Nuclear matter and surface clustering

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Abstract. We demonstrate that the binding energy per nucleon of symmetric nuclear matter (SNM) (with Coulomb interaction switched off and \( N = Z \)) in the limit of zero density approaches to its value, \( u_v \), at the saturation density, where \( u_v \) is the volume term of the Weizsäcker mass formula. This phenomenon is a direct result of the clustering of nuclei in the low density region of nuclear matter. We study the implications of this result on the properties of nuclei. We also study the properties of asymmetric nuclear matter. Because of clustering a provocative interpretation of the equation of state of asymmetric nuclear matter emerges which is at considerable variance at low densities with hitherto all the previous calculations. For nuclei, as a framework, an extended version of Thomas-Fermi theory is invoked. Calculations are performed for 2149 nuclei with \( N, Z \geq 8 \). The present scheme leads to a forceful interpretation of the low density asymmetry energy data of Natowitz et al. [1].

1. Introduction

In this paper we discuss the implication of clustering in nuclear matter at low densities. Properties of the nuclear matter play a very important role in shaping the structure of a nucleus, its energy and other properties. Here, we consider a hypothetical symmetric nuclear matter (SNM) where the Coulomb interaction is switched off. Large number of binding energy calculations of such a system have been carried out in the past with two and three-nucleon realistic or simplified potentials using either variational or different versions of Bruckner g-matrix techniques. A common feature of most of these calculations is that the binding energy per nucleon (\( BE/A \)) of the SNM approaches zero as the density approaches zero. The following thought experiment demonstrates that this feature is at a gross variance with clustering aspect of nuclear matter at low densities. We demonstrate that, based upon a quite general consideration, that in the limit of zero density the \( BE/A \) approaches \( u_v \), which corresponds to the value at the saturation density \( \rho_0 \). In [2], it was demonstrated that an idealized picture of \( \alpha \)-matter of SNM leads to \( BE/A \approx 7.3 \) MeV, which is roughly the binding energy of \( \alpha \)-particle per nucleon without the Coulomb interaction. But why \( \alpha \)-particles? Why not heavier nuclei since they have lower \( BE/A \) since the Coulomb interaction is switched off? One may thus consider SNM, in the limit of zero density, as an aggregate of heavier nuclei or large chunks of SNM itself. In the latter case the \( BE/A \) will then tend to its value at the saturation density which is \( u_v \). We thus obtain the exact relation

\[ E(\rho \to 0) \to E(\rho = \rho_0) = -u_v, \]

where, \( E \) is the energy per nucleon of SNM. The above considerations are based upon the concept of ideal cluster matter which do not interact in the limit of zero density. However, at somewhat higher but low densities the SNM will be a highly correlated system with complicated structure. We have shown elsewhere [3], that the equation of state (EOS) of SNM will have one maximum between 0 and...
\( \rho_n \). This claim along with the identity (1) leads to the possibility of the presence of clusters at low densities, which in turn then offers a force interpretation of the asymmetry energy data of Natowitz et al [1]. In addition, within the framework of an extended Thomas-Fermi model [4], we demonstrate that clustering is fully consistent with the static properties of nuclei, namely, the binding energies and rms radii. Because of the clustering the EOS of asymmetric nuclear matter (NM) is also found to be qualitatively different than all the previous studies.

In section 2, we give the formulations and show how the above presented picture of nuclear matter is incorporated in the theory to calculate the properties of the nuclei. Section 3 gives the results and discussion. Section 4 contains the conclusions.

2. Asymmetry Energy, EOS of Nuclear Matter and an Extended Tomas Fermi Model

The asymmetry energy \( E_{\text{asym}}(\rho) \) is defined as the difference between the \( E(\rho) \) of pure neutron matter (PNM) and the SNM

\[
E_{\text{asym}}(\rho) = E(\rho, \delta = 1) - E(\rho, \delta = 0)
\]

where the isospin asymmetry parameter is defined as \( \delta = (\rho_n - \rho_p)/\rho \) with \( \rho_n \) and \( \rho_p \) as the densities of neutrons and proton respectively. Neutron matter is a gas of neutrons at all densities, we obtain the exact result \( E_{\text{asym}}(\rho \rightarrow 0) \rightarrow u_c \), since \( E(\rho \rightarrow 0, \delta = 0) \rightarrow -u_c \). Also, the EOS of NM with arbitrary \( \delta \) can be expanded by Taylor series where we ignore the small charge symmetry breaking component:

\[
E(\rho, \delta) = E(\rho, \delta = 0) + S(\rho)\delta^2 + Q(\rho)\delta^4
\]

In the above expansion, we have retained terms up to the fourth power of \( \delta \). This was found necessary to obtain an adequate description of the static properties of nuclei when we use the EOS of PNM calculated using Diffusion Monte Carlo technique with realistic interactions [5]. We have no knowledge about the density dependence of \( Q(\rho) \). We make the simplifying assumption that \( Q(\rho) \) is proportion to \( S(\rho) \). We thus replace \( S(\rho) \) by \((1-q)E_{\text{asym}}\) and \( Q(\rho) \) by \( qE_{\text{asym}} \), where \( q \) is an input parameter which is determined from the fits to the static properties of nuclei.

For the EOS of SNM we use the following phenomenological form [3,6] which satisfy the identity (1) with a one maximum between 0 and \( \rho_0 \).

\[
E(\rho_\pm) = -u_c + \frac{K}{18} \left( \frac{\rho - \rho_0}{\rho_0} \right)^2 + M \left( \frac{\rho - \rho_0}{\rho_0} \right)^3, \quad \rho \geq \rho_\pm
\]

\[
E(\rho_\pm) = -u_c + A\rho + B\rho^2 + C\rho^3 + D\rho^4 + \frac{3h^2}{5m_N} \left( \frac{3\pi^2 / 2}{2} \right)^{2/3} \rho^{2/3}, \quad \rho \leq \rho_\pm
\]

where \( \rho_\pm \) is a parameter between 0 and \( \rho_0 \). It may be noted from (4a) and (4b) that as the density approaches \( \rho_0 \) and 0, \( E \) approaches \(-u_c \) in accordance with the identity (1). The constant terms \( A, B, C, \) and \( D \) are determined by equalizing \( E(\rho_+) \) and \( E(\rho_-) \) and their first three derivatives at \( \rho = \rho_\pm \). (4a) essentially contains two parameters, \( M \) and \( \rho_\pm \). The other parameters are consistent with generally accepted values, namely, \( u_c \approx 16\text{ MeV} \), the compression modulus \( K \approx 230\text{ MeV} \), and \( \rho_0 \approx 0.16\text{ fm}^{-3} \).

To calculate the properties of nuclei, we use an extended version of the Thomas-Fermi theory [3, 4] which is a precursor of density functional theories recently being developed under the SciDAC program [7]. Density Functional theories consist of terms pertaining to homogenous part of the nuclear matter and non-homogenous parts which controls the surface properties of the nucleus [4, 7]. We write the energy of a nucleus as a functional of neutron and proton densities:

\[
\varepsilon [\rho_n, \rho_p] = \int \left[ E(\rho, \delta)\rho + \frac{\hbar^2}{2m} \left( \tau_x(\rho_n, \rho_p) + \tau_x(\rho_p, \rho_n) \right) \right] + a_\rho (\nabla_\rho)^2 - a_{\rho p}(\nabla_\rho - \nabla_{\rho p})^2 \right] d\vec{r} + \frac{1}{2} e^2 \int \frac{\rho_p(\vec{r}^*) \rho_p(\vec{r}^*)}{\vec{r} - \vec{r}^*} d\vec{r} d\vec{r}^* - \frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} e^2 \left( \rho_p^{4/3}(\vec{r}) d\vec{r} + \text{Shell} + a_{\rho p} A^{-1/3} \Delta_{np} + E_W \right)
\]
The first line in (5) corresponds to volume and surface terms. The first and the second integrals in the second line are, respectively the direct and exchange Coulomb terms. The expressions for the kinetic energy densities can be found in Ref. [3]. The shell contribution is taken from Ref. [8], the pairing term is of some importance in the expansion (3). These results are discussed in details in Ref. [3].

\[
E_w = V_w \exp \left( -\lambda \frac{N-Z}{A} \right)^2 + W_w |N-Z| \exp \left( -\frac{A}{A_0} \right)^2.
\]

(6)

For neutron and proton densities we employ a three parameter modified Fermi distribution [2], we thus have a total of six variational parameters which were obtained by minimizing the density functional (5) for each nucleus. Fits to energies are obtained by minimizing the rms deviation

\[
\sigma(E) = \sum \frac{(E_{\text{theo}} - E_{\text{exp}})}{N} \right) \right)
\]

(7)

We similarly define the rms deviations \(\sigma(R)\), \(\sigma(S1)\), \(\sigma(S2)\), and \(\sigma(Q_p)\) for the point proton radii, one neutron, two neutron and \(\beta\)-decay energies, respectively. We minimize \(\sigma(E)\) by varying \(M, u_c, \rho_0, \alpha_p, q, \alpha_{pair}\) and the Wigner parameters \(V_w, \lambda, W_w\) and \(A_0\) for fixed values of \(\rho_c\). The value of the parameter \(\rho_c\) is sensitive to the asymmetry energy data of Natowitz et al., [1]. It is found to be around 0.05–0.06 \(\text{fm}^3\). The parameter searches were made through an automated procedure.

3. Results and Discussion

| Neutron Matter | Clustering | \(\sigma(E)\) MeV | \(\sigma(R)\) fm | \(\sigma(S1)\) MeV | \(\sigma(S2)\) MeV | \(\sigma(Q_p)\) MeV | \(q\) |
|----------------|------------|-----------------|----------------|-----------------|-----------------|-----------------|-----|
| AV8' + UX    | Yes        | 0.664           | 0.044          | 0.391           | 0.519           | 0.510           | 0.171|
| AV8' + UX    | No         | 0.671           | 0.042          | 0.419           | 0.564           | 0.557           | 0.151|
| AV8'         | Yes        | 0.637           | 0.043          | 0.381           | 0.508           | 0.506           | 0.097|

Table I: Results with 2149 nuclei. \(\rho_c = 0.06 \text{fm}^3\).

We have considered a total of 2149 nuclei [11]. Results are displayed in Table I. \(\sigma(R)\), \(\sigma(S1)\), \(\sigma(S2)\), \(\sigma(Q_p)\), are for the measured 799 [12], 1988, 1937, and 1868 nuclei, respectively. The column “Clustering” indicates that if the clustering has been taken into account or not. If we use the EOS (4) as it is we have the clustering indicated by “Yes”. If we make \(u_c = 0\) in (4b), it will correspond to no clustering in the surface region indicated by “No”. The non-zero values of \(q\) signify that the quartic isospin term is of some importance in the expansion (3). These results are discussed in details in Ref. [3].

| rms deviations | Present | Möller et al., Ref.[13] | Brussels-Montreal HFB-14 Ref.[10] | HFB-17 Ref.[10] |
|----------------|--------|------------------------|----------------------------------|----------------|
| \(\sigma(E)\) MeV | 0.637  | 0.669                  | 0.729                            | 0.581          |
| \(\sigma(R)\) fm | 0.043  | –                      | 0.031                            | 0.030          |
| \(\sigma(S1)\) MeV | 0.380  | 0.411                  | –                                | 0.506          |
| \(\sigma(S2)\) MeV | 0.505  | –                      | –                                | –              |
| \(\sigma(Q_p)\) MeV | 0.504  | –                      | –                                | 0.583          |
| \(\sigma(S_{nr})\) MeV | 0.561  | 0.910                  | 0.833                            | 0.729          |
| No. of Nuclei  | 2149   | 1654                   | 2149                             | 2149           |

Table II: Root mean square deviations in various approaches.

In Table II, we compare our results with some of the earlier authors where the clustering aspect demonstrates improvement, particularly in the one neutron separation energies \(\sigma(S1)\) and \(\sigma(S_{nr})\), where \(\sigma(S_{nr})\) is the one neutron separation energies which are less than 5 MeV (a subset of 186 neutron rich nuclei). These indeed are sensitive to surface properties. In Fig. 1, we plot the calculated and experimental differences for energies of 2149 nuclei for \(N, Z \geq 8\) in the left panel. The right panel gives the differences of proton point rms radii as a function of \(A\). The points are for AV8′ from table I.
Fig1: The calculated and experimental differences in energies and point proton rms radii as a function of $A$.

Fig2: Comparison of the calculated and experimental asymmetry energy data. For details see text.

Fig3: EOS of symmetric (left panel) and asymmetric (right panel) nuclear matter. For details see text.
In Fig. 2, we compare our asymmetry energy results with the experimental results of Natowitz et al., [1]. The up triangles represent the results after the medium modification is taken into account on the data represented by down triangles. The open circles and the dotted line are the results of Quantum Statistical calculations. The curves (with the same legend as in Fig3, see next paragraph) are the results of our calculations.

In the left panel of Fig 3, we plot the EOS for SNM. The long dashed line represents the results for AV8’+UIX, the solid line shows for AV8’. These curves are for $\rho_0 = 0.06$ fm$^{-3}$. The dashed-dot and short-short curves are for AV8’+UIX with $\rho_0 = 0.05$ fm$^{-3}$ and $\rho_0 = 0.07$ fm$^{-3}$, respectively. It is seen that for a change of $\rho_0$ by 0.02 fm$^{-3}$, the change in the location of maximum, $E_{\text{max}}$, in the EOS of SNM is only 0.005 fm$^{-3}$. It is fixed around $\rho = 0.025$ fm$^{-3}$. Also shown is the EOS of Akmal et al., (APR) [14]. The triangles are the results with AV18 +UIX with relativistic boost corrections. The dotted line is obtained by invoking heuristic corrections to account for the known empirical values of $\rho_0$, $K$ and $\alpha$. Below the spinodal density (0.05 fm$^{-3}$) most of the many body calculations of SNM become unreliable.

In the right panel, we plot the EOS of asymmetric NM for different values of the asymmetry parameter $\delta$. The vertical short lines represent the location of equilibrium densities. Note that all the curves meet the y-axis [$E(\rho, \delta\text{-axis})$] at nonzero negative values for $\delta < 1$. It is interesting to note that these negative values of energies are always less than the corresponding values of the minimum energies at the equilibrium densities. In fact they represent the ground state of the asymmetric NM; not the energies at the equilibrium densities. In earlier NM calculations all the energies approach zero as the density approaches zero for all values of $\delta$.

4. Conclusions
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 low densities significantly. It is demonstrated that clustering is consistent with the static properties of nuclei. Also, a forceful interpretation of the experimental asymmetry data emerges and the exact result that $E_{\text{asym}}(\rho \rightarrow 0) \rightarrow \alpha$.

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