2!(Z-2)!} = \frac{Z(Z-1)(Z-2)!}{2!(Z-2)!} = \frac{Z(Z-1)}{2}$$

and finally have the Coulomb energy which should vanish at $Z = 1$ as

$$E_{FN} = \frac{3}{5}\frac{ke^2}{12r_0}\frac{Z(Z-1)}{A^{\frac{1}{3}}} = \alpha\frac{Z(Z-1)}{A^{1/3}} \tag{20}$$

where

$$\alpha = \frac{3}{5}\frac{ke^2}{12r_0} \tag{21}$$

By substituting the values of constants in (21), the value of the constant was calculated as, $\alpha = 60\ keV$. Equation (20) gives the Coulomb energy of atomic nucleus due to the finite size of proton.

The values of the direct Coulomb energy E_{dir} of the atomic nuclei obtained from (7) and the coulomb energy (20) due to finite – size of protons E_{FN} are computed for light, medium and heavy atomic nuclei and denoting

$$\zeta = \left(1 - \frac{E_{FN}}{E_{dir}}\right) \tag{22}$$

as the deviation of Coulomb energy due to finite size of proton relative to the direct Coulomb energy. Then the results are presented in Table 1.

Table 1 showed that the values of finite-size Coulomb energy (calculated by taking into account the extended charge of protons) is found to be smaller than that of direct Coulomb energy by less than 2%. This is because the finite size of proton increases very slightly, the proton – proton distance and thus affects the values of the Coulomb energy.

Table 1: The values of the direct Coulomb energy E_{dir} from (7) and E_{FN} from (20)

Nuclide: $^{A}X_{Z}$	$E_{\text{dir}}(MeV)$	$E_{\text{FN}}(MeV)$	$(1-\zeta)$
$^{1}H_{1}$	0.0000	0.0000	0.0000
$^{4}He_{2}$	0.0055	0.0063	-0.1374
$^{6}Li_{3}$	0.0159	0.0165	-0.0390
$^{9}Be_{4}$	0.0288	0.0288	-0.0010
$^{10}B_{5}$	0.0467	0.0465	0.0033
$^{12}C_{6}$	0.0662	0.0655	0.0112
$^{14}N_{7}$	0.0884	0.0871	0.0145
$^{16}O_{8}$	0.1130	0.1111	0.0163
$^{19}F_{9}$	0.1372	0.1348	0.0176
$^{20}Ne_{10}$	0.1690	0.1661	0.0172
$^{23}Na_{11}$	0.1971	0.1937	0.0174
$^{24}Mg_{12}$	0.2332	0.2292	0.0173
$^{27}Al_{13}$	0.2646	0.2600	0.0172
$^{28}Si_{14}$	0.3046	0.2993	0.0172
$^{31}P_{15}$	0.3400	0.3344	0.0165
$^{32}S_{16}$	0.3848	0.3785	0.0162
$^{35}Cl_{17}$	0.4226	0.4159	0.0158
$^{36}Ar_{18}$	0.4710	0.4636	0.0156
$^{39}K_{19}$	0.5121	0.5044	0.0151
$^{40}Ca_{20}$	0.5640	0.5556	0.0149
$^{45}Sc_{21}$	0.5984	0.5899	0.0142
$^{46}Ti_{22}$	0.6543	0.6453	0.0139
$^{51}V_{23}$	0.6911	0.6819	0.0132
$^{50}Cr_{24}$	0.7601	0.7500	0.0132
$^{55}Mn_{25}$	0.7995	0.7895	0.0126
$^{54}Fe_{26}$	0.8709	0.8598	0.0128
$^{59}Co_{27}$	0.9133	0.9023	0.0121
$^{58}Ni_{28}$	0.9888	0.9767	0.0122
$^{63}Cu_{29}$	1.0321	1.0201	0.0116
$^{64}Zn_{30}$	1.1002	1.0875	0.0115
$^{69}Ga_{31}$	1.1467	1.1341	0.0110
$^{70}Ge_{32}$	1.2171	1.2039	0.0109
$^{75}As_{33}$	1.2644	1.2512	0.0104
$^{74}Se_{34}$	1.3499	1.3357	0.0105
$^{79}Br_{45}$	1.4010	1.3869	0.0100
$^{78}Kr_{36}$	1.4905	1.4754	0.0101
$^{85}Rb_{37}$	1.5283	1.5136	0.0096
$^{84}Sr_{38}$	1.6206	1.6050	0.0096
$^{89}Y_{39}$	1.6769	1.6614	0.0092
$^{90}Zr_{40}$	1.7572	1.7411	0.0092
$^{93}Nb_{41}$	1.8265	1.8102	0.0090
$^{92}Mo_{42}$	1.9264	1.9091	0.0090
$^{98}Tc_{43}$	1.9758	1.9588	0.0086
$^{100}Ru_{44}$	2.0563	2.0388	0.0085
$^{103}Rh_{45}$	2.1286	2.1109	0.0083
$^{102}Pd_{46}$	2.2350	2.2163	0.0084
$^{107}Ag_{47}$	2.2944	2.2758	0.0081
$^{106}Cd_{48}$	2.4044	2.3848	0.0081
$^{113}In_{49}$	2.4538	2.4348	0.0078
$^{112}Sn_{50}$	2.5616	2.5415	0.0078
$^{121}Sb_{51}$	2.5950	2.5758	0.0074
$^{120}Te_{52}$	2.7098	2.6897	0.0074
$^{127}I_{53}$	2.7593	2.7396	0.0071
$^{124}Xe_{54}$	2.8887	2.8677	0.0073
$^{133}Cs_{55}$	2.9319	2.9118	0.0069
$^{130}Ba_{56}$	3.0589	3.0375	0.0070
$^{139}La_{57}$	3.1017	3.0811	0.0067

$^{136}Ce_{58}$	3.2378	3.2160	0.0068
$^{141}Pr_{59}$	3.3121	3.2904	0.0066
$^{142}Nd_{60}$	3.4132	3.3908	0.0066
$^{145}Pm_{61}$	3.5083	3.4857	0.0064
$^{144}Sm_{62}$	3.6323	3.6088	0.0065
$^{151}Eu_{63}$	3.6872	3.6642	0.0063
$^{154}Gd_{64}$	3.7845	3.7612	0.0061
$^{159}Tb_{65}$	3.8608	3.8376	0.0060
$^{156}Dy_{66}$	4.0114	3.9870	0.0061
$^{165}Ho_{67}$	4.0582	4.0347	0.0058
$^{162}Er_{68}$	4.2046	4.1798	0.0059
$^{169}Tm_{69}$	4.2667	4.2423	0.0057
$^{168}Yb_{70}$	4.4003	4.3750	0.0057
$^{175}Lu_{71}$	4.4702	4.4454	0.0055
$^{176}Hf_{72}$	4.5896	4.5643	0.0055
$^{181}Ta_{73}$	4.6684	4.6431	0.0054
$^{180}W_{74}$	4.8067	4.7805	0.0054
$^{185}Re_{75}$	4.8945	4.8684	0.0053
$^{184}Os_{76}$	5.0357	5.0088	0.0053
$^{191}Ir_{77}$	5.1063	5.0799	0.0052
$^{192}Pt_{78}$	5.2315	5.2045	0.0052
$^{197}Au_{79}$	5.3207	5.2938	0.0051
$^{196}Hg_{80}$	5.4666	5.4389	0.0051
$^{203}Tl_{81}$	5.5375	5.5102	0.0049
$^{204}Pb_{82}$	5.6662	5.6384	0.0049
$^{209}Bi_{83}$	5.7663	5.7386	0.0048
$^{209}Po_{84}$	5.9070	5.8786	0.0048
$^{209}At_{85}$	6.0493	6.0202	0.0048
$^{222}Rn_{86}$	6.0590	6.0314	0.0046
$^{223}Fr_{87}$	6.2015	6.1733	0.0046
$^{226}Ra_{88}$	6.3142	6.2857	0.0045
$^{227}Ac_{89}$	6.4487	6.4197	0.0045
$^{232}Th_{90}$	6.5519	6.5228	0.0044
$^{231}Pa_{91}$	6.6991	6.6694	0.0044
$^{238}U_{92}$	6.7810	6.7516	0.0043
$^{237}Np_{93}$	6.9413	6.9111	0.0043
$^{244}Pu_{94}$	7.0234	6.9936	0.0042
$^{243}Am_{95}$	7.1860	7.1555	0.0043
$^{247}Cm_{96}$	7.2916	7.2611	0.0042
$^{247}Bk_{97}$	7.4451	7.4140	0.0042
$^{251}Cf_{98}$	7.5638	7.5325	0.0041
$^{252}Es_{99}$	7.7075	7.6756	0.0041
$^{257}Fm_{100}$	7.8148	7.7830	0.0041
$^{260}Md_{101}$	7.9348	7.9030	0.0040
$^{262}Lw_{102}$	8.0807	8.0484	0.0040
$^{261}Rf_{103}$	8.2408	8.2078	0.0040
$^{262}Db_{104}$	8.4023	8.3688	0.0040
$^{263}Sg_{105}$	8.5520	8.5179	0.0040
$^{262}Ns_{106}$	8.7302	8.6953	0.0040
$^{264}Hs_{107}$	8.8684	8.8333	0.0040
$^{266}Mt_{108}$	9.0077	8.9721	0.0040

The information represented in Table 1 is extended further by plotting a graph of two Coulomb energies (7) and (20) as a function of proton number, *Z* (Figure 4).

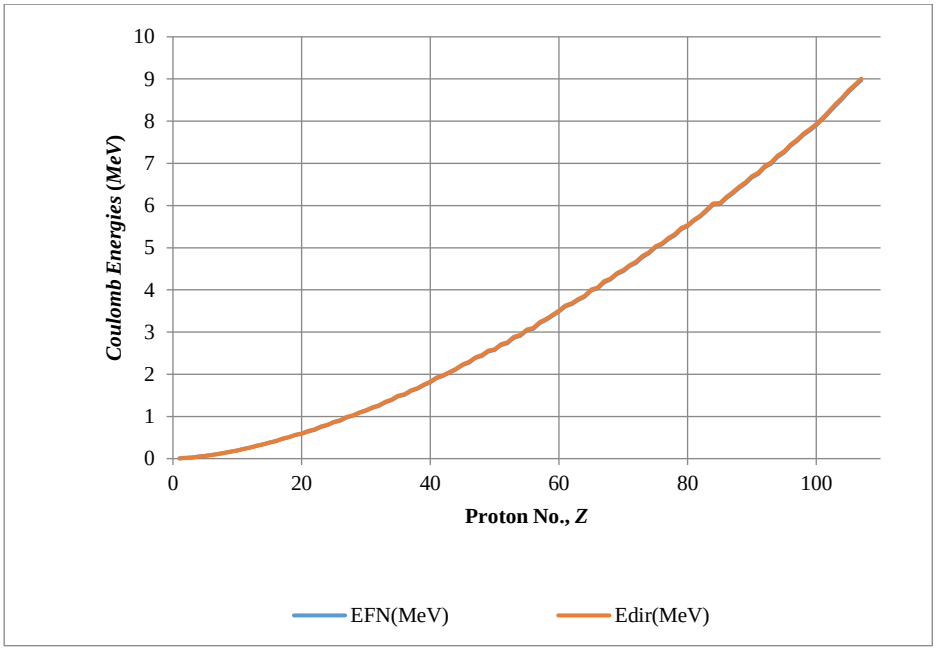

Figure 4: The Coulomb energies of atomic nuclei as functions of proton number, Z

Figure 4 represents a comparison of the results from Coulomb energy obtained by (7) using two-parameter Fermi distribution and (20) using extended proton charge distribution. The Figure showed that both direct Coulomb energy and the Coulomb energy due to finite size of proton are very closely related, both energies vanishes at $Z = 1$ (in case of hydrogen atom and its isotopes) and then gradually increases with the proton number, Z. Thus, the results obtained are in good agreement with the values of Coulomb energies calculated from the past.

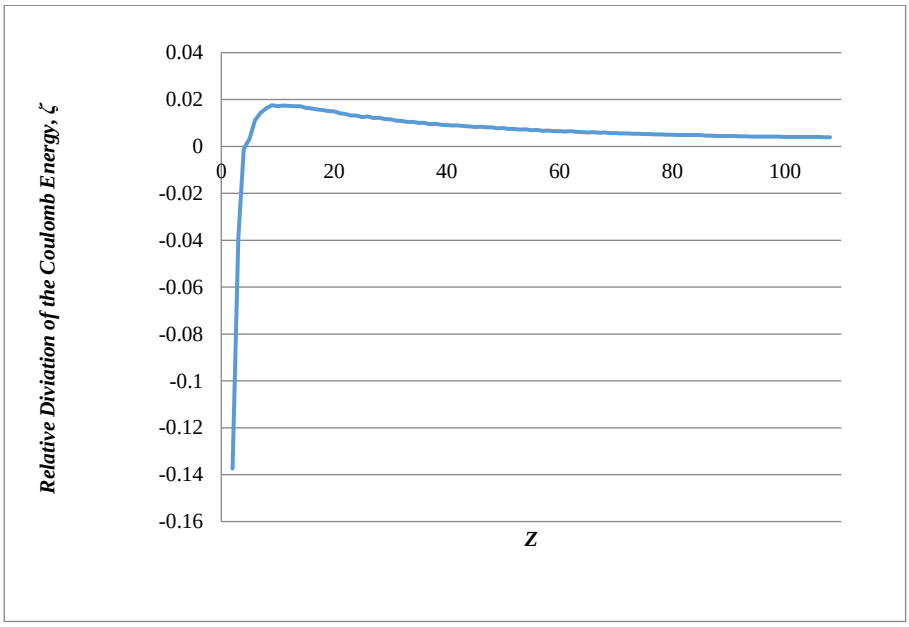

Figure 5: The relative Coulomb energies of atomic nuclei, ζ, as functions of Z

Figure 5 showed that the deviation of Coulomb energy due to finite size of proton (20) relative to direct Coulomb energy (7) increases rapidly with increasing Z up to about $Z \sim 10$ and then more slowly decreases with further increase in Z. Therefore, the values of the finite-sized Coulomb energy

are about 2% less than the previously calculated values of the Coulomb energies. This is because of the increase in proton – proton distance due to the finite size of proton and therefore changes the magnitude of the respective Coulomb energy. This seems to indicate that the coulomb energy calculated due to finite size of proton is even more consistent with the experimentally measured values.

5. Conclusion

A classical electrodynamics' approach has been investigated to determine the effect of finite size of proton on Coulomb energy of atomic nuclei. An exact analytical expression or result has been derived for the Coulomb energy potential for finite size protons. Results for different atomic number nuclei, ranging from light, medium and large have been plotted, and compared with the earlier theoretical values of Coulomb energy and found to be smaller by about 0% to a maximum of 2%. This is because of the consideration of the finite-size nature of protons instead of point-like protons, thus affecting the values of the Coulomb energy.

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