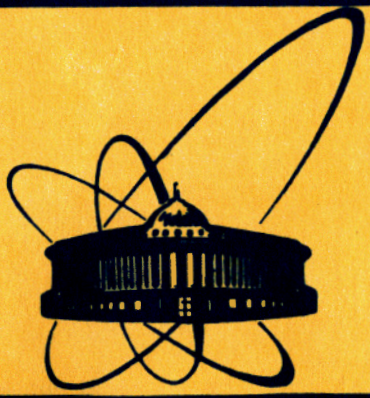

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I.Zh.Petkov, M.V.Stoitsov

A RELATION BETWEEN THE LOCAL SCALE TRANSFORMATION APPROACH AND THE NUCLEAR ENERGY DENSITY FORMALISM

1983

1. Lately, the Energy Density Formalism (EDF) has been oftenly used for a solution of different physical problems /1-5/. In EDF the energy of a many particle Fermi system is a functional $E[\rho]$ of the local particle density $\rho(\vec{r})$. The ground state energy E_0 results at a certain density, which minimizes the functional $E[\rho]$.

The possibility of expressing the energy as a functional only of the density follows from the Hohenberg-Kohn theorem /6/. The theorem is quite formal however and does not give a rule of constructing the explicit local density functional form of the energy.

Recently we have shown that there exists a rigorous approach for building up $E[\rho]$, which takes essentially use of the Local Scale Transformation Method (LSTM) /7,8/.

In the present note an expression of energy density functional is obtained by applying LSTM to the one-particle Dirac density matrix of a particular form. The structure of the expression occurs to be nearly the same as that of EDF functionals. The approach we develop is generally more informative as it gives the particle momentum distribution, as well.

2. We shall consider a nuclear A-particle system described by the Hamiltonian H with Skyrme's forces /9,10/. According to LSTM /8/ the expectation value of H with trial functions belonging to the certain determinant orbit $\bar{O} \subset \mathcal{H}_{HF}$ is s functional of the local scale transformation function $f(\vec{r})$:

$$E[f] = \int \mathcal{E}_f(\vec{r})\, d\vec{r}. \tag{1}$$

The energy density $\mathcal{E}_f(r)$ is given in terms of f(r) by

$$\mathcal{E}_f(r) = \frac{\hbar^2}{2M}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^3 + \frac{1}{16}(3t_1+5t_2)\rho\tau + \frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2, \tag{2}$$

where t_0, t_1, t_2, t_3 are Skarme's parameters ($W_0 = 0$).

The local density $\rho(\vec{r})$ and kinetic energy density $\tau(\vec{r})$ in eq. (2) are

$$\rho(\vec{r}) = \lim_{\vec{r}' \to r} \rho^{(1)}(\vec{r}, \vec{r}'; \vec{f}), \tag{3}$$

$$\tau(\vec{r}) = \lim_{\vec{r}' \to r} \nabla_{\vec{r}} \nabla_{\vec{r}'} \rho^{(1)}(\vec{r}, \vec{r}'; \vec{f}), \tag{4}$$

where $\rho^{(1)}(r, r'; f)$ is the local scale transformation of the one-particle "model" density matrix $\bar{\rho}^{(1)}(\vec{r}, \vec{r}')$. The last is given by

$$\bar{\rho}(\vec{r}, \vec{r}') = \sum_{\alpha=1}^{\infty} n_\alpha \overset{*}{\phi}_\alpha(\vec{r}) \phi_\alpha(\vec{r}'), \tag{5}$$

$$\bar{\rho}(r) = \lim_{\vec{r}' \to r} \bar{\rho}^{(1)}(\vec{r}, \vec{r}'), \tag{5a}$$

where the functions ϕ_α, $\alpha = 1, 2, 3, \ldots$ form a one-particle "model" bases, $n_\alpha / n_\alpha = 1$, $\alpha \le A$; $n_\alpha = 0$, $\alpha > A$; $A = N + Z$/are occupation numbers. The local density $\rho(\vec{r})$ and "model" density $\bar{\rho}(\vec{r})$ are connected by the equation

$$\rho(\vec{r}) = \frac{f^2}{r^2} \frac{\partial f}{\partial r} \bar{\rho}(\vec{f}), \quad \vec{f} = \frac{\vec{r}}{r} f(\vec{r}). \tag{6}$$

It was shown[8] that the relation (6) is a simple one. Therefore substituting the solution of eq. (6) into eqs. (2)-(5) we obtain eq. (1), which is the local density functional of the energy $E[\rho]$ constructed on a certain determinant class of orbits $\Theta \subset \mathcal{H}_{X\Phi}$

In general case it is not possible to find the functional $E[\rho]$ explicitly at any $\bar{\rho}^{(1)}(\vec{r}, \vec{r}')$ of the type (5). Therefore we consider a soluble model where we choose a certain self orbit representation form of the density matrix $\bar{\rho}^{(1)}(\vec{r}, \vec{r}')$.

3. We use the following model density matrix[11]:

$$\bar{\rho}^{(1)}(\vec{r}, \vec{r}') \equiv \rho^{(1)}(\vec{R}, \vec{S}) = \bar{\rho}(\vec{R}) \exp(-cS^2), \tag{7}$$

where $\vec{R} = \frac{1}{2}(\vec{r} + \vec{r}')$, $\vec{S} = \vec{r} - \vec{r}'$ and

$$\bar{\rho}(\vec{R}) = a \exp(-bR^2). \tag{8}$$

The coefficients

$$a = \frac{4\alpha^3}{\pi^{3/2}} \frac{1}{(1-t^2)^{3/2}}, \quad b = \alpha^2 \frac{1-t}{1+t}, \quad c = \frac{\alpha^2}{4} \frac{1+t}{1-t} \tag{9}$$

are expressed by the occupation number parameter $t / n_\alpha = t^{N_\alpha}$, $N_\alpha = n_X + n_Y + n_Z = 2n + \ell$ and oscillator parameter $\alpha = \left(\frac{M\omega}{\hbar}\right)^{1/2}$.

The normalization condition $\int \rho(\vec{r}) d\vec{r} = A$ gives the relation

$$A = 4(1-t)^{-3}; \qquad t = 1 - \left(\frac{4}{A}\right)^{1/3}. \tag{10}$$

Using the density matrix (7) and the method described above one can obtain the local and kinetic energy density

$$\tau(\vec{r}) = \frac{1}{4} \frac{(\nabla\rho)^2}{\rho} + \kappa^2(A) C_K \rho(\vec{r}) \left\{ \frac{2}{3} \frac{f^2}{r^2} + \frac{1}{3} (\nabla f)^2 \right\}, \tag{11}$$

$$\rho(\vec{r}) = \frac{f^2}{r^2} \frac{\partial f}{\partial r} \exp(-\epsilon f^2), \tag{12}$$

where $C_K = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}$, $\epsilon = \pi A^{-2/3}$ and $\kappa^2(A) = \frac{10}{(36\pi)^{1/3}}\left[1 - \left(\frac{4}{A}\right)^{1/3}\right]$.

The solution of eq. (12) with respect to $f(r)$ is:

$$f(\vec{r}) = f_0(\vec{r}) \left\{ 1 + \sum_{n=1}^{\infty} a_n (\epsilon f_0^2)^n \right\}, \tag{13}$$

where

$$f_0(\vec{r}) = \left\{ 3 \int_0^r \rho u^2 du \right\}^{1/3}. \tag{14}$$

The coefficients $\{a_n\}$ are to be obtained by the following recurrence link

$$C_0^{(m)} = 1,$$

$$C_n^{(m)} = \frac{1}{n} \sum_{\ell=0}^{n} (\ell m - n + \ell) a_\ell C_{n-\ell}^{(m)}, \qquad n \ge 1, \tag{15}$$

$$\sum_{n=0}^{k} \frac{(-1)^n C_n^{(2k-2n+3)}}{(k-n)!\,(2k-2n+3)} = 0, \qquad k \ge 1.$$

They prove to be sharply decreasing when the number n increases. First three coefficient values are $a_1 = \frac{1}{5}$, $a_2 = \frac{31}{350}$, $a_3 = \frac{89}{9450}$.

The decomposition (13) and eq. (11) result in

$$\tau(\vec{r}) = \tau_0(\vec{r}) + \kappa^2(A) \sum_{n=1}^{\infty} \epsilon^n \tau^{(n)}(\vec{r}), \tag{16}$$

where

$$\tau_0(\vec{r}) = \tau^{(W)} + \tau^{(GTF)} = \frac{1}{4}\frac{(\nabla\rho)^2}{\rho} + \kappa^2(A)\,C_K\{\frac{2}{3}\frac{f_0^2}{r^2} + \frac{1}{3}(\nabla f_0)^2\}\rho\,. \qquad (17)$$

Note that at $n \geq 1$ and $A > 5$ the parameter $\epsilon < 1$. At $A = 4$ or $A \to \infty$ the second term in (16) disappears. The explicit density functional is now readily obtained inserting eq. (16) into eq. (1).

4. It is essentially to mention that the main term of eq. (16) which is given by expression (17) can be obtained with a different choice of the density matrix

$$\rho^{(1)}(\vec{r}, \vec{r}'; f) = \sqrt{\rho(\vec{r})\,\rho(\vec{r}')}\;\hat{j}_1(\bar{\kappa}\,|\,\vec{f}(\vec{r}) - \vec{f}(\vec{r}')\,|), \qquad (18)$$

where $\vec{f}(\vec{r}) = \frac{\vec{r}}{r} f_0(\vec{r})$ and $\bar{\kappa} = (\frac{3\pi^2}{2})^{1/3}\kappa(A)$. This expression (18) results after local scale transformation of the nuclear matter density matrix [12]. The parameter $\kappa(A)$ in (12) limits to $\frac{10}{(36\pi)^{1/3}} \approx 2.008$ at $A \to \infty$. This limit disagrees with the correct value $\lim_{A\to\infty}\kappa(A) = 1$ following by the nuclear matter theory. Therefore we determine $\kappa(A)$ by equating the calculated binding energy with the experimental one.

Taking into account this obstacle, as well as the fact that $\tau(\vec{r}) \equiv \tau_0(\vec{r})$ at $A = 4$ or $A \to \infty$ we disregard the second term in eq. (16) to obtain an approximation for $E[\rho]$. Then the final result for $E[\rho]$ follows by the substitution of eq. (17) into eq. (1):

$$E[\rho] = \int \mathcal{E}_\rho(\vec{r})\,d\vec{r}\,, \qquad (19)$$

$$\mathcal{E}_\rho(\vec{r}) = \frac{\hbar^2}{2M}\tau + \frac{3t_2+t_1}{8}(\rho_p\tau_p^{(GTF)} + \rho_n\tau_n^{(GTF)}) +$$

$$+ t_0(\frac{1-x_0}{4})(\rho_p^2+\rho_n^2) + \frac{t_1}{8}((\nabla\rho_p)^2+(\nabla\rho_n)^2) +$$

$$+ t_0(\frac{2+x_0}{2})\rho_n\rho_p + \frac{t_3}{4}\rho\rho_n\rho_p + \frac{t_1+t_2}{4}(\rho_n\tau_p^{(W)} + \rho_p\tau_n^{(W)}) +$$

$$+ \frac{t_1+t_2}{4}(\rho_n\tau_p^{(GTF)} + \rho_p\tau_n^{(GTF)}) + \frac{3t_1-t_2}{8}\nabla\rho_p\,\nabla\rho_n + \mathcal{E}_C(\vec{r}), \qquad (19a)$$

where $\rho = \rho_p + \rho_n$ and $\tau = \tau_p + \tau_n$. From eq. (16):

$$\tau = \tau^{(W)} + \tau^{(GTF)}, \qquad (20)$$

$$\tau_\sigma^{(W)}(\vec{r}) = \frac{1}{4}\frac{(\nabla\rho_\sigma)^2}{\rho_\sigma}; \quad \sigma = p,n, \qquad (20a)$$

$$\tau^{(GTF)}(\vec{r}) = \kappa^2(A)\,C_K\,\rho_\sigma(r)\{\frac{2}{3}\frac{f_\sigma^2}{r^2} + \frac{1}{3}(\nabla f_\sigma)^2\}, \qquad (20b)$$

where $C_K = \frac{3}{5}(3\pi^2)^{1/3}$ and

$$f_\sigma(\vec{r}) = \{3\int_0^r \rho_\sigma u^2\,du\}^{1/3}; \quad \sigma = p,n, \qquad (21)$$

5. Analyzing the general expression (19) we will consider its particular features. As it is seen from (19)-(21) there appears an additional term to the kinetic energy $\tau^{(W)}$, widly known as Weizsecker's kinetic energy correction. As distinct from EDF phenomenological approaches [4] in which $\tau^{(W)}$ is multiplied by fitting numerical parameter, the LSTM leads to $\tau^{(W)}$ in its original form [5].

The second term of (20) at slowly varying local density is transformed into $\tau_{TF} \sim \rho^{5/3}$, that is Thomas-Fermi kinetic energy expression. At an arbitary density $\rho(\vec{r})$ can be considered as a generalized Thomas-Fermi Kinetic energy.

The stationary condition ($\delta_\rho E[\rho] = 0$, $\int \rho\,d\vec{r} = A$) is fulfilled when the density $\rho(\vec{r})$ satisfies the following integro-differential equation

$$\Delta\rho_\sigma + \frac{4M}{\hbar^2}(\lambda_\sigma + U_\sigma(\rho,\vec{r}))\,\rho_\sigma = 0, \qquad (22)$$

where a Lagrange multiplier λ_σ determines the nucleon separation energy. Note that eq. (22) gives a correct asymptotic behaviour of the density: $\rho(r \to 0) \sim \text{const}$, $\rho(r \to \infty) \sim \exp(-kr)$.

We are looking for a solution of eq. (22) with respect to $\rho_n(\vec{r})$ and $\rho_p(\vec{r})$ by applying a modification of the Core-spline method [13]. The obtained by this method nonlinear algebraical system of equations for the coefficients of the exponential core $p(x) = \exp(-kx)$ and the cubic spline $S_n^{(3)}(x)$ we solve by autoregularized iterative process of Gauss-Newton type [14]. Calculations are performed by REGN programme system [15] on the CDC-6500 at the Joint Institute for Nuclear Research, Dubna.

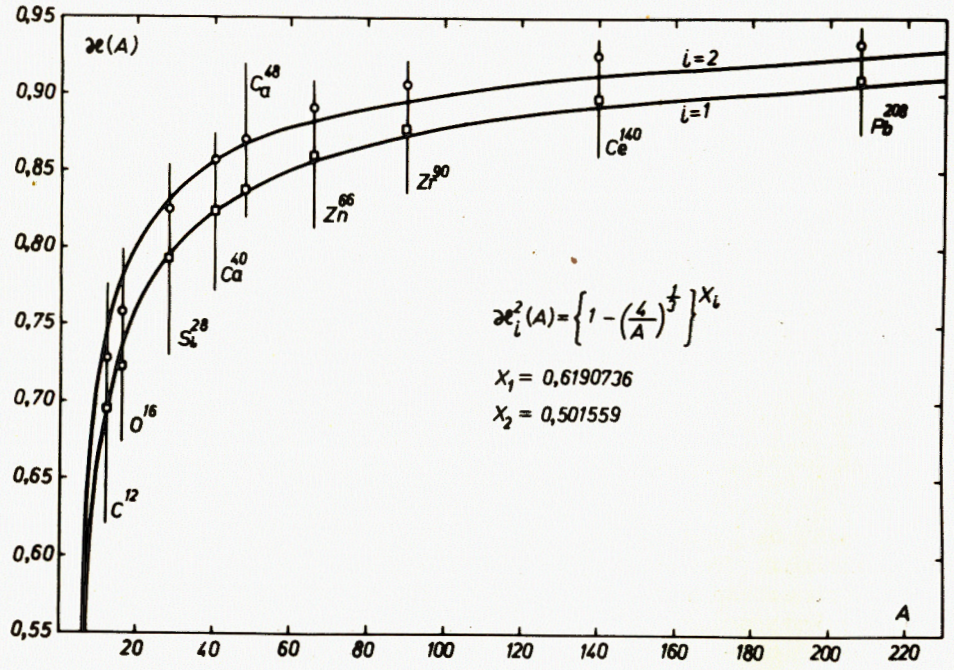

Fig.1. The value of $\varkappa(A)$ at different A.

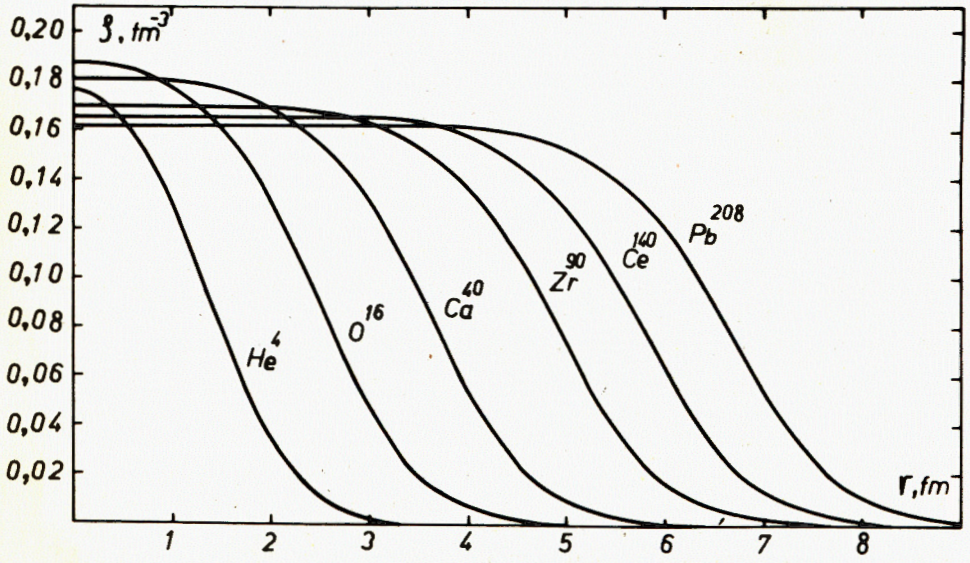

Fig.2. Mass density distributions in nuclei.

6. Numerical calculations are carried out for even-even nuclei: ^{12}C, ^{16}O, ^{32}S, ^{40}Ca, ^{48}Ca, ^{66}Zn, ^{90}Zr, ^{140}Ce, and ^{208}Pb. We take the same Skyrme-I force parameters, which are used in /9/. The fitting coefficient $\varkappa(A)$ at a given A is determined by a comparison between the calculated binding energy and the experimental one.

Figure 1 shows the value of $\varkappa(A)$ at different A. Two expressions of the kinetic energy are used: $\tau^{(GTF)}$ from eq.(20b) and the approximation

$$\tau_\sigma^{(AGTF)} = \varkappa^2(A)\, C_K \rho_\sigma^{5/3}; \qquad \sigma = p,n. \tag{23}$$

In the approximation (23) which results from (20b) at slowly varying densities, the energy density functional (19) does not contain the local scale transformation function (21) which essentially facilitates the calculations.

Figure 2 shows the mass distribution $\rho(r)$ calculated with $\tau^{(GTF)}$, when the proton and neutron densities are considered as proportional. The mass distribution of ^{40}Ca calculated with nonproportional densities is given in Fig.3. Sick's results /16/ for comparison are drawn as well.

The derivative of the distributions near the surface and the asymptotic behaviour compared with EDF densities are shown in Figs.4 and 5, respectively.

Table 1 contains r.m.s. of charge distributions, half-radius and diffuseness parameter. The separation energy values and the relevant experimental data are listed in Table 2. EDF results /3/ are given, as well.

7. In conclusion we mention that the results obtained in the present paper are indicative in two aspects. Firstly, it is seen, that the LSTM can be successfully used for finding the explicit energy density functionals. Secondly, the functional (19)-(21) constructed here, although derived from a rather non-realistic model density matrix (7) by means of LSTM, proves to be quite reasonable for the reproduction of the bulk characteristics of the nuclei.

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Table 1

Charge r.m.s. radii, half-radius and surface diffuseness parameters (in fm). The experimental values are taken from [16]

Nuclei	Charge r.m.s.			Half-radius			Diffuseness parameter		
	EXP	GTF	AGTF	EXP	GTF	AGTF	EXP	GTF	AGTF
C^{12}	2,49	2,64	2,67	2,214	2,17	2,12	0,488	0,498	0,507
O^{16}	2,71	2,73	2,77	2,526	2,45	2,40	0,497	0,505	0,518
Si^{28}	3,10	3,11	3,15	3,085	3,08	3,01	0,563	0,537	0,565
Ca^{40}	3,482	3,41	3,44	3,556	3,55	3,45	0,478	0,534	0,568
Ca^{48}	3,52	3,57	3,61	3,74	4,06	3,71	0,520	0,554	0,599
Zn^{66}	3,951	3,92	3,97	4,2	4,32	4,22	0,663	0,554	0,610
Zr^{90}	4,244	4,31	4,37	-	4,86	4,74	-	0,560	0,635
Ce^{140}	-	4,90	4,96	-	5,74	5,61	-	0,553	0,636
Pb^{208}	5,51	5,53	5,58	6,557	6,64	6,51	0,515	0,543	0,634

Table 2

Proton and neutron separation energies in nuclei

Nuclei	protons /Mev/			neutrons /Mev/		
	EXP	GTF	EDF	EXP	GTF	EDF
He^4	17,255	17,62	-	18,899	18,28	-
C^{12}	15,96	14,74	-	18,72	15,94	-
O^{16}	12,13	13,85	7,2	15,67	15,72	10,9
Ca^{40}	8,33	11,55	4,4	15,63	15,51	11,9
Ca^{48}	15,81	18,25	12,6	9,95	9,76	6,0

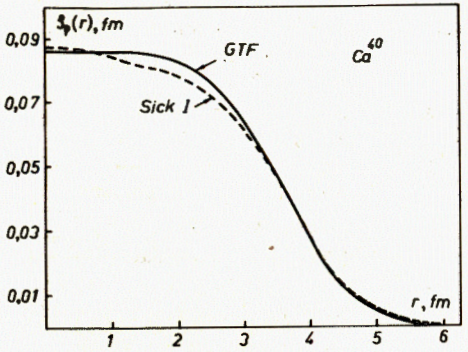

Fig.3. Proton density distributions in ^{40}Ca. The empirical distribution is from Refs. [16].

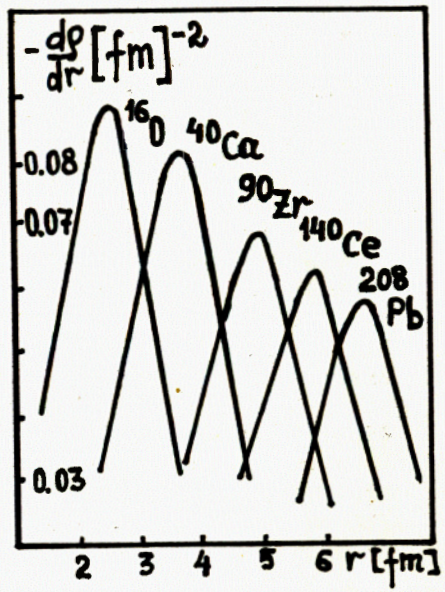

Fig.4. The derivative of the distributions given in Fig.2.

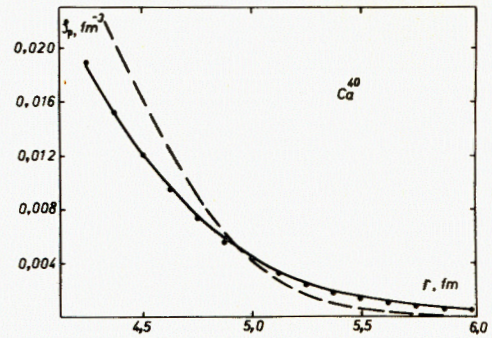

Fig.5. The asymptotic behavious of the ^{40}Ca proton distribution, compared with HF [8,9] and EDF [3] results.

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Петков И.Ж., Стойцов М.В. E4-83-282

Связь метода локально-масштабного преобразования с формализмом плотности энергии

Получено выражение для функционала плотности энергии. Для вывода использован метод локально-масштабного преобразования, применяемый к модельной одночастичной дираковской матрице плотности. Для описания ядерной системы выбран гамильтониан Скирма. В полученном выражении для плотности кинетической энергии выделяется член, известный как поправка Вайцзекера, а также член, который при медленно меняющихся плотностях переходит в томас-фермиевское выражение для кинетической энергии. Уравнение для плотности нуклонов ядра решается методом стержневых сплайнов. Приведены расчеты распределений плотности нуклонов и среднеквадратичных радиусов зарядовых распределений для ядер ^{12}C, ^{16}O, ^{32}S, ^{40}Ca, ^{48}Ca, ^{66}Zn, ^{90}Zr, ^{140}Ce, ^{208}Pb. Из результатов следует, что метод локально-масштабного преобразования можно успешно использовать для отыскания явного вида функционала плотности энергии. Построенный функционал плотности энергии хотя и выведен из нереалистической модельной матрицы плотности, удовлетворительно описывает объемные ядерные характеристики.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1983

Petkov I.Zh., Stoitsov M.V. E4-83-282

A Relation between the Local Scale Transformation Approach and the Nuclear Energy Density Formalism

An expression for the energy density functional is obtained. Local scale transformation method is applied to the one-particle Dirac density matrix of a particular form. A nuclear A-particle system is described by the Hamiltonian with Slyrme´s forces. An additional term, widely known as Weizsecker´s kinetic energy correction, appears as well as the term that is transformed into the Thomas-Fermi kinetic energy expression for slowly varying local density. The equation for the local density distribution is resolved by applying the Core-spline method. Numerical calculations of the density distributions and rms of charge distributions are carried out for ^{12}C, ^{16}O, ^{32}S, ^{40}Ca, ^{48}Ca, ^{66}Zn, ^{90}Zr, ^{140}Ce, and ^{208}Pb. It is seen from the results, that the local scale transformation method can be successfully used for finding the explicit form of the energy density functional. The constructed functional, although derived from a nonrealistic model density matrix proves to be quite reasonable for the reproduction of the bulk nuclear characteristics.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1983