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Modified Phenomenological Formula for the Ground State Energy of Light Nuclei

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ABSTRACT

A modified phenomenological formula for the ground state binding energy in the region of light nuclei is proposed. Since binding energy is proportional to the volume of a nuclide, the new formula contains a volume term proportional to the mass number A and expresses asymmetry energy and coulomb repulsion energy between protons in a much simpler form than the way it is presented in the liquid drop model. The formula is used to calculate nuclear binding energy using three terms only, namely mass number A , neutron number, N and atomic number, Z . The correspondence with the conventional Liquid drop model and with the experimental results is highly satisfactory for light nuclei. Considering a set of 60 light nuclei for $A \leq 55$, the formula yields root mean square deviation of 0.541 MeV, with respect to experimental values. This is better than conventional Liquid drop model which gives a root mean square deviation of 3.485 MeV over the same range of nuclei. The value of f is comparatively smaller for even-odd nuclei when compared to the corresponding even-even nuclei. Thus even-even nuclei are more strongly bound than odd-odd or even-odd nuclei making them more stable.

Keywords: binding energy, isotopes, liquid drop model, ground state energy, light nuclei

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1. INTRODUCTION

Nuclear binding energy formulation is a necessary step towards the proper understanding of the nature of atomic nucleus and its properties. Over the years a lot of effort has been made towards developing a standard model for obtaining ground state binding energy of a nucleus or its mass equivalent. One of the early fundamental nuclear models was the liquid drop model (LDM). This model which was first presented by Carl Friedrich Von Weizsäcker, [1] and later developed by Niels Bohr and John Archibald Wheeler was based upon the characteristics of the liquid drops [2, 3]. The liquid drop model succeeded in explaining some of the nuclear properties, such as mass parabola, correct binding energy for 200 stable and many unstable nuclei. The famous semi-empirical mass formula for nuclear binding energy is given as;

$$B(A, Z) = a_v A - a_s A^{2/3} - a_c Z(Z - 1)A^{-1} - a_a (N - Z)^2 A^{-1} \pm \delta + \eta \quad (1)$$

where A is the mass number, Z- proton number, N- neutron number; the constants $a_v = 15.77$ MeV, $a_s = 18.34$ MeV, $a_c = 0.71$ MeV, $a_a = 28.1$ MeV, δ and η are parameters.

However this model fails to predict other properties of nuclei such as, the magic numbers and nuclear magnetic moments.

Nuclear shell model is another well-established model proposed in the last century. In this model, the existence of harmonic oscillator potential along with spin-orbit coupling between nucleons is used to calculate the energy levels of a finite nuclear system [4-6]. The most successful achievement of the nuclear shell model was the explanation of magic numbers and nuclear magnetic moments. However this model was unable to gain much success in the calculation of nuclear binding energy.

There are other models in literature that have been presented to explain some other aspects of nuclei, like Alpha-Particle Model of Nuclei, Duflo and Zuker mass formula, Skyrme-HFB and Finite Range Droplet Model (FRDM) [7-9].

The nuclear mass models belong to two distinct categories namely; a) the microscopic models and b) the microscopic- macroscopic models. Microscopic approaches usually utilize mean field theories such as SkyrmeHartree-Fock or relativistic mean field approaches to calculate the mean field calculation. Microscopic-macroscopic methods usually use the liquid drop model (LDM) as the macroscopic part of the prescription and introduce different corrections based on microscopic models [10]. Fully microscopic approaches are yet to reach the accuracy achieved by microscopic-macroscopic mass formulas.

In this paper an improved phenomenological formula is developed for the ground state binding energy in the region of light nuclei. The formula is an improvement of integrated nuclear model, which is based on the quark model of nuclei and depends on three parameters only, namely A, N and Z.

2. PHENOMENOLOGICAL FORMALISM

In general, nuclear ground state energies of a system can be obtained from the general solutions of the many body problem by use of the many body Hamiltonian. This is not possible since the exact form of the Hamiltonian is not known. Therefore for any practical application, approximations, assumptions or models have been introduced. Alternately, instead of

introducing models or assumptions, Bao, et al. [11] proposed a formula based on the mass differences between any two neighboring nuclides.

For two neighboring nuclides, say of masses $M(Z, N)$ and $M(Z_0, N_0)$ or the nuclear binding energy $B(Z, N)$ and $B(Z_0, N_0)$ the mass difference or the nuclear binding energy difference can be expanded in power series in terms of $\Delta Z = Z - Z_0$ and $\Delta N = N - N_0$ and the formula for nuclear binding energy can be written as;

$$B(Z, N) = B(Z_0, N_0) + \Delta Z \frac{\partial B}{\partial N} + \Delta N \frac{\partial B}{\partial Z} + \frac{(\Delta Z)^2}{2!} \frac{\partial^2 B}{\partial Z^2} + \frac{(\Delta N)^2}{2!} \frac{\partial^2 B}{\partial N^2} + \Delta Z \Delta N \frac{\partial^2}{\partial Z \partial N} \left(\frac{\partial B}{\partial N} \right) + \dots \quad (2)$$

The second and higher terms do not contribute much to the value of $B(Z, N)$, hence only the linear terms in the binding energy, may be considered for the purpose of calculations.

It is to be emphasized that the nucleon asymmetry ($N \neq Z$) term is proportional to $\frac{(N-Z)^2}{A}$ and Coulomb term is proportional to $Z^2 A^{-1/3}$. These can be approximated as proportional to $\frac{N^2 - Z^2}{3Z}$, [12, 13].

The nuclear binding energy formula can then be written as;

$$B(N, Z) = \left(A - \left(\frac{(N^2 - Z^2) + \delta_0(N - Z)}{3Z} + \alpha \right) \right) \frac{M_N C^2}{100}; \quad 5 < A \leq 55 \quad (3)$$

where $M_N C^2 = 938 \text{ MeV}$; the mass of a nucleon and δ_0 stand for nuclear beta-stability line condition and is defined as;

$$\delta_0(N - Z) = \begin{cases} 0 & \text{for } N \neq Z \\ A & \text{for } N = Z \end{cases} \quad \text{And} \quad \alpha = \begin{cases} 2.25 & \text{for } N - Z \leq 1 \\ 1.75 & \text{for } N - Z = 2 \\ 1.25 & \text{for } N - Z = 3 \\ 0.65 & \text{for } N - Z = 4 \\ 0 & \text{for } N - Z = 5 \\ -1 & \text{for } N - Z \geq 6 \end{cases}$$

3. DISCUSSION AND RESULTS

Since binding energy is proportional to the volume of the nuclide [14, 15], the first term, in the formula represents the Volume term

The term $\frac{N^2 - Z^2}{3Z}$ represents a combined simpler form of asymmetry energy and Coulomb repulsion force between protons.

In the present formula, some significant changes have been made namely; instead of the constant 3, as used in the nuclear binding energy formula in Integrated nuclear model (INM), a stability coefficient α is introduced that has a range between -1 to 2.25. The stability coefficient α , depends on the difference between the number of neutrons and protons in the nucleus of an atom. A closer look also reveals that for isotopic nuclei, the coefficient α is inversely proportional to the mass number A, just like in the INM.

Another significant change is in the nuclear stability line condition such that instead of,

$$\delta_0(N - Z) = \begin{cases} 0 & \text{for } N \neq Z \\ 1 & \text{for } N = Z \end{cases}$$

As, presented in INM, we now have

$$\delta_0(N - Z) = \begin{cases} 0 & \text{for } N \neq Z \\ A & \text{for } N = Z \end{cases}$$

In this case, the value of A has been found to give better results than the constant 1 for light nuclei with N = Z.

For A < 5, the formula requires minor corrections namely; the adjusting coefficient, α simply changes to 1.

In order to test the validity of the formula in equation (3), the binding energy of each nucleus is calculated for given Z and N numbers and then compared with values from the LDM and the experimental values.

Table 1. Nuclear binding energy for light nuclei; $A \leq 55$, from the improved formula given by equation (3), LDM and experimental values.

Nucleus	A	Z	N	B (LDM) (MeV)	B/A (LDM) (MeV)	B (Exp.) (MeV)	B/A (Exp.) (MeV)	B (Improved Formula) (MeV)	B/A (Improved) (MeV)
H	1	1	0	-26.461	-26.461	0	0	0	0
H	2	1	1	-5.226	-2.6128	2.225	1.1125	3.127	1.5633
H	3	1	2	1.832	0.6105	8.482	2.8273	9.380	3.1267
He	3	2	1	0.353	0.1175	7.718	2.5727	18.760	6.2533
He	4	2	2	21.945	5.4863	28.296	7.0740	21.887	5.4717
Li	6	3	3	27.640	4.6067	31.994	5.3323	28.922	4.8203
Li	7	3	4	38.384	5.4834	39.244	5.6063	37.259	5.3228
Be	9	4	5	56.632	6.2924	58.165	6.4628	56.280	6.2533
B	10	5	5	63.094	6.3094	64.751	6.4751	66.442	6.6442
B	11	5	6	75.063	6.8239	76.205	6.9277	75.196	6.8360
C	12	6	6	87.749	7.3124	92.162	7.6802	85.202	7.1001

C	13	6	7	93.629	7.2022	97.108	7.4699	94.061	7.2354
N	14	7	7	99.661	7.1186	104.659	7.4756	103.962	7.4258
N	15	7	8	112.280	7.4854	115.492	7.6995	112.895	7.5263
O	16	8	8	123.714	7.7321	127.619	7.9762	122.722	7.6701
O	17	8	9	130.974	7.7044	131.763	7.7508	131.712	7.7477
O	18	8	10	141.250	7.8472	139.807	7.7671	138.355	7.6863
F	19	9	10	149.678	7.8778	147.801	7.779	150.514	7.9218
Ne	20	10	10	160.155	8.0078	160.645	8.0323	160.242	8.0121
Ne	21	10	11	168.363	8.0173	167.406	7.9717	169.309	8.0623
Ne	22	10	12	179.445	8.1566	177.77	8.0805	176.188	8.0085
Na	23	11	12	188.009	8.1743	186.564	8.1114	188.097	8.1781
Mg	24	12	12	196.686	8.1952	198.257	8.2607	197.762	8.2401
Mg	25	12	13	205.599	8.2240	205.588	8.2235	206.881	8.2752
Mg	26	12	14	217.267	8.3564	216.681	8.3339	213.916	8.2275
Al	27	13	14	224.119	8.3007	224.952	8.3316	225.661	8.3578
Si	28	14	14	233.089	8.3246	236.537	8.4478	235.282	8.4029
Si	29	14	15	242.558	8.3641	245.011	8.4487	244.438	8.4289
Si	30	14	16	254.675	8.4892	255.620	8.5207	251.585	8.3862
P	31	15	16	260.905	8.4163	262.917	8.4812	263.213	8.4907
S	32	16	16	269.232	8.4135	271.781	8.4932	272.802	8.5251
S	33	16	17	279.154	8.4592	280.422	8.4976	281.986	8.5450
S	34	16	18	291.632	8.5774	291.839	8.5835	289.217	8.5064
S	36	16	20	309.137	8.5872	308.714	8.5754	303.443	8.4290
Cl	35	17	18	297.298	8.4942	298.21	8.5203	300.758	8.5931
Cl	37	17	20	317.675	8.5858	317.101	8.5703	314.920	8.5113
Ar	36	18	18	305.028	8.4730	306.717	8.5199	310.322	8.6200
Ar	38	18	20	328.107	8.6344	327.343	8.6143	326.824	8.6006

Ar	40	18	22	343.739	8.6685	343.811	8.5953	341.310	8.5328
K	39	19	20	333.249	8.5449	333.724	8.5570	338.297	8.6743
K	40	19	21	342.621	8.5655	341.524	8.5381	345.620	8.6405
K	41	19	22	354.466	8.6455	351.619	8.5761	352.614	8.6003
Ca	40	20	20	340.419	8.5105	342.052	8.5513	347.842	8.6960
Ca	42	20	22	364.077	8.6685	361.896	8.6166	364.413	8.6765
Ca	43	20	23	372.638	8.6660	369.829	8.6007	371.448	8.6383
Ca	44	20	24	383.661	8.7197	380.96	8.6582	379.108	8.6161
Ca	46	20	26	399.706	8.6893	398.769	8.6689	397.712	8.6459
Sc	45	21	24	390.660	8.6813	387.848	8.6188	390.275	8.6728
Ti	46	22	24	399.525	8.6853	398.193	8.6564	401.990	8.7389
Ti	47	22	25	408.535	8.6922	407.073	8.6611	409.096	8.7042
Ti	48	22	26	419.927	8.7485	418.7	8.7229	416.856	8.6845
Ti	49	22	27	427.266	8.7197	426.842	8.7111	424.800	8.6694
Ti	50	22	28	437.024	8.7405	437.781	8.7556	435.744	8.7149
V	50	23	27	434.667	8.6934	434.794	8.6959	435.714	8.7143
V	51	23	28	445.416	8.7337	445.845	8.7421	443.715	8.7003
Cr	50	24	26	434.436	8.6887	435.049	8.7010	439.557	8.7911
Cr	52	24	28	455.553	8.7607	456.349	8.7759	454.565	8.7416
Cr	53	24	29	463.391	8.7432	464.289	8.7602	462.616	8.7286
Cr	54	24	30	473.570	8.7698	474.008	8.7779	473.690	8.7720
Mn	55	25	30	481.195	8.7490	482.075	8.765	481.507	8.7547

With the aid of the improved formula, the nuclear binding energy can be calculated more accurately for all isotopes for light nuclei in the region $A \leq 55$ as shown in Table 1.

As seen from the Table 1. Nuclear binding energies obtained from equation (3) are in good agreement with the existing experimental data and also with LDM values for light nuclides. The root mean square deviation for the binding energy per nucleon with respect to the experimental values for $A \leq 55$ is 0.541MeV. This is much better than the LDM, which gives a root mean square deviation of 3.485MeV for the same number of nuclides.

In order to confirm how well the improved formula can reproduce both experimental data and LDM data for nuclear binding energies, the comparison is also made graphically as shown in the following Figures 1 and 2.

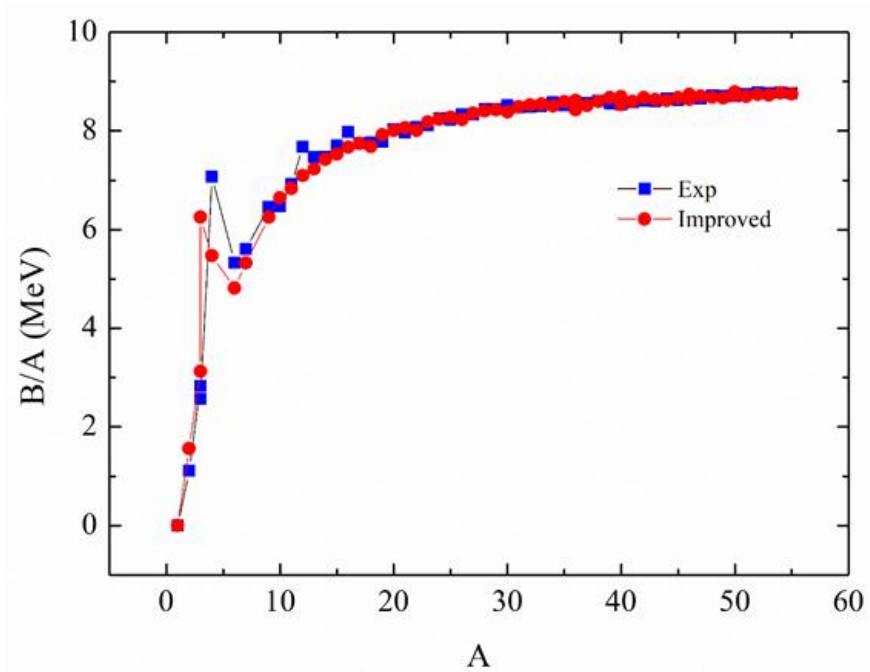


Figure 1. The Improved formula in comparison with the Experimental data of Nuclear binding energy per nucleon for mass number $A \leq 55$

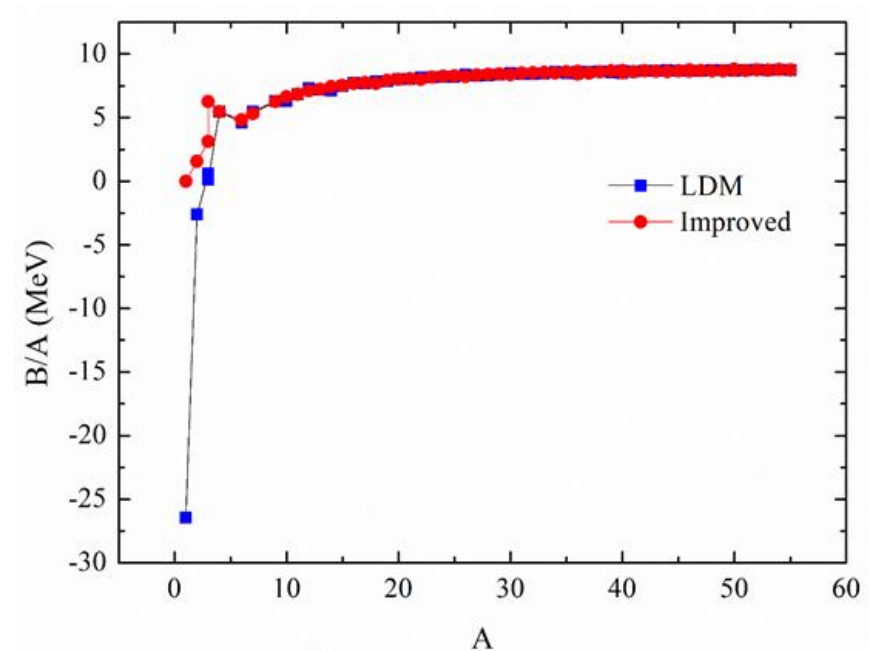


Figure 2. The Improved formula in comparison with the LDM data of nuclear binding energy per nucleon for mass number $A \leq 55$

In Figure 1, the blue curve shows the values of the binding energy per nucleon obtained from the experimental values, and the red curve indicate the phenomenological formula data.

As seen in the figure, the improved formula can reproduce data that agrees well with experimental data. It is thus concluded that the improved formula is sufficiently valid

In Figure 2, the blue curve shows the values of binding energy per nucleon obtained from the LDM data and the red curve indicate the phenomenological formula data.

As seen also in the figure, the improved formula can reproduce values that agree well with the values from the Liquid Drop Model. Thus the improved formula is quite accurate.

4. BINDING ENERGY OF EVEN-EVEN, EVEN-ODD, AND ODD-EVEN NUCLEI.

For a given isotope, the values of nuclear binding energy from the improved formula are calculated for even-even, even-odd, odd-even and odd-odd nuclei. The difference in binding energy between the isotopes is then studied. In this particular study we consider isotopes of Oxygen, Calcium and Molybdenum. The variation in binding energy per nucleon for the isotopes is then compared with experimental values and also with the values from the liquid drop model (LDM)

Table 2. Nuclear binding energy for isotopes of Oxygen, Calcium and Molybdenum from the improved formula, LDM and experimental values.

Nucleus	A	Z	N	B (LDM), MeV	B/A (LDM), MeV	B (EXP), MeV	B/A (EXP), MeV	B (MeV) (Improved formula)	B/A (Improved formula)
O	16	8	8	123.714	7.7321	127.619	7.9762	122.722	7.6701
O	17	8	9	130.974	7.7044	130.974	7.7508	131.712	7.7477
O	18	8	10	141.250	7.8472	139.807	7.7671	138.355	7.6863
Ca	40	20	20	340.419	8.5105	342.052	8.5513	347.842	8.6960
Ca	42	20	22	364.077	8.6685	361.896	8.6166	364.413	8.6567
Ca	43	20	23	372.638	8.6660	369.829	8.6007	371.448	8.6383
Ca	44	20	24	383.661	8.7196	380.960	8.6582	379.108	8.6161
Ca	46	20	26	399.706	8.6893	398.769	8.6689	397.712	8.6459
Mo	92	42	50	793.099	8.6206	796.508	8.6577	817.549	8.8864
Mo	94	42	52	812.607	8.6448	814.256	8.6623	821.122	8.7353
Mo	95	42	53	820.597	8.6379	821.625	8.6487	822.656	8.6598
Mo	96	42	54	830.485	8.6509	830.779	8.6540	824.100	8.5844

Mo	97	42	55	837.710	8.6362	837.600	8.6351	825.366	8.5089
Mo	98	42	56	846.834	8.6412	846.243	8.6351	826.482	8.4335
Mo	100	42	58	861.747	8.6175	860.458	8.6046	828.269	8.2827

From Table 2, it is observed that, the nuclear binding energy per nucleon for $^{17}_8O$ (even-odd nuclei) is less than that of $^{16}_8O$ (even-even nuclei). The same result is also obtained for $^{42}_{20}Ca$ (even-even nuclei) and $^{43}_{20}Ca$ (even-odd nuclei) nuclides. In Molybdenum, we have five even-even nuclides and two even-odd nuclides.

Even-even nuclides include $^{92}_{42}Mo$, $^{94}_{42}Mo$, $^{96}_{42}Mo$, $^{98}_{42}Mo$ and $^{100}_{42}Mo$ while even-odd nuclides are $^{53}_{42}Mo$ and $^{55}_{42}Mo$.

The nuclear binding energy per nucleon for $^{93}_{42}Mo$ which is an even-odd nuclide is less than that of $^{92}_{42}Mo$, (even-even) nuclei. Similarly the same result is obtained for $^{94}_{42}Mo$ and $^{95}_{42}Mo$.

It should also be noted, the values of binding energy per nucleon for Molybdenum obtained from the improved formula are not accurate, since the improved formula only applies to nuclides, $A \leq 55$.

Both protons and neutrons have an intrinsic angular momentum reflected in a quantity called spin. Both have spin $\frac{1}{2}$, but the direction can either be up or down. When a nucleus has an even number of protons and an even number of neutrons, the spin up protons are able to pair off with the spin down neutrons. This makes the nucleus more tightly bound, increasing binding energy, hence more stable. For a nucleus, with oddness of either, Z or N or both, the spin up protons do not completely pair off with spin down neutrons. This therefore lowers nuclear binding energy, making odd nuclei generally less stable. The effect of such pairing is displayed in the values of the binding energies of different nuclei in Table 2. The odd-even or even-even nuclei display different magnitudes for the binding energy.

5. CONCLUSIONS

An improved phenomenological formula has been proposed. The formula which is based on the Integrated Nuclear Model in the region of light nuclei contains a volume term proportional to the mass number, A. The formula also contains asymmetry energy and Coulomb repulsion between protons expressed in a combination form much simpler than the way it is presented in the liquid drop model. Unlike many derived global formulas with many parameters and several coefficients, the proposed formula calculates nuclear binding energy using three terms that depend only upon A, N and Z numbers only. The formula also has a single coefficient namely α compared to LDM which has several coefficients. The rms deviation for 60 light nuclei, for $A \leq 55$ with respect to experimental values is 0.541 MeV, which is better than the LDM which gives an rms deviation of 3.485 MeV for the same number of nuclei. From the results, it is found that the formula predicts nuclear binding energies for light nuclei to a good degree of accuracy which is an indication of validity of the formula.

Similar to LDM, deviations in this formula come from two extreme sides, the lightest nuclides and from the heaviest ones. For the heaviest ones the number of neutrons is much more than proton numbers, resulting in larger asymmetry.

Nuclear binding energy depends on evenness or oddness of its atomic number, Z neutron number, N and consequently their sum, the mass number, A . Oddness of either Z or N or both tends to lower binding energy, making odd nuclei generally less stable.

In any mass or nuclear binding energy formulation, the theoretical calculations will be extremely sensitive to the choice of parameters used. Hence the binding energies and one-neutron, one-proton, two-neutron etc., separation energies will stringently depend on the choice of parameters. There is still no exact agreement as to whether n-p, n-n, or p-p is the predominant pairing inside the nucleus. Such pairing will certainly determine the magnitude the magnitude of binding energy. As the neutron or proton number becomes abnormally large in a nucleus, the so called drip-line is reached when the last neutron or proton has practically zero binding fractions. Such situations cannot be explained by the binding energy formula proposed by the various authors from time to time. For instance, when the mass or binding energy formula was proposed in the beginning, concepts like shell structure of nuclei, pairing types, laboratory production of nuclei with abnormally large neutron or proton numbers called designer nuclei, and the concept of drip-line was not known. Hence binding energies formula may have to be modified as new properties of nuclei are discovered experimentally from time to time. Recent studies indicate that the Coulomb law inside the nucleus needs to be modified since the size of the nucleus is very small. Hence the proximity of protons and high mass density can result in a modified Coulomb law and also there may be a new role for gravitational forces [16].

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