STATISTICAL MODEL OF A NUCLEUS INCLUDING CORRELATIONS

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The constants appearing in the Weizsäcker formula for the binding energy of an atomic nucleus are calculated. To account for correlations the gas approximation with a changed dispersion law of nucleons, whose applicability was demonstrated in ^[2], is used. Inhomogeneity effects are taken into account in the Thomas-Fermi approximation (heavy nuclei). Agreement with the empirical values of the coefficients is achieved.

1. One can assume as established that the properties of nuclear matter are satisfactorily described through a pair interaction potential between the nucleons, which is derived from nucleon scattering experiments (cf., for example, [1,2]). Therefore the application of methods worked out in the theory of nuclear matter to the description of the fundamental properties of real nuclei is of definite interest.

Attempts to obtain integral characteristics of nuclei, starting only with a given pair potential, have already been carried out earlier [3-6]. We have in mind, in particular, the works of Gombás and co-workers [3], where the Thomas-Fermi model is used. However for agreement with experimental data a pair potential inconsistent with experiments on nucleon scattering had to be introduced in this connection. The application of the Bruckner method to the description of the properties of heavy nuclei makes the mathematical apparatus even more inconvenient. Only preliminary evaluations have been performed so far in this direction [5,6].

To account for the dynamical correlation effects, which play an essential role for realistic interaction potentials, a method proposed in a previous paper by the authors ^[2] is used in the present work. The essence of this method consists of the following. The pair interaction potential of the nucleons is split into a sum of two potentials. For one of them (the attractive one) which has a large range of action a (the parameter k_0a is $\gg 1$, where k_0 is the Fermi momentum) we assume the Hartree-Fock approximation. To the other one ('fhard core'') we apply the gas approximation (the parameter k_0c is $\ll 1$, where c is the radius of the 'fhard core''). The interference between these two potentials leads to a change

in the dispersion law of colliding nucleons at the expense of the self-consistent potential of the forces of attraction, as was shown in $[2].^{1)}$

In contradistinction to the case of uniform nuclear matter, in our case it is necessary to take the effects of nonuniformity into account. In general the kinetic energy of the system is some functional of the particle number distribution of the system $E_{kin} = E_{kin} \{p(\mathbf{r})\}^{2}$ This functional can often be expressed in the form of an expansion in the derivatives of the function ρ^{3} :

 $E_{\mathbf{kin}} = \int d\mathbf{r} f_0(\rho(r)) + \int d\mathbf{r} f_1(\rho(r)) (\nabla \rho(r))^2 + \ldots$

Here the functions f_0 , f_1 , etc contain the density values at the considered point \mathbf{r} only.

Let us further introduce the quantity $k_0(r) = (3\pi^2\rho(r)/2)^{1/3}$; in the uniform case it coincides with the limiting momentum k_0 while in the nonuniform case it coincides with limiting momentum of the usual Thomas-Fermi method, if the correlation interaction is not taken into account there. In the general case $k_0(r)$ is the limiting momentum of the motion in some effective field including the correlation effects.

We must emphasize that these statements are only true in the case that the ratio of the second term in the expansion of E_{kin} to the first one is

¹⁾Strictly speaking, the applicability of the method considered was demonstrated only for uniform nuclear matter. In the case of a realistic nucleus, whose density distribution has the shape displayed in Fig. 1, this proof is applicable as before to the central part of the nucleus. As to its surface, the estimates given in ^[2] warrant the applicability of the method even there, except for an inessential region of very small density.

 $^{^{\}mbox{2}}$ The expressions for the remaining parts of the energy are given below.

³We consider a spherically symmetrical system.

small. An estimate of this ratio from simple dimensional arguments gives the quantity $(\nabla \rho)^2 / \rho^{8/3}$. Introducing the wavelength $\lambda(\mathbf{r}) \sim 1/k_0(\mathbf{r})$ of a particle moving in the effective field mentioned above the ratio considered takes the form

$$(d\lambda / dr)^2 \sim 1 / k_0^2 r_0^2$$

where r_0 is the distance over which k_0 changes by a noticeable amount.

Thus, if $d\lambda/dr \ll 1$, i.e., the wavelength varies little over distances of the order of a wavelength itself (this corresponds to a quasiclassical character of the motion of the particle in the effective field), then the second term in the expansion of E_{kin} can be neglected. By the same token one can use the expression for the energy of a uniform system with the constant k_0 replaced by the function $k_0(r)$.

The empirical results concerning the function $\rho(\mathbf{r})$ in the nucleus show that the nucleus can be divided into two parts. In the central part of the nucleus the density distribution varies noticeably over distances of the order of the nuclear radius, i.e., ~ $aA^{1/3}$, where a is the range of the forces. In this region $(d\lambda/dr)^2 \sim A^{-2/3}/k_0^2a^2 \sim A^{-2/3}$, since $k_0 \sim a^{-1}$. In the surface region of the nucleus $r_0 \sim a$ and therefore $(d\lambda/dr)^2 \sim 1$.

Thus for sufficiently heavy nuclei the quantity $(dt/dr)^2$ is small in the central part of the nucleus and of order unity on the surface. The effective contribution of the second term in the expansion of E_{kin} is therefore of order $A^{-1/3}$. We have to remark that the numerical coefficient in the corresponding expression turns out to be very small, which in general allows us to discard the correction considered.⁴⁾ The same applies also to the quantity E_c [cf. (7) below].

The determination of the function $\rho(\mathbf{r})$ [and $k_0(\mathbf{r})$] and also the value of the system energy can be most simply effected using a variational principle, i.e., requiring a minimum of the energy relative to a change of $\rho(\mathbf{r})$. We use below a direct variational method, in which we essentially substitute into the expression for the energy trial functions ρ that depend on some parameters, and then minimize with respect to these parameters.

These trial functions are chosen of the following form:

$$\begin{aligned} \rho_{(p, n)}(r) &= \rho_{0}(p, n) \Big| \begin{cases} 1, & r < R - d/2 \\ (R + d/2 - r)/d, & R - d/2 < r < R + d/2 \end{cases} \end{aligned}$$
(1)

⁴⁾The expression for this correction (called the quantum correction) has the form $(\hbar^2/72M) \int dr (\nabla \rho)^2 / \rho$. The coefficient in the well known Weizsäcker formula, as will be shown, is too large by a factor of nine^[7].

The indices p and n correspond respectively to the proton and neutron distributions. It follows from the normalization conditions

$$\int d\mathbf{r} \,\rho_{(p)}(r) = Z, \qquad \int d\mathbf{r} \,\rho_{(n)}(r) = A - Z$$

(Z is the charge of the nucleus) that the nuclear radius R is determined by the relations $\label{eq:radius}$

$$R \approx (9\pi A)^{1/3} / 2k_0 \tag{2}$$

and

$$\rho_{0(p)} \approx \rho_{0}(1-\varepsilon), \qquad \rho_{0(n)} \approx \rho_{0}(1+\varepsilon), \qquad (3)$$

where $\epsilon = (A - 2Z)/A$. Here and below it is assumed that the width of the surface layer d is small compared to the nuclear radius (cf. the figure). The quantity k_0 entering into (2) is $k_0 = (3\pi^2\rho_0)^{1/3}$.



The trial function (1) thus contains three variational parameters (for given mass number A). In the first place there is the nuclear radius R (or the limiting momentum k_0 in the core of the nucleus). Second, there is the parameter ϵ determining the relative excess of neutrons. Third and last is the width of the surface layer d.

The variation of the energy with respect to these parameters can, naturally, give only a relative minimum. The reason for this is that we are considering a comparatively narrow class of trial functions, albeit in agreement with the experimental data on the shape of the nucleus. Therefore the energy value obtained below turns out to be somewhat exaggerated.

The use of a wider class of functions would lead to a considerable complication of the calculations. Therefore we limit ourselves to the statement of qualitative expressions, corresponding to the use of the chosen class of trial functions. Moreover we can point to the results of the numerical calculations of Gombás^[3] and Cameron^[8], who investigated convergent problems and obtained an almost uniform density distribution.

We mention in this connection two factors contributing to the relative uniformity of the density distribution in the core of the nucleus. On the one hand, the different forces create opposite tendencies in the particle distribution: the Coulomb and repulsive forces tend to create an excess density at the surface of the nucleus, while at the same time the attractive forces lead to a concentration of matter in the center. On the other hand, the sharp density dependence of the repulsive forces that make a positive contribution to the energy plays an important role. Therefore a noticeable deviation of the particle distribution from the uniform one proves to be energetically unfavored. It is precisely for this latter reason that Cameron (cf. above) obtained a practically uniform particle distribution in the neutron gas.

In view of the fact that the direct variational method leads to too high a value for the energy it is necessary to dwell especially on the problem of the stability of the nucleus against its collapse to a point. The situation is in that sense more favorable in the theory of a realistic nucleus than in the theory of nuclear matter, since the additional terms in the energy, corresponding to the Coulomb interaction, symmetry energy, and surface effects give according to their physical meaning a positive contribution. Therefore as soon as the stability of nuclear matter is established the stability of a realistic nucleus follows automatically from it.

Variation of the expression for the energy yields a relation which agrees in form with the semiempirical Weizsäcker formula.⁵⁾ Therefore the comparison of the results obtained here with experiment causes no difficulty and indicates a sufficiently good agreement (at least with a 20 per cent accuracy). Thus the model in which an empirical nucleon pair interaction is used can describe a whole series of characteristics of a realistic atomic nucleus in the ground state. This circumstance apparently indicates that the role of many-body forces in nuclear matter is not as large as could be concluded from general arguments.

2. We choose the same nuclear pair interaction potential as in [2]:

$$v(r) = v_{c}(r) + v_{a}(r)\hat{S};$$

$$v_{c} = \infty \text{ for } r < c, \quad v_{c} = 0 \text{ for } r > c;$$

$$v_{a} = -V_{0} \text{ for } c < r < a, \quad v_{a} = 0 \text{ for } r < c, r > a;$$

$$c = 0.4 \text{ F}, \quad a = 2.3 \text{ F}, \quad V_{0} = \pi^{2}/4M (a - c)^{2};$$

Ŝ is the Serber exchange operator.

In the approximation considered the total energy of the nucleus can be written down in the form of a sum:

$$E = E_{\rm kin} + E_a + E_c + E_{\rm Coul}.$$
 (4)

Here the kinetic energy of the nucleons has the form $(k_{0(p,n)}(r) = (3\pi^2 \rho_{(p,n)}(r))^{1/3})$

$$E_{\rm kin} = \frac{1}{20\pi^2 M} \int d\mathbf{r} \; (k_0^5_{(p)}(r) + k_0^5_{(n)}(r)). \tag{5}$$

In the Hartree-Fock approximation the energy corresponding to the attractive potential $\ensuremath{v_a}$ has the form

$$E_{a} = \frac{1}{8} \int d\mathbf{r}_{1} d\mathbf{r}_{2} v_{a} (r_{12}) \{ \rho_{(p)} (r_{1}) \rho_{(p)} (r_{2}) + \rho_{(n)} (r_{1}) \rho_{(n)} (r_{2}) \\ + 4\rho_{(p)} (r_{1}) \rho_{(n)} (r_{2}) \} + \frac{1}{2 (2\pi)^{6}} \int d\mathbf{r}_{1} d\mathbf{r}_{2} v_{a} (r_{12}) \\ \times \left\{ \int_{1}^{1} d\mathbf{p}_{1} d\mathbf{p}_{2} + \int_{11}^{1} d\mathbf{p}_{1} d\mathbf{p}_{2} + 4 \int_{111}^{1} d\mathbf{p}_{1} d\mathbf{p}_{2} \right\} \\ \times \exp \left[i (\mathbf{p}_{1} - \mathbf{p}_{2}) \mathbf{r}_{12} \right],$$
(6)

where the integration regions I, II, and III are defined respectively by the inequalities

$$p_{1,2} < k_{0(p)}(r_{1}); \qquad p_{1,2} < k_{0(n)}(r_{1});$$

$$p_{1} < k_{0(p)}(r_{1}), \quad p_{2} < k_{0(n)}(r_{2}). \tag{6'}$$

The correlation energy E_c is calculated in the gas approximation taking the changed nucleon dispersion law into account and has the form (cf. [2]):

$$E_{c} = \frac{4\pi c}{(2\pi)^{n}} \int \frac{d\mathbf{r}}{M^{*}(r)} \left\{ \int_{\mathbf{l}} d\mathbf{p}_{1} d\mathbf{p}_{2} + \int_{\mathbf{1I}} d\mathbf{p}_{1} d\mathbf{p}_{2} + 4 \int_{\mathbf{1II}} d\mathbf{p}_{1} d\mathbf{p}_{2} \right\} + \frac{2c^{2}}{3\pi^{2}M} \int d\mathbf{r} \left\{ \frac{6(11-2\ln 2)}{35\pi^{2}} \left(\frac{M}{M^{*}(r)} \right)^{2} \left(\frac{M_{0}(r)}{M} \right) k_{0}^{7}(r) + 0.13c \left(\frac{M}{M^{*}(r)} \right)^{3} \left(\frac{M_{0}(r)}{M} \right)^{2} k_{0}^{8}(r) + \frac{c}{2\pi} k_{0}^{8}(r) \right\}.$$
(7)

Here the integration regions I, II, and III are defined by (6'), where one only has to replace r_1 and r_2 by r; $k_0(r) = [3\pi^2(\rho_{(p)} + \rho_{(n)})/2]^{1/3}$; $M^*(r)$ and $M_0(r)$ are effective masses, which in contradistinction to the corresponding quantities in ^[2] depend on the coordinates of r. In the derivation of this formula we did not consider the dependence of the effective masses on the difference between the densities $\rho_{(p)}$ and $\rho_{(n)}$. Moreover we neglected this difference in the terms of second and third order in c. The contribution of the terms not accounted for here is very small.

The expression for the Coulomb energy will be given below for a specific function $\rho(\mathbf{r})$.

3. Substituting the trial function (1) into the expression for the energy (4) we can represent the latter in the form of an explicit function of the variational parameters k_0 , d, and ϵ . Here we neglect from the very beginning terms giving a contribution of the order of $(a/R)^2 \sim A^{-2/3}$, which is equivalent to considering heavy nuclei. Assuming that the thickness of the surface layer is d ~ a (this will be verified by the calculation), we also omit terms of the order of $(d/R)^2$. Furthermore the quantity ϵ , in which an expansion to second

⁵⁾The pairing effect, which requires different methods for its description, is of course, not taken into account here.

order inclusively will be carried out, turns out to be comparatively small. Terms giving a contribution of the order of $\epsilon^2(a/R)$ as well as the mentioned interference of surface effects and the symmetry effect will likewise not be taken into account.

In the calculation of the integrals in (7) we replace the functions $M^{*}(r)$ and $M_{0}(r)$ on the surface layer by the constants M_1^* and M_{01} , which are defined in the same way as in [2] but are referred to the density $\rho = \rho_0/2$. This replacement does not lead to a significant error, since M* and M_0 depend very weakly on r. Numerically M_{10}/M = 1.47, $M_1^*/M = 1.3$ (with the equilibrium value of the parameter k_0).

As the result of easy but lengthy calculations one obtains for the energy per nucleon the expression

$$\frac{E}{A} = U_{\text{vol}} + \varepsilon^2 U_{\text{sym}} + \frac{Z^2}{A^{4/3}} U_{\text{Coul}} + \frac{U_{\text{surf}}}{A^{1/3}}, \quad (8)$$

coinciding in form with the Weizsäcker formula without the correction for the pairing energy.

In formula (8) the expression for the volume energy $\,U_{vol}\,$ coincides with the one obtained in $^{[2]}$ for the case of nuclear matter. The second term in (8) corresponds to the symmetry energy due to deviation in the proton and neutron numbers from the mean (it vanishes for Z = A/2). For U_{sym} one obtains the expression

$$U_{\rm sym} = \frac{k_0^2}{6M} \left[1 - \frac{2}{\pi} \gamma \frac{M}{M^*} + \frac{\pi \xi^2}{12 \, (\xi - \gamma)^2} \left(1 + \frac{6}{\xi^2} + \frac{3 \sin 2\xi}{2\xi^3} \right) \right]. \tag{9}$$

Here we dropped the correlation correction of second order in γ , which is equal to

$$-\frac{4}{9}\frac{k_0^2}{M}\gamma^2\frac{2\ln 2-1}{\pi^2}\left(\frac{M}{M^*}\right)^2\frac{M_0}{M}\approx-0.5\,\mathrm{MeV}.$$

Here and below $\gamma = k_0 c$, $\xi = k_0 a$, and M* is the effective mass for $\rho = \rho_0$.

The expression for the Coulomb energy is calculated with sufficient accuracy from the model of a uniformly charged sphere

$$U_{\text{Coul}} = \frac{2e^2k_0}{5} \left(\frac{3}{\pi}\right)^{1/3}.$$
 (10)

Finally for the surface term U_{surf} we obtain the expression

$$U_{\text{surf}} = 2.95 \ \alpha + \beta + (1.3 \ \alpha + \beta) \ y + 0.45 \ \alpha \ y^2 + o(y^3).$$
(11)

We introduced here the notation

$$y = \frac{d}{a} - 1, \qquad \alpha = \frac{k_0^2}{M} \left(\frac{3}{\pi}\right)^{1/3} \frac{\pi \xi^4}{144 (\xi - \gamma)^2},$$
$$\beta = \frac{k_0^2}{M} \left(\frac{3}{\pi}\right)^{1/3} \left\{\frac{9\pi}{32 (\xi - \gamma)^2} \left[\frac{2}{\xi^2} + \frac{2}{5} + \frac{4}{\xi^2} \cos 2\xi\right]\right\}$$

$$+ \left(\frac{1}{\xi} - \frac{7}{\xi^3}\right)\sin 2\xi \Big] - \frac{3}{40}\xi - \frac{\gamma\xi}{\pi} \Big[\frac{M}{M^*} - \frac{2}{3}\frac{M}{M_1^*}\Big] \\ - \gamma^2\xi \frac{6(11 - 2\ln 2)}{35\pi^2} \Big[\Big(\frac{M}{M^*}\Big)^2\frac{M_0}{M} - \frac{3}{5}\Big(\frac{M}{M_1^*}\Big)^2\Big(\frac{M_{10}}{M}\Big)\Big] \\ - \gamma^3\xi \Big[0.13\Big(\Big(\frac{M}{M^*}\Big)^3\Big(\frac{M_0}{M}\Big)^2 - \frac{6}{11}\Big(\frac{M}{M_1^*}\Big)\Big(\frac{M_{10}}{M}\Big)^2\Big) + \frac{5}{22\pi}\Big]\Big\}.$$

It is assumed that y < 1; this permits us to limit ourselves to the terms written down in (11). For the equilibrium value of k_0 we have $\alpha \approx 27$ MeV and $\beta \approx -50$ MeV.

4. We proceed to the variation of the expression obtained for the energy. We begin with the variation with respect to k_0 . In the previous paper ^[2], where an analogous procedure was carried out for the first term of formula (8), the equilibrium value of k_0 equal to $k_{00} = 1.4 \text{ F}^{-1}$ was found. Writing the equilibrium value of k_0 for a realistic nucleus in the form

$$k_0 = k_{00} + \delta k_0,$$

it is easy to see that δk_0 can be put into the form of a sum⁶) $\delta_1 \epsilon^2 + \delta_2 A^{-1/3}$, where δ_1 and δ_2 are certain coefficients. Substituting the expression obtained into (8), expanding it in powers of ϵ^2 and $A^{-1/3}$, and allowing for the minimum condition $\partial U_{vol} / \partial k_1 \Big|_{k_{00}} = 0$ we verify that within the accuracy limits taken we can put

$$k_0 = k_{00} = 1.4 \,\mathrm{F}^{-1}$$
. (12)

The equilibrium value of k_0 is thus determined by the first term of formula (8) alone. The value of the nuclear radius corresponding to (12) [cf. (2)] turns out to be equal to $1.1 A^{1/3} F$, which almost coincides with the experimental value.

Only the quantity U_{surf} depends on the parameter d. Its variation with respect to y = d/a - 1gives

$$U_{\rm surf} \approx 23$$
 MeV, $y = 0.6$. (13)

The thickness of the surface layer is defined as the distance over which the nucleon density drops from 90 to 10% of its value at the center. For y = 0.6 the thickness of the surface layer turns out to equal to roughly 3 F (the experimental value is 2.4 F).

The symmetry energy U_{sym} can be gotten directly from the relation (9). One obtains for it the value of $U_{svm} \approx 33$ MeV. The variation with respect to the parameter ϵ is easily carried out if one expresses the factor Z^2 in the Coulomb energy

⁶In this analysis we do not take into account Coulomb effects, whose contribution turns out to be very small.

through ϵ . As the result one obtains the following equilibrium value:

$$\frac{Z}{A} = 2\left(4 + \frac{U_{\rm Coul}}{U_{\rm sym}}A^{2/3}\right)^{-1}.$$
 (14)

Using the fact that $U_{Coul} = 0.71$ MeV we obtain for uranium Z/A = 0.41 (the actual value is Z/A = 0.39).

In conclusion we compare the values obtained above of the coefficients of U in formula (8) with their empirical values. Two variants of the semiempirical Weizsäcker formula [9] can be used for such a comparison.

In the simplified variant the coefficients U have the following values 7 :

$$U_{\rm surf} \approx 18 \, {\rm MeV}, \qquad U_{\rm sym} \approx 24 \, {\rm MeV}.$$

In the second variant of the Weizsäcker formula we take into account the mutual influence of the surface effects and the symmetry effect; this influence contributes the additional term $U' \epsilon^2 A^{-1/3}$. Then

$$U_{\rm surf} \approx 21 \, {\rm MeV}, \qquad U_{\rm sym} \approx 30 \, {\rm MeV}, \qquad U' \approx -36 \, {\rm MeV}.$$

The values of the coefficients U_{surf} and U_{sym} obtained in this work correspond more closely to the second variant, even though these variants do not differ strongly from each other. A detailed comparison with the second variant could not be

achieved in here, owing to the neglect of the mutual influence of the surface effects and the symmetry effects. To account for this influence we must introduce different trial functions for the protons and neutrons in the surface layer, which will be done in a separate paper.

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⁷⁾The coefficient U_{vol} was considered in^[2]; the coefficient U_{Coul} , which has a simple meaning, coincides with its empirical value.