

SEMI-CLASSICAL, MICROSCOPIC APPROACH TO THE LIQUID DROP MODEL — A POSSIBLE WAY OF THE DESCRIPTION OF HEAVY ION REACTIONS

ZBIGNIEW SOSIN[†], JINESH KALLUNKATHARIYIL

The Marian Smoluchowski Institute of Physics, Jagiellonian University
Reymonta 4, 30-059 Kraków, Poland

(Received October 29, 2013; revised version received November 26, 2013)

An isospin and spin dependent form of the equation of state for nuclear matter is presented. This form is used for the description of nucleon interaction in a new dynamical model. Preliminary calculations show that the new approach makes possible predicting the alpha-like structures appearing in the case of the even–even nuclei ground state.

DOI:10.5506/APhysPolB.45.925

PACS numbers: 21.60.Gx, 21.65.Mn, 21.10.Dr, 21.65.–f

1. Introduction

Although nuclei are close to 55 orders of magnitude lighter than a typical neutron star, it seems that the state of the above two objects can be determined by the same equation, which is the equation of state (EOS) of nuclear matter. In this case, EOS is defined as the average energy per baryon expressed as a function of thermodynamic variables. It seems that the above statement can be more easily justified for heavy nuclei but, as can be shown, using an appropriate form of the equation of state can give good results also for the ground states of lighter nuclei. We arrived at these conclusions using semi-classical, microscopic version of the liquid drop model in which dynamics is governed by EOS.

The description of the nuclear dynamics, which uses the concept of the equation of state, can be found in the reaction models referring to the liquid drop model (LDM) [1]. In this description, it is assumed that the energy of the system is determined mainly by the following three components:

- the volume energy defined by the kinetic energy related to internal, fermionic motion and respective potential interactions for infinite nuclear matter in equilibrium,

[†] ufsosin@cyf-kr.edu.pl

- the surface energy, which in classical description could be treated as a result of the surface tension action,
- the Coulomb energy associated with the proton charge.

Such models typically assume one body dissipation and incompressibility of nuclear matter. In such an approach, the volume energy together with energies which are corrections related to a not equal number of protons and neutrons and a non-zero spin of the system may be treated as the 0th term of the expansion of the energy density function (given by EOS). An incompressibility assumed in this model introduces additional constraints on the global coordinates which describe the system shape and its evolution.

In our microscopic description of the system evolution, we take into account also the next term in the expansion of the equation of state as a function of the density of nuclear matter. The presented approach treats the local density of the nuclear matter as a result of the aggregation of partial densities given by Gaussian packets which represent the nucleons forming the system. As a result, the local density of a matter is explicitly given by the position of these packages and their variance. In our approach, we describe the volume energy as the respective functional (volume integral of the energy density given by the equation of state multiplied by the density of the nuclear matter).

The nuclear EOS describes equilibrated, infinite nuclear matter and is used in the calculations of the properties of the astronomical objects as, for example, neutron stars or supernovae [2]. In such large objects, the surface effect in the description of the total energy is negligible. For small objects, such as atomic nuclei, the energy due to interactions at the surface, cannot be ignored and in such case the system energy must have additional contributions, corresponding to this additional surface energy. In the presented approach, the surface energy is related to the dispersion of the energy density in the nucleon's environment and also to the increase of the diffuseness of the nucleon momentum caused by nucleon location at the surface (see in [3]).

In the interaction description which is applied in the model presented here, one can distinguish ingredients related to the volume, surface and Coulomb energy, which are the essence of the description used in the LDM model.

In our approach, all the mentioned types of energy are functionals expressed by integrals determined by the distribution of nuclear matter. Since these densities are here uniquely determined by the position and other parameters of wave packets (spin, isospin and variance), the description can be interpreted as the Microscopic LDM model (MLDM).

As we know, the equation of state of nuclear matter is still not well established and its determination is one of the most important tasks of the experimental and theoretical nuclear physics. In the presented approach, the equation of state plays a very important role and in this way the described model has an opportunity to contribute in the EOS investigation. It is also important to use a convenient form of the EOS suitable for efficient description of the heavy ion reactions as well as for the description of the ground state properties of the reacting nuclei. This form of the EOS should fulfil the following requirements:

1. The compression part of the equation of state, in the neighbourhood of saturation density ρ_0 (where ρ_0 is the density of the matter which is equilibrated in isospin and spin, and for which the density of energy reaches a minimum) can be written as a sum of the two types of energy:
 - e_0 : energy related to symmetric nuclear matter (SNM);
 - e_{sym} : energy produced by the nuclear matter symmetry disorders, which is called a symmetry energy (see Section 2).

It turns out that adopting certain simplifying assumptions (see Appendix A), these energies can be expressed as a function of the total density ρ . The expectation which is in line with a mean field theory (*e.g.* with the Skyrme–Hartree–Fock model) determine the zero energy density in the case where density of matter tends to zero (it is in contrast with some other models like, for instance, an idealized alpha-mater picture [4]).

2. For the saturation density, we require:
 - a defined value of the energy density;
 - a defined values of the first and the second derivatives (slope and curvature) of the energy density (defined by EOS);
 - and for density $\rho \rightarrow 0$ the additional requirement is $e(\rho) \rightarrow 0$;

then the simplest form of a polynomial, which can meet all these requirements can be expressed as

$$e = \alpha\rho + \beta\rho^2 + \gamma\rho^3. \quad (1)$$

The method of determining the coefficients alpha, beta, gamma is given in Section 2 and Appendix A. As it is shown [3], form (1) is suitable for different theoretical descriptions of the EOS. It is also worth noting that this form of the EOS allows us to find the respective mean energy values in an analytical way (in the case when the density is expressed by partial density, taken as the Gaussian functions).

A modified equation of state in a form suitable for the MLDM calculations is defined in the next section. In the third section, we will present the application of the proposed form of the EOS together with an additional surface energy term in the MLDM model. The obtained preliminary results in this model are related to the properties of nuclei in their ground states and are presented in Section 4. Since in our description we use EOS, in which energy symmetry is associated with spin and isospin asymmetry (see the next section), the geometric structure defined by the position of the centres of the wave packets can be interpreted as clusters. For the nuclei with even and equal number of neutrons and protons, these clusters appear as alpha particles. In Section 5 we present such alpha structures, which appear in model calculations for light nuclei. In the last chapter, conclusions and future plans are presented.

2. An equation of state given by the third-degree polynomials

The concept of the EOS of the nuclear matter in the case of two-component proton–neutron gas has been discussed in many articles. This equation as well as a form based on the use of the third-degree polynomials is described in [3] and works cited therein. In the next section, we present the ground state properties of nuclei which are obtained by the microscopic, density-functional approach. The EOS plays a key role in this approach.

This model is designed to explore the dependence of the dynamics on wave packets, isospin and spin of nucleons, which these packets represent. By isospin dependence, we mean the dependence on the charge of the nucleon (third component of the isospin vector).

If the isospins, spins and variances of wave packets are variables affecting the mutual interaction of nucleons, then appropriate equations of state must describe a gas consisting of four components:

- protons with spin up — density $\rho_{p\uparrow}$;
- protons with spin down — density $\rho_{p\downarrow}$;
- neutrons with spin up — density $\rho_{n\uparrow}$;
- neutrons with spin down — density $\rho_{n\downarrow}$.

In our considerations, by ‘nucleons with spin up’ or ‘nucleons with spin down’ we mean nucleons having spin projections ‘up’ or ‘down’ on the chosen quantization axis. Now the EOS can be formally written

$$e = e(\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}) . \quad (2)$$

According to symmetries characterizing the nuclear interaction, the system energy is conserved during mutual exchange of neutrons and protons, and also when changing projections of the spin of all particles to the opposite projections. To allow us to use these symmetries, we define new coordinates:

$$\xi = \frac{\rho - \rho_0}{\rho_0}, \quad (3)$$

$$\delta = \frac{\rho_n - \rho_p}{\rho}, \quad (4)$$

$$\eta_n = \frac{\rho_{n\uparrow} - \rho_{n\downarrow}}{\rho}, \quad (5)$$

$$\eta_p = \frac{\rho_{p\uparrow} - \rho_{p\downarrow}}{\rho}, \quad (6)$$

where ρ is the total nuclear matter density, and ρ_0 is the density of the isospin and spin equal to zero matter at saturation. We find that during the above-mentioned operation (mutual conversion of neutrons into protons and the change of spin projections of all nucleon) the sign of the coordinates: neutron-proton asymmetry δ and spin asymmetry η_n and η_p are respectively changed. Therefore, in order to assure energy conservation, in the expression which defines the system energy, quantities δ , η_n and η_p can occur only as products with the respective even number of factors. Using these symmetries one can show (see Appendix A) that the equation of state can be written with the components having an extended form of symmetry energy:

$$\begin{aligned} e = & e_{00} + \frac{K_0}{18}\xi^2 \\ & + \delta^2 \left(e_{I0} + \frac{L_I}{3}\xi + \frac{K_I}{18}\xi^2 \right) \\ & + (\eta_n^2 + \eta_p^2) \left(e_{ii0} + \frac{L_{ii}}{3}\xi + \frac{K_{ii}}{18}\xi^2 \right) \\ & + 2\eta_n\eta_p \left(e_{ij0} + \frac{L_{ij}}{3}\xi + \frac{K_{ij}}{18}\xi^2 \right). \end{aligned} \quad (7)$$

The first two lines in the sum (7) represent a well-known form of the equation of state. The first line describes the matter in a balanced system (zero isospin and spin), where K_0 is the coefficient of compressibility of the nuclear matter and the second one describes the isospin interaction

$$e_I = e_{I0} + \frac{L_I}{3}\xi + \frac{K_I}{18}\xi^2 \quad (8)$$

which is called the symmetry energy for which e_{I0} is the Wigner constant, and the coefficients L_I and K_I are the slope and curvature respectively.

In equation (7), by analogy to the isospin symmetry energy, one can distinguish the spin symmetry energies for neutrons and protons separately

$$e_{ii} = e_{ii0} + \frac{L_{ii}}{3}\xi + \frac{K_{ii}}{18}\xi^2, \quad (9)$$

and energy

$$e_{ij} = e_{ij0} + \frac{L_{ij}}{3}\xi + \frac{K_{ij}}{18}\xi^2 \quad (10)$$

for the mutual, spin interaction of protons and neutrons. The expansion coefficients: e_{ii0} , L_{ii} and K_{ii} , (constant slope and curvature) with indices ii , describe the energy related to the proton or neutron gas, while the respective indices ij indicate that the symmetry energy refers to the mutual interaction of protons and neutrons.

All types of the symmetry energy describe the influence of the spin and isospin polarization of the matter on the average energy of the nucleon (EOS). According to the observations presented in the introduction, we assume that the energy associated with the SNM as well as all types of symmetry energy should disappear as the density of matter tends to zero. Therefore, to ensure zero values for all energies occurring in equation (7) at $\rho = 0$ and to get the proper slope and curvature of the saturation density ρ_0 , we use the form of the third-degree polynomial proposed in [3]. As mentioned in [3], if the density of matter is described by the sum of Gaussian distributions, then such a form of the EOS allows us to calculate the average energy analytically.

Any type of energy found in (7) may be written as

$$e_k = \alpha_k \rho + \beta_k \rho^2 + \gamma_k \rho^3, \quad (11)$$

and the index k can take values 0, I , ii , and ij . Here, the coefficients α_k , β_k , γ_k are determined by the relations:

$$\alpha_k = \left(3e_{k0} - \frac{2}{3}L_k + \frac{K_k}{18} \right) / \rho_0, \quad (12)$$

$$\beta_k = - \left(3e_{k0} - L_k + \frac{K_k}{9} \right) / \rho_0^2, \quad (13)$$

$$\gamma_k = \left(e_{k0} - \frac{L_k}{3} + \frac{K_k}{18} \right) / \rho_0^3. \quad (14)$$

3. Application of the proposed EOS form to the MLDM calculations

The proposed MLDM, similarly like in other models [9–11], describe the time evolution of the wave function represented by the product of M

Gaussian wave packets, which represent the nucleons forming the system

$$\Phi = \prod_{k=1}^M {}^k\phi_{I_k S_k}, \quad (15)$$

$${}^k\phi_{I_k S_k} = \frac{1}{(2\pi\sigma_k^2(r))^{3/4}} \exp\left(\frac{-(\mathbf{r}_k - \langle\mathbf{r}_k\rangle)^2}{4\sigma_k^2(r)} + \frac{i}{\hbar}\mathbf{r}_k\langle\mathbf{p}_k\rangle\right), \quad (16)$$

where $\sigma_k^2(r)$, $\langle\mathbf{r}_k\rangle$, $\langle\mathbf{p}_k\rangle$, are the width (the position variance of the k^{th} nucleon) of a Gaussian wave functions, and centres of its position and associated momentum for each of the M nucleons. Also every partial wave function (15) has a label $I_k = n$ or $I_k = p$ and $S_k = \uparrow$ or $S_k = \downarrow$, informing us about isospin and spin associated with the given nucleon and determine the kind of density ($\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}$) to which given wave packet participate. In our approach, the variables $\langle\mathbf{r}_k\rangle$, $\langle\mathbf{p}_k\rangle$ and $\sigma_k^2(r)$ are time-dependent parameters describing the wave functions. In addition, we assume that with every wave packet for each of M nucleons, isospin and spin are related and that they remain fixed during the interaction (in this way, index k inform us about the parameters of the given nucleon).

Equations of motion of variables $\langle\mathbf{r}_k\rangle$, $\langle\mathbf{p}_k\rangle$ and $\sigma_k^2(r)$ are derived using the time-dependent variational principle (see *e.g.* [5]) based on the action minimization. For this purpose, we define the action as

$$S = \int_{t_1}^{t_2} L(\Phi, \Phi^*) dt, \quad (17)$$

with the Lagrange functional given as

$$L = \left\langle \Phi \left| i\hbar \frac{d}{dt} - H \right| \Phi \right\rangle = \left\langle \Phi \left| i\hbar \frac{d}{dt} \right| \Phi \right\rangle - \langle \Phi | H | \Phi \rangle. \quad (18)$$

Now, we will concentrate on the determination of the average value of Hamiltonian $\langle \Phi | H | \Phi \rangle$. As usual, the Hamiltonian can be written as a sum of the kinetic energy T and the potential interaction V . To determine the average kinetic energy, we assume that each wave packet has a momentum dispersion $\sigma_k(p)$ around its mean value $\langle\mathbf{p}_k\rangle$, ($\sigma_k(r)\sigma_k(p) = \hbar/2$ is assumed). Then the average kinetic energy is given by

$$\langle \Phi | T | \Phi \rangle = \sum_{k=1}^M \left[\frac{\langle\mathbf{p}_k\rangle^2}{2m} + \frac{3\sigma_k^2(p)}{2m} \right]. \quad (19)$$

We assume also that the interaction between nucleons can be described by the potential given in the form

$$V(\{\mathbf{r}_k\}, \{\sigma_k(r)\}) = V_N(\{\mathbf{r}_k\}, \{\sigma_k(r)\}) + V_S(\{\mathbf{r}_k\}, \{\sigma_k(r)\}) + V_{\text{Coul}}(\{\mathbf{r}_k\}, \{\sigma_k(r)\}), \quad (20)$$

where V_N is the nuclear interaction, V_S is the modification of the interaction induced by changing the density of matter around the nucleon (surface energy) and V_{Coul} consists of the Coulomb interaction. If the nuclear matter is characterized by non-zero spin polarization, then there is a magnetic field. This field can also be generated by the motion of protons. In such a case, the Hamiltonian should be corrected for the magnetic interaction.

Now, the average value of the Hamiltonian can be expressed by

$$\langle \Phi | H | \Phi \rangle = \sum_{k=1}^{k=M} \left[\frac{\langle \mathbf{p}_k \rangle^2}{2m} + \frac{3\sigma_k^2(p)}{2m} \right] + \langle \Phi | V_N | \Phi \rangle + \langle \Phi | V_S | \Phi \rangle + \langle \Phi | V_{\text{Coul}} | \Phi \rangle + \langle \Phi | M | \Phi \rangle. \quad (21)$$

In our further considerations, we ignore magnetic interaction. The crucial assumption of the present approach is that the energy of the fermionic internal motion can be described by $\frac{3\sigma_{p_k}^2}{2m}$, so the sum

$$B_V = \sum_{k=1}^{k=M} \frac{3\sigma_k^2(p)}{2m} + \langle \Phi | V_N | \Phi \rangle = \int e(\rho, \delta, \eta_n, \eta_p) \rho(\mathbf{r}) d^3\mathbf{r} \quad (22)$$

can be treated as a volume term of binding energy. As we know, the ground state energy of the nuclear matter is described by the EOS, which considers the energy density as a sum of the kinetic energy, associated with the internal fermionic motion, and energy given by the potential interaction. Therefore, in our approach we do not have to find the appropriate distribution of the nucleon momenta, provided that a correct description is given by the selection of appropriate EOS parameters. Such an EOS parametrization replaces the potential parametrization normally used.

As in [3], the surface energy is defined as

$$B_{\text{surf}} = \langle \Phi | V_S | \Phi \rangle = s_0 \sum_{i=1}^{i=M} \frac{\sigma_i(e)}{\sigma_i^2(r)}, \quad (23)$$

where in this semi-empirical part s_0 is the surface energy coefficient. In this formula, the variance $\sigma_k(e)$ denotes the variance of energy $e(\rho, \delta, \eta_n, \eta_p)$ with respect to the probability ${}^k\rho(\mathbf{r})$ of finding the k^{th} nucleon

$$\sigma_k(e) = \left[\int (\bar{e}_k - e(\rho, \delta, \eta_n, \eta_p))^2 {}^k\rho(\mathbf{r}) d^3\mathbf{r} \right]^{\frac{1}{2}}, \quad (24)$$

where \bar{e}_k is the average energy given by

$$\bar{e}_k = \int e(\rho, \delta, \eta_n, \eta_p) {}^k\rho(\mathbf{r}) d^3\mathbf{r}. \quad (25)$$

In Appendix A, we describe the method of calculation used for variance $\sigma_k(e)$ calculations.

Let us discuss briefly the description of the surface energy given by formula (23). In our approach, we consider drops of the nuclear matter shown in Fig. 1. The density of matter $\rho(r) = \rho_n(r) + \rho_p(r)$ is a function of the distance r , where $\rho_n(r) = \rho_{n\uparrow} + \rho_{n\downarrow}$ and $\rho_p(r) = \rho_{p\uparrow} + \rho_{p\downarrow}$. If the k^{th} packet is in the region of fixed energy $e(\rho, \delta, \eta_n, \eta_p)$, then its variance $\sigma_k(e)$, associated with this package ${}^k\rho(\mathbf{r})$, is equal to zero. If the package ${}^l\rho(\mathbf{r})$ is in the change of the energy, then the variance $\sigma_l(e)$ is greater than zero. According to the formula (23), the surface energy associated with the i^{th} packet is inversely proportional to the uncertainty of location, which means that it is proportional to the indetermination of the package momentum. Now, the formula (23) can be understood as follows. The variation of energy $\sigma_i(e)$ (and associated forces) describes the possibility of localization of the i^{th} nucleon in the case of its entering the alternating field. Such a localization results in an increase of indetermination of the momentum and an increase of the average kinetic energy associated with the i^{th} package.

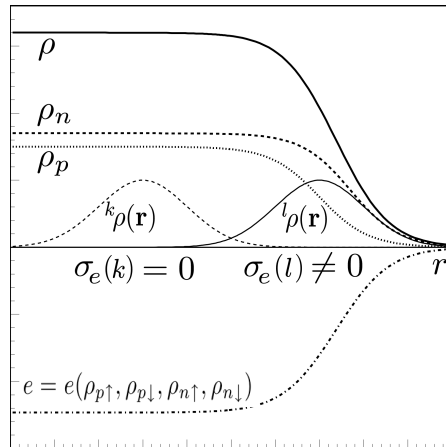


Fig. 1. An example of the position of the partial density function and associated energy variance. As one can see for a position close to the center, variance of the energy (24) vanishes. See the text for more details.

The last term in (20) is the Coulomb energy (for protons only) and is given in the form

$$\langle \Phi | V_{\text{Coul}} | \Phi \rangle = \frac{1}{2} \sum_{k \neq l} \int k \rho(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} l \rho(\mathbf{r}') d^3 \mathbf{r} d^3 \mathbf{r}' . \quad (26)$$

This integral can be calculated analytically as (see *e.g.* [6])

$$e^2 \sum_{k \neq l} \frac{\text{erf} \left(\frac{r_{kl}}{\sqrt{2} \sigma_{kl}(r)} \right)}{r_{kl}} , \quad (27)$$

where $r_{kl} = |\langle \mathbf{r}_k \rangle - \langle \mathbf{r}_l \rangle|$ and $\sigma_{kl}(r) = \sqrt{\sigma_k^2(r) + \sigma_l^2(r)}$.

The average Hamiltonian can be written in a form which is analogous to the description given by the LDM

$$\begin{aligned} \langle \Phi | H | \Phi \rangle = & \sum_{k=1}^{k=M} \frac{\langle \mathbf{p}_k \rangle^2}{2m} + B_V (\{\langle \mathbf{r}_k \rangle\}, \{\sigma_k(r)\}) + B_S (\{\langle \mathbf{r}_k \rangle\}, \{\sigma_k(r)\}) \\ & + V_{\text{Coul}} (\{\langle \mathbf{r}_k \rangle\}, \{\sigma_k(r)\}) . \end{aligned} \quad (28)$$

Based on the Euler–Lagrange equations, one can find the corresponding equations of motion for coordinates $\langle \mathbf{p}_k \rangle$, $\langle \mathbf{r}_k \rangle$ and $\sigma_k(r)$ (see the Euler–Lagrange equations). This will be described in a forthcoming paper.

Here, as the first test of the new form of the equation of state, based on the MLDM model, we will try to describe the ground state properties of a selected set of nuclei. In our very preliminary approach, we will focus on the binding energies and nuclear charge radii (RMS).

4. The MLDM calculations for describing the ground state properties of nuclei

In the MLDM model, the ground state of a nucleus is a many-body state which is an absolute minimum with respect to variations of $\langle \mathbf{r}_k \rangle$, $\sigma_k(r)$. Additionally, in the ground state, for every k the average momentum $\langle \mathbf{p}_k \rangle = 0$, which means that for MLDM particles will be essentially at rest and the system corresponds to a solid one. In order to determine the nuclear ground state wave function, the following procedure of searching the set $\{\langle \mathbf{r}_k \rangle, \sigma_k(r)\}$ is used:

1. In a limited space, we choose a random position of the wave packet together with a certain initial variance. In order to accelerate calculations for even–even nuclei, we can also assume a correlation (mating) of packets describing nucleons of the same type and differing only in the direction of the spin projection. In such a case, we assume that positions of centres and variances of a spin pair are equal.
2. Using a selected set of parameters describing the interaction (type EOS), we search for such values of these parameters for which the energy of the system is minimal. One should also be careful to avoid emerging local minima. Wave functions found in this way are characterized by certain symmetries, which may be helpful in assessing the resulting minimum. In the next chapter, we will discuss types of symmetry, emerging especially for even–even nuclei with an equal numbers of protons and neutrons.

To use the presented model for calculating the ground state properties of nuclei, we have to select specific values of parameters describing the equation of state. For this purpose, a global search for optimal parameter values should be used. This will be done in the next paper, here we apply only a very simplified search method based on the following assumptions:

In the first step, we try to determine the ρ_0 , e_{00} , K_0 and s_0 parameters. In our preliminary estimations, we assume that $\rho_0 = 0.159 \text{ nucl/fm}^3$ and $K = 300 \text{ MeV}$, which has to be in an agreement with the experiment and theoretical calculations. Then, we use the binding energies and RMS radii for ^4He and ^{12}C nuclei to determine e_{00} and s_0 by the trial and error method. In this way, we obtain $e_{00} = -12.9 \text{ MeV}$ and $s_0 = 0.09 \text{ fm}^2$. For these nuclei, due to the matter gathering in clusters which are equilibrated in spin and isospin coordinates, corrections arising due to the symmetry energies appear to be negligibly small. Note that the obtained parameters e_{00} and s_0 differ from standard values (in particular, the typical value of $e_{00} = -16 \text{ MeV}$). This is the result of their assessment for very light nuclei. In the future, it will be necessary to determine these parameters based on a larger database (the set of energies and radii of the nuclei in their ground states).

In the next step, we use the binding energies and RMS radii of ^2H , ^3H , ^3He , to obtain an estimate of the isospin and spin polarization parameters. Our rough estimate gives $e_{I0} = 30 \text{ MeV}$, $L_I = 123 \text{ MeV}$, $K_I = 500 \text{ MeV}$ for isospin parameters and $e_{ii0} = 65 \text{ MeV}$, $L_{ii} = 300 \text{ MeV}$, $K_{ii} = 300 \text{ MeV}$ for the spin interaction in gas of neutrons (the same parameters for the proton gas). The mutual spin interaction of protons and neutrons are described by parameters $e_{ij0} = -1 \text{ MeV}$, $L_{ij} = 20 \text{ MeV}$, $K_{ij} = 300 \text{ MeV}$.

With such parameters, the dependence of energies e_0 , e_I , e_{ii} and e_{ij} , on the density are presented in Fig. 2.

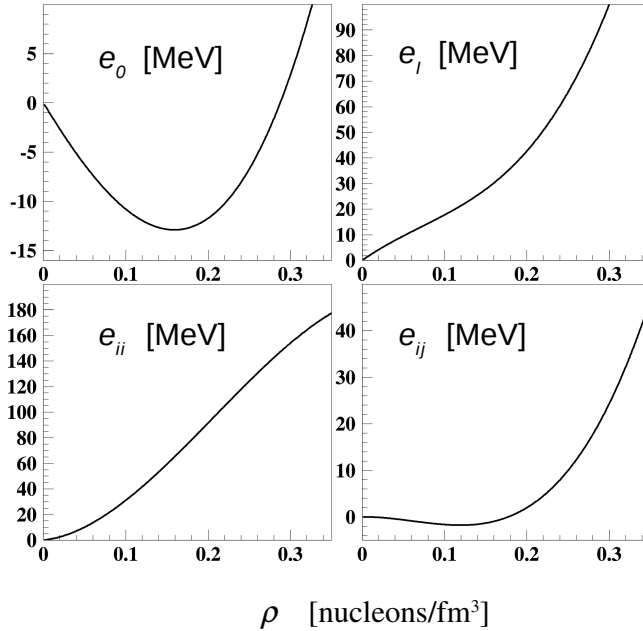


Fig. 2. The dependence on the density of nuclear matter: e_0 in an isospin and spin balanced state, the symmetry energy e_I for isospin, the symmetry energy e_{ii} for the spin polarization for proton or neutron matter and the symmetry energy e_{ij} for spin polarization for proton–neutron matter (see the text).

In this simple analysis, the ${}^2\text{H}$, ${}^3\text{H}$, ${}^3\text{He}$, ${}^4\text{He}$ and ${}^{12}\text{C}$ nuclei can be treated as generators of the EOS parameters. Reproduced by MLDM model, binding energies and RMS radii are for these generators arranged together with the experimental data in Table I.

TABLE I

MLDM calculation results (for preliminary EOS parameters selection). Binding energies and RMS charge radii of nuclei are compared with the experimental data.

Nuclei	Binding energy data [MeV]	Binding energy MLDM [MeV]	RMS charge radius data [fm]	RMS charge radius MLDM [fm]
${}^2\text{H}$	−1.112	−1.104	2.14	2.196
${}^3\text{H}$	−2.827	−2.809	1.759	1.824
${}^3\text{He}$	−2.572	−2.571	1.945	1.974
${}^4\text{He}$	−7.074	−7.062	1.676	1.727
${}^{12}\text{C}$	−7.68	−7.719	2.47	2.466

For such choice of the EOS parameters (and the coefficient of surface tension $s_0 = 0.09 \text{ fm}^2$), we obtain predictions for the binding energies per nucleon and RMS charge radii which are presented together with the experimental data in Table II.

TABLE II

MLDM calculation results (prediction, preliminary). Binding energies and RMS charge radii of nuclei are compared with the experimental data.

Nuclei	Binding energy data [MeV]	Binding energy MLDM [MeV]	RMS charge radius data [fm]	RMS charge radius MLDM [fm]
^{16}O	-7.976	-7.84	2.701	2.613
^{20}Ne	-8.032	-7.908	3.005	2.774
^{24}Mg	-8.261	-7.953	3.056	2.874
^{32}S	-8.493	-7.929	3.261	3.127
^{36}Ar	-8.520	-7.896	3.39	3.227
^{40}Ca	-8.551	-7.85	3.476	3.336

The data in Table I and Table II should be treated as very preliminary predictions of the MLDM code based on a roughly chosen equation of state. For heavier nuclei, one can see quite large deviations of the calculated and experimental data. In order to achieve greater consistency with the description of the experimental data, all EOS parameters should be re-adjusted.

5. The alpha structure of even-even nuclei with equal number of protons and neutrons

The concept of nuclear clusters appeared along with the quantum description of nuclei (and even before the discovery of the neutron in 1932 by James Chadwick). In article [7], many experimental arguments are presented for the possible existence of alpha clusters, as a matter substructures in forming nuclei. We present here only two of them, both taken from [8].

(i) The binding energy of even-even nuclei with an equal number of protons and neutrons appears to be a linear function of the number of bonds in alpha-particle model, where the number of bonds is equal to: $k = 1$ for ^8Be , $k = 3$ for ^{12}C , $k = 6$ for ^{16}O , $k = 9$ for ^{20}Ne , etc. (see Fig. 9). In the cited work, this phenomenon is explained on the basis of the proposed form of the potential interaction between the alpha particles, however there is no justification for increase in the number of bonds, with an increasing number of alpha particles.

(ii) The binding energy of nuclei with an even number of protons Z and an odd, higher by 1 number of neutrons $N = Z + 1$. In this case, we assume that the additional neutron is interacting with multi-centrist potential defined by the system of the appearing alpha particles. Let the binding energy for each nuclide X be defined by the function $b(X)$. If the neutron binding energy in ${}^5\text{He}$ is denoted by B , then we get the following scheme:

$$\begin{aligned} b({}^5\text{He}) - [b({}^4\text{He}) + b(n)] &= B, \\ b({}^9\text{Be}) - [b({}^8\text{Be}) + b(n)] &= B + (R + Q), \\ b({}^{13}\text{C}) - [b({}^{12}\text{C}) + b(n)] &= B + 2(R + Q), \\ b({}^{17}\text{O}) - [b({}^{16}\text{O}) + b(n)] &= B + 3(R + Q), \end{aligned} \quad (29)$$

where constants R and Q are the result of reasoning, which below is presented in the case of ${}^9\text{Be}$. If a $|\psi_1\rangle$ and $|\psi_2\rangle$ denote the neutron wave functions corresponding to the interaction with a given alpha particle, then the two-centre wave function for ${}^8\text{Be}$ can be expressed approximately as a linear combination of the single center ones ($|\psi_1\rangle$ and $|\psi_2\rangle$). Now, the average binding energy of a neutron, in two-center potential, can be expressed as

$$b({}^9\text{Be}) - [b({}^8\text{Be}) + b(n)] = \frac{\langle \psi_1 + \psi_2 | T + V_1 + V_2 | \psi_1 + \psi_2 \rangle}{\langle \psi_1 + \psi_2 | \psi_1 + \psi_2 \rangle}, \quad (30)$$

where in the Hamiltonians $H = T + V_1 + V_2$ operator T describes the kinetic energy and the V_1 and V_2 are related to the neutron interaction with the corresponding alpha particle. As can be seen, the following expressions occur twice in the numerator:

- $\langle \psi_1 | T + V_1 | \psi_1 \rangle = B$, which is the neutron binding energy in ${}^5\text{He}$, and
- $\langle \psi_1 | V_2 | \psi_1 \rangle = R$, which describes the additional energy associated with the presence of the second alpha particle, and
- $\langle \psi_1 | H | \psi_2 \rangle = Q$ as the energy associated with the exchange process.

If the wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$ are normalized, then the denominator in (30) is equal to $2(1 + \langle \psi_1 | \psi_2 \rangle)$. Usually, it can be assumed that $\langle \psi_1 | \psi_2 \rangle = S$ is small compared to 1, and therefore (30) tends to the corresponding part of the expression (29).

The systematics presented in Eq. (29) shows an important role of the alpha structure in nuclei.

The report [7] describes also some of alpha cluster models. Our approach is based on single nucleons and in this way it is similar to QMD (Quantum Molecular Dynamics) [9], AMD (Antisymmetric Molecular Dynamics) [10] and FMD (Fermionic Molecular Dynamics) [11], in which a dynamics is based on variational principle.

Since our model includes isospin and spin interactions occurring between different types of nucleons with densities $\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}$, nucleons are grouped in order to minimize this additional symmetry energy. As we know, in the case of fermions this causes the binding of particles into pairs. For nuclear matter, an additional positive energy is associated with the lack of isospin balance. To minimize both of these symmetry energies, nucleons create alpha clusters. This phenomenon is included in our model, so one can observe the alpha structure in the resulting nuclear matter distribution, particularly for even-even nuclei with equal proton and neutron numbers. To show this, we present in Figs. 3–6 results of calculations for nuclei ^{16}O , ^{24}Mg , ^{36}Ar and ^{40}Ca .

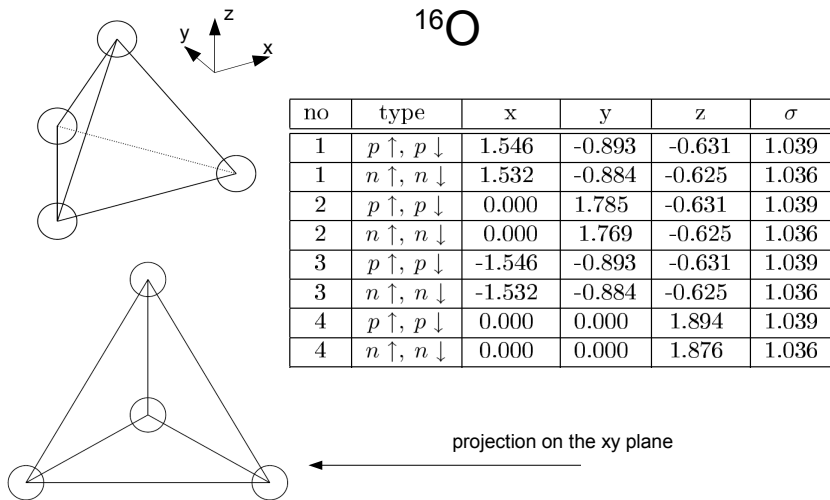


Fig. 3. The position and the variance of the wave packet for the nucleons in the nucleus ^{16}O . In the first column of the table, there are the numbers of groups of nucleons, which are correlated in the alpha particle. The second column indicates spins and a type of nucleons creating given pairs. The common position and variance of the two wave packets are presented.

The alpha structures obtained in our calculations are identical with structures presented in papers [8, 12] up to the silicon and the number of alpha-alpha bonds are the same as that proposed by [13] (after ^{16}O , there is an increment of three bonds for each additional alpha particle). Thus, we have 15 bonds for ^{28}Si instead of 16 [8]. The justification for this selection can be understood from Fig. 7 for alpha-alpha distance distribution.

This distribution presented in Fig. 7, shows that the countable alpha-alpha bond distances are centred around 3.23 fm up to 3.5 fm. In the case of ^{28}Si , distances associated with 15 bonds lie below this value and the rest

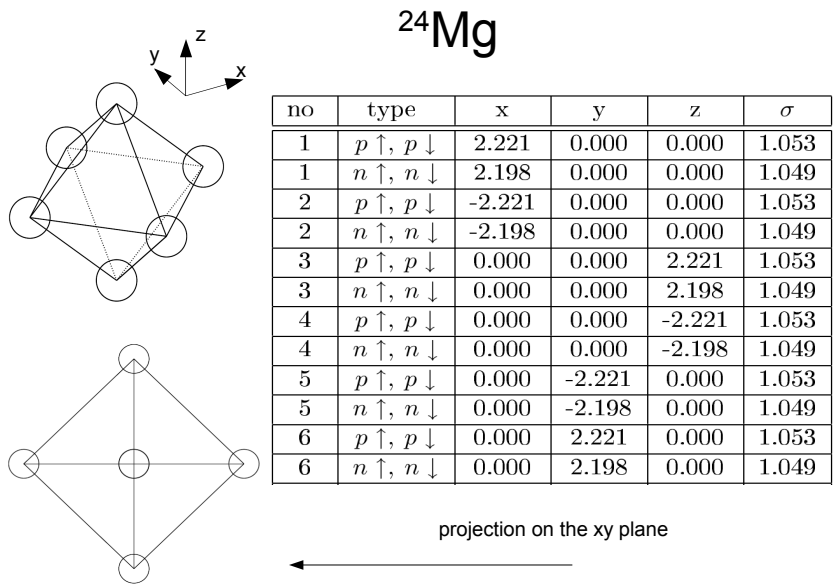


Fig. 4. The position and the variance of the wave packet for the nucleons in the nucleus ^{24}Mg . Notation is the same as in Fig. 3.

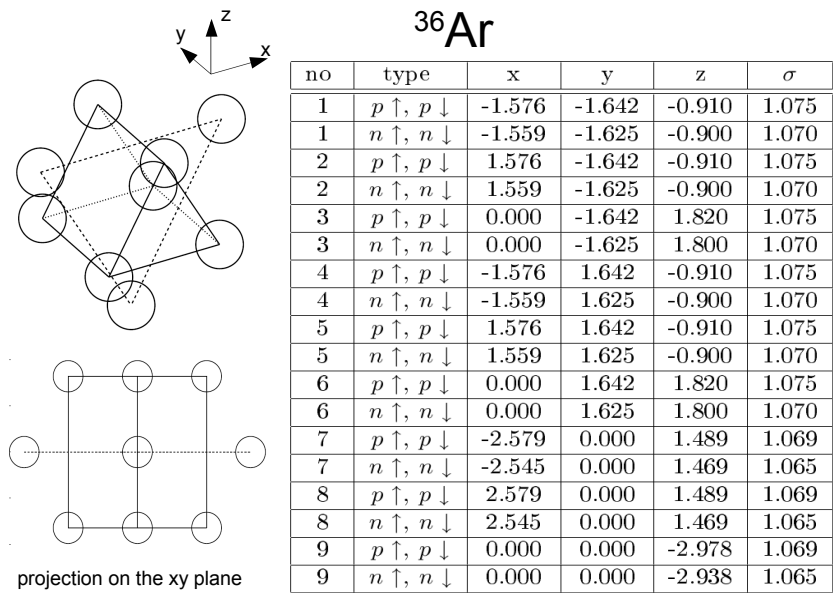


Fig. 5. The position and the variance of the wave packet for the nucleons in the nucleus ^{36}Ar . Notation is the same as in Fig. 3.

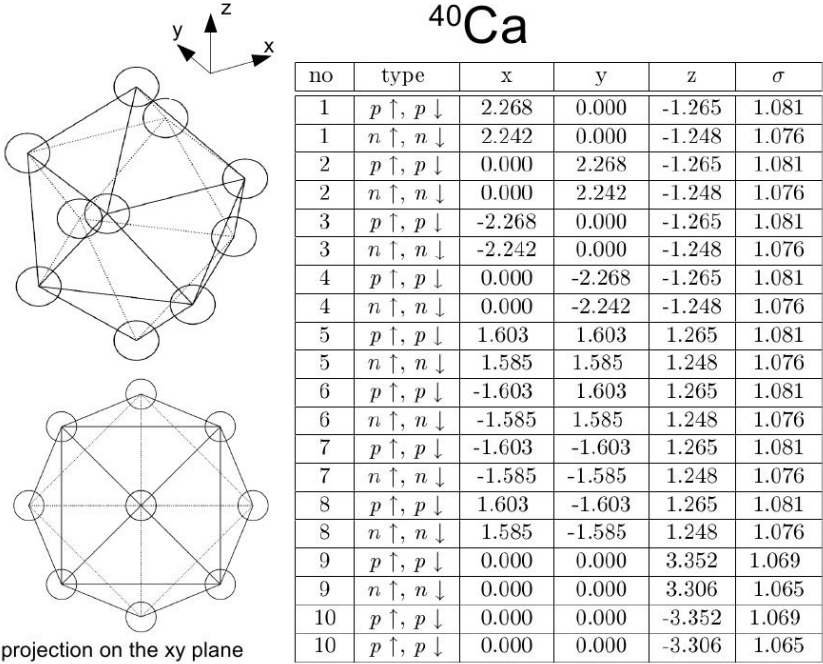


Fig. 6. The position and the variance of the wave packet for the nucleons in the nucleus ^{40}Ca . Notation is the same as in Fig. 3.

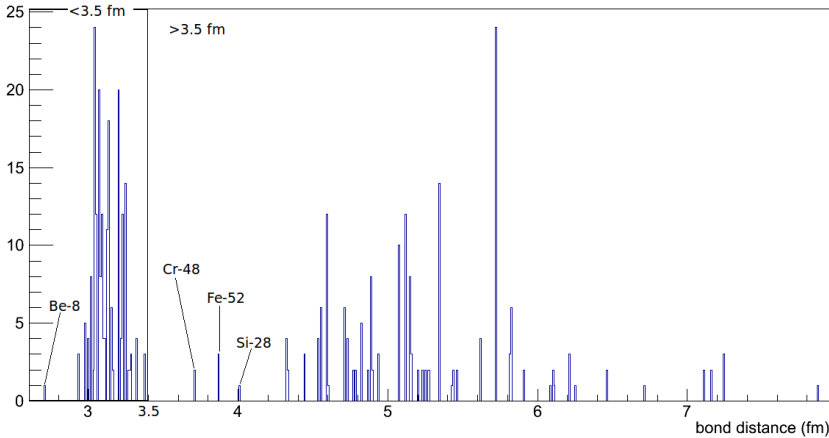


Fig. 7. The distribution alpha-alpha inter-particle distance calculated with MLDM is plotted (up to ^{60}Zn). Most of the countable distances lies below 3.5 fm. For ^{28}Si , 16th bond length is shown.

has distances larger than 4.0 fm. In our model calculations, a systematic increase in the binding energy can be observed up to ^{56}Ni . For small Z , we obtained structures identical to that of Bethe's prediction [13]. Results of the model also indicate that the first nucleus for which the change of systematic increase in the number of bonds with an increase in the number of alpha particles in the structure is ^{60}Zn (see Fig. 8). This results in a departure from the systematic increase in energy presented in Fig. 9.

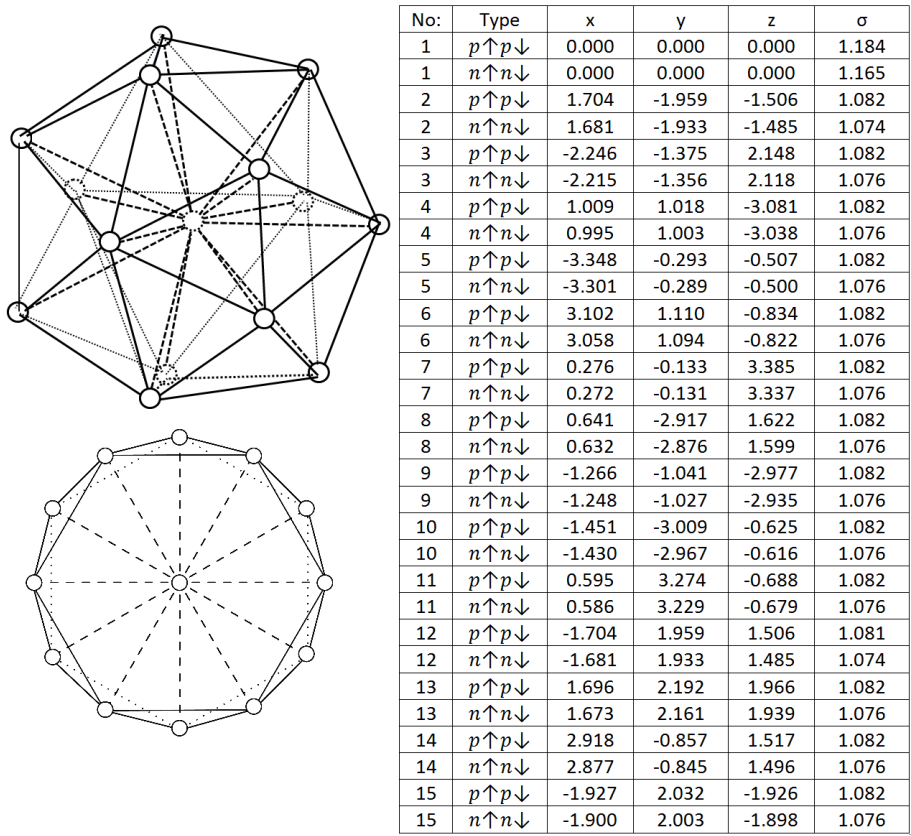


Fig. 8. The alpha particle structure of ^{60}Zn obtained via MLDM calculation (the systematic shift in the increase of the binding energy starts from this element, see the text for detail).

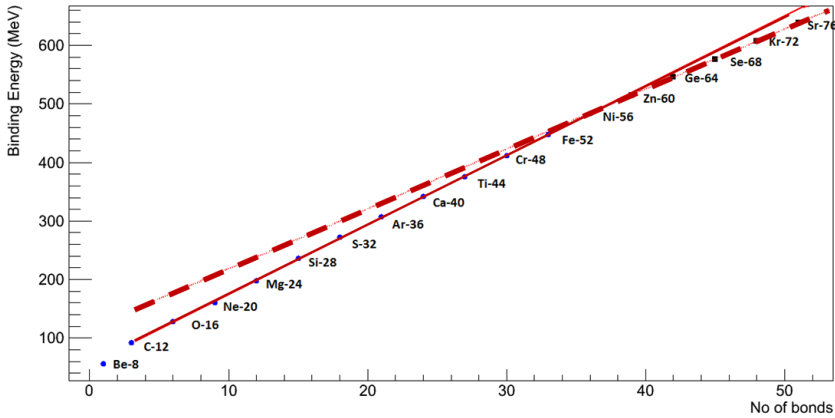


Fig. 9. Total binding energy of nuclei *versus* number of bonds. From ^{12}C to ^{56}Ni , it follows the same linear relationship, according to obtained structures. From ^{60}Zn , the slope has a new linear relationship reflecting change occurring in the nuclei structures, (see the text for details).

6. Conclusions

A new form of the EOS suitable for the MLDM model calculations is presented. Preliminary results show that the MLDM model is able to reproduce the basic properties of atomic nuclei. We see also that MLDM describes properties of the very light nuclei fairly well. Because light nuclei are usually populated with the highest probability, this is important for a correct description of the reaction dynamics.

Another important property of the model, resulting from taking into account the mutual interaction related to the spin and isospin of nucleons, is the existence of the alpha structures which is particularly noticeable for even-even nuclei with equal numbers of protons and neutrons. This formation of alpha clusters is in line with considerations of the total binding energy gain associated with the resulting increase in the number of bonds between alpha particles. It seems that the model can be helpful in explaining the change of the total binding energy increase occurring close to the nucleus $Z > 28$. This creates an additional branch in the scheme of the binding energy growth as can be seen in the experimental systematics.

A detailed analysis of the binding energy (as energy per nucleon) and analysis of the nuclear density profiles show that the structures described herein for certain nuclei may vary. This is due to the existence of various structures that minimize the energy of the ground state. For some nuclei, the binding energy differences related to the various structures are sometimes very small and subtle effects can lead to selection of one of them. This also

shows that the number of alpha bonds may differ slightly in each individual case. The analysis of this behaviour as well as restrictions on the applicability of the present simple model will be presented in the forthcoming paper.

We need to emphasize the very preliminary character of these results. In order to predict better values of the EOS parameters, further work is needed and we have to perform a global search in which we will take into account all available experimental data. It would also help to compare the model results, describing the basic observables for heavy ion reactions (particularly for the compressibility factor K_0) in the low energy region where the impact of the nucleon–nucleon collisions can be neglected.

Authors are indebted to Professors L. Jarczyk and R. Płaneta for reading the manuscript and a fruitful discussion. This work was supported in part by the Foundation for Polish Science MPD program, co-financed by the European Union within the European Regional Development Fund and also by the IN2P3 grant number 08-128.

Appendix A

In this appendix, the form of the EOS is derived. We start from the expansion of the energy density function and we use the symmetry which exists in nuclear interactions. According to this symmetry, in the expansion (up to the 4th order) of the $e(\xi, \delta, \eta_n, \eta_p)$ around the point: $\xi = 0$, $\delta = 0$, $\eta_n = 0$, $\eta_p = 0$ only the following terms appear:

$$\begin{aligned}
 e = & e_0 + \frac{1}{2}e_{\xi\xi}\xi^2 \\
 & + \delta^2 \left(\frac{1}{2}e_{\delta\delta} + \frac{1}{4}e_{\delta\delta S_n S_n}\eta_n^2 + \frac{1}{2}e_{\delta\delta S_n S_p}\eta_n\eta_p + \frac{1}{4}e_{\delta\delta S_p S_p}\eta_p^2 + \frac{1}{2}e_{\xi\delta\delta}\xi + \frac{1}{4}e_{\xi\xi\delta\delta}\xi^2 \right) \\
 & + \eta_n^2 \left(\frac{1}{2}e_{\eta_n\eta_n} + \frac{1}{24}e_{\eta_n\eta_n\eta_n\eta_n}\eta_n^2 + \frac{1}{4}e_{\eta_n\eta_n\eta_p\eta_p}\eta_p^2 + \frac{1}{2}e_{\xi\eta_n\eta_n}\xi + \frac{1}{4}e_{\xi\xi\eta_n\eta_n}\xi^2 \right) \\
 & + \eta_p^2 \left(\frac{1}{2}e_{\eta_p\eta_p} + \frac{1}{24}e_{\eta_p\eta_p\eta_p\eta_p}\eta_p^2 + \frac{1}{2}e_{\xi\eta_p\eta_p}\xi + \frac{1}{4}e_{\xi\xi\eta_p\eta_p}\xi^2 \right) \\
 & + \eta_n\eta_p \left(e_{\eta_n\eta_p} + e_{\xi\eta_n\eta_p}\xi + \frac{1}{2}e_{\xi\xi\eta_n\eta_p}\xi^2 \right). \tag{31}
 \end{aligned}$$

The symbol e with the index constituting one of the variables of the equation denotes a derivative of the energy density with respect to this variable. We neglect the dependence on δ^4 and for small spin polarization terms in brackets containing η_n^2 , η_p^2 , $\eta_n\eta_p$ can be neglected. Finally, one can write

$$\begin{aligned}
 e = & e_0 + \frac{1}{2}e_{\xi\xi}\xi^2 + \delta^2 \left(\frac{1}{2}e_{\delta\delta} + \frac{1}{2}e_{\xi\delta\delta}\xi + \frac{1}{4}e_{\xi\xi\delta\delta}\xi^2 \right) \\
 & + \eta_n^2 \left(\frac{1}{2}e_{\eta_n\eta_n} + \frac{1}{2}e_{\xi\eta_n\eta_n}\xi + \frac{1}{4}e_{\xi\xi\eta_n\eta_n}\xi^2 \right) + \eta_p^2 \left(\frac{1}{2}e_{\eta_p\eta_p} + \frac{1}{2}e_{\xi\eta_p\eta_p}\xi + \frac{1}{4}e_{\xi\xi\eta_p\eta_p}\xi^2 \right) \\
 & + 2\eta_n\eta_p \left(\frac{1}{2}e_{\eta_n\eta_p} + \frac{1}{2}e_{\xi\eta_n\eta_p}\xi + \frac{1}{4}e_{\xi\xi\eta_n\eta_p}\xi^2 \right). \tag{32}
 \end{aligned}$$

Replacing symbols of derivatives $e_{\lambda\dots}$ by variables defined in the following relations:

$$\begin{aligned} \frac{K_0}{18} &= \frac{1}{2}e_{\xi\xi}, \\ e_{I0} &= \frac{1}{2}e_{\delta\delta}, & \frac{L_I}{3} &= \frac{1}{2}e_{\xi\delta\delta}, & \frac{K_I}{18} &= \frac{1}{4}e_{\xi\xi\delta\delta}, \\ e_{ii0} &= \frac{1}{2}e_{\eta_n\eta_n}, & \frac{L_{ii}}{3} &= \frac{1}{2}e_{\xi\eta_n\eta_n}, & \frac{K_{ii}}{18} &= \frac{1}{4}e_{\xi\xi\eta_n\eta_n}, \\ e_{ij0} &= \frac{1}{2}e_{\eta_n\eta_p}, & \frac{L_{ij}}{3} &= \frac{1}{2}e_{\xi\eta_n\eta_p}, & \frac{K_{ij}}{18} &= \frac{1}{4}e_{\xi\xi\eta_n\eta_p} \end{aligned} \quad (33)$$

and taking into account the mentioned symmetries of nuclear interactions (the derivatives $(e_{\eta_p\eta_p}, e_{\eta_n\eta_n})$, $(e_{\xi\eta_p\eta_p}, e_{\xi\eta_n\eta_n})$ and $(e_{\xi\xi\eta_p\eta_p}, e_{\xi\xi\eta_n\eta_n})$ are pairwise equal, and this means that the respective symmetry energy associated with the spin is identical for protons and neutrons), we obtain equation (7).

Appendix B

In this appendix, we present the method of calculation of the variance of energy given by the EOS in the neighbourhood of the center of the packet k . In the first step, we calculate the average energy density of matter at random points with the distribution of ${}^k\rho(\mathbf{r})$

$$\bar{e}_k(k) = \int e(\rho, \delta, \eta_n, \eta_p) {}^k\rho(\mathbf{r}) d^3\mathbf{r}. \quad (34)$$

If we use the equation of state in the form of an expansion (7) and (11), the derived term for the isospin part cannot be solved analytically

$$\begin{aligned} \int \delta^2 \alpha_I \rho {}^k\rho(\mathbf{r}) d^3\mathbf{r} &= \alpha_I \int \left(\frac{\rho_n - \rho_p}{\rho} \right)^2 \rho {}^k\rho(\mathbf{r}) d^3\mathbf{r} \\ &= \alpha_I \int \frac{\rho_n \rho_n - 2\rho_n \rho_p + \rho_p \rho_p}{\rho} {}^k\rho(\mathbf{r}) d^3\mathbf{r}. \end{aligned} \quad (35)$$

In order to avoid this problem, we can use the following approximations

$$\alpha_I \int \frac{\rho_n \rho_n}{\rho} {}^k\rho(\mathbf{r}) d^3\mathbf{r} \cong \alpha_I \frac{N}{A} \int \rho_n {}^k\rho(\mathbf{r}) d^3\mathbf{r}, \quad (36)$$

where N and A are the total number of neutrons and nucleus, respectively. As we can see, after removing ρ from the denominator, the integral can be solved analytically. Similarly, we can find the remaining ingredients (35) (with $\rho_n \rho_p$ and $\rho_p \rho_p$).

In the next step, we assume that the δ , η_n , η_p are established in the vicinity of the nucleon k as $\bar{\delta}(k)$, $\bar{\eta}_n(k)$, $\bar{\eta}_p(k)$ (we replace them by the corresponding average values) and we determine the effective density of $\rho_{ef}(k)$ based on the equation

$$\bar{e}_k = e(\rho_{ef}(k), \bar{\delta}(k), \bar{\eta}_n(k), \bar{\eta}_p(k)) . \quad (37)$$

In further considerations, we replace the set $\rho_{ef}(k)$, $\bar{\delta}(k)$, $\bar{\eta}_n(k)$, $\bar{\eta}_p(k)$ by $\tilde{\rho}_{p\uparrow}(k)$, $\tilde{\rho}_{p\downarrow}$, $\tilde{\rho}_{n\uparrow}(k)$, $\tilde{\rho}_{n\downarrow}(k)$. To calculate the variance $\sigma_k^2(e)$, we develop the integral expression

$$\sigma_k^2(e) = \int (\bar{e}_k - e(\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}))^2 {}^k\rho(\mathbf{r}) d^3\mathbf{r} \quad (38)$$

around $\tilde{\rho}_{p\uparrow}(k)$, $\tilde{\rho}_{p\downarrow}$, $\tilde{\rho}_{n\uparrow}(k)$, $\tilde{\rho}_{n\downarrow}(k)$. This allows the analytical calculation of the considered integral. In our calculations, we limited ourselves to the first order expansion. So, because $e(\tilde{\rho}_{p\uparrow}(k), \tilde{\rho}_{p\downarrow}(k), \tilde{\rho}_{n\uparrow}(k), \tilde{\rho}_{n\downarrow}(k)) = \bar{e}_k$ this choice of expansion gives a very simple form of the integrand.

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