

## Self-Consistent Nuclear Model\*

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A Hamiltonian proposed by Duerr is applied to carry out self-consistent calculations for atomic nuclei. Average exchange forces, calculated from a plane-wave model, are included in the Hartree potential. In order to obtain agreement with the empirical data, two coupling constants and one constant representing the range of the interaction have to be adjusted. The range turns out to be  $3.23 \times 10^{-14}$  cm. Because this range is very short the calculations may not be justified and must be considered as a formal procedure. Having adjusted the three parameters, reasonable neutron and proton binding energies and nucleon densities are obtained for the nuclei  $O^{16}$ ,  $Ca^{40}$ ,  $Ce^{140}$ , and  $Pb^{208}$ .

### I. INTRODUCTION

THE purpose of this paper is to present a simple nuclear model which mathematically leads to the self-consistent state of atomic nuclei.

Recently the Brueckner theory<sup>1</sup> achieved considerable success in explaining the properties of finite nuclei, although complete quantitative agreement has not been found as yet. Considering the difficulties of the formalism and the ambitious purpose of the theory this is not surprising.

The Brueckner theory has the disadvantage that its mathematical language is highly complex and thus presents great difficulties in actual computation. Therefore, it is of interest to make an attempt to solve the self-consistent problem in the framework of the much easier to handle independent-particle model. It has to be pointed out that the independent-particle model contains inherent inaccuracy, namely, the two-particle correlations are neglected. Since in case of short range forces they may be important the present paper should be regarded as a formal mathematical procedure.

We shall attempt to obtain a self-consistent single-particle potential using a Hamiltonian proposed by

Duerr.<sup>2</sup> We limit ourselves to spherically symmetric fields and use as specific examples the nuclei  $Pb^{208}$ ,  $Ce^{140}$ ,  $Ca^{40}$ , and  $O^{16}$ . The Duerr-Hamiltonian looks as follows:

$$H = \sum_i \psi_i^* c \alpha \cdot \mathbf{p} \psi_i + \beta M c^2 \sum_i \psi_i^* \psi_i - a M c^2 \varphi \sum_i \psi_i^* \beta \psi_i + b M c^2 \varphi_0 \sum_i \psi_i^* \psi_i + \frac{c^2}{2} [(\nabla \varphi)^2 + \mu_1^2 \varphi^2] - \frac{c^2}{2} [(\nabla \varphi_0)^2 + \mu_2^2 \varphi_0^2], \quad (1.1)$$

where  $\alpha$  and  $\beta$  are the Dirac matrices,  $\varphi$  represents an attractive scalar field and  $\varphi_0$  a repulsive field which transforms like the fourth component of a vector field,  $a$  and  $b$  are coupling constants. It was pointed out earlier in a paper by Johnson and Teller<sup>3</sup> that a pseudo-scalar field gives zero average in the interior of a nucleus which is built up of shell model states. On the other hand this is not so in the case of a scalar field. Thus the Hamiltonian (1.1) is the most general type which gives nonzero average potential in the interior of a large nucleus. In the nonrelativistic limit both  $\varphi$  and  $\varphi_0$  behave like scalars. As we shall see, it is necessary to have two fields because an attractive field alone yields a collapsed state. The Hamiltonian (1.1) represents a velocity dependent field because at high nucleon velocities the expectation value of  $\beta$  tends to zero. The effective velocity dependent potential is  $M c^2 (-a \langle \beta \rangle \varphi + b \langle I \rangle \varphi_0)$  where  $I$  is the unit matrix.

Unfortunately the Duerr-Hamiltonian leads to wrong predictions for high-energy scattering. It has, however, the advantage that it gives a closed and handy formalism which leads to stable states of nuclei. Actually we shall attempt an approximation to a Hartree-Fock model by introducing the exclusion principle into the statistical formulation.

### II. DERIVATION OF THE SELF-CONSISTENT FORMALISM

In the nonrelativistic limit ( $p \ll M c$ ) the Hamiltonian (1.1) becomes after a Foldy-Wouthuysen transformation (see reference 2)

<sup>3</sup> M. H. Johnson and E. Teller, Phys. Rev. **98**, 783 (1955).

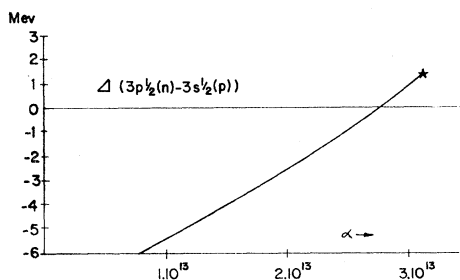


FIG. 1. Difference between the calculated last proton and last neutron binding energy in case of the  $Pb^{208}$  nucleus as a function of the range. The star means the experimental value.

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<sup>1</sup> K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961).

<sup>2</sup> Hans-Peter Duerr, Phys. Rev. **103**, 469 (1956).

$$\begin{aligned}
 li = \sum_i \psi_i^* \beta \left\{ \frac{1}{2Mg} \mathbf{p}^2 - \frac{i\hbar}{2M^2c^2} (\nabla V/g^2) \cdot \mathbf{p} \right. \\
 \left. - \frac{\hbar^2}{8M^2c^2} \nabla \cdot \left[ \frac{\nabla(V-V_0)}{g^2} \right] \right\} \psi_i \\
 + \sum_i \psi_i^* \left\{ V_0 - \beta V + \beta M c^2 \right. \\
 \left. + \frac{\hbar^2}{4M^2c^2g^2} \frac{1}{r} \frac{d}{dr} (\beta V + V_0) (\boldsymbol{\sigma} \cdot \mathbf{l}) \right\} \psi_i \\
 + \frac{1}{2a^2M^2c^2} [(\nabla V)^2 + \mu_1^2 V^2] \\
 - \frac{1}{2b^2M^2c^2} [(\nabla V_0)^2 + \mu_2^2 V_0^2], \quad (2.1)
 \end{aligned}$$

where

$$V = aM c^2 \varphi; \quad V_0 = bM c^2 \varphi_0; \quad g = 1 - V/Mc^2.$$

It is tacitly assumed in (2.1) that the time derivatives  $\partial V/\partial t$  and  $\partial V_0/\partial t$  are zeros. We see that in the positive energy states ( $\langle \beta \rangle = 1$ ) there is a large spin-orbit interaction. In previous models this large spin-orbit interaction has been generally taken as a Thomas-type interaction in which a phenomenological factor occurred.

Formula (2.1) is the Hamiltonian in the Hartree approximation.

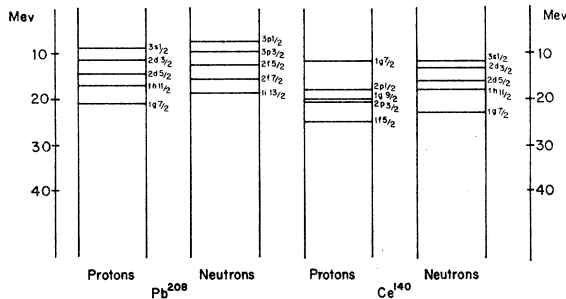


FIG. 2. Top energy levels in self-consistent fields.  $\alpha = 3.10 \times 10^{13} \text{ cm}^{-1}$ ,  $g_1 = 2.3g \times 10^{-8} \text{ cgs}$ ,  $g_2 = 1.80 \times 10^{-8} \text{ cgs}$ .

The Pauli exclusion principle requires that the total wave function of the  $N$ -particle system be antisymmetric which leads to the determinant form for the total wave function and to the Hartree-Fock equations for the single-particle functions. Instead of solving the complicated Hartree-Fock equations we try to modify the Hartree equations in such a way that these modified Hartree equations should yield approximately the same single-particle functions and energies as the correct Hartree-Fock equations. We can do that by introducing an exchange potential  $V_{\text{ex}}$  which results from the average exchange effects. We shall add this potential to the simple Hartree potentials to obtain the collective potential to be used in the modified Hartree approximation.

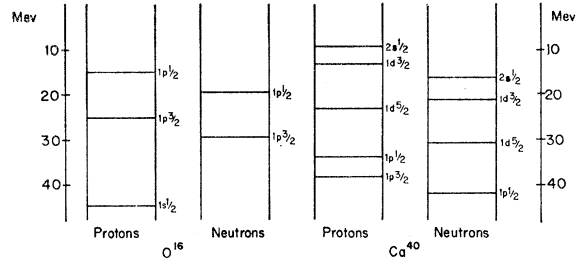


FIG. 3. Top energy levels in self-consistent fields.  $\alpha = 3.10 \times 10^{13} \text{ cm}^{-1}$ ,  $g_1 = 2.3g \times 10^{-8} \text{ cgs}$ ,  $g_2 = 1.80 \times 10^{-8} \text{ cgs}$ .

We assume that  $V_{\text{ex}}$  satisfies a Yukawa type equation

$$\nabla^2 V_{\text{ex}} - \mu^2 V_{\text{ex}} = -\frac{g^2 \mu^2}{2\pi} f(\rho; \mu), \quad (2.2)$$

where  $f(\rho; \mu)$  is given by (A1.9) in Appendix I. (For detailed discussion of the exchange potential see Appendix I.) We have to keep in mind that the exchange effect acts only between particles having the same spin and isotopic spin state. The proton and neutron distributions are in general different in a nucleus and the exchange potentials acting on them will be different as well.

Because of this difference between the proton and neutron exchange effects the effective meson potential acting on a single proton and neutron in a nucleus will be different. Since in most cases there are more neutrons than protons in a nucleus the meson well for protons will be deeper. This difference is counteracted by the Coulomb repulsion.

The inclusion of the Pauli principle in the above discussed way yields the total Hamiltonian for a system

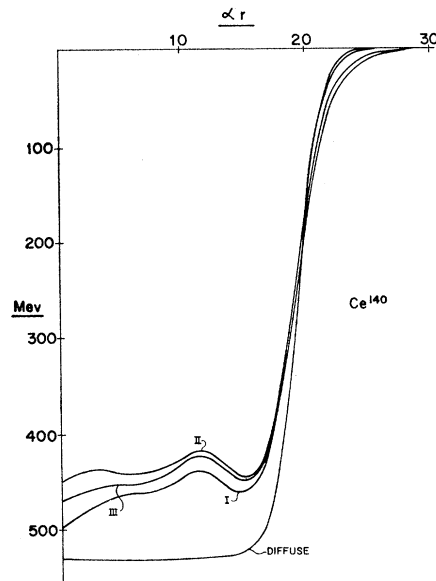


FIG. 4. The "big" scalar potential for protons ( $V_p$ ) in the  $\text{Ce}^{140}$  nucleus belonging to different iterations.

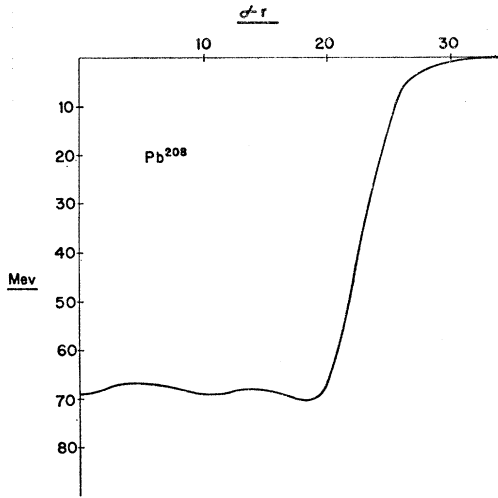


FIG. 5. Self-consistent neutron potential ( $V_n - V_{n0}$ ) for the  $\text{Pb}^{208}$  nucleus.

consisting of  $Z$  protons and  $N$  neutrons

$$H = \sum_{i=1}^Z H_{p_i} + \sum_{i=1}^N H_{n_i} + H_{\text{scalar meson}} + H_{\text{vector meson}}. \quad (2.3)$$

Here the Hamiltonian for a single proton is

$$H_{p_i} = \psi_i^* \left\{ \frac{1}{2M(1-V_p/Mc^2)} \mathbf{p}^2 - \frac{i\hbar}{2M^2c^2(1-V_p/Mc^2)^2} \nabla V_p \cdot \mathbf{p} - \frac{\hbar^2}{8M^2c^2} \nabla \cdot \left( \frac{\nabla(V_p - V_{p0})}{(1-V_p/Mc^2)^2} \right) + Mc^2 - (V_p - V_{p0}) + \left[ \frac{\hbar^2}{4M^2c^2} \left( \frac{1}{(1-V_p/Mc^2)^2} \frac{1}{r} \frac{d}{dr} (V_p + V_{p0}) - \frac{1}{r} \frac{dV_c}{dr} \right) \times \epsilon \right] + V_c \right\} \psi_i, \quad (2.4)$$

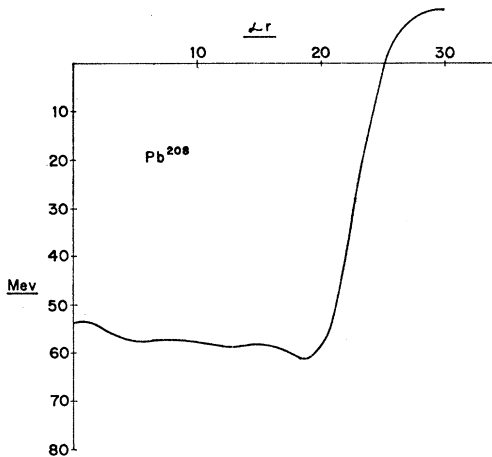


FIG. 6. Self-consistent proton potential ( $V_p - V_{p0} - V_c$ ) for the  $\text{Pb}^{208}$  nucleus.

where  $\epsilon = l$  for  $j = l + \frac{1}{2}$ ,  $\epsilon = -l - 1$  for  $j = l - \frac{1}{2}$ . The last two terms in (2.4) are the spin-orbit interaction and the Coulomb repulsion  $V_c$ . The two collective meson potentials for protons  $V_p$  and  $V_{p0}$  correspond to  $V$  and  $V_0$  in the formula (2.1), and they are given by

$$V_p = V - V_{\text{ex}} \text{ for protons,}$$

$$V_{p0} = V_0 - V_{0\text{ex}} \text{ for protons.}$$

Similarly the collective neutron potentials are

$$V_n = V - V_{\text{ex}} \text{ for neutrons,}$$

$$V_{n0} = V_0 - V_{0\text{ex}} \text{ for neutrons.}$$

In the single-particle Hamiltonian for neutrons  $V_c$  is obviously omitted.

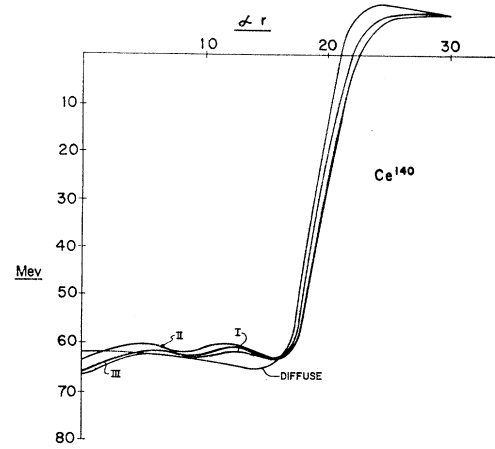


FIG. 7. Proton potentials ( $V_p - V_{p0} - V_c$ ) for the  $\text{Ce}^{140}$  nucleus belonging to different iterations. For starting potential the diffuse type  $V = D/[1 + \exp(\alpha(r-R))]$  was used. III can be considered as the self-consistent potential.

The Hamiltonian (2.3) combined with (2.2) for the exchange part yields the field equations for the collective potentials and the single-particle equations as well:

$$\nabla^2 V_p - \mu_1^2 V_p = -4\pi g_1^2 \{ \rho_p [1 - K\rho_p^3/M^2c^2g_p^2] + \rho_n [1 - K\rho_n^3/M^2c^2g_n^2] - (\mu_1^2/8\pi) f(\rho_p; \mu_1) \}, \quad (2.5)$$

$$\nabla^2 V_{p0} - \mu_2^2 V_{p0} = -4\pi g_2^2 \{ \rho_p + \rho_n - (\mu_2^2/8\pi) f(\rho_p; \mu_2) \}, \quad (2.6)$$

$$H_p \psi_i = E_i \psi_i. \quad (2.7)$$

In (2.5) and (2.6),

$$\rho_p = \sum_{i=1}^Z |\psi_i|^2; \quad \rho_n = \sum_{i=1}^N |\psi_i|^2;$$

$$g_p = 1 - V_p/Mc^2; \quad g_n = 1 - V_n/Mc^2;$$

$$K = (3/10M)(3\pi^2)^{2/3} \hbar^2.$$

We redefine the coupling constants in a more familiar

way,

$$a^2 M^2 c^2 = 4\pi g_1^2; \quad b^2 M^2 c^2 = 4\pi g_2^2.$$

In (2.5) we used the approximation

$$\frac{\hbar^2}{2M} \sum_{i=1}^Z \psi_i^* \nabla^2 \psi_i \approx K \rho_p^{5/3},$$

which is good only in the case where the wave functions can be represented by plane waves.

The equations for the collective neutron potentials can be obtained in the same way, the only difference is that we have there  $f(\rho_n; \mu)$ . Finally the Coulomb potential  $V_c$  is determined by the Laplace equation

$$\nabla^2 V_c = 4\pi e^2 \rho_p, \tag{2.8}$$

where  $e$  means the elementary charge ( $4.8024 \times 10^{-10}$  cgs).

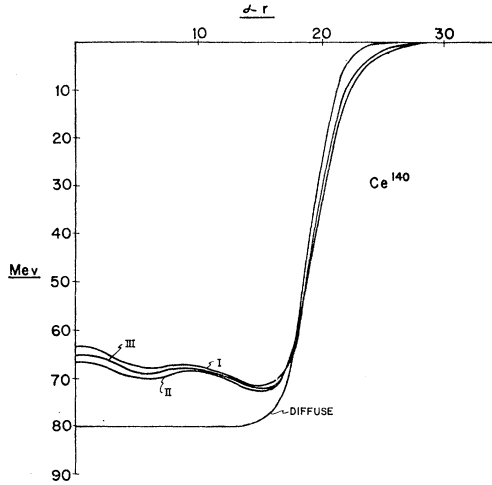


FIG. 8. Neutron potentials ( $V_n - V_{n0}$ ) for the  $\text{Ce}^{140}$  nucleus belonging to different iterations. For starting potential the diffuse type  $V = D/[1 + \exp\alpha(r - R)]$  was used. III can be considered as the self-consistent potential.

We observe that the repulsion which eventually keeps the nucleus at a finite size appears both in the single-particle Hamiltonian (2.4) and in the equation for the attractive potential (2.5). In (2.4) it appears in the form of an increased kinetic energy because of the effective mass

$$M_p^* = M(1 - V_p/Mc^2).$$

We also see from (2.5) that in case of high momenta the attractive potential becomes small whereas the repulsive part in (2.6) remains large. This latter effect corresponds to the relativistic case where  $\beta V$  tends to zero with increasing momenta.

### III. DISCUSSION OF THE RESULTS

The Eqs. (2.5)–(2.7) form the basis for the self-consistent calculations which were carried out for the

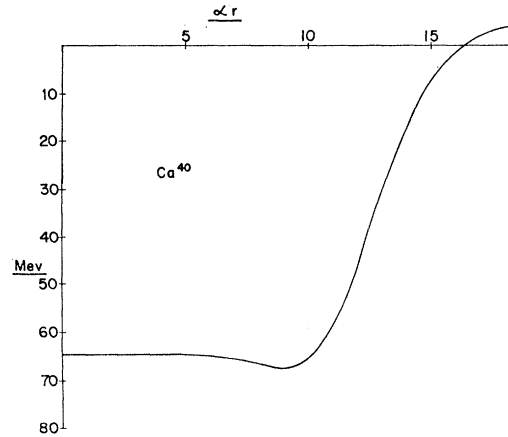


FIG. 9. Self-consistent proton potential ( $V_p - V_{p0} - V_c$ ) for the  $\text{Ca}^{40}$  nucleus.

$\text{O}^{16}$ ,  $\text{Ca}^{40}$ ,  $\text{Ce}^{140}$ , and  $\text{Pb}^{208}$  nuclei. Since we do not assume that the two-particle interaction is represented by the exchange of single  $\pi$  mesons, the Compton wavelength of the fields  $V$  and  $V_0$  was taken as a free parameter. We shall call it briefly the range of the potentials. The range of  $V$  and  $V_0$  has to be taken as equal. Otherwise the effective potential  $V - V_0$  oscillates at the nuclear surface. The nuclear radius, or in other words  $r_0$  in the nuclear radius expression  $R = r_0 A^{1/3}$  is known from the experiments with limited accuracy. According to these  $r_0$  is likely to be between  $1.2$  and  $1.4 \times 10^{-13}$  cm. The nuclear size, the binding energy of the last neutron and proton can be reproduced by varying three parameters which are the range of the potentials and the coupling constants  $g_1$  and  $g_2$ . The ratio of the last proton and last neutron binding energies is a function mainly of the range. The calculations for the  $\text{Pb}^{208}$  nucleus were carried out with several ranges and it was found that the correct last proton and last neutron binding ratio was reproduced by taking  $\alpha = 3.10 \times 10^{13} \text{ cm}^{-1}$  ( $\alpha = \mu_1 = \mu_2$ ).

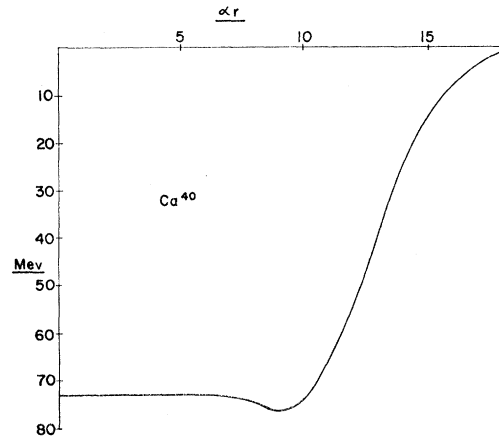


FIG. 10. Self-consistent neutron potential ( $V_n - V_{n0}$ ) for the  $\text{Ca}^{40}$  nucleus.

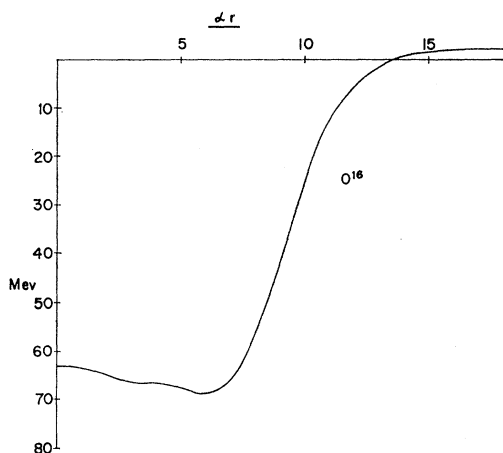


FIG. 11. Self-consistent proton potential ( $V_p - V_{p0} - V_c$ ) for the  $O^{16}$  nucleus.

### A. Self-Consistency

The self-consistent state was obtained usually after the third or fourth iteration regardless of the range of the potentials. For starting potentials the diffuse type  $V = D/[1 + \exp\alpha(r - R)]$  was used, where the potential depths had to be chosen adequately. As mentioned above the correct  $\beta^+$  and  $\beta^-$  stabilities for the neighboring nuclei of the  $Pb^{208}$  nucleus were reproduced with a potential range  $1/\alpha = 3.23 \times 10^{-14}$  cm (see Fig. 1). This short range was needed in order to produce a sufficiently great difference between the interactions of like and unlike nucleons. The small value of the range raises serious doubt as to the validity of the use of average potentials. Actually the exchange forces are substitutes for the more usual symmetry forces. It is possible that the former results of our calculations correspond to a physical situation in which the range is longer and symmetry forces are added.

### B. Top Levels

The correctness of the top level system can be checked from the experimentally known  $(\gamma, n)$  threshold energies

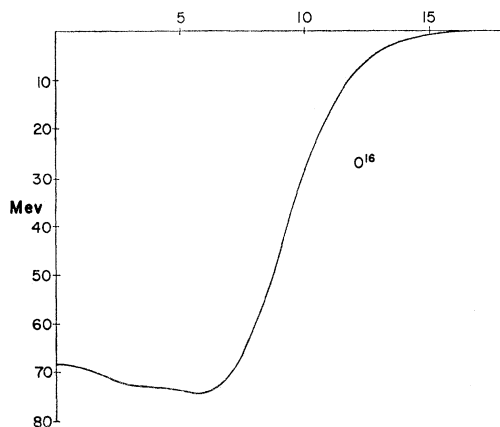


FIG. 12. Self-consistent neutron potential ( $V_n - V_{n0}$ ) for the  $O^{16}$  nucleus.

and from the  $\beta^+$  and  $\beta^-$  decay energies and angular momentum states of the neighboring nuclei.

The stability of the  $Pb^{207}$  nucleus and the activity of  $AcC^{207}$  with 1.47-Mev  $\beta^-$  energy indicates that in the case of  $Pb^{208}$  nucleus we can expect the top neutron level ( $3p_{3/2}$ ) to be about 1.47 Mev higher than the top proton level ( $3s_{3/2}$ ). The coupling constants were adjusted to reproduce the nuclear radius and the experimentally measured  $(\gamma, n)$  threshold energy for the top neutron level, which in the case of the  $Pb^{208}$  nucleus is 7.4 Mev. The sequence of the top proton and neutron levels can be checked by the angular momentum states of the neighboring odd  $Z$  and odd  $N$  nuclei, respectively. As we go away from the magic shells we go from the spherically symmetric state to the deformed core state, consequently our level system which was calculated in spherically symmetric fields cannot be trusted quantitatively. Nevertheless, the  $Tl^{205}$ ,  $Tl^{208}$ ,  $Au^{197}$  nuclei confirm that the  $3s_{3/2}$  and  $2d_{3/2}$  levels are the top proton levels, similarly the  $Pb^{207}$  and  $Hg^{201}$  nuclei show the  $3p_{3/2}$  and  $3p_{3/2}$  levels as top neutron levels.

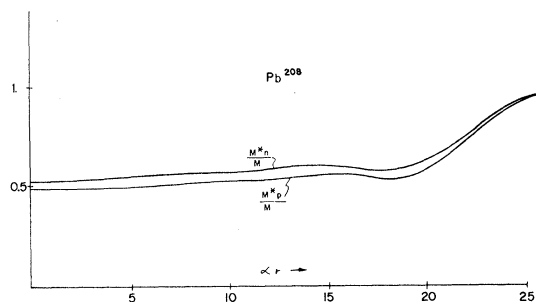


FIG. 13. Effective nucleon mass in the self-consistent field of the  $Pb^{208}$  nucleus.  $\alpha = 3.10 \times 10^{13}$  cm $^{-1}$ .

The above discussions seem to indicate that the parameter set  $\alpha = 3.10 \times 10^{13}$  cm $^{-1}$ ,  $g_1 = 2.39 \times 10^{-8}$  cgs,  $g_2 = 1.80 \times 10^{-8}$  cgs yields the self-consistent state for the  $Pb^{208}$  nucleus and predicts top levels for the neighboring nuclei with fairly good accuracy (see Fig. 2). We may observe that the magnitude of the coupling constants are enormous,  $g_1^2/\hbar c \sim 18$ ,  $g_2^2/\hbar c \sim 10$ . This is the result of the short range interaction alone. Taking the range as a variable the same magnitude for the potential depth can be obtained by keeping  $g/\alpha$  constant. Thus the  $\pi$  meson range would result  $g_1^2/\hbar c \sim 0.95$ ,  $g_2^2/\hbar c \sim 0.53$ .

TABLE I. Comparison of calculated and experimental neutron separation energies.

Nucleus	$(\gamma, n)$ threshold (Mev) <sup>a</sup>	Last neutron binding (Fig. 1-2)
$O^{16}$	$16.3 \pm 0.4$	19.25
$Ca^{40}$	$15.9 \pm 0.4$	16.25
$Ce^{140}$	$9.05 \pm 0.2$	11.5
$Pb^{208}$	$7.4 \pm 0.1$	7.4

<sup>a</sup> Taken from: *Experimental Nuclear Physics*, edited by E. Segrè (John Wiley & Sons, Inc., New York, 1953), Vol. II.

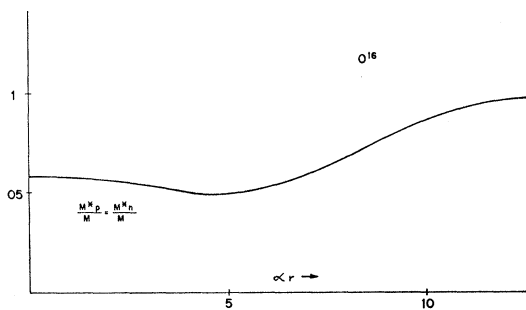


FIG. 14. Effective nucleon mass in the self-consistent field of the  $O^{16}$  nucleus.  $\alpha = 3.10 \times 10^{13} \text{ cm}^{-1}$ .

This range however does not give the empirical  $\beta^+$  and  $\beta^-$  stabilities.

Having fixed these parameters for the  $Pb^{208}$  nucleus the calculations were carried out for the  $Ce^{140}$ ,  $Ca^{40}$  and  $O^{16}$  nuclei. Table I shows that the obtained last neutron binding energies are in close agreement with the experimental  $(\gamma, n)$  threshold energies.

The stable  $La^{139}$  nucleus with  $J = \frac{7}{2}$  and the unstable  $Ce^{139}$  nucleus which transforms with  $K$  capture to  $La^{139}$  indicate that the top proton level is about 0.5 Mev higher than the top neutron level in the case of the  $Ce^{140}$  nucleus (see Fig. 2). The  $O^{16}$  and  $Ca^{40}$  nuclei have equal numbers of protons and neutrons, consequently the top proton level must be considerably higher than the top neutron level (see Fig. 3). This is proved by the short half-life of  $\beta^+$ -unstable  $O^{15}$  and  $Ca^{39}$  nuclei.

There is one remarkable difference between the level system shown in Figs. 2 and 3 and the empirical data. The  $1d_{3/2}$  level has to be above the  $2s_{3/2}$  level both in the proton and neutron case, and similarly the  $2d_{3/2}$  level is above the  $3s_{3/2}$  level for neutrons. (The only case where the  $3s_{3/2}$  level is above the  $2d_{3/2}$  level happens in the proton case in accordance with the level system of  $Pb^{208}$ .) The reason for this discrepancy lies partly in the inaccurate way of calculating the exchange effect. The average exchange effect has been calculated assuming for the wave functions plane waves. This is a good approximation for

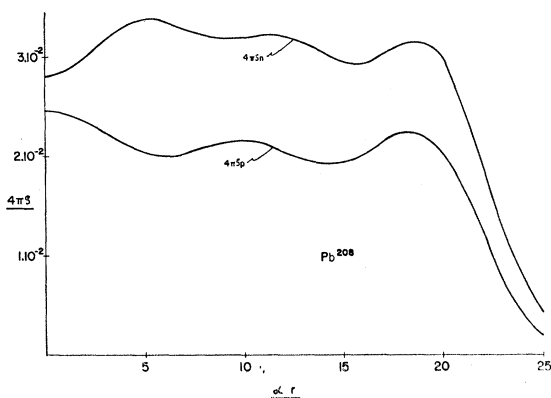


FIG. 15. Proton and neutron densities in the  $Pb^{208}$  nucleus.

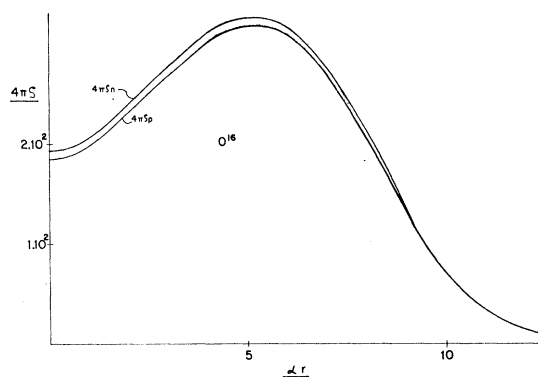


FIG. 16. Proton and neutron densities in the  $O^{16}$  nucleus.

heavy nuclei as in the case of  $Pb^{208}$ ; however for light nuclei it is inaccurate. Furthermore, the exchange effects are different for different nucleon states and we calculated the exchange potential in an average way.

#### IV. CONCLUSION

We saw that the Hamiltonian (1.1) in Sec. I yields saturation and it also has the nice property that it automatically gives a large spin-orbit interaction. However, this Hamiltonian predicts wrong nucleon-nucleus scattering data at high energies. In case of high energies it predicts a net repulsion which is in contradiction with the experiments. On the other hand, at low energies as in the ground state of the nucleus it works surprisingly well.

The magnitude of the coupling constants  $g_1$  and  $g_2$  had to be chosen in such a way that there should be enough repulsion to produce the right nuclear radii and that, furthermore, the depth of the effective potential  $V - V_0$  should give the correct binding energy for the top neutron. The result is that the potentials  $V$  and  $V_0$  have the order of magnitude 450 and 390 Mev, respectively

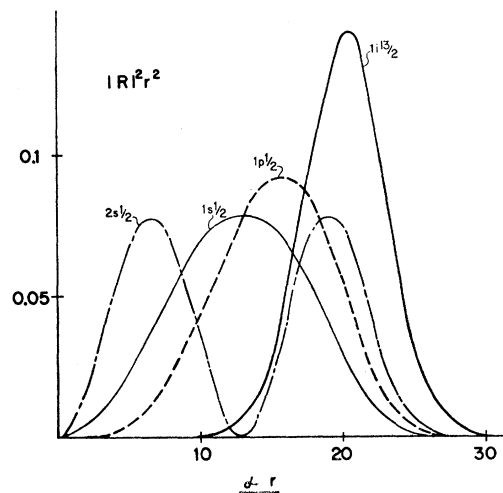


FIG. 17. Single-particle radial distributions in the  $Pb^{208}$  nucleus.  $R$  is the radial part of the single particle wave function,

(see Fig. 4); therefore, the effective potential is the net difference of the two nearly canceling fields (see Figs. 5–12). Thus, our model is a rather drastic device which keeps the nucleus at a finite size. What really matters is the velocity dependent difference between the large potentials. It can be expected that any velocity dependent potential of similar strength, such as following from the Brueckner theory, would give similar results. One of the consequences of the model is that the nucleons inside the nucleus have an effective mass of the magnitude 0.5 times the bare mass (see Figs. 13 and 14). Figures 15 and 16 represent the density profile of the  $\text{Pb}^{208}$  and  $\text{O}^{16}$  nuclei, respectively. We may notice that in case of equal number of protons and neutrons as in the case of  $\text{O}^{16}$  the Coulomb repulsion pushes the protons somewhat outward. Figure 17 shows the radial part of some wave functions for the  $\text{Pb}^{208}$  nucleus.

The scalar field corresponding to the range that we found might be represented by mesons having the mass 4.43 times the mass of the  $\pi$  meson. This is in the range of a  $K$ -meson Compton-wavelength. The range, however, can not be established accurately by our calculations, and its physical reality is doubtful.

It is of some interest that by the use of three adjustable parameters a wide variety of nuclear binding energies and levels could be reproduced within limited errors.

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#### APPENDIX

##### I. Exchange Potential in a Nucleon Gas

In this section we calculate the exchange energy of a nucleon having the wave vector  $\mathbf{k}$  moving in a nucleon gas. We assume that the wave functions can be represented by plane waves. This is a fairly good approximation for heavy nuclei. We also assume a Yukawa type interaction between two particles,

$$V(1,2) = -g^2 [\exp(-\alpha|\mathbf{r}_1 - \mathbf{r}_2|)] / (|\mathbf{r}_1 - \mathbf{r}_2|). \quad (\text{A1.1})$$

Let us calculate first the exchange term between two particles:

$$A_{ji} = - \int \int \rho_{ji}(\mathbf{r}_1) \rho_{ji}^*(\mathbf{r}_2) V(1,2) dv_1 dv_2, \quad (\text{A1.2})$$

where  $\rho_{ji}(\mathbf{r}) = \psi_j(\mathbf{r}) \psi_i^*(\mathbf{r})$ . Using (A1.1) for A(1.2) we have

$$A_{ji} = \int \rho_{ji}(\mathbf{r}_1) V_{ji}(\mathbf{r}_1) dv_1, \quad (\text{A1.3})$$

where

$$V_{ji}(\mathbf{r}_1) = g^2 \int \rho_{ji}^*(\mathbf{r}_2) [\exp(-\alpha|\mathbf{r}_1 - \mathbf{r}_2|)] / (|\mathbf{r}_1 - \mathbf{r}_2|) dv_2.$$

$V_{ji}(\mathbf{r})$  also satisfies the differential equation

$$\nabla^2 V_{ji} - \alpha^2 V_{ji} = -4\pi g^2 \rho_{ji}^*. \quad (\text{A1.4})$$

Using plane waves we have

$$\rho_{ji}^*(\mathbf{r}) = (1/\Omega) \exp[-i(\mathbf{k}_j - \mathbf{k}_l) \cdot \mathbf{r}].$$

( $\Omega$  = volume occupied.)

The solution of (A1.4) is given by

$$V_{ji}(\mathbf{r}) = [(4\pi g^2)/(\alpha^2 + |\mathbf{k}_j - \mathbf{k}_l|^2)] \rho_{ji}^*(\mathbf{r}). \quad (\text{A1.5})$$

Replacing (A1.5) into (A1.3) we obtain

$$A_{ji} = 4\pi g^2 \Omega^{-1} / (\alpha^2 + |\mathbf{k}_j - \mathbf{k}_l|^2). \quad (\text{A1.6})$$

Formula (A1.6) gives the exchange energy of two nucleons. The total exchange energy of a nucleon having a momentum  $\hbar\mathbf{k}_j$  in a nucleon gas is given by

$$V_{\text{ex}} = 4\pi g^2 \Omega^{-1} \int_0^N (\alpha^2 + |\mathbf{k}_j - \mathbf{k}_l|^2)^{-1} dn;$$

$$dn = (1/4\pi^2) \Omega k_l^2 dk_l d(\cos\vartheta),$$

thus

$$V_{\text{ex}} = (g^2/\pi) \int_0^{K_{\text{max}}} \int_{-1}^{+1} (\alpha^2 + k_j^2 + k_l^2 + 2k_j k_l \cos\vartheta)^{-1} \\ \times k_l^2 dk_l d(\cos\vartheta) \\ = (g^2/2\pi) \int_0^{K_{\text{max}}} k_j^{-1} \ln \frac{\alpha^2 + (k_j + k_l)^2}{\alpha^2 + (k_j - k_l)^2} k_l dk_l. \quad (\text{A1.7})$$

The integral in (A1.7) can be carried out in a long but straightforward way and it yields

$$V_{\text{ex}} = \left(\frac{g^2}{2\pi}\right) \left\{ \left(\frac{1}{2k_j}\right) (K_{\text{max}}^2 - k_j^2 + \alpha^2) \ln \frac{(K_{\text{max}} + k_j)^2 + \alpha^2}{(K_{\text{max}} - k_j)^2 + \alpha^2} \right. \\ \left. + 2K_{\text{max}} - 2\alpha \tan^{-1} \frac{K_{\text{max}} + k_j}{\alpha} \right. \\ \left. - 2\alpha \tan^{-1} \frac{K_{\text{max}} - k_j}{\alpha} \right\}. \quad (\text{A1.8})$$

Formula (A1.8) gives the exchange energy of one nucleon with all the nucleons in a nucleon gas. It contains the self-exchange energy too which in the Hartree-Fock method cancels the self energy appearing in the Hartree method. We see from (A1.8) that the exchange potential depends on the momentum  $\hbar k_j$  of the nucleon in question. For a nucleon having the average mo-

mentum  $\frac{3}{4}K_{\text{max}}$  (A1.8) yields

$$V_{\text{ex}} = \left(\frac{g^2}{2\pi}\right) \left\{ \left(\frac{2}{3}\right) (3\pi^2\rho)^{-\frac{1}{3}} \left[ \left(\frac{7}{16}\right) (3\pi^2\rho)^{\frac{2}{3}} + \alpha^2 \right] \right. \\ \times \ln \frac{49(3\pi^2\rho)^{\frac{2}{3}} + 16\alpha^2}{(3\pi^2\rho)^{\frac{2}{3}} + 16\alpha^2} + 2(3\pi^2\rho)^{\frac{1}{3}} \\ \left. - 2\alpha \tan^{-1}[(7/4)(3\pi^2\rho)^{\frac{1}{3}}\alpha^{-1}] \right. \\ \left. - 2\alpha \tan^{-1}[(1/4)(3\pi^2\rho)^{\frac{1}{3}}\alpha^{-1}] \right\}. \quad (\text{A1.9})$$

In (A1.9) we used the relation  $K_{\text{max}} = (3\pi^2\rho)^{\frac{1}{3}}$ , where  $\rho$  is the nucleon density. It is assumed that half of the nucleons are in the state spin up and half of them in spin down.

Formula (A1.9) is valid for an infinitely large nucleus. In that case, the potential energy is a function of the nucleon density alone, which is a constant. In analogy with the equation which holds for the classical type direct potential we assume that for finite size nuclei the exchange potential also satisfies a Yukawa type equation

$$\nabla^2 V_{\text{ex}} - \alpha^2 V_{\text{ex}} = - (g^2\alpha^2/2\pi) f(\rho; \alpha), \quad (\text{A1.10})$$

where  $f(\rho; \alpha)$  is the expression in the parenthesis on the right side of (A1.9). We observe that in the interior of the nucleus where  $\nabla^2 V_{\text{ex}}$  can be neglected formula (A1.10) goes over to (A1.9). Near the surface the term  $\nabla^2 V_{\text{ex}}$  becomes important. No justification of this term

is known to us beyond the statements that a surface term of this order of magnitude is reasonable and that the introduction of this term greatly simplifies the treatment of the expression for  $V_\rho$  and  $V_{\rho 0}$  in Sec. II.

## II. Computational Methods

The equation for the radial part of the wave function has the form

$$R'' + f(x)R' + [k_{njl}(x) - \lambda_{njl}g(x)]R = 0, \quad (\text{A2.1})$$

where the functions  $f(x)$  and  $k(x)$  contain the potentials and spin-orbit term,  $g(x)$  is the effective mass function defined in Sec. II, and  $\lambda_{njl}$  is the eigenvalue in dimensionless units.

(A2.1) was solved step by step using the approximation

$$R'(x) \sim [R(x+\Delta x) - R(x-\Delta x)]/2\Delta x,$$

$$R''(x) \sim [R(x+\Delta x) - 2R(x) + R(x-\Delta x)]/(\Delta x)^2.$$

The solution of the field Eqs. (2.5) and (2.6) was performed by simple integration<sup>4</sup> using the Weddle numerical integration method.

The IBM 704 electronic computer was programmed to solve (A2.1) and the field equations and the solutions were carried out until the self-consistent state was reached.

<sup>4</sup> For details see R. Mises: *Differential and Integral Gleichungen der Mechanik and Physik* (Friedrich Vieweg und Sohn, Braunschweig, 1930), Vol. 1.