

Relevance of infinite nuclear matter quantities in finite nuclei

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Abstract. The density-dependent symmetry energy depicts the energy difference between the binding energy of symmetric nuclear matter and pure neutron matter, which is associated with various phenomena such as exotic nuclei, heavy ion-collision experiments, supernovae, and gravitational collapse in neutron stars. In this theoretical work, we study the isospin-dependent properties of finite nuclei, namely symmetry energy, surface symmetry energy, volume symmetry energy, and their ratio κ from their corresponding components available in the infinite nuclear matter using the coherent density fluctuation model. We have performed the calculations for a few $even - even$ isotopes of Titanium for the non-linear NL3 parameter set within the purview of relativistic mean-field formalism. This study provides theoretical understanding and computational steps for analyzing the magicity of Titanium nuclei which can be extended to different sets of nuclei across the nuclear landscape.

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1. INTRODUCTION

While moving across from nuclear landscape from stable to unstable exotic nuclei, the appearance of newer magic numbers and the disappearance of others can be observed owing to the distinct constituents of the nucleon-nucleon interaction. Some of these nuclei have widely different nuclear configurations than those predicted from early nuclear models. These nuclei can have extreme values of neutron-proton asymmetry (also referred as isospin-asymmetry) which is given as $\delta = (\rho_n - \rho_p)/\rho$, where ρ_n and ρ_p are the neutron and proton densities respectively and $\rho = \rho_n + \rho_p$ is the baryon density. The $\rho-$ meson term handles the density type isospin, whereas the $\delta-$ meson handles the mass asymmetry.

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The fundamental problem of understanding nuclear physics involving isospin is describing the equation of states (EOS) in terms of binding energy per nucleon

$$E(\rho,\delta) = E(\rho,0) + E_{sym}(\rho)\delta^2 + \mathcal{O}(\delta^{\triangle}).....,\tag{1}$$

The term $E(\rho, 0)$ refers to energy in a symmetric nuclear matter which depends on the total density, i.e., the sum of neutron and proton densities. $E_{sym}(\rho)$ refers to the density-dependent nuclear symmetry energy (NSE). δ^4 is found to be very small and can be safely ignored [1,2] and thus, the EOS can be described using the parabolic equation. The study of NSE has a profound research interest in the field of nuclear astrophysics. It is used to characterize both the finite and infinite asymmetric nuclear matter. However, proper study related to the density-dependence of symmetry energy is still in a nascent stage. Recently Bhuyan *et al.* [3-7] have successfully studied various density-dependent symmetry energy properties using the relativistic mean-field formalism, providing a newer direction in this field. Moreover, the availability of radioactive ion beam (RIB) and its advances in measurements of exotic nuclei has given experimental support and stimulated theoretical research projects towards understanding the properties related to nuclear symmetry energy.

The structure of the paper is as follows: The theoretical formalism pertaining to the relativistic mean-field formalism is discussed in Section 2.1. We then present the need and derivation for calculating the symmetry energy and its related parameter using the coherent density fluctuation model in Section 2.2. Section 3 provides a flowchart detailing the steps for creating the required program. Finally, we present the calculations and a brief discussion of the result for nuclear symmetry energy, surface, and volume symmetry energy for Titanium nuclei in Section 4.

2. METHODOLOGY

2.1 Relativistic mean-field formalism

The relativistic mean-field (RMF) formalism has various advantages corresponding to its non-relativistic counterparts [8-12]. The RMF formalism includes the presence of spin-orbit interaction in the relativistic equations. This method has successfully reproduced the bulk properties of finite nuclei such as binding energy, quadrupole moment, charge radius, etc., throughout the mass table. It also considers some of the meson-nucleon coupling parameters, which successfully reconciles with the experimental data. Moreover, the nuclear equation of state and properties associated with neutron stars can be studied using this formalism. A generalized expression of non-linear finite-range RMF model having typical Lagrangian density takes the form as

$$\begin{aligned}\mathcal{L} = {} & \overline{\psi}\{i\gamma^{\mu}\partial_{\mu} - M\}\psi + \frac{1}{2}\partial^{\mu}\sigma\partial_{\mu}\sigma - \frac{1}{2}m_{\sigma}^2\sigma^2 - \frac{1}{3}g_2\sigma^3 - \frac{1}{4}g_3\sigma^4 - g_s\overline{\psi}\psi\sigma \\ & -\frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_w^2\omega^{\mu}\omega_{\mu} - g_w\overline{\psi}\gamma^{\mu}\psi\omega_{\mu} - \frac{1}{4}\vec{B}^{\mu\nu}.\vec{B}_{\mu\nu} + \frac{1}{2}m_{\rho}^2\vec{\rho}^{\mu}.\vec{\rho}_{\mu} \\ & -g_{\rho}\overline{\psi}\gamma^{\mu}\vec{\tau}\psi\cdot\vec{\rho}^{\mu} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - e\overline{\psi}\gamma^{\mu}\frac{(1-\tau_3)}{2}\psi A_{\mu}.\end{aligned}\tag{2}$$

Here the fields for the electromagnetic, ρ, σ and ω meson is depicted as A_μ, $\vec{\rho}_\mu$, σ and ω_μ respectively. Moreover, $\vec{B}_{\mu\nu}$, $\Omega^{\mu\nu}$ and $F^{\mu\nu}$ are the field tensors corresponding to the $\vec{\rho}_\mu$, ω^μ and photon fields respectively.

Within RMF formalism, the simplistic expression of nuclear symmetry energy can be written as:

$$S^{NM}(\rho) = \frac{1}{2}\frac{\partial^2(\mathcal{E}/\rho)}{\partial\alpha^2}\bigg|_{\alpha=0}, \tag{3}$$

where $\mathcal{E}$ is the energy density and α corresponds to the neutron-proton asymmetry in terms of baryon density. Following Ref. [3, 13-16] the mesons coupling corresponding to the fields of nucleons can be given as

$$g_i(\rho) = g_i(\rho_{sat})f_i(x)|_{i=\sigma,\omega}. \tag{4}$$

Here

$$f_i(x) = a_i\frac{1+b_i(x+d_i)^2}{1+c_i(x+d_i)^2}, \tag{5}$$

and

$$g_\rho = g_\rho(\rho_{sat})e^{a_\rho(x-1)}, \tag{6}$$

where $x = \rho/\rho_{sat}$. The term ρ_{sat} refers to saturation density of nuclear matter.

This project involves the use of baryon densities from the relativistic mean-field approach for a specific parametrization to calculate the value of symmetry energy. We have chosen the most popular and well-known NL3 parameter set for our endeavour because it has proven to reproduce nuclear saturation properties that are in excellent agreement with the present experimental data throughout the periodic table [4-5, 17-19] and references therein. The main task was then to create a program from scratch which could calculate the isospin dependent properties of finite nuclei such as symmetry energy and the different parameters directly associated with it, namely volume symmetry energy, surface symmetry energy, and their ratios κ at local density.

2.2 Coherent density fluctuation model

The symmetry energy is a property associated with infinite nuclear matter which is defined in momentum space, whereas finite nuclei is defined in coordinate space [20-24]. Experimentally it is not possible to observe the symmetry energy. However, we can evaluate this property using observables related to it. For this task, different models were proposed, including liquid drop model (LDM) [25], coherent density fluctuation model (CDFM) [21,22], etc. The nuclei in the LDM are assumed to be macroscopic drops of nuclear matter in the form of liquid which is incompressible. This model accounts for the short-range nuclear interactions as well as the nuclear matter saturation property.

According to this, for a finite nucleus, the symmetry energy is strongly correlated with the surface contribution, which implies that a single parameter for all nuclei that are fitted may yield only the average values. Therefore, for evaluating symmetry energy, one needs to take into account the contribution owing to the mass number. However, using additional parameters turns out to be a difficult task in known nuclei, which has a constrained range. Therefore, alternative models for symmetry energy calculation are much needed. The CDFM is one such model that is built upon the Fermi gas model, which has the generator coordinate with long-range collective type correlations. This model was developed by Antonov *et al.* [20,21]. It has successfully calculated the density distribution, ground and excited state root-mean-square (*rms*) radius for different nuclei, namely ^{4}He, ^{16}O, ^{40}Ca, etc. There are many advantages attributed to using CDFM. Firstly, CDFM automatically accounts for fluctuations present due to the density distribution by using the weight function. Secondly, the fluctuations attributed to momentum distribution close to the surface are taken care of using the Wigner distribution function (or mixed density matrix). The one-body density matrix (OBDM) $\rho(\mathbf{r},\mathbf{r})$ can be represented by another OBDM that has coherent superposition $\rho_x(\mathbf{r},\mathbf{r})$ corresponding to the fluctons (spherical pieces of nuclear matter).

$$\rho_x(\mathbf{r}) = \rho_0(x)\Theta(x - |\mathbf{r}|), \tag{7}$$

Here, $\rho_x(r)$ is the diagonal part of the OBDM and $\rho_0(x)$ is the spherical flucton density which is expressed as $\rho_0(x) = \frac{3A}{4\pi x^3}$. According to the definition of density matrix, one particle density is given by its diagonal elements [26]: $\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r'})|_{\mathbf{r'}\to\mathbf{r}}$. Thus, the infinite superposition of spherical fluctons defined for generator coordinate with radius x containing the Fermi gas of all uniformly distributed nucleons with mass A, the OBDM then takes the form as [22,26]:

$$\rho(\mathbf{r},\mathbf{r'}) = \int_0^\infty dx|\mathcal{F}(\S)|^\in \rho_\S(\mathbf{r},\mathbf{r'}). \tag{8}$$

The term $\mathcal{F}(\S)|^\in$ is called as the weight function where $\rho_x(\mathbf{r},\mathbf{r}')$ depicts the coherent OBDM superposition which is described as:

$$\rho_x(\mathbf{r},\mathbf{r}') = \mathbf{3}\rho_\mathbf{0}(\mathbf{x})\frac{\mathbf{J_1}(\mathbf{k_F}(\mathbf{x})|\mathbf{r}-\mathbf{r}'|)}{(\mathbf{k_F}(\mathbf{x})|\mathbf{r}-\mathbf{r}'|)} \times \Theta\left(x - \frac{|\mathbf{r}+\mathbf{r}'|}{2}\right). \tag{9}$$

The Bessel function J_1 has the order as one. The term $k_F(x)$ depicts Fermi momentum for radius x of the flucton given as

$$k_F(x) = \left(\frac{3\pi^2}{2}\rho_0(x)\right)^{1/3} \equiv \frac{\beta}{x}, \tag{10}$$

where

$$\beta = \left(\frac{9\pi A}{8}\right)^{1/3} \simeq 1.52A^{1/3}. \tag{11}$$

The Wigner distribution function corresponding to OBDM is given as

$$W(\mathbf{r},\mathbf{k}) = \int_0^\infty dx|\mathcal{F}(\S)|^{\in}\mathcal{W}_{\S}(\mathbf{r},\mathbf{k}), \tag{12}$$

where $W_x(\mathbf{r},\mathbf{k}) = \frac{4}{8\pi^3}\Theta(x - |\mathbf{r}|)\Theta(k_F(x) - |\mathbf{k}|)$. Similarly applying the CDFM approach, the density term $\rho(r)$ can be stated as

$$\begin{aligned} \rho(r) &= \int d\mathbf{k}W(\mathbf{r},\mathbf{k}) \\ &= \int_0^\infty dx|\mathcal{F}(\S)|^{\in}\frac{\ni\mathcal{A}}{\triangle\pi\S^{\ni}}\times(\S - |\mathbf{r}|). \end{aligned} \tag{13}$$

$$|\mathcal{F}(\S)|^{\in} = -\left(\frac{\infty}{\rho_{\prime}(\S)}\frac{\lceil\rho(\nabla)}{\lceil\nabla}\right)_{\nabla=\S}. \tag{14}$$

The normalization of weight function is given as $\int_0^\infty dx|\mathcal{F}(\S)|^{\in} = \infty$. Using Ref. [3, 22, 27, 28], the expression of symmetry energy for asymmetric nuclear matter as a function of $\rho_0(x)$ takes the form

$$S^{NM} = 41.7\rho_0^{2/3}(x) + b_1\rho_0(x) + b_2\rho_0^{4/3}(x) + b_3\rho_0^{5/3}(x). \tag{15}$$

Here b_1, b_2 and b_3 are constants derived from the method of Bruckner *et al.* [29, 30] having the values given as

$$\begin{aligned} b_1 &= 148.26, \\ b_2 &= 372.84, \\ b_3 &= -769.57. \end{aligned} \tag{16}$$

The expression for effective symmetry energy for asymmetric nuclear matter S from CDFM can be stated as [3, 22, 27, 28]:

$$S = \int_0^\infty dx|\mathcal{F}(\S)|^{\in}\mathcal{S}^{\mathcal{NM}}(\S). \tag{17}$$

Brueckner's energy density functional method suggests that in some areas the symmetry energy shows negative values, which is physically not possible. So to avoid such non-physical negative values of symmetry energy, one needs to set proper limits of integration in the Eq. 17. This is one of the most crucial parts of programming. Following Ref. [23], we first introduce the minimum value of nuclear distance x_{min} at which symmetry energy for asymmetric nuclear matter changes sign from negative value (at $x < x_{min}$) to positive value (at $x > x_{min}$). For $x < x_{min}$ the value of weight function is nearly zero, which implies that no contribution to the symmetry energy is supplied in this region. Moreover, it is required to introduce the value of x_{max} beyond which the weight function contribution to symmetry energy is negligible. This is done by first defining $\Delta x = x_{max} - x_{min}$.

Later we put the constraint for the value of x_{max} to be the point at which $S - S_{\Delta x} \leq 0.1$ MeV. Here the term $S_{\Delta x}$ is evaluated using the Eq. 17. Thus, the expression in Eq. 17 can be better written as

$$S = \int_{x_{min}}^{x_{max}} dx |\mathcal{F}(§)|^{\in} \mathcal{S}^{\mathcal{NM}}(§). \tag{18}$$

Using the Bethe-Weizsãcker LDM, the symmetry energy can be expressed in terms of surface and volume components which can be stated as [31],

$$S = \frac{S_V}{1 + \frac{S_S}{S_V} A^{-1/3}} = \frac{S_V}{1 + \frac{1}{\kappa A^{1/3}}} \tag{19}$$

The term $\kappa \equiv \frac{S_V}{S_S}$ is defined as the ratio of volume and surface symmetry energy. One can evaluate the volume and surface components of symmetry energy separately as

$$S_V = S\left(1 + \frac{1}{\kappa A^{1/3}}\right) \tag{20}$$

and

$$S_S = \frac{S}{\kappa}\left(1 + \frac{1}{\kappa A^{1/3}}\right), \tag{21}$$

Following Ref. [32,33] it is possible to find the expression of symmetry energy S and κ as a function of nuclear saturation density ρ_0 within the CDFM formalism as

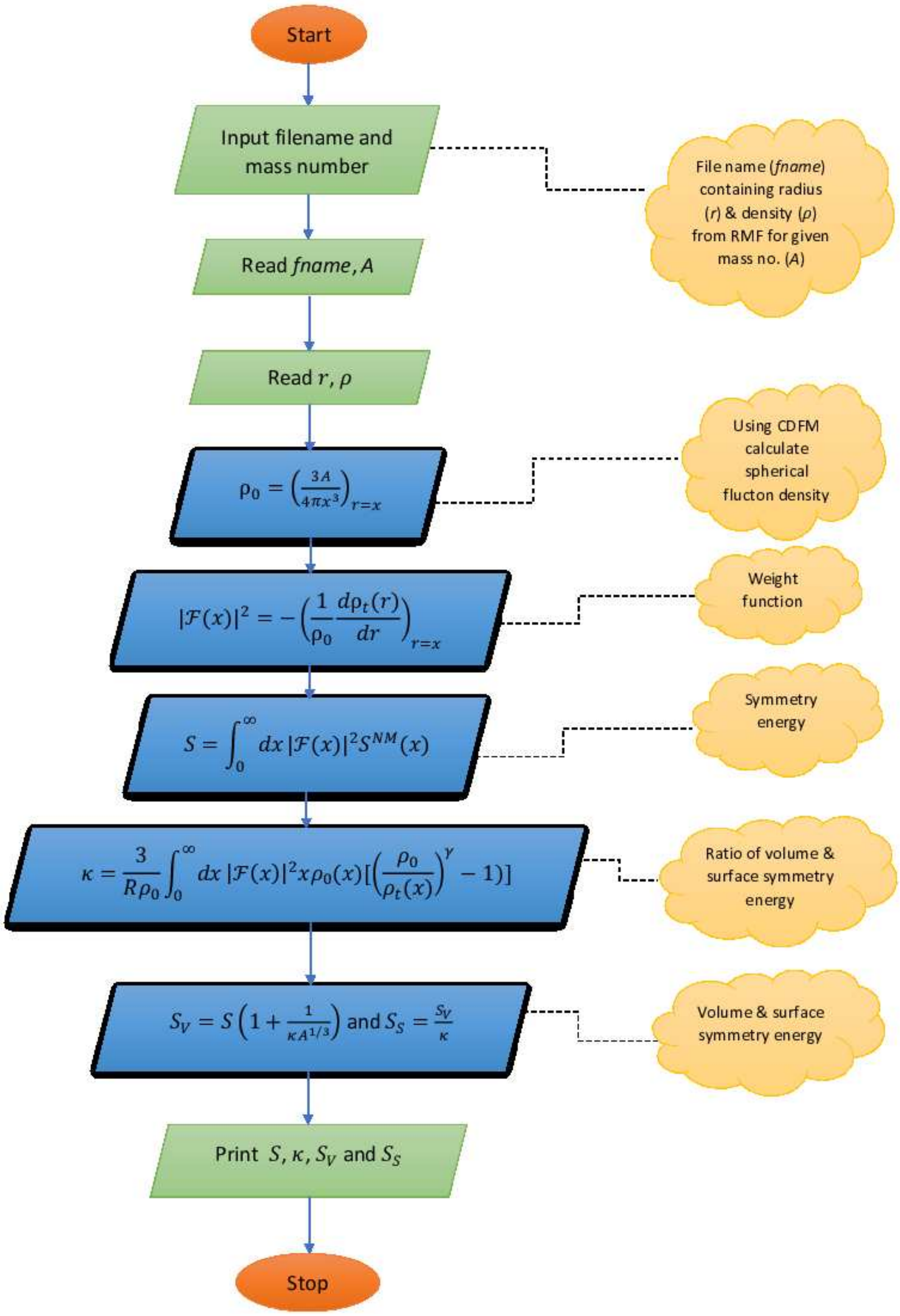
$$S = S(\rho_0) \int_0^{\infty} dx |\mathcal{F}(§)|^{\in} \left[\left(\frac{\rho(§)}{\rho_{\prime}}\right)^{\gamma}\right], \tag{22}$$

and

$$\kappa = \frac{3}{R\rho_0} \int_0^{\infty} dx |\mathcal{F}(§)|^{\in} §\rho_{\prime}(§) \left[\left(\frac{\rho_{\prime}}{\rho(§)}\right)^{\gamma} - \infty\right]. \tag{23}$$

The term $S(\rho_0)$ is the symmetry energy at saturation density, and R is the nuclear matter radius. It is crucial to note here that the term ρ_0 corresponds to nuclear saturation density, whereas $\rho_0(x)$ corresponds to spherical flucton density as a function of nuclear distance (x). Here γ parameter is chosen to be 0.3, as it is consistent with the various experimental results [32-34]. Using the same integration limits of symmetry energy i.e. x_{min} and x_{max}, we next evaluate the value of κ from Eq. 23. This permits us to finally evaluate the value of volume symmetry energy and surface symmetry energy by following Eqs. 20, 21 respectively. Thus, the computational steps can be summarized as follows: first, one needs to evaluate the symmetry energy within the proper limits using Eq. 18. Subsequently, one needs to find the κ using the Eq. 23. Finally, volume and surface symmetry energy can be evaluated using Eq. 20 and 21 respectively.

3. Flowchart


Start
Input filename and mass number
File name (fname) containing radius (r) & density (ρ) from RMF for given mass no. (A)
Read fname, A
Read r, ρ
$\rho_0 = \left(\frac{3A}{4\pi x^3}\right)_{r=x}$
Using CDFM calculate spherical flucton density
$|\mathcal{F}(x)|^2 = -\left(\frac{1}{\rho_0}\frac{d\rho_t(r)}{dr}\right)_{r=x}$
Weight function
$S = \int_0^\infty dx\,|\mathcal{F}(x)|^2 S^{NM}(x)$
Symmetry energy
$\kappa = \frac{3}{R\rho_0}\int_0^\infty dx\,|\mathcal{F}(x)|^2 x\rho_0(x)[\left(\frac{\rho_0}{\rho_t(x)}\right)^\gamma - 1)]$
Ratio of volume & surface symmetry energy
$S_V = S\left(1+\frac{1}{\kappa A^{1/3}}\right)$ and $S_S = \frac{S_V}{\kappa}$
Volume & surface symmetry energy
Print S, κ, S_V and S_S
Stop

4. RESULTS AND CONCLUSION

In this section, we provide the results and brief discussions related to symmetry energy and its related components, namely volume and surface symmetry energy along with their ratio κ for neutron-rich $even - even$ Titanium isotopes using the relativistic mean-field model for the NL3 parameter set. The coherent density fluctuation model is used to translate the nuclear matter quantities at local density. In other words, the CDFM is used to obtain a transparent relationship for the quantities corresponding to the intrinsic analytical equation of states while using a simple approach to the weight function [24]. The expression of weight function $\mathcal{F}(\S)^{\in}$ given in Eq. 14, may seem to be of simple nature. However, this expression provides a pathway to correlate the infinite matter quantities such as symmetry energy and its related surface and volume components existing in momentum space to that of the corresponding finite nuclear quantities in the coordinate space. Within the relativistic mean-field model, the symmetry energy, which is a quantity of infinite nuclear matter, can directly be calculated for any finite nucleus from the difference of isoscalar and isovector parts of the energy density functional. This questions the need to implement the CDFM model instead of the relativistic mean-field equation to calculate the symmetry energy for finite nuclei. It can be owed to the fact that many parameters such as pairing, shell corrections and other meson interactions are unaccounted for when performing the calculations for the finite nuclei, which leads to poor description of the symmetry energy in finite nuclei. To counter this problem, CDFM provides a uniform description of finite nuclei similar to infinite nuclear matter through the primary assumption of nuclear matter as spherical pieces of nuclear matter known as fluctons [35]. For calculating the value of symmetry energy at local density, we need to obtain the values of total density (sum of neutron and proton density) as a function of nuclear distance. We have plotted the total baryon density distribution, i.e., the sum of proton density ρ_p and neutron density ρ_n as a function of nuclear distances, for few Titanium nuclei based on NL3 parameter in Fig 1. A similar characteristic of nuclear density is observed for all the presented nuclei.

After finding the values of total baryon density as a function of nuclear distance, we use the CDFM to find the value of weight function $\mathcal{F}(\S)^{\in}$ from Eq. 14 for each of the isotopic nuclei. It can be observed that the magnitude of the weight function is always less than one. The plot of total densities as a function of nuclear distance for some of the nuclei is given in Fig. 1. A thorough investigation of Fig. 1 suggests that an increase in proton number (Z) yields slight enhancement in the surface region. Hence, effective nuclear matter quantities can be understood by using the total density distribution. The plot of weight function $\mathcal{F}(\S)^{\in}$ as a function of nuclear distance is provided in Fig. 2. Some inference based on Fig. 2 can be drawn, which states that the shape of weight function corresponds to a bell shape having maximum density near the middle of flucton radius which is not necessarily the center of flucton. Since the weight function is dependent on total density, the increase or decrease in the value of total density leads to the corresponding increase or decrease in the weight function.

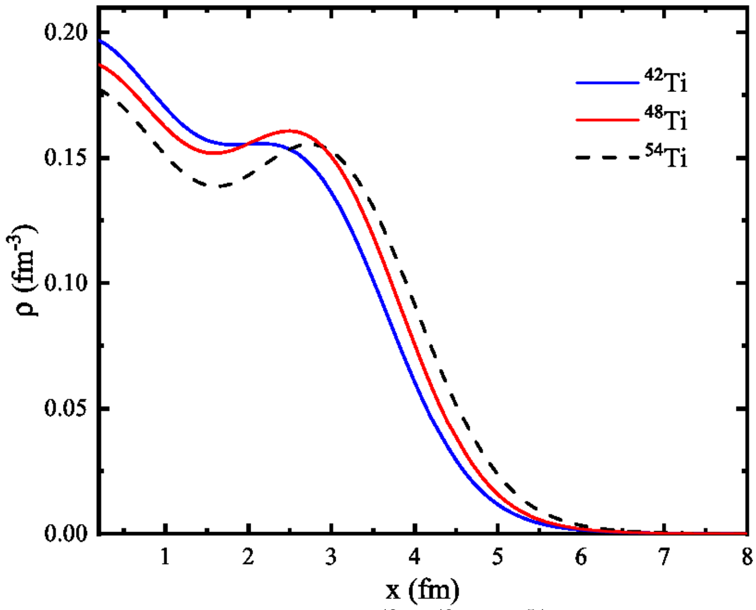


Figure 1. Total density distribution for ^{42}Ti, ^{48}Ti and ^{54}Ti isotopes from NL3 as a function of nuclear distances. Follow the text for details.

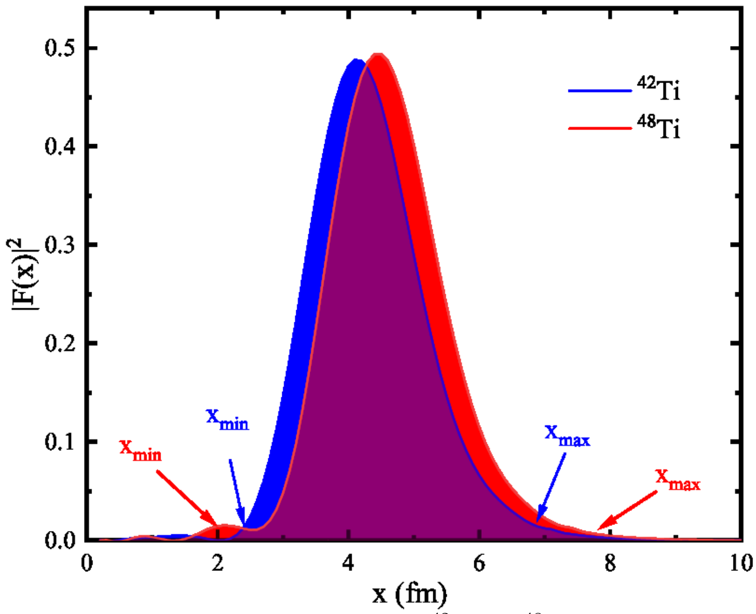


Figure 2. Weight function corresponding to ^{42}Ti and ^{48}Ti isotopes from NL3 as a function of nuclear distance. Follow the text for details.

The principal aim of this project involved the calculations pertaining to the symmetry energy and its volume and surface components. Symmetry energy being a quantity of infinite nuclear matter, cannot be measured directly. However, it is possible to measure it using other observables which share some indirect relationship with it. The isospin asymmetry is the difference in the densities of neutrons and protons. The symmetry energy, which is defined as the energy density derivative with respect to isospin asymmetry, plays a significant role in a range of nuclear physics branches involving the study of ground-state nuclear structure [36-38], heavy-ion reaction dynamics [39,40] and study related to neutron stars [2, 41-43].

Using the value of symmetry energy, we compute the value of its components, namely surface and volume symmetry energy, which are usually calculated at saturation based on the properties of nuclear matter. Based on the method of Brueckner's energy density functional [29,30], some non-physical (negative values) of nuclear symmetry energy were observed. Therefore, this method requires assigning a proper limit to the integration for the calculation of symmetry energy and its related parameter based on the change in sign from negative to positive value detailed in Section 2.2.

We have provided a detailed flowchart as a means of simplifying the whole process of programming for calculating the symmetry energy and its related parameters in Section 3. Moreover, Fig. 2 shows the calculated weight function as a function of nuclear distance for two Titanium isotopes namely ^{42}Ti and ^{48}Ti nuclei. The points x_{min} and x_{max} signify the integration limits for each of the nuclei taken while calculating the value of symmetry energy. Using Titanium isotopic chain and following Eq. 17, 20, 21, and 23, we have calculated the symmetry energy, volume symmetry energy, surface symmetry energy and their ratio κ, respectively, for the NL3 parameter set within the RMF formalism. The values corresponding to these parameters are given in Table 1. The present calculation can be extended to more isotopic chains, including light, heavy and super-heavy regions. The symmetry energy co-efficient, namely, neutron pressure and curvature, can also be incorporated based upon the model of CDFM. These nuclear matter quantities can be treated as primary observable for shell/sub-shell closure (s) at and/or near the drip-line region of the nuclear chart.

Table 1. The calculated symmetry energy (S), volume symmetry energy (S_V), surface symmetry energy (S_S) and their ratio κ for Titanium isotopic chain from non-linear NL3 parameter set is shown in the table

Nucleus	Symmetry energy	Volume symmetry energy	Surface symmetry energy	κ
^{42}Ti	26.54807791	31.80804655	21.90635807	1.452000668
^{44}Ti	26.89762324	32.16993464	22.26152446	1.44509127
^{46}Ti	27.2649504	32.56214504	22.66766852	1.43650173
^{48}Ti	27.60654222	32.88987599	22.87557569	1.437772602
^{50}Ti	27.87674081	33.17500314	23.22874705	1.428187369
^{52}Ti	27.81287292	32.99695584	22.95625787	1.437383916
^{54}Ti	27.75016038	32.85276579	22.83300272	1.438828094

From the Table 1 at ^{50}Ti, which corresponds to N = 28, one can observe a significant increase in the symmetry energy along with its surface and volume components while showing a decrement in κ value, which altogether indicates higher stability of isotopes and a possible shell closure. This will open the path for a better understanding of the properties across the nuclear landscape. A few investigations in the direction of isospin dependent effective nuclear surface quantities for possible signature of magicity or shell/subshell closure are already established in Ref. [3] and references therein.

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