

Density Functional Theory Calculation in Nuclei Cluster

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Abstract: In this study, a nuclei phenomenological theory that includes a general form of clustering at the nuclear surface is presented. Different clusters with different shapes and sizes with medium alterations are involved in a phenomenological way. Arguments brought to an equation of state for nuclear matter consistent with clustering in the low-density region are stated. Due to the clustering, an interesting interpretation of the equation of state for asymmetric nuclear matter comes into view. A prolonged Thomas-Fermi theory version is assumed as a framework for nuclei where it contains Wigner contributions and the phenomenological pairing. Clustering in nuclei is being related with the nuclear matter equation of state at the nuclear surface, in this theory, including low density clustering. Calculations are conducted for diverse nuclear matter state equations. Binding energies of 2149 nuclei for $N, Z \geq 8$ are taken into account by this study.

Keywords: nuclei cluster, equation of state.

1. Introduction

Density functional theory has become a popular method in computational chemistry and physics in the past two decades. The theory mainly gained its popularity due to low computational cost and its simple theory. The continuous developments of high-quality exchange-correlation functionals (xcFs) has enabled chemists and physicists to study the large as well as complex systems at low-to-moderate computational expense with high accuracy.

Density functional theory (DFT) is based on the theorem by P. Hohenberg and W. Kohn [1] that for a molecule, electron density $\rho(\mathbf{r})$, where \mathbf{r} is the spatial coordinates can be utilized to determine all properties of the molecular systems. DFT is almost always applied in its Kohn-Sham formalism (KS-DFT) [2] at present. The so called formalism represents the density of the system under consideration by a single Slater determinant [3] of a fictitious non-interacting system.

In this work, we present a thermodynamically consistent phenomenology. The possibility of clusters' forming in various sizes and shapes accompanied by medium modifications are included through this phenomenology. We start with the statement that the binding energy of symmetric nuclear matter (SNM) per nucleon in the limit of zero density must get near u_v (≈ 16 MeV) at the saturation density ρ_0 (≈ 0.16 fm⁻³), where u_v is the Weizsäcker mass formula's volume term. The previous statement is based upon the

theory that nuclear matter at a given density in its ground state ($T=0$ MeV) will achieve the minimum possible energy. The following procedure demonstrates our statement. It is explained in [4] that an idealized α -matter picture of SNM in the zero density neighbourhood provides energy per nucleon, $E/A \approx -7.3$ MeV, which is the α -particle's energy per nucleon considering that the Coulomb interaction is turned off. The previous conclusion is at variance with the results of mean field theories where $E(\rho) \rightarrow 0$ as the density $\rho \rightarrow 0$, for instance, in the calculations of Skyrme-Hartree-Fock.

SNM might be looked at as a perfect gas of hunks of very heavy nuclei or nuclear matter (NM) where the surface effects can be neglected consequently. The densities are considered low enough so that interactions amongst clusters is negligibly small and the perfect cluster - matter idea is valid. Consequently, the exact result is acquired as $E(\rho) \rightarrow -u_v$ as $\rho \rightarrow 0$. Therefore, we have the relation

$$E(\rho \rightarrow 0) \rightarrow E(\rho = \rho_0) = -u_v. \quad (1)$$

Relation (1) is counter intuitive and, seemingly, has not been applied in any nuclear physics computations. The usage of relation (1) will be extended in our formulation. We do not consider the SNM as an ideal cluster matter at finite but low densities since it should occur just in the zero density limit. Nuclear matter will be highly associated with complex structure at low densities.

2. Methodology and Computational Considerations

An Extended Thomas-Fermi (ETF) method established on the density functional method [5-9], will be applied. The process with widely utilization in nuclear physics, metallic clusters and atomic [6] is considered that exactly conveys the average energy part. As a result, the quantal shell effects are handled in line with Strutinsky's calculations [10] or the liquid drop model and the spin-orbit densities is neglected. In recent exploratory research, this issue has been adequately discovered. The inclusion part has been left for the future and is likely to further progress the results. Yet, its effects have been involved, nearly through shell correction.

$E[\rho_n, \rho_p]$, spherical symmetry and the energy of a nucleus,

are assumed and expressed as the neutron and proton densities functional:

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

where τ_2 and τ_4 are the kinetic energy densities

$$\tau_2(\rho_n, \rho_p) = \sum_{k=n,p} \left(\frac{1}{36} \frac{(\nabla \rho_k)^2}{\rho_k} + \frac{1}{3} \Delta \rho_k \right), \quad (3)$$

$$\begin{aligned} \tau_4(\rho_n, \rho_p) = & \frac{1}{6480} (3\pi^2)^{-2/3} \times \\ & \sum_{k=n,p} \rho_k^{1/3} \left[8 \left(\frac{\nabla \rho_k}{\rho_k} \right)^4 - 27 \left(\frac{\nabla \rho_k}{\rho_k} \right)^2 \frac{\Delta \rho_k}{\rho_k} \right. \\ & \left. + 24 \left(\frac{\Delta \rho_k}{\rho_k} \right)^2 \right]. \end{aligned} \quad (4)$$

In equation (2) and (3), the summation k is over the proton and neutron densities. The $\hbar^2 / 2m$ factor that increases τ_2 and τ_4 contains the bare nucleon mass m . These have been presented taking a cue from Skyrme density functional [11]. The parameter a_{np} multiplying $(\nabla \rho_n - \nabla \rho_p)^2$ has been the subject of an attractive recent *ab initio* study of drops of neutron matter caught in an external field [12]. It was found that the term is reduced ineffective through the quartic isospin term in the symmetry energy. The shell contributions also incorporate deformation energies. The last two terms represent the pairing energy and Wigner (E_W) contributions, respectively.

For Δ_{np} , according to [13,14], we apply

$$\Delta_{np} = \begin{cases} 2 - |I| : N \text{ and } Z \text{ even} \\ |I| : N \text{ and } Z \text{ odd} \\ 1 - |I| : N \text{ even } Z \text{ odd and } N > Z \\ 1 - |I| : N \text{ odd } Z \text{ even and } N < Z \\ 1 : N \text{ even, } Z \text{ odd and } N < Z \\ 1 : N \text{ odd, } Z \text{ even and } N > Z \end{cases} \quad (5)$$

with $|I| = |N - Z|/A$.

We use a phenomenological Wigner term

$$\begin{aligned} E_W = & V_W \exp \left\{ -\lambda \left(\frac{N - Z}{A} \right)^2 \right\} \\ & + W_W |N - Z| \exp \left\{ -\left(\frac{A}{A_0} \right)^2 \right\} \end{aligned} \quad (6)$$

Goriely *et al.* [15] in their Skyrme-Hartree-Fock-Bogoliubov microscopic-macroscopic mass formula presented this structure..

According to this study perspective, the Wigner, pairing and shell terms do not have significant roles. Nevertheless, the findings are improved, i.e. quantitatively accompanies with energies and rms radii, and cause we differentiate our outcomes with other microscopic/macroscopic theories. The liquid drop model is the same as the shell, pairing and Wigner terms inclusion..

Three-parameter modified Fermi distribution parameter for each category [6,16] is applied for variational neutron (proton) densities:

$$\rho_{n(p)}(r) = \frac{N_{n(p)}}{(1 + \exp((r - R_{n(p)})/t_{n(p)}))^{\gamma_{n(p)}}} \quad (7)$$

with $R_{n(p)}$, $t_{n(p)}$ and $\gamma_{n(p)}$ that represent variational parameters for neutrons (protons) and $N_{n(p)}$ that is the normalization constant that guarantees the right neutron (proton) numbers. The six parameters are varied for each nucleus to lessen the energy.

One of the advantages of this approach can be the application of microscopically calculated homogeneous equation of state (EOS) of neutron matter. the recently calculated values [17,18] are used in this research. It can be obtained through applying a precise secure phase auxiliary field diffusion Monte Carlo (AFDMC) process with 66 neutrons encased in a periodic box with Argonne *AV8'* [19] and Urbana three-nucleon *UIX* [20] interactions. Between the neutron matter for *AV8'* results and *AV18'* in the low density region there is some differences. However if the more realistic Illinois (IL) three-body interaction [21] is used there should be some differences, as needed for generating the ground and excited state energies of p-shell nuclei in the Green's function Monte Carlo (GFMC) calculations [22]. In Figure 1 we illustrate the results of [17], indicated by filled circles for *AV8' + UIX*. The solid line is the fit acquired by

$$E(\rho) = \sum_{i=1}^3 y_i \rho^i / \left(1 + \sum_{i=1}^4 z_i \rho^i \right) \quad (8)$$

where the parameter values are $y_1 = 0.331 \times 10^4 \text{ MeV fm}^3$, $y_2 = 0.632 \times 10^7 \text{ MeV fm}^6$, $y_3 = 0.259 \times 10^9 \text{ MeV fm}^9$, $z_1 = 0.948 \times 10^4 \text{ fm}^3$, $z_2 = 0.192 \times 10^7 \text{ fm}^6$, $z_3 = 0.772 \times 10^7 \text{ fm}^9$, $z_4 = -0.323 \times 10^8 \text{ fm}^{12}$.

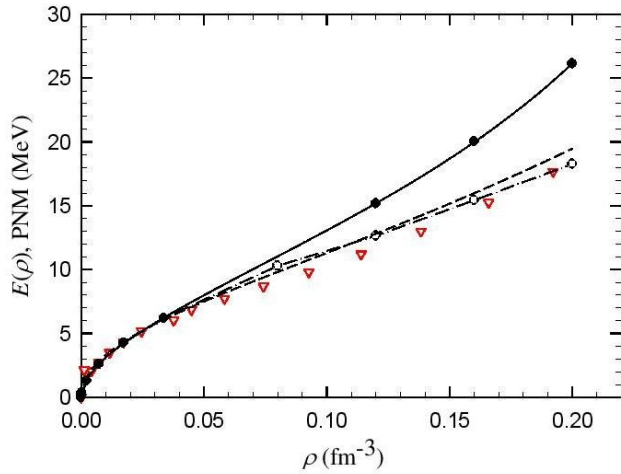


Figure 1. Equation of State of neutron and neutron matter as function of density

The results of AFDMC computations with AV8'+UIX of [17] are represented by the filled circles. Contrastively, the open circles show outcomes with AV8' alone; to aid the eye, dot-dashed line (to combine with the open circles) is demonstrated. The solid line is the fit achieved by Pade approximation. The dashed line is the outcomes for AV8' + $V_{2\pi}^{PW} + V_{\mu=300}^R$ as presented in [18]. The inverted triangles (FP) are the results from [23].

The open circles represent the outcomes with AV8' alone and can be acquired by reproducing the solid curve with a fudge factor $\exp(-2.615(\rho - 0.05))$ for $\rho > 0.05 \text{ fm}^{-3}$. We use these fits in our computations of $E_{sym}(\rho)$. [17] have given an alternate parameterized structure for $E(\rho)$ of neutron matter

$$E(\rho) = a \left(\frac{\rho}{\rho_0} \right)^\alpha + b \left(\frac{\rho}{\rho_0} \right)^\beta \quad (9)$$

This form is also used in one specific case, but equation (7) provides a better parameterization for $\rho < 0.04 \text{ fm}^{-3}$. The root mean square deviations is defined for energies and radii

$$\sigma(E) = \sqrt{\sum_{i=1}^N (E_{theo}^i - E_{exp}^i)^2 / N}, \quad (10)$$

with a parallel definition for $\sigma(R)$,

$$\sigma(R) = \sqrt{\sum_{i=1}^{N'} (R_{theo}^i - R_{exp}^i)^2 / N'}, \quad (11)$$

where N and N' show the numbers of nuclei included. For every value, the *rms* deviations $\sigma(S1)$, $\sigma(S2)$, and $\sigma(Q_\beta)$ for the one and two neutron separation and β -decay energies are defined analogously.

3. Results and Discussion

In the first place, to prepare the computations comparatively less extensive, the study limits to 367 spherical nuclei [24] from ^{38}Ca to ^{220}Th . They consist of the chains $^{38-52}\text{Ca}$,

$^{42-54}\text{Ti}$, $^{100-134}\text{Sn}$ and $^{178-214}\text{Pb}$. These are the same set of nuclei demonstrated [24]. The electronic binding energy take $1.433 \times 10^{-5} Z^{2.39} \text{ MeV}$ away from the binding energies of [25]. For the charge *rms* radii we have considered all the 149 nuclei of the 799 nuclei [26], common to the set of 367 nuclei. The point proton *rms* radii, r_p , are achieved through

the relation $r_p = \sqrt{r_c^2 - 0.64}$, where r_c is the charge *rms* radius.

We have a total of twelve parameters (which in the long run is reduced to eleven), to be specific, u_v , ρ_0 , M , ρ_x , a_ρ , a_{np} , q and a_{pair} , and the four parameters V_W , λ , W_W and A_0 in the Wigner term, in equation (3). Computed energies are obtained variationally through differentiating the density by the six variational parameters of equation (4). The task starts with the setting $q = 0$, i.e. no isospin quartic term, and minimize $\sigma(E)$, for fixed values of ρ_x , changing the other parameters. Minimization is achieved by an automated method of searching.

The enhanced values of $\sigma(E)$ will be $\leq 0.6 \text{ MeV}$ consistent with the present microscopic-macroscopic theories. Wigner parameters also convert rational. This seems to be logical reason for the presence of the quartic isospin term.

It has been also reported by Brussels-Montreal group [27] that if they adjust the Skyrme density functional parameters to mimic the APR [28] EOS of neutron matter, they gain through AV18+UIX, the quality of fits to masses deteriorates. A large quartic isospin term is induced by UIX that cannot be emulated through the isovector gradient term. An older neutron matter EOS by Friedman-Pandharipande (FP) [23] is applied by the Brussels-Montreal group. Although calculations have not been made with this EOS, it is believed that if clustering is not included a quartic isospin term to a good approximation will not be required. The EOS of neutron matter for FP and AV8' are near, as shown in Figure 1, however at the same time, AV8' is steeper than FP. The common Skyrme density functionals will be appropriate in this condition. This responses the question asked previously as "why the quartic isospin term is not necessary in earlier microscopic-macroscopic theories".

4. Concluding Remarks

The Hohenberg and Kohn theorem [1] holds for an exact density functional. The estimated ETF functional will result in a slight over binding problem, progressively, when shell effects are not designed in a self-consistent manner, mainly through the "expectation value method" as clarified by Brack *et al.* [6], in spite the fact that we have applied a phenomenological pairing and Wigner terms. It is believed that this slight over binding, some parts in 10^4 for heavy nuclei [6], is easily remunerated through the small change in the theory parameters possibly indicated by the overall good fits to the nuclei's static properties. Additionally, there exists

a connection between macroscopic phenomenological models and the ETF energy functional in such a way as the droplet model and liquid drop model [6]. There has been made a quantitative connection between the parameters of Skyrme forces which appear in the density functional with the parameters of the macroscopic models. The ETF energy functional is more common and acceptable because it embodies the macroscopic models. As explained before, some of the macroscopic models with microscopic corrections [14, 24, 29–33] may have the inconsistency problem too. Exceptions in [34] microscopic mass formula, newly established fully microscopic density functional theories [35–38] (the nuclei spectroscopic properties are described in the latter too), and microscopic-macroscopic theories, for instance in [6, 7, 27]. The $\sigma(E)$ values strive well with the majority of the other approaches. We have invoked the ETF density functional to show that the low density symmetry energy data of [39] is constant with the nuclei static properties. This goal has been achieved successfully.

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