Modified Fermi-Gas Model to Calculate the Nuclear Quantities

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Abstract: Due to the unknown nature of nuclear forces, using nuclear models for different purposes of nuclear usage, as explanation of the interactions between nuclear particles are remarkable. In this study, by introducing a density and nucleus parameterization; we modify the Fermi gas model, and calculate nuclear quantities based on the modified model. For the first time, according to properties of the nuclear density, we consider it as an error function, then, parameterize nuclear density based on the known properties of nucleus. According to the modified Fermi gas model, we calculate quantities of density, radius and find the relationship between them. Then, we calculate the surface thickness of the nucleus and the nucleus radius, average radius of the nucleus, volumetric energy, surface energy and the Coulomb energy with the Pauli correction effect, asymmetric energy of nucleons, the nuclear compressibility; binding energy is obtained using outcomes too. At last Coefficients of Binding Energy is compared with previous studies; the result of formulation and error in the Tablecurve software shows that error calculated by the program was too little so we concluded that the formula presented to calculate the nuclear energy is appropriate to interpret nuclear properties.

[Reshadatiyan M, Tahmasebi Birgani M J, Ghasemi F, Kazeminejad I. **Modified Fermi-Gas Model to Calculate the Nuclear Quantities.** *Academ Arena* 2013;5(10):1-7] (ISSN 1553-992X). http://www.sciencepub.net/academia. 1

Keywords: Nuclear quantities; Fermi gas model; Nucleus density; Error function.

1. Introduction

Nuclei have a certain time–independent properties such mass, size, charge, intrinsic angular momentum and certain time–dependent properties such as radioactivity and artificial transmutations (nuclear reactions). The mass of a nucleus is related to the mass summation of the protons and neutrons which constitute it and nuclear binding energy is the energy required to split a nucleus of an atom into its component parts (Serway and Vuille, 2010); the binding energy is also reduced by Coulomb repulsion forces between the protons (Jevremovic, 2009). The electron scattering experiment could reliably use for measuring nuclear radius (Povh, 2008). The nucleon density distribution has been measured in scattering experiments too (Sitenko and Tartakovskii, 1977); heavy nuclei have a uniform central density, surrounded by a diffuse surface region. The shape of the nucleon density distributions (Woods-Saxon distributions) is described by a Fermi function. A Woods-Saxon distribution is an accurate one as its nuclear potential does not have a sharp edge as indicated by Moharram et al. (1980), and Srokowski et al. (1995).

The nuclear force (nucleon–nucleon interaction) is very powerful, but extremely short-range; the range of the nuclear force is < 2 fm (Bolonkin, 2009). There are many different nucleus models that scientists have used to explain the nature of the nuclear force in order to employ of nuclear energy since 1934 (Sutton, 1992); to this day proposed models can not completely alone explain all nuclear properties. These models include some that are based on the three phases of ordinary matter: solid, liquid, and gaseous, and some that are based on atomic molecules. One of an independent particle models is Fermi gas model (semi-classical); due to the lack of experimental data, this model is still not completed. However it is a statistical model of the nucleus; this model pictures the nucleus as a degenerate gas of protons and neutrons as nucleons move freely inside the nucleus (Sharma, 2008).

In the present study we modified Fermi gas model considering effect of the nuclear surface and calculate the surface thickness of the nucleus and the nucleus radius, average radius of the nucleus, kinetic energy and the Coulomb energy with the Pauli correction effect, asymmetric energy of nucleons, the nuclear compressibility and binding energy based on the modified model as well as comparing the findings with results of other studies.

2. Material and Methods

Due to the different approximations for the nuclear density, Woods-Saxon distribution considered more accurate than other approximations.

This function should be expressed by series in order to use in calculations; consequently, it would be more complicated. So firstly we introduce a simple function which is similar to this distribution curve and represents nuclear density; finally nuclear quantities will be calculated using this novel function. The error function is suggested for nuclear density and is defined as follows (Weber et al., 2003):

$$\left[1-erf(x)\right]=\left[1-\frac{2}{\sqrt{\pi}}\int_{0}^{x=\alpha r}e^{-u^{2}}du\right] \quad (1)$$

Figure 1 presents error function, this graph plots in Matlab Software. For similarity between Woods-Saxon distribution and 1-erf(x) curves, we ourselves propose density function as the follows:

$$\rho(x)=\rho_{0}\left[1-\frac{2}{\sqrt{\pi}}\int_{0}^{x=\alpha r}e^{-u^{2}}du\right] \quad (2)$$

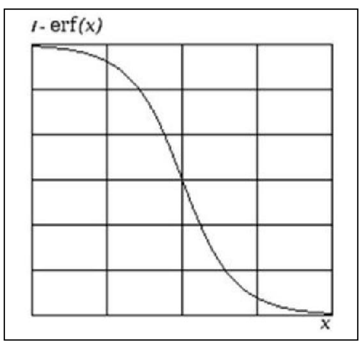

Figure 1. $\left[1-erf(x)\right]$ curve is similar to Woods-Saxon distribution

2.1 The average radius of the nucleus

Radius of the nucleus can be calculated from the knowledge of mass number (Hobbie et al., 2007) and accordingly density, so in the following equation ρ_0 is the density where $\overline{R}$ is the average radius of the nucleus and we have:

$$\overline{R}=\langle r\rangle=\frac{\int\rho(r)r\,dv}{\int\rho(r)dv} \quad (3)$$

After substituting Eq. (2) in Eq. (3) and solving integrals by the Derive 6 software, $\overline{R}^{3}$ is obtained as:

$$\overline{R}^{3}=1.66(\overline{R})^{3} \quad (4)$$

2.2 ρ_0 in density function

Since in the Fermi gas model, we consider nuclear shape as spherical (Wong, 2004); in calculating ρ_0 the volume of a sphere is used:

$$A=\int_{0}^{\infty}\rho(r)dV \quad (5)$$

After substituting Eq. (2) in Eq. (5) and solving integrals, ρ_0 will be 3ρ.

If we consider Hauser-Feshbach nuclear density which is $\rho=1/72\times10^{38}$ we have:

$$\rho_{0}\cong 0.52\,Particle\;/\;cm^{3} \quad (6)$$

2.3 The average kinetic energy of a nucleon

Number of counted balances in interval k to k+dk at momentum space (k) is obtained by:

$$dn(k)=\frac{1}{8}(4\pi k^{2}dk)\frac{1}{(\frac{\pi}{a})^{3}} \quad (7)$$

To modify this model, counting balances on three surfaces $k_x=0, k_y=0, k_z=0$ (Surface effect) and counting balances on axis (linear effect), should be moved out of the volume.

Surface linear effect is defined:

$$\frac{1}{2}\frac{dk}{\left(\frac{\pi}{a}\right)} \quad (8)$$

By substitution volume and surface area formula of sphere, the correct counted balances in momentum space are obtained:

$$dn=(0.36(\overline{R})^{3}k_{F}^{2}-0.4(\overline{R})^{2}k_{F}-0.45\overline{R})dk \quad (9)$$

According to the Pauli exclusion principle which illustrate state of electrons in the same orbit, (Godse and Bakshi, 2009) we have:

$$\int dn(k)=\frac{A}{4} \quad (10)$$

By substitution Eq. (9) in Eq. (10) and solving the integral we obtain:

$$A=0.48(\overline{R})^{3}k_{F}^{3}-0.8(\overline{R})^{2}k_{F}^{2}-1.8\overline{R}k_{F} \quad (11)$$

For Average kinetic energy of the nucleons we can use this formula:

$$\left\langle\frac{E}{A}\right\rangle=\frac{\int_{0}^{k_F}\varepsilon(k)\frac{dn(k)}{dk}dk}{\int_{0}^{k_F}dn(k)} \quad (12)$$

Where

$$\varepsilon_{F}=\frac{(\hbar K_{F})^{2}}{2M} \quad (13)$$

Eq. (13) is fermi energy of the last balance. After solving the integral respect to K_F we have:

$$\left\langle \frac{E}{A} \right\rangle = E_F \left(0.6 + \frac{0.17}{X} + \frac{1.27}{(X)^2} \right) \quad (14)$$

Based on the results of Feshbach calculations, Experimental value for $K_F \cong 1.4\, fm^{-1}$ and E_F will be $40 MeV$ where M is the proton mass.

Kinetic energy in Eq. (14) can be obtained as a function of A in Eq. (11). For this we use change of variable $X = \bar{R}K_F$ and approximation method to solve the problem which is $X = y + 0.55$ and the other one $y(y^2 - 3.6) = 2A + 2.4$. This equation can be solved using Cardan method too (Nickalls, 2008). For nuclei with different Nucleons numbers, we put y and X values in Table 1.

Table 1. Values of the third-order in Eq. (11)

A	Y*	X*
27	4.2	4.75
64	5.3	5.85
125	6.5	7.05
216	7.7	8.2
342	7.8	9.5

Values calculated in solving the third order equation (Eq. (11)) for different numbers of nucleons were inserted in the software Tablecurve shows in Figure 2 and amid numerous formulas, a formula that had the lowest standard error was determined that is:

$$\bar{R}k_F = 2.08 + 0.7A^{0.4} \quad (15)$$

We know (Bartke, 2009):

$$R = R_0 A^{\frac{1}{3}} \quad (16)$$

And in Fermi gas model $K_F \cong 1.4\, fm^{-1}$ so by substituting in Eq. (15), R_0 can be calculated as a function of A:

$$R_0 = 1.48A^{-1/3} + 0.5A^{0.07} \quad (17)$$

Furthermore, by inserting $\bar{R}K_F$ and R_0 values in Eq. (14) we have:

$$\left\langle \frac{E}{A} \right\rangle = E_F \left(0.6 + \frac{0.17}{2.08 + 0.7A^{0.4}} + \frac{1.27}{(2.08 + 0.7A^{0.4})^2} \right) \quad (18)$$

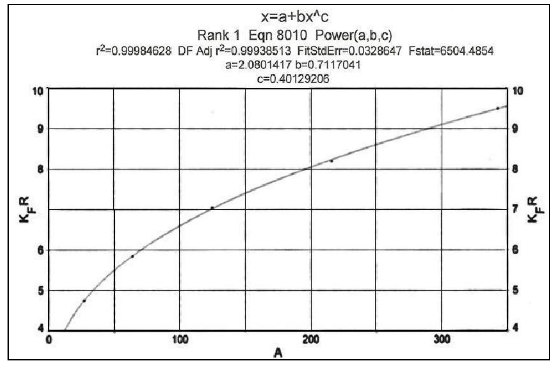

Figure 2. Graph of $K_F\bar{R}$ as a function of A

2.4 The Coulomb energy

The shape of the nucleus is determined mainly by three factors, the volume energy, the surface energy, and the coulomb energy (Aruldhas and Rajagopal, 2005); Nuclear Coulomb energy according to the Pauli Exclusion Principle is obtained by:

$$C.E = \frac{A(A-1)}{2} \times \int \rho_{00}(r_1, r_2) v_{12}(r_1, r_2) dr_1 dr_2 \quad (19)$$

Where

$$v_{12} = \frac{e^2}{r_{12}} \left[\frac{1 + \tau_3(1)}{2} \right] \left[\frac{1 + \tau_3(2)}{2} \right] \quad (20)$$

After putting the proposed density function in the formula, the integral equation is split into two separate integrals; the first integral gives classical Coulomb energy of a sphere; the second integral gives corrections of the Pauli principle on the nuclear Coulomb energy.

The answer to the first integral for $Z \succ\succ 1$ is:

$$C.E = 0.65 \frac{Z^2 e^2}{R} \quad (21)$$

And the solution for the second integral is:

$$(C.E)_{ex} = \frac{9\pi}{4} \frac{z^2 e^2}{\Omega k_F^2} \quad (22)$$

And finally total coulomb energy is:

$$C.E = \frac{3}{5} \frac{Z^2 e^2}{R} - (C.E)_{ex} \quad (23)$$

By substitution Eq. (22) in to Eq. (23) we can write:

$$C.E = 0.83 \frac{Z^2}{A^{\frac{1}{3}}} \left(1 - \frac{1}{A^{\frac{2}{3}}} \right) \quad (24)$$

2.5 The asymmetry energy

Asymmetry energy (also called Pauli Energy) is an energy associated with the Pauli

Exclusion Principle. To calculate this energy it is sufficient to calculate the energy difference between two symmetry and asymmetry nucleus. So by assuming $E_F \cong 40MeV$ In the following expression $\frac{N-Z}{A}$ is called neutron excess ratio which decrease nuclear stability (Singh, 2008).

We have:

$$\Delta E = \frac{1}{3}\frac{\varepsilon_F (N'-Z')^2}{A} \cong 1.32\frac{(N'-Z')^2}{A} Mev \qquad (25)$$

2.6 The binding energy

Nuclear energy is the summation of kinetic energy and the binding energy of the nucleus that is $\langle U\rangle = \langle T\rangle + \langle B.E\rangle$; as we know $\langle U\rangle \cong 40MeV$

Consequently, the whole binding energy is obtained using U and T which was calculated lately (Eq. (18)), and by subtracting relations of the Coulomb energy, asymmetry energy and the coupling energy we can write the following equation,

$$\langle B.E.\rangle = 16A - \frac{6.8A^{\frac{2}{3}}}{2.08A^{\frac{-1}{3}} + 0.7A^{0.07}} - \frac{50.8A^{\frac{1}{3}}}{(2.08A^{\frac{-1}{3}} + 0.7A^{0.07})^2}$$
$$-0.83\frac{Z^2}{A^{\frac{1}{3}}}\left(1 - \frac{1}{A^{\frac{2}{3}}}\right) - 1.32\left(\frac{N'-Z'}{A}\right) \pm \gamma \qquad (26)$$

2.7 The Nuclear compressibility

The curvature of the shape of the volume energy as a function of the density in the vicinity of the equilibrium value defines the nuclear compressibility K (Hornyak, 1975):

:

$$K_{Com} = R_0^2 \frac{\partial^2 E}{\partial R_0^2} \qquad (27)$$

We can write Eq. (15) in form of:

$$K_F = \frac{f(A)}{R_0} \qquad (28)$$

By substitution Eq. (28) in to Eq. (14) we have:

$$\langle E\rangle = \frac{\hbar^2}{2M}\frac{f^2(A)}{R_0^2}\left(0.6 + \frac{0.17}{X} + \frac{1.27}{(X)^2}\right)A \qquad (29)$$

In Eq. (29) by taking two derivatives with respect to R_0, considering $E_F \cong 40MeV$ and substitution in Eq. (27) we obtain:

$$K_{Com} = 144A + \frac{40.8A^{\frac{2}{3}}}{2.08A^{\frac{-1}{3}} + 0.7A^{0.07}} + \frac{304.8A^{\frac{1}{3}}}{(2.08A^{\frac{-1}{3}} + 0.7A^{0.07})^2} \qquad (30)$$

While Berg and Lawrence's achieved relation for K_{Com} is $125A + 210A^{\frac{2}{3}}$ (Berg and Wilets, 1956).

Finally considering Eq. (27), the compressibility of nuclear is:

$$b_{Com} = 16A + \frac{4.53A^{\frac{2}{3}}}{2.08A^{\frac{-1}{3}} + 0.7A^{0.07}} + \frac{33.86A^{\frac{1}{3}}}{(2.08A^{\frac{-1}{3}} + 0.7A^{0.07})^2} \qquad (31)$$

2.8 The nuclear electric quadrupole moment

The nuclear electric quadrupole moment is a parameter which describes the effective shape of the ellipsoid of nuclear charge distribution (Cottingham and Greenwood, 2001).

The nuclear electric quadrupole moment is defined as:

$$Q = K_C \int \frac{r^2}{2}\left(3\cos^2\theta - 1\right)\rho dV \qquad (32)$$

Note that the nucleus assumed spherical, now we write spherical polar coordinates for Eq. (32):

$$Q = \int_0^r \int_0^\pi \int_0^{2\pi} \frac{K_C r^2}{2}\left(3\cos^2\theta - 1\right)\rho r^2 \sin\theta d\theta d\phi dr = 0 \qquad (33)$$

As it is obvious the calculated value is equal to zero, Of course the above integral was expected, because the nuclear electric quadrupole moment depends on the nucleus shape and it's symmetric and asymmetric with respect to axes and in this spherical shell nuclear model the nuclear electric quadrupole moment is equal to zero due to symmetry of the sphere with respect to axes (McParland, 2010).

2.9 The Thickness of the nuclear surface

The surface thickness is defined to be the change in radius required to reduce $\rho(r)/\rho_0$ from 0.9 to 0.1 (ρ_0 is the density in the center of the nucleus).

Using Eq. (2) the following result are obtained by Derive 6 software; if we consider:

$\rho(x) = 0/9\rho_0$ So we have $x = 0.088$, and for $\rho(x) = 0/1\rho_0$ we have $x = 1.163$

On the other hand, as regards $X = \alpha r$ and $\bar{R} = \frac{1}{\alpha}$ so the surface thickness will be:

$$t = R_2 - R_1 = \frac{1.163 - 0.088}{\alpha} = 1.075 R_0 A^{\frac{1}{3}} \quad (34)$$

As a result, the thickness of the nuclear surface is obtained as a function of A using Eq. (17):

$$t = 1.59 + 0.53 A^{0.4} \quad (35)$$

In Table 2 we calculated the thickness of the surface for a number of heavy and semi-heavy nuclei with respect to the relation obtained for surface thickness of the nucleus.

Table 2. Surface thickness value for heavy and semi-heavy nuclear obtained by Eq. (35)

Nucleus	t*(fm)
$^{56}_{26}Fe$	4.24
$^{75}_{33}As$	4.57
$^{88}_{38}Sr$	4.76
$^{130}_{54}Xe$	5.3
$^{206}_{82}Pb$	6.05
$^{238}_{92}U$	6.32

3. Results

The calculations result of the nuclear quantities was showed in this project. Among the proposed models, the Fermi gas model as a selected model in this project is a proper model for calculating the properties and factors of nucleus.

The advantage of this model is that by investigating variety of approximation for nuclear density, we could introduce a function (Error function) for the nucleus density, and with employing it; we could find, firstly, a relation for the average radius $\bar{R}$ with respect to α, which is a coefficient of the nucleus radii (X=αr) also, we calculated $\bar{R}^3$.

We could find ρ_0 in the proposed density function (nuclear density, when the nucleus radius is equal to $\bar{R}$). We obtain the average kinetic energy of the nucleons with respect to A; after that we gain binding energy by reducing surface effects, asymmetry, Coulomb and coupling of nucleons.

In binding energy, the term with coefficients A is the volume energy term; the term with a coefficient $A^{\frac{2}{3}}$ is the surface energy term; and the term with a coefficient $A^{\frac{1}{3}}$ is the radial. The next term is the Coulomb energy; then, asymmetry energy; and γ is the coupling energy. By different values for A, we collect values X, and Y in Table 1. And then, best curve fit to the data which is shown in Figure 2, is plotted using the Tablecurve software.

4. Discussions

Considering the calculated surface thickness values, it can be seen, this quantity can be increased by increasing the number of nucleons. Based on the binding energy significance in splitting a nucleus of an atom into its component parts; a comparison of experimental and theoretical of binding energy coefficients of this study with others has shown in Table 3. This table show, the volumetric energy coefficient values which have been calculated in this study is very close to values obtained by others. Surface energy coefficient calculated in the present study is as a function of the nucleon number of the nucleus (A) while other studies have obtained a constant numerical value for this coefficient. With paying more attention in the binding energy formula, it can be seen that this relation has a term A-dependent compared to the relations calculated by others and the result will be a modified Fermi gas model for nucleus. A comparison between the nuclear compressibility calculated in this study and the results of others indicate that there has not been found an experimental procedure for the determination of this quantity until now; however Berg and Wilets (1956) obtained the relation $K_{com} = 125A + 210A^{\frac{2}{3}}$, Brueckner and Gammel (1958) achieved k=172, Molitoris and Stöcker (1985) attained k=380MeV, Danielewicz (1994) acquired k=215, and we obtained the value of k=148 for A=100 based on Eq. (30). Results of formulation and partial error in the Tablecurve software show minor error and indicates the formula presented to calculate the nuclear energy is appropriate; so that By finding a relation for the nuclear fixed radius amount R_0 with respect to atomic number, we can calculate the mean radius of the nuclear, the volumetric energy, surface energy, and coulomb energy along with the Pauli effect, asymmetry energy of nucleons, compressibility of nuclear and Fermi energy. The advantage of this method is that it can calculate the entropy and the thermodynamics of nuclear will be achieved consequently; we will consider calculation this for our future work. In future relativistic case can be discussed and evaluated; nucleus can consider in adiabatic state and thermodynamic calculations can be carried out on the basis of this assumption; also as we assumed two-particle interacts in here (proton - proton or protons - neutrons or neutrons - neutrons), in future three-particle interacts (protons - neutrons - neutrons) also can be studied in order to find modified quantities. Regarding the fact that fossil fuels are coming to an end soon, the use of nuclear energy for peaceful purposes is getting a big deal of attention (Esrafilian and Maghamipour, 2012).

Table 3. Coefficients of binding energy formula (semi-empirical formula of mass) based on the various theories and experiment.

Ref.	$a_V(MeV)$ Coefficient of volumetric energy	$a_S(MeV)$ Surface energy coefficient	$a_C(MeV)$ Coulomb energy coefficient	$a_{asym}(MeV)$ Asymmetry energy coefficient			
(Green and Engler, 1957)	-15.58	17.23	0.698	23.3			
(Brueckner et al., 1961)	-15.642	19.23	20	0.727			
(Myers and Swiatecki, 1966)	-15.68	18.56	7.17	28.1			
(Wang and Hwang, 1972)	-15.68	18.56	0.717	1.79			
(Seeger and Howard, 1976)	-15.25	17.07	33.16	1.22			
(Sapershtein and Khodel, 1977)	-14.9	19	30,3	1.17			
(Fewell, 1995)	14	-13	-0.585	-19.3			
(Yang and Hamilton, 2010)	15.8	-18.3	-0.72	-23.2			
Current study	16	-6.8f(A)	-0.83	-1.32			

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