

Symmetry Energy of Nuclear Matter at Low Densities and Clustering at the Nuclear Surface

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Abstract. We present a density functional theory which connects nuclear matter equation of state, which incorporates clustering at low densities, with clustering in medium and heavy nuclei at the nuclear surface. This explains the large values of symmetry energy reported by Natowitz *et al* for densities $< 0.01 \text{ fm}^{-3}$, in addition to the binding energies and charge rms radii of 367 spherical nuclei. The present theory which is partly macroscopic competes with other high quality microscopic-macroscopic approaches. Merits of the results with clustering and no-clustering are discussed. We also make connection with realistic interactions (AV18+UIX/IL2) which have been used in *ab initio* calculations in s- and p-shell nuclei and neutron matter. Theory predicts new situations and regimes to be explored both theoretically and experimentally. It is demonstrated that, due to clustering, the neutron skin thickness reduces significantly.

1. Introduction

In this paper we present a phenomenological theory of nuclei which incorporates clustering at the nuclear surface in the most general form. The theory explains the recently extracted large symmetry energy at low densities of symmetric nuclear matter (SNM) by Natowitz *et al* [1] as well as the static properties of nuclei, namely, the binding energies and root mean square radii. Two new ideas are introduced:

1. In a phenomenological way cluster of all sizes, shapes along with medium modifications are included. This modifies the equation of state (EOS) of nuclear matter at sub-nuclear densities significantly.
2. The importance of quartic term in symmetry energy is demonstrated at and below the saturation density in nuclear matter. It is shown that it is due to use of realistic EOS of neutron matter particularly the contribution arising due to three-nucleon interaction and also due to clustering. This is also a significant departure from the normal practices.

We postulate that the energy per nucleon $E(\rho)$ of nuclear matter at zero density is equal to its value, $-u_v$ ($\approx -16 \text{ MeV}$), at the saturation density ρ_0 ($\approx 0.16 \text{ fm}^{-3}$), where u_v is the coefficient of the volume term in the Weizsäcker mass formula. This can be shown in the following way. In the limit of zero density, consider that SNM consists of an ideal gas of α -particles [2]. Then $E(\rho)$ of SNM $\approx -7.3 \text{ MeV}$, energy per nucleon of the α -particles, since Coulomb interaction is switched off and density is low enough so that mutual interaction between α -particles can be ignored. This energy is lower than the energy of the gas of nucleons in the limit of zero density, e.g., in mean field theories where $E(\rho) \rightarrow 0$ as $\rho \rightarrow 0$. But why α -particles; instead we may consider heavy nuclei, in fact large chunks of SNM where we can ignore surface effects. The energy per nucleon of these large chunks of SNM

approach $-u_v$. We keep the densities low enough so that these chunks do not interact with each other. The central densities of these large chunks themselves approach ρ_o , the saturation density. It then follows that $E(\rho \rightarrow 0) \rightarrow -u_v$. This leads to the identity

$$E(\rho \rightarrow 0) \rightarrow E(\rho_o) = -u_v \quad (1)$$

We shall incorporate the above identity in our calculations and demonstrate its effect on the symmetry energy and the static properties of nuclei. The identity (1) may also affect the dynamic properties of nuclei; but we do not address to these in the present study. They shall be taken up elsewhere. Another important aspect of the study is the use of realistic EOS of neutron matter [3,4] obtained with *ab initio* calculations using Argonne AV8' [5] and UIX [6]. Use of these *ab initio* calculations strongly indicates the presence of quartic term in symmetry energy. Though our theory is mostly phenomenological, but it maintains a close and direct connection with bare and realistic two- and three-nucleon interactions. This again is quite in contrast to earlier such studies which have either very little or no connection with realistic interactions [7-12]. In the following sections we describe our methodology and results followed by conclusions.

2. Nuclear Matter Properties and Extended Thomas-Fermi Theory

The EOS of nuclear matter, $E(\rho, \delta)$, with arbitrary isospin, can be expanded by Taylor series

$$E(\rho, \delta) = E(\rho, \delta = 0) + S(\rho)\delta^2 + Q(\rho)\delta^4 \quad (2)$$

where δ is the isospin variable $(\rho_n - \rho_p)/\rho$ and ρ_n , ρ_p and ρ are the neutron, proton and total densities, respectively. Because of charge symmetry the odd powers of δ does not contribute. In expansion (2), we have retained terms up to 4th power of δ . The density dependent coefficient of the quadratic term is the familiar symmetry energy. At present, we have no idea about the density dependence of the quartic term $Q(\rho)$. We make the simplifying assumption that $S(\rho)$ and $Q(\rho)$ are proportional to each other, i.e., they have the same density dependence. We put $S(\rho) = (1-q) E_{sym}(\rho)$ and $Q(\rho) = q E_{sym}(\rho)$ where we exploit the assumption that $Q(\rho)$ is proportional to $S(\rho)$. The density independent parameter q is found to play important role when realistic EOS of neutron matter is employed. From now onwards we shall assume that these substitutions have been implemented in (2). The first term on the *rhs* of (2) is the EOS of SNM, i.e., $E(\rho, \delta = 0) \equiv E(\rho)$.

In density functional theories (DFT), EOS of nuclear matter enters in an essential way [12-15]. In most of these studies Skyrme density functional [12] has been employed. Clearly it does not satisfy the identity (1). We use quite general density functional, independent of any specific interaction, which incorporates (1). This is in line with DFT theories, where effective interactions are secondary to the theory. It is the density functional that defines the force [16]. Following [17-19], we write

$$E(\rho_{\geq}) = -u_v + \frac{K}{18}((\rho - \rho_o)/\rho_o)^2 + M((\rho - \rho_o)/\rho_o)^3, \quad \text{for } \rho \geq \rho_x \quad (3a)$$

$$E(\rho_{\leq}) = -u_v + A\rho + B\rho^2 + C\rho^3 + D\rho^4 + 3\hbar^2(3\pi^2\rho/2)^{2/3}/5m, \quad \text{for } \rho \leq \rho_x \quad (3b)$$

Notice in (3a) and (3b) when ρ approaches ρ_o and 0, respectively, $E(\rho)$ approaches $-u_v$ satisfying the identity (1). K is the compression modulus which we assume 230 MeV [20]. M is anharmonicity parameter to be determined. ρ_x is a density parameter between 0 and ρ_o . The constants A , B , C and D are determined by equalizing $E(\rho_{\geq})$ and $E(\rho_{\leq})$ and their first three derivatives at $\rho = \rho_x$. u_v and ρ_o stay close to generally accepted values of 16 MeV and 0.16 fm^{-3} , respectively. Thus (3) contains essentially two parameters, namely M and ρ_o . if we drop the $-u_v$ term in (3b) we get the result of mean field theories that $E(\rho \rightarrow 0) \rightarrow 0$. In this situation there will be no clustering at the nuclear surface. We consider both the situations.

The symmetry energy, $E_{sym}(\rho)$, is defined as the difference between the energy per particle of pure neutron matter, $E(\rho, \delta = 1)$ and the SNM. A positive feature of the present approach is that the microscopically calculated homogeneous EOS of neutron matter can be directly employed. We use the recently calculated values [3]. This has been obtained by employing an accurate fixed phase AFDMC technique with 66 neutrons enclosed in a periodic box with Argonne AV8' [5] and Urbana three-

nucleon *UIX* [6] interactions. In Fig. 1, left panel, we plot the results of Ref. [3,4] which we use in our calculations.

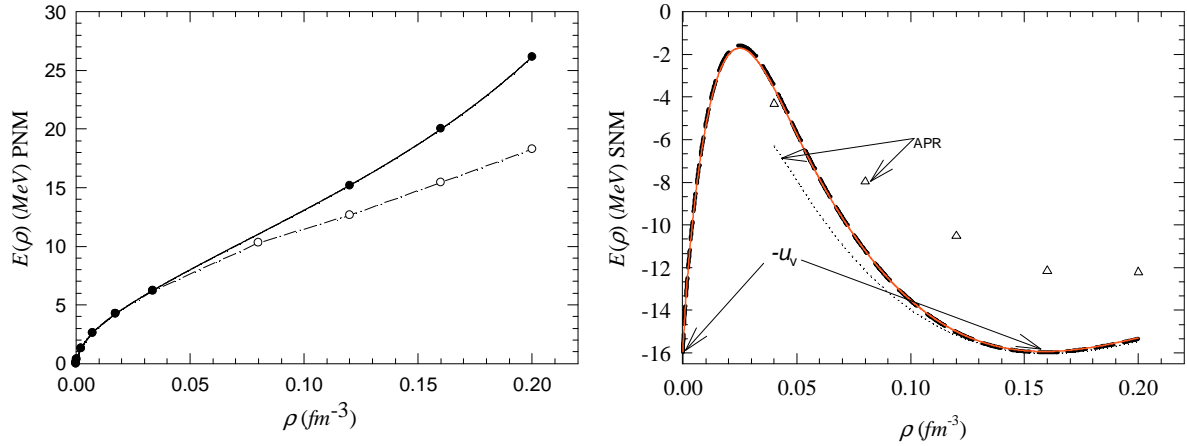


Fig. 1: EOS of neutron matter, left panel. The solid line is with AV8'+UIX and dashed line with AV8' alone. In the right panel EOS of symmetric nuclear matter is plotted. For details see text.

For calculating the energies of nuclei, we use an extended version of Thomas-Fermi theory [12]. In addition, we include the shell correction, which we extract from Ref. [21], pairing from Ref. [10], and a Wigner contribution similar to Refs. [8, 9]. We thus write the energy as a functional of neutron and proton densities:

$$\begin{aligned} \mathcal{E}[\rho_n, \rho_p] = & \int [E(\rho)\rho + (\hbar^2/2m)(\tau_2(\rho_n, \rho_p) + \tau_4(\rho_n, \rho_p)) + a_\rho(\nabla\rho)^2] d\vec{r} \\ & + \int [(1-q)E_{sym}(\rho)\delta^2 + qE_{sym}(\rho)\delta^4] \rho d\vec{r} \\ & + (1/2)e^2 \int \rho_p(\vec{r})\rho_p(\vec{r}')/|\vec{r} - \vec{r}'| d\vec{r}' d\vec{r} - (3/4)(3/\pi)^{1/3} e^2 \int \rho_p^{4/3}(\vec{r}) d\vec{r} \\ & + Shell + a_{pair} A^{-1/3} \Delta_{np} + E_W \end{aligned} \quad (4)$$

The integral in the first line can be identified as the volume and surface term. Next integral (second line) is the contribution due to symmetry energy. Third line is the Coulomb, direct and exchange terms. Details regarding the kinetic energy densities τ_2 and τ_4 can be found in Ref. [12]. For Δ_{np} we use the prescription as given in Ref. [10]. E_W is the Wigner contribution defined as

$$E_W = V_W \exp\{-\lambda((N-Z)/A)^2\} + W_W |N-Z| \exp(-(A/A_0)^2) \quad (5)$$

Our parameter values V_W , λ , W_W and A_0 are consistent with Refs. [8, 9]. For the neutron and proton variational densities, we use three parameter modified Fermi distribution;

$$\rho_{n(p)}(r) = N_{n(p)} / (1 + \exp((r - R_{n(p)})/t_{n(p)}))^{\gamma_{n(p)}} \quad (6)$$

where $R_{n(p)}$, $t_{n(p)}$, and $\gamma_{n(p)}$ are variational parameters. $N_{n(p)}$ is the normalization constant which takes into account the correct number of neutrons(protons). We vary the six parameters for each nucleus to minimize the density functional (4). Fits to energies or nuclear masses are obtained by minimizing the *rms* deviation $\sigma(E)$ defined as

$$\sigma(E) = \sqrt{\sum_i (E_{theo}^i - E_{exp}^i)^2 / N}, \quad (7)$$

where N is the total number of nuclei included in the fit and rest of the symbols are self evident. We similarly define the *rms* deviations $\sigma(R)$. We minimize $\sigma(E)$ by varying the parameters of the theory, namely, M , u_v , ρ_o , a_ρ , q , a_{pair} and the parameters in the Wigner term V_W , λ , W_W and A_0 for specific values of ρ_x . The parameter ρ_x is sensitive to the symmetry energy data of Natowitz *et al.* It fixes it around 0.05–0.06 fm^{-3} .

3. Results and Discussion

Neutron Matter	Clustering	$\sigma(E)$	$\sigma(R)$	q
AV8'+UIX	Yes	1.489	0.022	0.0
AV8'+UIX	Yes	0.589	0.020	0.168
AV8'+UIX	No	0.637	0.024	0.150
AV8'	Yes	0.570	0.020	0.082
AV8'	No	0.622	0.019	0.062

Table I: $\sigma(E)$ is in units of MeV and $\sigma(R)$ in fm^{-3} . See text for details.

We consider 367 spherical nuclei [22]. These are the same set of nuclei as considered by Bhagwat *et al* [23]. For the *rms* radii, we consider all the 149 nuclei out of the 799 nuclei of Ref. [24] which are common to the set of 367 nuclei. Calculated energies are obtained variationally by varying the density through the six variational parameters of (6). We adopted an automated technique to search for the parameters of the theory while minimizing $\sigma(E)$. We display our results for $\sigma(E)$ and $\sigma(R)$ in Table I. All the entries in this table are for $\rho_x = 0.06 fm^{-3}$. The first column specifies the use of the neutron matter EOS – AV8'+UIX which stands for the solid curve of the left panel of Fig.1, and AV8', the dashed curve. “Yes” in the second column of the table implies that calculations have been performed using (3b), and “No” implies that they have been carried out by dropping the $-u_v$ term in (3b), i.e., no clustering. The first row gives result with $q = 0$, i.e. no isospin quartic term for fixed values of ρ_x , varying the other parameters. It seen that $\sigma(E)$ is quite large ≈ 1.5 MeV. When we vary q , second line of results, we observe a dramatic reduction in $\sigma(E)$, almost by a factor of three. This sufficiently justifies inclusion of the isospin quartic term. When we drop u_v in (3b), i.e. no clustering, we find an increase in $\sigma(E)$ by $\approx 7.6\%$. A similar situation is encountered with AV8'. Here the increase in $\sigma(E)$ is around 9%. Thus clustering does affect the $\sigma(E)$ values though by a modest amount. However, as we shall see, its impact on symmetry energy is quite significant. We also notice that q values for both AV8'+UIX and AV8' decreases in the no clustering situation. Thus our results demonstrate that quartic isospin term plays a significant role. It arises particularly due to UIX in the EOS of neutron matter and clustering also contributes to it. Our values of $\sigma(E)$ are quite close to the value obtained in Ref. [9], 0.581 MeV, where they use Hartree-Fock-Bogoliubov approach using Skyrme interaction and a few phenomenological prescriptions. This comparison has to be made in a proper perspective. In Ref. [9], the authors consider 2149 nuclei. When we include 2149 nuclei our $\sigma(E)$ values become 0.664 and 0.637 MeV for AV8'+UIX and AV8' respectively. Reasons for this increase are following. Firstly, density functional (4) with the densities (6) is spherical. Many of the 2149 nuclei have regions of deformation. In our case this deformation is contained in the microscopic shell correction which we have taken from Ref. [21]. Thus our calculations lack a certain amount of self consistency; though we expect its effect to be small. The second reason lies with the calculations of Ref. [9]. The Brussels-Montreal group uses an effective Skyrme interaction which mimics or rather coincides with the Friedman-Pandharipande [25] EOS of neutron matter which is softer compared to EOS of Ref. [3] which we have employed. According to Ref. [9], the use of a stiffer EOS, for example of APR [26], deteriorates the value of $\sigma(E)$ which is with AV18+UIX. We may point out that in the density region 0 to ρ_0 there are only small differences between the EOS of neutron matter of AV18+UIX and AV8'+UIX [3] which we have used. This apparent increase in $\sigma(E)$ of the Brussels-Montreal group, we think, is due to absence of the quartic isospin term in the Skyrme density functional.

Our parameter values are as follows: (A) For AV8'+UIX, corresponding to result line 2 of Table I, $a_\rho = 38.709$ MeV fm^5 , $a_{pair} = -5.912$, $M = -13.410$ MeV, $\rho_0 = 0.1586$ fm^{-3} , $u_v = 15.970$ MeV, $V_w = -2.98$ MeV, $\lambda = 200$, $W_w = 0.343$ MeV and $A_0 = 68$. (B) For AV8', corresponding to result line 4, $a_\rho = 38.178$ MeV fm^5 , $a_{pair} = -5.76$, $M = -13.093$ MeV, $\rho_0 = 0.1585$ fm^{-3} , $u_v = 15.935$ MeV, $V_w = -2.60$ MeV, $\lambda = 347$, $W_w = 0.320$ MeV and $A_0 = 68$.

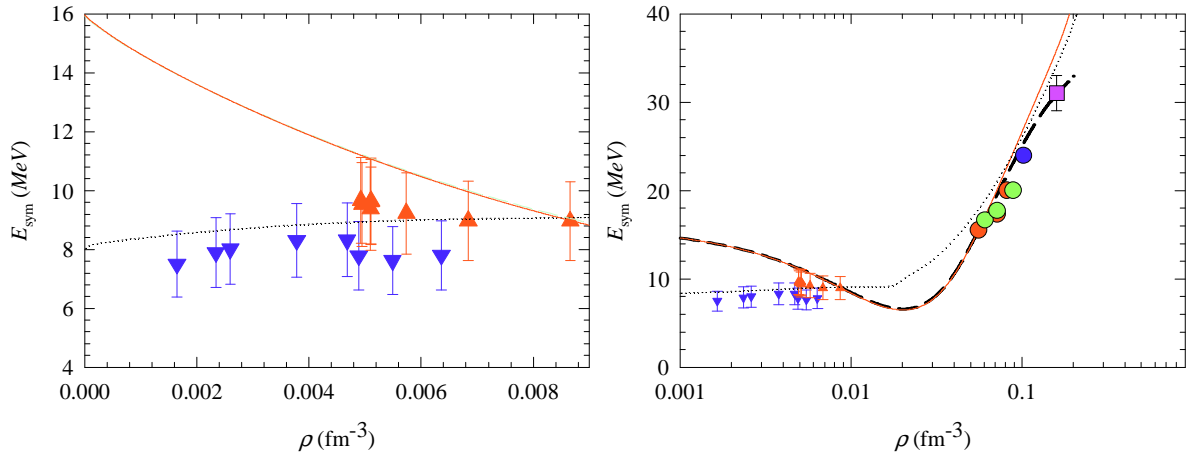


Fig. 2 (color online): Solid curve (red) corresponds to parameter set (A) and the dashed (black) curve to the set (B). For details, see text.

In the right panel of Fig. 1, we give the results for EOS of SNM. The solid (red) curve is with parameter set (A) and the dashed (black) curve with (B). The dotted line and the triangles are the calculations of APR [26].

In Fig. 2, we give results for the symmetry energy. The color code and legends for the various curves are same as those described above for Fig. 1 (right panel). The dotted curve represents the quantum statistical (QS) calculation at $T = 1$ MeV. The down blue triangles are the data from [1] without correction to medium effects. The up red triangles are the data with medium corrections which is quite significant. The down blue triangles have downward trend with decreasing densities, whereas the up red triangles have upward trend. Our calculations distinguish between the two sets of data, the up red triangles and the down blue triangles. Our symmetry energy shows a distinct minimum at $\rho \approx 0.02 \text{ fm}^{-3}$. Above this density the quasi particle picture is dominant and below this density clustering plays the crucial role. In QS approach this minimum is not seen. This is because heavier clusters are not included in this approach. It is therefore important that this region of the density should be experimentally explored. The right panel of Fig. 2 gives the overall picture. The data points represented with circles are from [27].

Neutron skin thickness [28] is usually defined as the difference between the *rms* radii of neutrons and protons. We expect the clustering to affect δR significantly as it is a direct surface phenomenon. We find that for ^{208}Pb $\delta R = 0.10 \text{ fm}$ with clustering. Its value without clustering is 0.16 fm .

The above considerations have consequences for neutron star studies and hypernuclei [29]. For example, in case of hypernuclei, because of cluster formation, the Λ -binding to nuclear matter in the vicinity of zero density will approach to its value at the saturation density which is around 30 MeV. This will have interesting consequences for Λ -single particle energies. We may also point out that we have constrained our theory with the realistic two- and three-nucleon interactions which explain the s- and p-shell nuclei [30] and the NN scattering data [5] below 340 MeV.

4. Conclusions

We close the foregoing presentation with the following remarks. We have developed a theory of nuclei which explains the low energy symmetry energy data of Natowitz *et al.* at low densities of nuclear matter and at the same time consistent with the static properties of nuclei. We find that the slope of the symmetry energy curve is negative at low densities which leads to a minimum in the symmetry energy at $\rho \approx 0.02 \text{ fm}^{-3}$, below which clustering starts dominating and above which the quasi particle picture prevails. We have also demonstrated that quartic term in isospin plays an important role. It arises due

to use of realistic EOS of neutron matter, mainly due to three-nucleon interaction. Some of the isospin quartic contribution also originates from clustering.

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