СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА

E4 - 9456

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ENERGY DENSITY FORMALISM CALCULATIONS WITH FERMI-TYPE DISTRIBUTION OF THE NUCLEONS

1976

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1. INTRODUCTION

It was demonstrated in a number of works [1-3] that the energy density formalism /EDF/ yields satisfactory results for the basic bulk properties of nuclei. Recently the EDF was applied to the determination of the ion-ion interaction in the sudden collision approximation and the study of nuclear properties away from the stability line. The methods developed in [1-3] give numerical solution for the nuclear density distribution through a system of differential equations. For lack of an analytic expression for the density distribution one faces certain difficulties and is practically involved in time- consuming computations. Furthermore Hartree-Fock calculations and experiments on electron scattering on nuclei favour Fermi type distribution of the nucleons. We, naturally, come to the question whether it is possible to make the EDF compatible with the well known Fermi density distribution ρ_F, the latter is in good agreement with the experimental data. The present work gives a positive answer to that problem.

A short survey of the EDF and a formulation of the problem are carried out in section 2. The method of the determination of the basic coefficients that enter the energy functional is given in section 3. The obtained numerical results about the binding energies and the equilibrium parameters of the symmetrized Fermi density distribution of a wide range of nuclei are presented and discussed in section 4.

2. THE ENERGY DENSITY

According to Kohn and coworkers' theorem[4] the ground state energy of a system of Fermi particles can be written as a functional of the local density.

$$E = \int \mathcal{E}(\rho)\, d\tau \,. \qquad (1)$$

Furthermore the expression for E is stationary with respect to variations of the density ρ. $\mathcal{E}(\rho)$ has been specified in[1]:

$$\mathcal{E}(\rho) = 0.3\frac{h^2}{M}\left(\frac{3}{2}\pi^2\right)^{2/3}\left(1-\frac{1}{A}\right)\frac{1}{2}\left[(1+\alpha)^{5/3}+\right.$$

$$\left.+(1-\alpha)^{5/3}\right]\rho^{5/3} + \rho V(\rho,\alpha) + \frac{1}{2}e\rho_p\Phi_c -$$

$$-0.7386\, e^2 \rho_p^{4/3} + \frac{h^2\eta}{8M}(1-k\alpha^2)(\nabla\rho)^2 + \frac{h^2}{72M}\frac{(\nabla\rho)^2}{\rho}\,, \qquad (2)$$

where

$$V(\rho,\alpha) = b_1(1+a_1\alpha^2)\rho + b_2(1+a_2\alpha^2)\rho^{4/3} + b_3(1+a_3\alpha^2)\rho^{5/3}, \qquad (3)$$

and

$$\rho = \rho_n + \rho_p\,,\ \int\rho_n\, d\tau = N\,,\ \int\rho_p\, d\tau = Z\,,\ \alpha = \frac{\rho_n - \rho_p}{\rho}\,,$$

$\rho_{n,p}$ are the neutron and proton distributions, respectively, and the Coulomb potential generated by ρ_p in (2) and (3). The choice of the basic coefficients b_i and a_i in (3) depends on the nuclear matter saturation properties, the latter being determined by the particular type of nucleon-nucleon interaction. Obviously, the b_i and a_i values deduced on the basis of nuclear matter calculations by Brueckner et al.[1,2], contain an amount of uncertainties. So it is quite reasonable to determine the b_i and a_i coefficients by comparison of bulk properties calculations about definite nuclei of known nucleon distribution with the experimental data.

For the purpose it is necessary to minimize the functional (1) with respect to the parameters R and b of the symmetrized Fermi distribution[5]

$$\rho_F(r) = \rho_0\left(\frac{1}{1+e^{\frac{r-R}{b}}} + \frac{1}{1+e^{\frac{-r-R}{b}}} - 1\right), \qquad (4)$$

where

$$\int\rho\, d\tau = A\,.$$

The b_i coefficients are the consequent solutions of the following system of linear algebraic equations:

$$E = E_{exp}\,,$$

$$\frac{\partial E}{\partial R} = 0\,, \qquad (5)$$

$$\frac{\partial E}{\partial b} = 0\,,$$

R and b which enter (5) are the experimentally deduced parameters of the density distribution[5].

The a_i coefficients are determined through an analogous to (5) system for the $\alpha \neq 0$ case. The analysis of the solutions to the above mentioned system for certain selected nuclei gives the optimal set of basic coefficients b_i and a_i. Thus, the functional density (2) is fully determined and it becomes possible to look for the binding energy and the equilibrium parameters of the density distribution for any given nucleus.

3. PARAMETER SEARCH AND APPROXIMATIONS

A simplifying assumption about the proportionality between the neutron and proton density distributions is employed in the present work. The coefficients are found by means of (5) in the case of ^{40}Ca for which $\alpha = 0$. The

obtained sets of b_i values are used in search for the binding energy and equilibrium density parameters of ^{16}O. The following set of values: $b_1 = -787.7$, $b_2 = 1337$, $b_3 = -627.1$ is in the best agreement with the experimentally found values of the binding energies, half-value radii and diffuseness parameters of ^{16}O and ^{40}Ca. These results are obtained using a value of η equal to 13 ($k = 2.15$) the surface correction term in (2) which agrees with the estimates of /1-3/.

The Coulomb energy entering (1) is calculated by the following approximate formula/6/ :

$$E_{Coul} = \frac{3}{5}\frac{(Ze)^2}{R_c}\left[1 + 18.03\left(\frac{b}{R}\right)^3 - \frac{7}{8}\pi^4\left(\frac{b}{R}\right)^4\right] -$$

$$-3\left(\frac{3}{16\pi}\right)^{2/3}\frac{e^2 Z^{4/3}}{R_c}\left[1 - 1.336\frac{b}{R} + 7.127\left(\frac{b}{R}\right)^2 -\right.$$

$$\left. -18.21\left(\frac{b}{R}\right)^3 + 83.406\left(\frac{b}{R}\right)^4\right], \qquad (6)$$

where

$$R_c = R\left[1 + \frac{7}{6}\pi^2\left(\frac{b}{R}\right)^2 - \frac{49}{72}\pi^4\left(\frac{b}{R}\right)^4\right] \qquad (7)$$

and R, b are the parameters of the symmetrized Fermi density distribution.

The determination of the binding energy, in such a way, leads to a minimization of the functional (2) with respect to the two parameters R and b. It is interesting to juxtapose the saturation curve for $\alpha = 0$ corresponding to the set of values found in the present paper and the respective result given by Brueckner et al./2/. This juxtaposition is clearly seen in *Fig. 1* where our saturation curve yields greater value of the binding energy per nuclei (≈ -18.8 *MeV*) and greater value of the equilibrium Fermi momentum ($\approx 1.54\ F^{-1}$ or $\rho_0 \approx 0.24\ F^{-3}$). The stiffness parameter deduced here is of the order of magnitude of 280 which differs substantially from the result of Brueckner et al./1/ but is very close to the estimate of Myers and Swiatecki/7/.

The method of determination of the α_i set of values is analogous to that employed in the b_i case. The unproportionality between the proton and neutron density distributions is effectively taken into account through a modification of R_c ($R_c \to 0.92\,R_c$) in the expression for the Coulomb energy (6). Naturally one should expect better results when considering this unproportionality in a more precise manner. The following α_i values are obtained: $\alpha_1 = 0.3118$, $\alpha_2 = 0.377$, $\alpha_3 = -0.8297$.

4. *RESULTS AND DISCUSSION*

The functional (2) specified according to section 2 is made use of in computing the values of the binding energies and density distribution parameters for a number of nuclei. *Table 1* gives the binding energies for spherical nuclei from ^{16}O to ^{208}Pb. One can see that the difference between the experimental and theoretical values is not greater than 0.1 *MeV* per nucleon for all nuclei under consideration with the exception of ^{16}O where the error amounts to 0.5 *MeV* per nucleon. *Table 2* gives the results about the binding energies of nuclei where the number of protons and neutrons differs from the magic numbers. The agreement with the experiment is again within the same bounds. There is a certain discrepancy in ^{12}C and ^{238}U where the inclusion of deformation effects seems essential. The values of the half-radii, rms radii, diffuseness parameters for the considered nuclei are reported in *Table 3*. It is clear that the half-radii are in good agreement with experiment, while we get systematically lower values of about 15% on the average for the diffuseness parameter. This difference can be attributed to factors of a different origin. On the one hand, that is the Thomas-Fermi approximation for the kinetic energy and the character of the surface correction term which influences strongly the resulting value of the diffuseness parameter. On the other hand, it can be the type of a two parameter Fermi density distribution employed in the present paper.

Table 1

Experimental and present results for the binding energies of some spherical nuclei.

Nucleus	Experiment	Present work
^{16}O	127.6	120.4
^{40}Ca	342.1	342.2
^{48}Ca	416.0	413.8
^{56}Ni	484.0	487.4
^{90}Zr	783.9	787.3
^{116}Sn	988.7	996.6
^{140}Ce	1172.7	1175.0
^{208}Pb	1636.6	1618.0

Table 2

The same as Table 1. The nuclei are not necessarily spherical.

Nucleus	Experiment	Present work
^{12}C	92.2	85.3
^{24}Mg	198.3	193.4
^{28}Si	236.5	230.6
^{32}S	271.8	267.9
^{56}Fe	492.3	489.6
^{58}Ni	506.5	501.5
^{60}Ni	526.9	524.8
^{66}Zn	578.2	580.4
^{238}U	1801.7	1731.2

Table 3

Half-value and rms radii, and surface diffuseness parameters in F. Experimental values are taken from Rfs. /1,2/

Nucleus	Half-radius		Rms radius		Diff.parameter	
	Exp.	Pres.work	Exp.	Pres.work	Exp.	Pres.work
^{12}C	2.214	2.5	2.496	2.487	0.488	0.42
^{16}O	2.562	2.7	2.71	2.65	0.497	0.44
^{24}Mg	2.934	3.05	3.105	2.92	0.569	0.46
^{28}Si	3.085	3.2	3.175	3.01	0.563	0.46
^{32}S	3.255	3.35	3.37	3.11	0.6	0.46
^{40}Ca	3.556	3.6	3.493	3.29	0.578	0.47
^{48}Ca	3.74	3.91	3.49	3.496	0.52	0.48
^{56}Fe	4.054	4.01	3.853	3.582	0.6	0.48
^{56}Ni		4.0		3.58		0.48
^{58}Ni	4.153	4.07	3.844	3.604	0.566	0.47
^{60}Ni		4.11	3.82	3.649		0.48
^{66}Zn	4.2	4.28	4.081	3.747	0.663	0.48
^{90}Zr		4.76	4.265	4.096		0.48
^{116}Sn	5.486	5.21	4.55	4.443	0.56	0.5
^{140}Ce		5.67		4.741		0.49
^{208}Pb	6.557	6.63	5.427	5.449	0.515	0.49
^{238}U		6.8		5.573		0.49

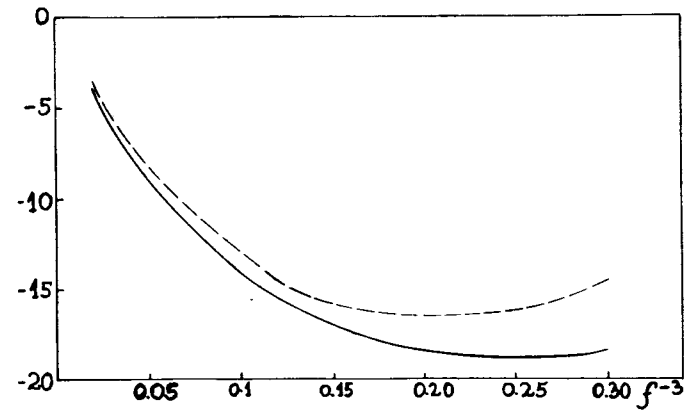

Fig. 1. Nuclear matter saturation curves for $\alpha = 0$ *. Full line corresponds to our results. Dashed line is the result of Brueckner et al.*/2/.

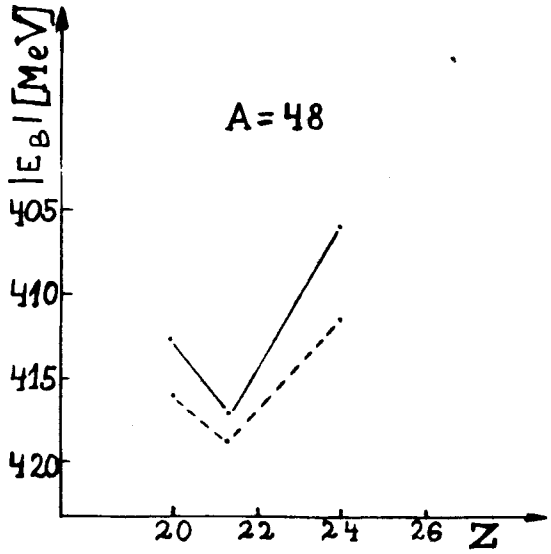

Fig. 2. Binding energies for the isobare A = 48. Full line corresponds to our results. Dashed line is the experimental sequence.

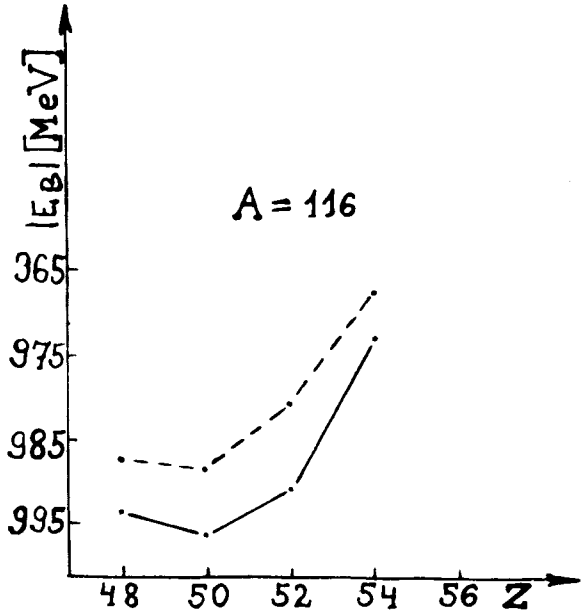

Fig. 3. The same as Fig. 1 for A = 116.

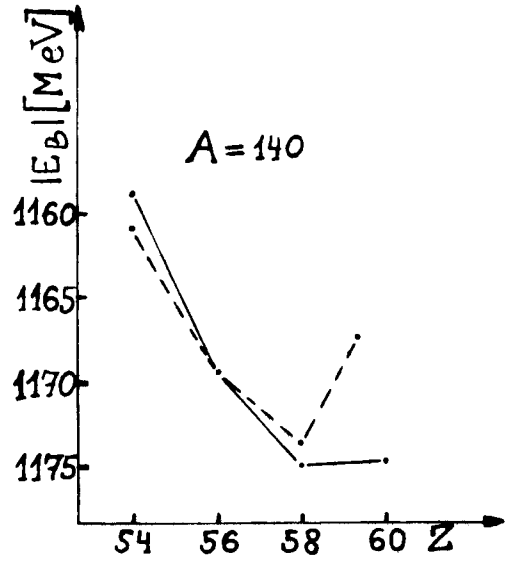

Fig. 4. The same as Fig. 1 for A = 140.

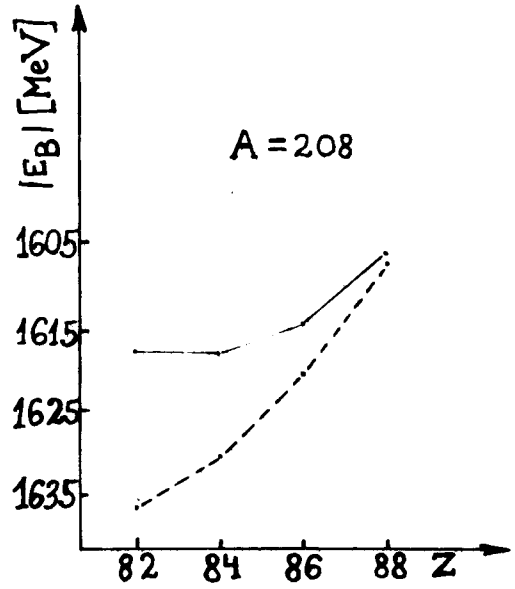

Fig. 5. The same as Fig. 1 for A = 208.

Figs. 2-5 show the binding energies of nuclei for A = 48, 116, 140, 208 isobare sequences. The position of the minimum of the symmetry energy comes out at the right value of a.

The results obtained in the present paper show that the proposed procedure, rather simple and convenient for practical computation, may prove suitable in the determination of the ion-ion interaction, and in different applications where realistic symmetrized Fermi type distribution should be employed.

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Received by Publishing Department on January 14, 1976.