Relativistic Hartree-Fock description of nuclei*

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A relativistic nuclear Hamiltonian is constructed, from which the relativistic Hartree and Hartree-Fock equations are derived. Then the Hartree equations are applied to 16 O and 40 Ca nuclei taking as input different relativistic one-boson-exchange potentials as well as the effective interaction of Walecka, introduced in his theory of highly condensed matter. Single-particle energies turn out to be of the correct magnitude. In particular, it is possible to explain the magnitude of the spin-orbit splitting without any free parameter.

NUCLEAR STRUCTURE ¹⁶O, ⁴⁰Ca; calculated single-particle binding energies. Relativistic Hartree-Fock method.

I. INTRODUCTION

This paper presents an approach to a relativistic description of bound nuclei. The strong interaction between the nucleons is generated by the exchange of mesons. For the description of nucleon-nucleon scattering one-boson-exchange potentials (OBEP) have turned out to be very useful. Recently developed relativistic boson exchange potentials¹ are used successfully to reproduce the experimental nucleon-nucleon scattering phase shifts. A survey on the situation in the nucleonnucleon scattering can be found, for example, in the review article by Erkelenz.²

While there exist many calculations with OBEP for the two-nucleon problem and nuclear matter, there are only a few such calculations for finite nuclei.³ In this series of papers Miller has set up the relativistic Hamiltonian for an A-body system with two-body interactions, which are given by the r-space OBEP derived in the review article of Green and Sawada.⁴ The variational approach was used to obtain from this Hamiltonian the relativistic Hartree-Fock (RHF) equations. Then Miller solved the Hartree and, within certain approximations, also the Hartree-Fock equations numerically.

In the present paper the relativistic Hamilton operator for bound nucleons, which interact strongly through meson exchange, is rederived in a simple manner; it is shown, in particular, how to include derivative coupling and retardation effects. (The Hartree equations derived in this way differ from Miller's Hartree equations only by a self-energy term, which is not subtracted in Miller's approach.) In his derivation of the RHF

equations, Miller uses a specific (spherical coordinate) representation of γ matrices right from the beginning, while in this work a somewhat simpler approach has been used which leads to practical simplifications in setting up the RHF equations. These equations are then solved to explore the extent to which a relativistic description of the nucleus is relevant for low-energy properties of nuclei, as Miller has already pointed out. For example, the spin-orbit interaction is usually treated in a purely phenomenological way in a nonrelativistic theory, whereas it should emerge naturally in a relativistic description. In addition, it is certainly desirable to obtain relativistic single-nucleon wave functions, in order to describe typical medium-energy processes such as (p, π^+) etc.⁵ We shall proceed as follows: In Sec. II the field theoretical Hamiltonian will be set up for nucleons bound in a nucleus. The relativistic Hartree and Hartree-Fock equations for closed shell nuclei are given in Sec. III. In Sec. IV the results of the Hartree calculations are discussed for nucleons in oxygen and calcium, respectively. A conclusion is then presented in Sec. V.

II, RELATIVISTIC HAMILTONIAN FOR A SYSTEM OF MANY NUCLEONS

We start with an exposition of the basic meson theoretic ingredients of the free nucleon-nucleon interaction. For our purposes the relativistic OBEP of Gersten, Thompson, and Green (GTG)⁶ or the more refined one of Erkelenz, Holinde, and Machleidt (EHM)⁷ are most useful. The physical properties of the exchanged mesons are displayed in Table I. We now proceed to construct

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		5 5 1 1 1	GTG					EHM			
Meson	T	J^{P}	m (MeV)	$\frac{g^2}{4^{\pi}}$	$\frac{f}{g}$	Λ (MeV)	т (MeV)	$\frac{g^2}{4^{\pi}}$	$\frac{f}{g}$	Λ (MeV)	$\frac{g_{\mathbf{R}^2}}{4\pi}$
π	1	0-	138.7	14.19		1414	138	14.4		1265	14.06
η	0	0	548.5	3.09		1414	548.5	6		1530	4.56
σ	0	0*	570.	6.97		1414	550	8.67		1530	6.57
δ	1	0+	960.	0.33		1414	960	2.88		1530	1.059
ρ	1	1	763.	0.43	6.38	1414	712	0.77	6.6	1530	0.37
ω	0	1	782.8	9,92		1414	782.8	23		1530	9.25
Þ	0	1	•••	•••		•••	1020	5		1530	0.86

(2)

TABLE I. The meson parameters for the OBEP of Gersten, Thompson, and Green $(GTG)^6$ and Erkelenz, Holinde, and Machleidt $(EHM)^7$. The definition of the renormalized coupling constants for the OBEP of EHM is given by Eq. (37) of Sec. II.

the Hamiltonian for nuclei consisting of A nucleons, which for simplicity we assume to interact only by the exchange of σ , π , ρ , and ω mesons. We start with the following effective Lagrangian:

$$\mathfrak{R} = \mathfrak{P}_{N}^{\text{free}} + \mathfrak{P}_{\pi}^{\text{free}} + \mathfrak{P}_{\rho}^{\text{free}} + \mathfrak{P}_{\omega}^{\text{free}} + \mathfrak{P}_{\omega}^{\text{free}} + \mathfrak{P}_{\omega}^{\text{free}} + \mathfrak{P}_{NN\pi}^{\text{int}} + \mathfrak{P}_{NN\pi}^{\text{int}} + \mathfrak{P}_{NN\sigma}^{\text{int}} + \mathfrak{P}_{NN\omega}^{\text{int}} + \mathfrak{P}_{NN\omega}^{\text{int}} , \qquad (1)$$

where *Lagrangian* densities

$$\mathfrak{g}_{N}^{\text{free}} = -\frac{1}{2}\overline{\psi}(x) [(-i\gamma^{\mu}\overline{\partial}_{\mu} + M) + (i\overline{\partial}_{\mu}\gamma^{\mu} + M)]\psi(x),$$

$$R_{\text{free}}^{\text{free}} = -\frac{1}{2} \left[m^2 \alpha^2(x) - \partial_{-} \alpha(x) \partial^{\mu} \alpha(x) \right]$$
(3)

$$c_{\sigma} = -\frac{1}{2} [m_{\sigma} \psi(x) - \delta_{\mu} \psi(x) + \delta_{\mu} \psi(x)], \qquad (0)$$

$$g_{\mu} = -\frac{1}{2} [m_{\pi} \phi^{-}(x) - \partial_{\mu} \phi(x) \partial^{\pi} \phi(x)], \qquad (4)$$

$$\vec{x}_{p}^{\text{nee}} = -\frac{1}{4} G_{\mu\nu}(x) G^{\mu}(x) + \frac{1}{2} m_{p}^{\mu} \rho_{\nu}(x) \rho^{\mu}(x), \quad (5a)$$

$$G_{\mu\nu}(x) \equiv \partial_{\mu}\rho_{\nu}(x) - \partial_{\nu}\rho_{\mu}(x), \qquad (5D)$$

$$\Re_{\omega}^{\text{free}} = -\frac{1}{4} F_{\mu\nu}(x) F^{\mu\nu}(x) + \frac{1}{2} m_{\omega}^{2} \omega_{\nu}(x) \omega^{\nu}(x)$$
(6a)

$$F_{\mu\nu}(x) \equiv \partial_{\mu}\omega_{\nu}(x) - \partial_{\nu}\omega_{\mu}(x).$$
 (6b)

 $M, m_{\sigma}, m_{\pi}, m_{\rho}, m_{\omega}$ are the rest masses of the nucleons and of the corresponding mesons. $[\psi(x) \text{ denotes the nucleon field operator and } \overline{\psi} \text{ its adjoint,}$ i.e., $\overline{\psi} = \psi^{\dagger} \gamma^{0}$.] $\varphi(x), \overline{\phi}(x), \overline{\rho}^{\nu}(x), \omega^{\nu}(x)$ are the σ -, π -, ρ -, and ω - meson field operators. Note that $\overline{\phi}$ and $\overline{\rho}^{\nu}$ are vectors in isospin space. The arrows on top of the ϑ_{μ} operators indicate the direction of action of these operators. For $\mathfrak{L}^{\text{int}}$ we choose the following local interaction Lagrangians (the effect of form factors will be dealt with later):

$$\mathfrak{R}_{NN\sigma}^{\text{int}} = g_{\sigma} \overline{\psi}(x) \varphi(x) \psi(x) , \qquad (7)$$

$$\mathfrak{L}_{NN\pi}^{\text{int}} = i g_{\pi} \overline{\psi}(x) \overline{\phi}(x) \overline{\tau} \gamma_5 \psi(x), \qquad (8)$$

$$\mathfrak{X}_{NN\rho}^{\text{int}} = -g_{\rho}\overline{\psi}(x)\overline{\rho}^{\nu}(x)\overline{\tau}\gamma_{\nu}\psi(x)$$

$$+ \frac{f_{\rho}}{4M} \,\overline{\psi}(x) \sigma^{\mu\nu} \tau \vec{G}_{\mu\nu}(x) \psi(x), \qquad (9)$$

$$\mathfrak{Q}_{NN\omega}^{\text{int}} = -g_{\omega}\overline{\psi}(x)\omega^{\nu}(x)\gamma_{\nu}\psi(x)$$

$$-\frac{f_{\omega}}{4M}\overline{\psi}(x)\sigma^{\mu\nu}F_{\mu\nu}(x)\psi(x).$$
(10)

 $\bar{\tau}$ are the Pauli isospin matrices. (The notation of the γ matrices and the Pauli matrices is that of Bjorken and Drell.⁸) We now wish to construct the Hamilton operator in nucleon space starting with the Lagrangian (1), i.e., eliminate the meson fields.

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First \mathfrak{X} is varied with respect to $\overline{\psi}$ and $\partial_{\mu} \overline{\psi}$ to obtain the Euler-Lagrange equation, which is the usual Dirac equation with source terms:

$$(-i\gamma^{\mu}\partial_{\mu} + M)\psi(x) = g_{\sigma}\varphi(x)\psi(x) + ig_{\pi}\overline{\phi}(x)\overline{\tau}\gamma_{5}\psi(x)$$
$$-g_{\rho}\overline{\rho}^{\nu}(x)\overline{\tau}\gamma_{\nu}\psi(x)$$
$$+\frac{f_{\rho}}{4M}\sigma^{\mu\nu}\overline{\tau}\vec{G}_{\mu\nu}(x)\psi(x)$$
$$-g_{\omega}\omega^{\nu}(x)\gamma_{\nu}\psi(x). \qquad (11)$$

 $[f_{\omega}$ is small, so the corresponding term in Eq. (11) has been neglected.] It should be noted that the nucleon current satisfies the continuity equation

$$\partial_{\mu} \left[\overline{\psi}(x) \gamma^{\mu} \psi(x) \right] = 0.$$
 (12)

The meson field equations are given by

$$(\Box + m_{\sigma}^{2})\varphi(x) = g_{\sigma}\overline{\psi}(x)\psi(x), \qquad (13)$$

$$(\Box + m_{\pi}^{2})\overline{\phi}(x) = i g_{\pi}\overline{\psi}(x)\overline{\tau}\gamma_{5}\psi(x), \qquad (14)$$

$$\partial^{\mu} \vec{G}_{\mu\nu}(x) + m_{\rho}^{2} \vec{p}_{\nu}(x) = g_{\rho} \vec{\psi}(x) \vec{\tau} \gamma_{\nu} \psi(x)$$
(15)

$$+\frac{f_{\rho}}{2M}\,\partial^{\mu}[\,\overline{\psi}(x)\overline{\tau}\sigma_{\mu\nu}\,\psi(x)]\,,$$

$$\partial^{\mu}F_{\mu\nu}(x) + m_{\omega}^{2}\omega_{\nu}(x) = g_{\omega}\overline{\psi}(x)\gamma_{\nu}\psi(x).$$
(16)

Equations (13) and (14) are both inhomogeneous Klein-Gordon equations, while the other equations (15) and (16) are Proca equations with source terms. Taking into account that the nucleon current is conserved [Eq. (12)] Eqs. (15) and (16) are

equivalent to Klein-Gordon equations with source terms:

$$(\Box + m_{\rho}^{2})\bar{\rho}_{\nu}(x) = g_{\rho}\bar{\psi}(x)\bar{\tau}\gamma_{\nu}\psi(x) + \frac{f_{\rho}}{2M}\partial^{\mu}[\bar{\psi}(x)\bar{\tau}\sigma_{\mu\nu}\psi(x)], \qquad (17)$$

 $(\Box + m_{\omega}^{2})\omega_{\nu}(x) = g_{\omega}\overline{\psi}(x)\gamma_{\nu}\psi(x).$ (18)

Equations (13, (14), (17), and (18) can be solved for the meson field operators:

$$\psi(x) = g_{\sigma} \int D_{\sigma}(x - y)\overline{\psi}(y)\psi(y)d^{4}y, \qquad (19)$$

$$\overline{\phi}(x) = i g_{\pi} \int D_{\pi}(x - y) \overline{\psi}(y) \overline{\tau} \gamma_5 \psi(y) d^4 y , \qquad (20)$$

$$\vec{\rho}_{\nu}(x) = g_{\rho} \int D_{\rho}(x-y)\overline{\psi}(y)\overline{\tau}\gamma_{\nu}\psi(y)d^{4}y + \frac{f_{\rho}}{2M} \int D_{\rho}(x-y)\partial^{\mu}[\overline{\psi}(y)\overline{\tau}\sigma_{\mu\nu}\psi(y)]d^{4}y ,$$
(21)

$$\omega_{\nu}(x) = g_{\omega} \int D_{\omega}(x-y)\overline{\psi}(y)\gamma_{\nu}\psi(y)d^{4}y.$$
⁽²²⁾

 $D_i(z)$ is the retarded propagator of the Klein-Gordon equation

$$D_{i}(z) = \frac{1}{2\pi} \Theta(z) \delta(z_{\mu} z^{\mu}) - \frac{m_{i}}{4\pi} \frac{\Theta(z_{\mu} z^{\mu})}{(z_{\mu} z^{\mu})^{1/2}} \Theta(z) J_{1}(m_{i}(z_{\mu} z^{\mu})^{1/2}).$$

Here $\Theta(z)$ is the unit step function defined by

$$\Theta(z) = \begin{cases} 1, & z_0 > 0 \\ 0, & z_0 < 0. \end{cases}$$

 J_1 (z) is the Bessel function of integer order, while m_i defines the mass of the propagating meson.

With the aid of the explicit expression of the meson field operators (19) to (22) it is possible to eliminate the meson fields in the Dirac equation (11):

$$(-i\gamma_{\mu}\partial_{1}^{\mu} + M)\psi(x_{1}) = g_{\sigma}^{2} \int D_{\sigma}(x_{1} - x_{2})\overline{\psi}(x_{2})\psi(x_{2})d^{4}x_{2}\psi(x_{1}) - g_{\pi}^{2}\overline{\tau}_{1}\cdot\overline{\tau}_{2} \int D_{\pi}(x_{1} - x_{2})\overline{\psi}(x_{2})\gamma_{5}\psi(x_{2})d^{4}x_{2}\gamma_{5}\psi(x_{1}) - g_{\rho}^{2}\overline{\tau}_{1}\cdot\overline{\tau}_{2} \int D_{\rho}(x_{1} - x_{2})\overline{\psi}(x_{2})\gamma^{\nu}\psi(x_{2})d^{4}x_{2}\gamma_{\nu}\psi(x_{1}) - g_{\omega}^{2} \int D_{\omega}(x_{1} - x_{2})\overline{\psi}(x_{2})\gamma^{\nu}\psi(x_{2})d^{4}x_{2}\gamma_{\nu}\psi(x_{1}).$$
(23)

Additional pieces from tensor couplings have been omitted here for simplicity. This Dirac equation leads to the Hamiltonian in nucleon space

$$H \equiv H^{N} = \int_{x_{1}^{0} = i}^{\infty} \overline{\psi}(x_{1})(-i\,\vec{\gamma}\cdot\vec{\nabla}_{1}+M)\psi(x_{1})d^{3}x_{1} + \frac{1}{2}\sum_{i=\sigma, \pi, \rho, \omega}^{\infty} g_{i}^{2}(\vec{\tau}_{1}\cdot\vec{\tau}_{2})^{T_{i}}\int_{x_{1}^{0} = i}^{\infty} \overline{\psi}(x_{1})\overline{\psi}(x_{2})\Gamma_{i}(1,2)D_{i}(x_{1}-x_{2})\psi(x_{2})\psi(x_{1})d^{3}x_{1}d^{4}x_{2}.$$
(24)

 $T_i = 0, 1$ indicates the isospin of the mesons, while the Γ_i denote Dirac matrices

$$\Gamma_{\sigma}(1,2) = -1,$$
(25)

$$\Gamma_{\sigma}(1,2) = \gamma_{\sigma}(1)\gamma_{\sigma}(2).$$
(26)

$$\Gamma_{n}(1,2) = \gamma_{\nu}(1)\gamma^{\nu}(2).$$
(20)
$$\Gamma_{0,\nu}(1,2) = \gamma_{\nu}(1)\gamma^{\nu}(2).$$
(27)

The $\psi(x)$ and $\psi^{\dagger}(x)$ are expanded in a complete set of functions. The stationary solutions for the nucleon fields can then be written:

$$\psi(x) = \sum_{\alpha} f_{\alpha}(\vec{x}) e^{-iE_{\alpha}t} b_{\alpha} + \sum_{\alpha} g_{\alpha}(\vec{x}) e^{iE_{\alpha}t} d_{\alpha}^{\dagger}, \qquad (28)$$

$$\psi^{\dagger}(\mathbf{x}) = \sum_{\alpha} f^{\dagger}_{\alpha}(\vec{\mathbf{x}}) e^{i E_{\alpha} t} b^{\dagger}_{\alpha} + \sum_{\alpha} g^{\dagger}_{\alpha}(\vec{\mathbf{x}}) e^{-i E_{\alpha} t} d_{\alpha}.$$
⁽²⁹⁾

 $f_{\alpha}(\vec{\mathbf{x}})$ and $g_{\alpha}(\vec{\mathbf{x}})$ are complete sets of Dirac spinors in coordinate space. b_{α} and b_{α}^{\dagger} are annihilation and creation operators for nucleons in the state α , respectively. d_{α} and d_{α}^{\dagger} are annihilation and creation operators for antinucleons in the state α , respectively.

Now the expansions (28, (29) and the retarded propagator are inserted into the Hamilton operator (24) and we obtain

$$H = \sum_{\alpha,\alpha'} \int f_{\alpha'}^{\dagger} (\vec{\mathbf{x}}) (-i \gamma^{0} \vec{\gamma} \cdot \vec{\nabla} + \gamma_{0} M) f_{\alpha}(\vec{\mathbf{x}}) d^{3} \mathbf{x} \ b_{\alpha'}^{\dagger} \ b_{\alpha}$$

$$+ \frac{1}{2} \sum_{\alpha,\alpha',\beta,\beta'} \int f_{\alpha'}^{\dagger} (\vec{\mathbf{x}}_{1}) f_{\beta'}^{\dagger} (\vec{\mathbf{x}}_{2}) V_{\alpha,\alpha'} (|\vec{\mathbf{x}}_{1} - \vec{\mathbf{x}}_{2}|) f_{\beta}(\vec{\mathbf{x}}_{2}) f_{\alpha}(\vec{\mathbf{x}}_{1}) d^{3} x_{1} d^{3} x_{2} \ b_{\alpha'}^{\dagger} \ b_{\beta} \ b_{\alpha}, \qquad (30)$$

$$V_{\alpha,\,\alpha'}\left(\left|\vec{x}_{1}-\vec{x}_{2}\right|\right) \equiv V_{\alpha,\,\alpha'}(r) = \sum_{i=\sigma_{i},\,\pi_{i},\,\rho,\,\omega} \frac{g_{i}^{\,2}}{4\pi} \left(\vec{\tau}_{1}\cdot\vec{\tau}_{2}\right)^{\tau_{i}} \gamma_{0}(1)\gamma_{0}(2) \Gamma_{i} \left(1,\,2\right) \frac{\exp\left\{-r\left[m_{i}^{\,2}-\left(E_{\alpha}-E_{\alpha'}\right)^{2}\right]^{1/2}\right\}}{r} \right). \tag{31}$$

Terms with antiparticle annihilation or creation operators have been omitted since they are of no interest in this work. Furthermore, it is noted that the potentials are energy dependent (state dependent), which is a consequence of retardation. If meson-nucleon vertex form factors of the type

$$F_{i}(q) = \left(\frac{\Lambda_{i}^{2}}{\Lambda_{i}^{2} - q^{2}}\right)^{1/2}, \quad i = \sigma, \pi, \rho, \omega$$
(32)

are introduced, the Hamiltonian in coordinate space is of the same form as Eq. (30), but with a modified potential:

$$V_{\alpha, \alpha'}(r) = \sum_{i = \sigma, \pi, \rho, \omega} \frac{g_i^2}{4\pi} \frac{\Lambda^2}{\Lambda^2 - m_i^2} (\tilde{\tau}_1 \cdot \tilde{\tau}_2)^{T_i} \gamma_0(1) \gamma_0(2) \Gamma_i(1, 2) \\ \times \left(\frac{\exp\{-r[m_i^2 - (E_\alpha - E_{\alpha'})^2]^{1/2}\}}{r} - \frac{\exp\{-r[\Lambda^2 - (E_\alpha - E_{\alpha'})^2]^{1/2}\}}{r} \right).$$
(33)

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The potentials of GTG and EHM involve different meson-nucleon form factors. The form factors of GTG are of the form

$$F(\mathbf{\ddot{q}}) = \frac{\Lambda^2}{\Lambda^2 + \mathbf{\ddot{q}}^2} , \qquad (34)$$

where Λ is the cutoff mass. The fact that

$$F(\mathbf{\dot{q}}=0)=1 \tag{35}$$

is convenient for nuclear physics purposes, since normally q^2 is small compared to Λ^2 , so that the effect of the form factor is small.

EHM use different form factors for the various mesons. Their form factors have the following structure:

$$F_{\alpha}(q) = \left(\frac{\Lambda_{\alpha}^{2} - m_{\alpha}^{2}}{\Lambda_{\alpha}^{2} - q^{2}}\right)^{n}$$
(36)

normalized at the meson poles $q^2 = m_{\alpha}^2$, with n = 1 for $\alpha = \pi, \eta, \sigma, \delta$ and $n = \frac{3}{2}$ for $\alpha = \rho, \omega, \phi$. In order to compare the OBEP of GTG and EHM we introduce "renormalized" EHM coupling constants defined by

$$\frac{g_{\alpha}^{2}}{4\pi} F_{\alpha}^{2}(q) = \frac{g_{\alpha}^{2}}{4\pi} \left(\frac{\Lambda_{\alpha}^{2} - m_{\alpha}^{2}}{\Lambda_{\alpha}^{2}} \right)^{2n} \left(\frac{\Lambda_{\alpha}^{2}}{\Lambda_{\alpha}^{2} - q^{2}} \right)^{2n}$$
$$= \frac{g_{R_{\alpha}}^{2}}{4\pi} \left(\frac{\Lambda_{\alpha}^{2}}{\Lambda_{\alpha}^{2} - q^{2}} \right)^{2n} .$$
(37)

The connection between $F_i(q)$ of Eq. (32) and the form factors used in the OBEP is easily made by expanding in powers of q^2 / Λ^2 for $q^2 \ll \Lambda^2$.

III. RELATIVISTIC HARTREE-FOCK METHOD FOR NUCLEI WITH CLOSED SHELLS

In order to obtain approximate solutions for the Hamilton operator (30), the Hartree-Fock approach will be discussed in this section. First the expectation value of the ground state energy is calculated for nuclei with an equal number of neutrons and protons. As the approximate state vector for the A nucleons we take

$$|\Psi\rangle = b^{\dagger}_{\alpha_1} b^{\dagger}_{\alpha_2} \cdots b^{\dagger}_{\alpha_A} |0\rangle, \qquad (38)$$

where $\alpha_1, \ldots, \alpha_A$ denote the single-particle orbits and $|0\rangle$ is the vacuum. Single-particle energies and wave functions are then generated by minimization of the ground state energy in the Hartree-Fock approximation. We start from

$$= \langle \Psi | H | \Psi \rangle$$

$$= \sum_{\alpha=1}^{A} \int f_{\alpha}^{\dagger}(\vec{\mathbf{x}}) (-i\gamma^{0}\vec{\gamma} \cdot \vec{\nabla} + \gamma^{0}M) f_{\alpha}(\vec{\mathbf{x}}) d^{3}x + \frac{1}{2} \sum_{\alpha, \alpha'=1}^{A} \int f_{\alpha}^{\dagger}(\vec{\mathbf{x}}_{1}) f_{\alpha}^{\dagger}(\vec{\mathbf{x}}_{2}) V_{\alpha, \alpha'}(|\vec{\mathbf{x}}_{1} - \vec{\mathbf{x}}_{2}|) f_{\alpha}(\vec{\mathbf{x}}_{1}) f_{\alpha'}(\vec{\mathbf{x}}_{2}) d^{3}x_{1} d^{3}x_{2}$$

$$- \frac{1}{2} \sum_{\alpha, \alpha'=1}^{A} \int f_{\alpha'}^{\dagger}(\vec{\mathbf{x}}_{1}) f_{\alpha}^{\dagger}(\vec{\mathbf{x}}_{2}) V_{\alpha, \alpha'}(|\vec{\mathbf{x}}_{1} - \vec{\mathbf{x}}_{2}|) f_{\alpha}(\vec{\mathbf{x}}_{1}) f_{\alpha'}(\vec{\mathbf{x}}_{2}) d^{3}x_{1} d^{3}x_{2}, \qquad (39)$$

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where the spinors $f_{\alpha}(\vec{\mathbf{r}})$ are given by⁸

$$f_{\alpha}(\mathbf{\hat{r}}) = \begin{pmatrix} \frac{iG_{n1j}(r)}{r} & \varphi_{1jm}(\hat{r}) \\ \frac{F_{n1j}(r)}{r} & \overline{\sigma} \cdot \mathbf{\hat{r}} \varphi_{1jm}(\hat{r}) \end{pmatrix} \xi_{1/2,\lambda}, \quad (40)$$

with

$$\varphi_{IJm}(\vec{\mathbf{r}}) = \sum_{m_{I}, \mu} (lm_{I} \frac{1}{2} \mu | jm) Y_{Im_{I}}(\hat{r}) \chi_{1/2, \mu}.$$
(41)

Here $\xi_{1/2}$ and $\chi_{1/2}$ are the isospin and spin wave functions, respectively. Explicit calculation of the expectation value of Eq. (39) is given in Appendix A. Single-particle wave functions and energies are obtained by requiring that independent variation of $F_{\alpha}(r)$ and $G_{\alpha}(r)$ under the restriction

$$N = \int f_{\alpha}^{\dagger}(\vec{\mathbf{r}}) f_{\alpha}(\vec{\mathbf{r}}) d^{3}r$$
$$= \int \left[G_{\alpha}^{2}(r) + F_{\alpha}^{2}(r) \right] dr = 1$$
(42)

leaves the expectation value of the Hamilton oper-

ator stationary:

$$\delta \langle \Psi | H | \Psi \rangle + \epsilon \, \delta N = 0. \tag{43}$$

The resulting Hartree-Fock equations for closed shell N = Z nuclei are

$$\frac{dF_{a_1}(r_1)}{dr_1} = G_{a_1}(r_1) [M - E_{a_1} + Y^{\sigma}_{a_1}(r_1) + Y^{\omega}_{a_1}(r_1) + Y^{\rho}_{a_1}(r_1)] + F_{a_1}(r_1) \left[\frac{\kappa_1}{r_1} + \tilde{Y}^{\sigma}_{a_1}(r_1) + \tilde{Y}^{\omega}_{a_1}(r_1) + \tilde{Y}^{\rho}_{a_1}(r_1) \right] + W^{\sigma}_{a_1}(G, r_1) + W^{\sigma}_{a_1}(F, r_1) + W^{\omega}_{a_1}(G, r_1) + W^{\rho}_{a_1}(G, r_1) + \tilde{W}^{\omega}_{a_1}(F, r_1) + \tilde{W}^{\rho}_{a_1}(F, r_1), \quad (44)$$

$$\frac{dG_{a_1}(r_1)}{dr_1} = F_{a_1}(r_1)[M + E_{a_1} + Y^{\sigma}_{a_1}(r_1) - Y^{\omega}_{a_1}(r_1) - Y^{\rho}_{a_1}(r_1)]
- G_{a_1}(r_1) \left[\frac{\kappa_1}{r_1} + \tilde{Y}^{\pi}_{a_1}(r_1) + \tilde{Y}^{\omega}_{a_1}(r_1) + \tilde{Y}^{\rho}_{a_1}(r_1) \right]
+ W^{\sigma}_{a_1}(F, r_1) - W^{\pi}_{a_1}(G, r_1) - W^{\omega}_{a_1}(F, r_1)
- W^{\rho}_{a_1}(F, r_1) - V^{\omega}_{a_1}(G, r_1) - V^{\rho}_{a_1}(G, r_1), \quad (45)$$

where

$$K_{a_{1}}^{K}(r_{1}) = \pm m_{K} \frac{g_{K}^{2}}{4\pi} \left[\sum_{a_{2}} (1 - T_{K}) 2(2j_{2} + 1) I_{a_{2},0}^{K}(r_{1}) - (2T_{K} + 1)(2j_{1} + 1) \sum_{L \text{ even}} \hat{L}^{2} \binom{j_{1} \quad j_{1} \quad L}{\left(\frac{1}{2} - \frac{1}{2} \quad 0\right)^{2}} I_{a_{1},L}^{K} \right],$$
(46)

with

$$I_{a,L}^{K}(r_{1}) = \int_{0}^{\infty} dr_{2} j_{L}(im_{K}r_{2})h_{L}^{(+)}(im_{K}r_{2})$$
$$\times [G_{a}^{2}(r_{2}) \mp F_{a}^{2}(r_{2})], \quad K = \sigma, \rho, \omega.$$
(47)

Here a_1 and a_2 denote the quantum numbers nlj, while T_K and m_K are the isospins and masses of the corresponding mesons. The different signs in Eqs. (46) and (47) refer to the σ and (ρ or ω) meson, in that order. j_0 and $h_0^{(+)}$ are the usual spherical Bessel and Hankel functions and $r_{<}(r_{>})$ is the smaller (larger) value of either r_1 or r_2 . The other ingredients Y, W, etc. of the Hartree-Fock equations are given in Appendix B. We note that retardation effects leading to the state dependence of $V_{\alpha,\alpha}$, are absent in the Hartree approximation and lead to corrections of at most 10% (for the lightest meson) in the Fock terms.

In this work we would like to concentrate on the Hartree approximation only and leave the more complicated Fock terms to a forthcoming paper. To obtain the Hartree equation, we start with the

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expectation value without exchange term:

$$\begin{split} \tilde{I} &= \sum_{\alpha=1}^{A} \int f_{\alpha}^{\dagger}(\vec{\mathbf{x}}) (-i\gamma^{0}\vec{\gamma} \cdot \vec{\nabla} + \gamma^{0}M) f_{\alpha}(\vec{\mathbf{x}}) d^{3}x \\ &+ \frac{1}{2} \sum_{\alpha=1}^{A} \int f_{\alpha}^{\dagger}(\vec{\mathbf{x}}_{1}) V_{\alpha}^{\text{Hart}}(\vec{\mathbf{x}}_{1}) f_{\alpha}(\vec{\mathbf{x}}_{1}) d^{3}x_{1} , \end{split}$$

with

$$V_{\alpha}^{\text{Hart}}(\mathbf{\tilde{x}}_{1}) = \sum_{\substack{\alpha'=1\\\alpha\neq\alpha'}}^{A} \int f_{\alpha'}^{\dagger}(\mathbf{\tilde{x}}_{2}) V(|\mathbf{\tilde{x}}_{1} - \mathbf{\tilde{x}}_{2}|) \times f_{\alpha'}(\mathbf{\tilde{x}}_{2}) d^{3}x_{2}.$$
(49)

The Hartree potential is obtained by first summing unrestrictedly over α' and then subtracting for α = α' a term which is averaged over angular momentum projections of the orbit α ,

$$V^{\text{Hart}}(\vec{x}_{1}) = \sum_{\alpha'=1}^{A} \int f_{\alpha}^{\dagger} \cdot (\vec{x}_{2}) V(|\vec{x}_{1} - \vec{x}_{2}|) f_{\alpha} \cdot (\vec{x}_{2}) d^{3}x_{2}$$
$$- \frac{1}{\hat{j}_{\alpha}^{-2}} \sum_{m_{\alpha}} \int f_{\alpha}^{\dagger} (\vec{x}_{2}) V(|\vec{x}_{1} - \vec{x}_{2}|) f_{\alpha}(\vec{x}_{2}) d^{3}x_{2}.$$
(50)

The second term of the potential represents a selfenergy term averaged over spins. Since the full Hartree-Fock equations automatically treat this term correctly, we have chosen to subtract this term in the restricted Hartree framework. This turns out to be a small correction to the dominant term (except for the binding energy per nucleon to be discussed later); Miller³ has neglected this term altogether. The resultant coupled equations for the large and small components are

$$\frac{dF_{a_1}(r)}{dr_1} = [M - E_{a_1} + U_{a_1}^{(+)}(r_1)]G_{a_1}(r_1) + \frac{\kappa_1}{r_1}F_{a_1}(r_1), \qquad (51)$$

$$\frac{dGa_1(r_1)}{dr_1} = [M + E_{a1} + U_{a_1}^{(-)}(r_1)]F_{a_1}(r_1) - \frac{\kappa_1}{m}G_{a_1}(r_1), \qquad (52)$$

with

$$U_{a_{1}}^{(\pm)}(r_{1}) = W_{a_{1}}^{\sigma}(r_{1}) \pm (W_{a_{1}}^{\omega}(r_{1}) + W_{a_{1}}^{\rho}(r_{1}))$$
(53)

and

$$W_{a_{1}}^{\kappa}(r_{1}) = \pm m_{\kappa} \frac{g_{\kappa}^{2}}{4\pi} \left[\sum_{a_{2}} (1 - T_{\kappa}) 2(2j_{a_{2}} + 1) I_{a_{2}}^{\kappa}(r_{1}) - I_{a_{1}}^{\kappa}(r_{1}) \right],$$

$$(k = \sigma, \rho, \omega), \quad (54)$$

where

$$I_{a}^{\kappa}(r_{1}) = \int_{0}^{\infty} dr_{2} j_{0}(im_{K}r_{\zeta})h_{0}^{(*)}(im_{K}r_{\zeta})$$
$$\times [G_{a}^{2}(r_{2}) \mp F_{a}^{2}(r_{2})].$$
(55)

The same notation is used as for the Hartree-Fock equations. We note that the π meson in lowest order does not contribute at all, which we can understand from Eq. (A8) and the remarks beyond (A9). The ρ meson contributes very little, (A14), and (A15). This does not change, if derivative coupling is included, since it involves spin structures of similar type as the π exchange. We note for later purposes that the vector meson contributions enter with different sign in Eqs. (51) and (52).

The method for numerical solution of the Dirac-Hartree equation is presented in Appendix C.

IV. RESULTS AND DISCUSSION OF THE HARTREE CALCULATION FOR NUCLEI

We present first the results of the Hartree calculations for ¹⁶O and ⁴⁰Ca nuclei using the nucleonnucleon interactions of EHM and GTG. In Table II single-particle energies, root mean square radii, and the binding energies per nucleon³ are given for ¹⁶O and ⁴⁰Ca. Experimental data¹¹ are also shown as a guideline. Although in the Hartree approximation the Pauli principle and higher order terms of the type described in Brueckner theory are neglected, the single-particle energies, root mean square radii, and the binding energies per nucleon of the lowest order relativistic Hartree calculations are in qualitative agreement with experimental values, at least in the EHM model. Note that the GTG potential ususally gives underbinding, while this is not so much the case for the EHM potential. We also remark that, by excluding the self-energy term of Eq. (50), E_B/A is raised considerably (by 15% for 40 Ca and 60% for 16 O in the case of EHM, and 20% for 40 Ca and a factor more than 3 for ¹⁶O in the case of GTG), while single-particle energies and rms radii are only moderately affected (less than about 15%). The relativistic model reproduces the correct magnitude of the spin-orbit splitting both in the p and d shell without any free parameter. Although Miller^{3,12} has already discussed that adequately adjusted relativistic OBEP lead to the correct magnitude of the spin-orbit splitting, we find it appropriate to elaborate on this fact from a somewhat different point of view. We transform the two Hartree equations (51) and (52) to a second order equation (of Schrödinger type). With the notation of Appendix C we obtain

TAB.	LE 11. Single-particle energies ($\epsilon_a = E_a - M$), root mean square radii,	and binding energies per nucleon of ¹⁶ O and
⁴⁰ Ca. 7	The experimental data in the last two rows are taken from Ref. 11.	

Element	$\substack{\epsilon_{1s(3/2)}\\(\mathrm{MeV})}$	€µ(3/2) (MeV)	$\epsilon_{1 \neq (1/2)}$ (MeV)	€ 1d (5/2) (MeV)	$\overset{\epsilon_{2s(i/2)}}{(\mathrm{MeV})}$		rms [fm]	E _B /A (MeV)	OBEP
¹⁶ O	-40.8	-19.2	-12.1	•••	•••	• • •	2.3	3.2	EHM ⁷ (Ref. 7)
¹⁶ O	-30.2	-12.1	- 7.7	•••	•••	• • •	2.6	0.5	$GTG^6(Ref. 6)$
⁴⁰ Ca	-58.2	-41.	-35.7	-22.	-11.8	-13.0	3, 0	6.1	EHM ⁷ (Ref. 7)
⁴⁰ Ca	-47.4	-31.4	-27.3	-14.9	- 9.4	- 8.6	3.2	2.8	$GTG^{6}(Ref. 6)$
¹⁶ O	-43 ± 9	-19 ± 2	-12 ± 1	•••	• • •	• • •	2.73	8.0	
⁴⁰ Ca	-50 ± 8	-34	4 ± 5	-14 ± 2	-10 ± 1	-7 ± 1	3. 5	8.5	

$$g''(r) = \left[-\frac{D''(r)}{2D(r)} + \frac{3}{4} \frac{D'^2(r)}{D^2(r)} + \frac{D'(r)}{D(r)} \frac{\kappa}{r} + D(r)H(r) + \frac{l(l+1)}{r^2} \right] g(r) ,$$

where

$$D(r) = 2M + \epsilon_a + U_a^{(-)}(r), \quad H(r) = -\epsilon_a + U_a^{(+)}(r), \quad (56)$$

and

 $\epsilon_a = E_a - M$

is the single-particle energy.

We obtain the following equivalent Schrödinger

$$g''(r) = \left[\frac{l(l+1)}{r^2} + 2M(V_a(r) + V_a^{so}(r) - \epsilon_a)\right]g(r)$$
(57)

with

$$V_{a}(r) = U_{a}^{(+)}(r) + \Delta U_{a}^{(+)}(r), \qquad (58)$$

$$U_{a}^{(+)} = \frac{(U_{a}^{(+)}(r) + \epsilon_{a})}{2M} (U_{a}^{(+)}(r) - \epsilon_{a}) - \frac{D'(r)}{2MD(r)} \frac{1}{r} - \frac{D''(r)}{4MD(r)} + \frac{1}{2M} \frac{3D'^{2}(r)}{4D^{2}(r)} ,$$

(59)

$$V_a^{\rm so}(r) = -\frac{(d/dr)U_a^{(-)}(r)}{2M(M+E_a+U_a^{(-)}(r))} \frac{\vec{1}\cdot\vec{\sigma}}{r} .$$
 (60)

The last three terms in Eq. (59) are negligible. (They are smaller than 4 MeV.) Figure 1 shows the potential $U_{1s(\alpha/2)}^{(+)}(r)$ in comparison with the Woods-Saxon potential for ¹⁶O. $U_{1s(\alpha/2)}^{(+)}(r)$ is somewhat narrower (0.5 fm) and deeper (40 MeV). The two main components of this potential are an attractive part, which originates in the σ -meson exchange and has a depth of 400 MeV, and a repulsive piece of 300 MeV strength from the ω -meson exchange (Fig. 2). The contributions of the other mesons to the Hartree potential are so small com-

pared to the σ and ω meson that they cannot be illustrated in that figure. One consequence of the considerable magnitude and the different signs of the σ and ω meson is that the potential $U_a^{(-)}(r)$ has the enormous strength of 700 MeV. The consequence of this is that the relativistic effects associated with $U^{(-)}$ are large. In Figs. 3-5 the difference between $V_a(r)$ and $U_a^{(*)}(r)$ is shown and compared with the Woods-Saxon potential for ¹⁶O. It is striking that $V_a(r)$ is nearly state independent and similar to the Woods-Saxon potential, whereas the state dependence of the Dirac single-particle potential $U_a^{(+)}(r)$ is considerable. $V_a(r)$ and $U_a^{(+)}(r)$ differ from each other by between 10 and 30 MeV. This shows that relativistic corrections for the single-particle potential are in general not negligible.

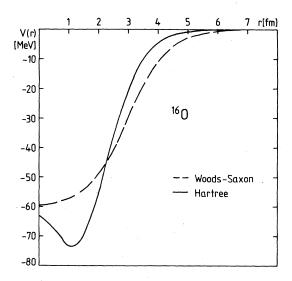


FIG. 1. Comparison between the Woods-Saxon potential and the self-consistent Hartree potential $[U_{1(2)}^{(+)}(r)]$ of the 1s(1/2) state for ¹⁶O. The parameters of the NN interaction are taken from EHM (Ref. 7, Table I), while the Woods-Saxon parameters are given in Eq. (C4).

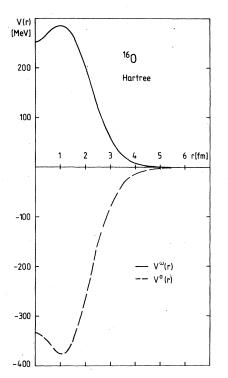


FIG. 2. Contributions of the σ and ω meson to the selfconsistent Hartree potential $U_{1s(1/2)}^{(+)}(r)$ for the 1s(1/2)state of ¹⁶O. The contributions of the other mesons (e.g. ρ meson) are so small that they cannot be illustrated in this figure. The parameters of the NN interaction are taken from EHM (Ref. 7, Table I) again.

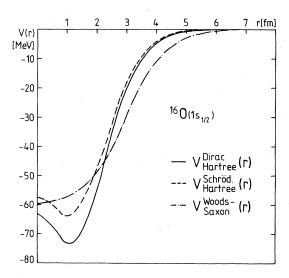


FIG. 3: Comparison between the Schrödinger potential $V_{\text{Hartree}}^{\text{Schröd}}(r) \equiv V_a(r)$ and the Dirac single-particle potential $V_{\text{Hartree}}^{\text{frac}}(r) \equiv V_a^{(+)}(r)$ for the 1s (1/2) level of ¹⁶O. The parameters of the NN interaction are taken from EHM (Ref. 7, Table I).

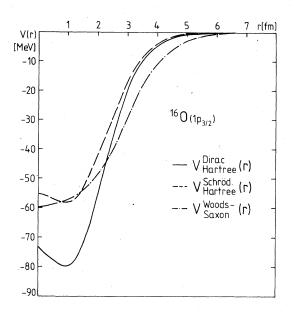


FIG. 4. The same as Fig. 3 for the 1p(3/2) level.

Since $U_a^{(-)}(r)$ has a strength of 700 MeV, the spin-orbit potential is sizable, too, even though the nucleon mass enters twice in the denominator. In the case of the Dirac equation with a Woods-Saxon potential $V_{\rm WS}(r)$ [compare Eqs. (C1) and (C2)] the potential $U_a^{(-)}(r)$ has to be replaced by $V_{\rm WS}(r)$, which is weaker by more than a factor of 10. The spin-orbit splitting reduces to only about 0.2 MeV. Note also that the spin-orbit force is confined to the nuclear surface, as it should be, and that in

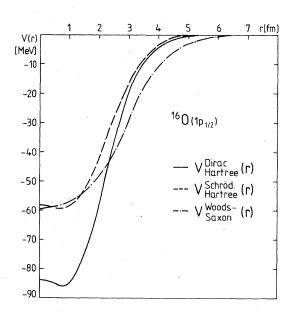


FIG. 5. The same as Fig. 3 for the 1p(1/2) level.

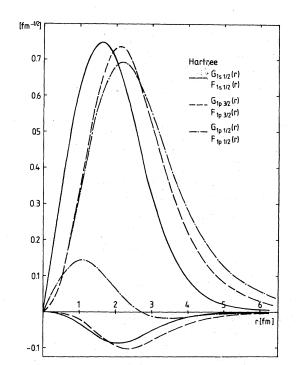


FIG. 6. Radial dependence of the relativistic Hartree wave functions after convergence of the procedure. EHM constants of Table I are taken for this calculation.

the limit $E_a \rightarrow M$, $U_a^{(-)} \ll M$, Eq. (60) reduces to the usual interaction of the Thomas type.

Figure 6 illustrates the wave functions (spinors) for 16 O obtained in the relativistic Hartree model.

Up to now free one-boson-exchange interactions were used as input in a Hartree scheme to describe the relativistic single-particle motion in nuclei. But a realistic description will have to go beyond lowest order OBEP and has to include higher order ladder summations (e.g., in the sense of Brueckner Hartree-Fock theory). In the context of this paper, we shall not touch these problems, but rather make contact, as in Ref. 14, with an effective relativistic boson-exchange interaction introduced by Walecka¹³, who used a relativistic Hartree model of nucleons interacting via exchange of (isoscalar) effective scalar and vector bosons (without form factors) to reproduce the properties of nuclear matter. The coupling strength of the effective scalar and vector bosons is introduced by two parameters

$$c_s = g_s \frac{M}{m_s}$$
 and $c_v = g_v \frac{M}{m_v}$, (61)

where *M* is the nucleon mass, while m_s and m_v are the scalar and vector boson masses, respectively. These parameters are adjusted to reproduce the binding energy $E_B/A = 15.75$ MeV and Fermi momentum $K_F = 1.42$ fm⁻¹ for nuclear matter. The result is

$$c_s^2 = 266.9 \text{ and } c_y^2 = 195.7.$$
 (62)

If we choose

 $m_s = m_{\sigma} = 550 \text{ MeV}$ and $m_v = m_{\omega} = 780 \text{ MeV}$ (63)

and so identify the effective vector boson with the ω meson and the effective scalar boson with the σ meson, although there is no particular reason to do so, we obtain

$$\frac{g_s^2}{4\pi} = 7.3$$
 and $\frac{g_v^2}{4\pi} = 10.8$. (64)

These coupling constants are remarkably close to those used in relativistic free OBEP. Since the masses of the effective scalar and vector meson in Walecka's model are *a priori* not given, the results of the Hartree calculations for ¹⁶O are presented as functions of m_s (Fig. 7) and m_v (Fig. 8) with fixed ratios g_s^2/m_s^2 and g_v^2/m_v^2 . The singleparticle energies depend relatively strongly on the scalar boson mass,¹⁴ while the results are nearly independent of the vector boson mass. But the basic conclusions about the single-particle energies, which we discussed above, remain unchanged.

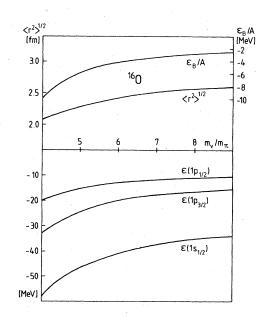


FIG. 7. Single-particle energies (lower section), root mean square radius, and binding energy per nucleon (upper section) of ¹⁶O as function of the mass m_S of the effective scalar boson mass, calculated in a Hartree-Dirac model. Scalar and vector boson exchange parameters have been fixed according to Walecka (Ref. 13) as in Eqs. (61) and (62). For the vector boson mass, $m_V = 783$ MeV was used. This figure is taken from Ref. 14.

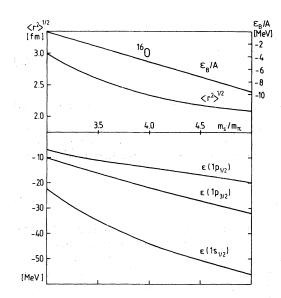


FIG. 8. Single-particle energies (lower section), root mean square radius and binding energy per nucleon (upper section) of ¹⁶O as a function of the mass m_V of the effective vector boson. Again the parameters have been fixed according to Walecka (Ref. 13) [see Eqs. (61) and (62)]. A scalar boson mass of 550 MeV was used.

Finally let us mention that the Hartree and Hartree-Fock procedures of Sec. III converge without form factor. This is an important property, which most of the nonrelativistic Hartree-Fock calculations do not have. In order to get an idea of the effect of form factors in our Hartree scheme we introduced form factors of Eq. (34) for both the scalar and vector boson. Variation of the cutoff parameter Λ between 500 and 1000 MeV lowers the single-particle energies less than 10%. So the results of the Hartree calculations are very insensitive to form factors, if the cutoff parameters are not too small.

V. CONCLUSION

In this paper a relativistic Hamiltonian for nuclei has been developed, and the Hartree and Hartree-Fock equations have been derived. The Hartree equations were applied to ¹⁶O and ⁴⁰Ca nuclei. As input the coupling constants and masses of relativistic (free) OBEP were taken. We were able—surprising enough—to reproduce with this very simple model the single-particle energies and root mean square radii for ¹⁶O and ⁴⁰Ca including the spin-orbit splitting reasonably well without any free parameter. Form factors turned out to be unimportant in this Hartree scheme.

Such Hartree calculations were also performed by Miller,³ who fitted the coupling constants and partly the masses of the mesons to reproduce the binding energies and root mean square radii of several nuclei as well as possible.

Finally we took the effective interaction of Walecka's theory of highly condensed matter. The parameters of this interaction are again quite close to the corresponding ones in the free NN interaction. Therefore we obtained with this effective interaction similar results as with the OBEP. On the basis of these results, namely the qualitative reproduction of single-particle energies already in the Hartree approximation, it might be indicative that there should be a tendecy of cancellation between higher order ladder sums and Fock terms, if relativistic OBEP are used as a starting point. The fact that such a one-boson-exchange potential binds the nucleus already in the simplest Hartree picture is quite surprising (see also Ref. 3); usually "strong core" interactions (such as Reid's soft core potential) do not give binding in lowest order. Such aspects are currently being investigated.

ACKNOWLEDGMENTS

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APPENDIX A: EXPECTATION VALUE OF THE HAMILTON OPERATOR

The expectation value of the kinetic energy for the Hamilton operator (30) yields⁸

$$\begin{split} \langle T \rangle &= \sum_{a_1} 2 \hat{j}_1^2 \int dr_1 \left\{ G_{a_1}(r_1) \left[M G_{a_1}(r_1) - \frac{dF_{a_1}(r_1)}{dr_1} + \frac{\kappa_1}{r_1} F_{a_1}(r_1) \right] \right. \\ &+ F_{a_1}(r_1) \left[\frac{dG_{a_1}(r_1)}{dr_1} + \frac{\kappa_1}{r_1} G_{a_1}(r_1) - M F_{a_1}(r_1) \right] \right\}, \end{split}$$

(A1)

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with

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$$\kappa_1 := \mp (j_1 + \frac{1}{2}) \text{ for } j_1 = l_1 \pm \frac{1}{2},$$
(A2)
$$a_1 := (n_1 l_1 j_1),$$
(A3)

$$\hat{j}_1^2 := 2j_1 + 1.$$

The expectation value of the potential energy, which originates from the direct term of the σ -meson exchange, is given by

$$\langle V_{\sigma}^{D} \rangle = 2 \frac{g_{\sigma}}{4\pi} m_{\sigma} \sum_{a_{1}} \sum_{a_{2}} \hat{j}_{1}^{2} \hat{j}_{1}^{2} \int dr_{1} dr_{2} U_{0}(im_{\sigma}, r_{<}, r_{>}) [G_{a_{1}}^{2}(r_{1}) - F_{a_{1}}^{2}(r_{1})] [G_{a_{2}}^{2}(r_{2}) - F_{a_{2}}^{2}(r_{2})].$$
(A4)

 a_2 is defined analogously to a_1 ; furthermore,

$$U_{L}(im, r_{\varsigma}, r_{\varsigma}) \equiv j_{L}(imr_{\varsigma})h_{L}^{(\star)}(imr_{\varsigma}), \qquad (A5)$$

~

where j_L and $h_L^{(+)}$ are the usual spherical Bessel and Hankel functions and $r_{<}(r_{>})$ is the smaller (larger) value of either r_1 or r_2 .

For the exchange term we obtain

$$\langle V_{\sigma}^{E} \rangle = -\frac{g_{\sigma}^{2}}{4\pi} \sum_{a_{1}} \sum_{a_{2}} \sum_{\substack{p_{1} + e_{2} + L \\ e_{1} + e_{2} + L \\ even}} M_{a_{1}, a_{2}}^{\sigma} \hat{f}_{1} \hat{f}_{2} \hat{f}_{2} \hat{L}^{2} \binom{f_{1}}{1} \hat{f}_{2} L}{\frac{1}{2} - \frac{1}{2} - 0} \right)^{2} \\ \times \int dr_{1} dr_{2} U_{L} (iM_{a_{1}, a_{2}}^{\sigma}, r_{2}, r_{2}) [G_{a_{1}}(r_{1})G_{a_{2}}(r_{1}) - F_{a_{1}}(r_{1})F_{a_{2}}(r_{1})] \\ \times [G_{a_{1}}(r_{2})G_{a_{2}}(r_{2}) - F_{a_{1}}(r_{2})F_{a_{2}}(r_{2})]$$
(A6)

with

 $\langle V_{\bullet}^{D}\rangle = 0$,

$$M_{a_1,a_2}^{\kappa} \equiv \left[m_{\kappa}^2 - (E_{a_1} - E_{a_2})^2\right]^{1/2} \text{ for } K = \sigma, \pi, \omega, \rho.$$
(A7)

In an analogous way the contribution of the π meson is

$$\begin{split} \langle V_{\pi}^{E} \rangle &= -3 \frac{g_{\pi}^{2}}{4\pi} \sum_{a_{1}} \sum_{a_{2}} \sum_{\substack{L \\ I_{1} + I_{2} + L \\ \text{odd}}} M_{a_{1}, a_{2}}^{\pi} \hat{f}_{1}^{2} \hat{f}_{2}^{2} \hat{L}^{2} \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} - \frac{1}{2} & 0 \end{pmatrix}^{2} \\ & \times \int dr_{1} dr_{2} U_{L} (i M_{a_{1}, a_{2}}^{\pi}, r_{<}, r_{>}) [G_{a_{2}}(r_{1}) F_{a_{1}}(r_{1}) + G_{a_{1}}(r_{1}) F_{a_{2}}(r_{1})] \\ & \times [G_{a_{2}}(r_{2}) F_{a_{1}}(r_{2}) + G_{a_{1}}(r_{2}) F_{a_{2}}(r_{2})]. \end{split}$$

One reason for the vanishing of the direct matrix element is that after summation over the angular momentum projection quantum numbers m_1 or m_2 , the matrix element (A8) is zero. Another reason is the isospin 1 of the π meson, since the isospin matrix element of the direct term yields

$$\sum_{\mu_1\mu_2} \langle \xi_{1/2,\mu_1} \xi_{1/2,\mu_2} | \vec{\tau}_1 \cdot \vec{\tau}_2 | \xi_{1/2,\mu_1} \xi_{1/2,\mu_2} \rangle = 0.$$
(A10)

For calculating the expectation values of the ρ - and ω -meson exchange the interaction is divided into two parts:

$$V_{a_1,a_2}^{\rho,\omega}(r) = \overline{V}_{a_1,a_2}^{\rho,\omega}(r) + \overline{\overline{V}}_{a_1,a_2}^{\rho,\omega}(r) , \qquad (A11)$$

with

<u>18</u>

(A8)

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$$\overline{V}_{a_{1},a_{2}}^{\rho,\omega}(r) = \frac{g_{\rho,\omega}^{2}}{4\pi} (\tau_{1} \cdot \tau_{2})^{T_{\rho}}, \omega\gamma_{0}(1)\gamma_{0}(2)\gamma_{0}(1)\gamma_{0}(2) \frac{\exp(-M_{a_{1},a_{2}}^{\rho,\omega} \cdot r)}{r}, \qquad (A12)$$

$$\overline{\overline{V}}_{a_1,a_2}^{\rho,\omega}(r) = \frac{g_{\rho,\omega}^2}{4\pi} (\tau_1 \cdot \tau_2)^{T_{\rho,\omega}} \gamma_0(1) \gamma_0(2) \gamma_k(1) \gamma^k(2) \frac{\exp(-M_{a_1,a_2}^{\rho,\omega} \cdot r)}{r}, \quad k = 1, 2, 3.$$
(A13)

With this notation we get for the expectation values

$$\langle \overline{V}_{\rho}^{D} \rangle = 0, \tag{A14}$$

$$\langle \overline{V}_{\rho}^{D} \rangle = 0$$

$$\langle \overline{V}_{\rho}^{D} \rangle = 0.$$
 (A15)

These expectation values are zero because the ρ meson has isospin one. The second expectation value (A15) is already zero after summation over one of the angular momentum projection quantum numbers m_1 or m_2 . Therefore we conclude that

$$\langle \overline{V}_{\omega}^{D} \rangle = 0. \tag{A16}$$

The remaining direct matrix element yields

$$\langle \overline{V}_{\omega}^{D} \rangle = 2 \frac{g_{\omega}^{2}}{4\pi} m_{\omega} \sum_{a_{1}} \sum_{a_{2}} \hat{j}_{1}^{2} \hat{j}_{2}^{2} \int dr_{1} dr_{2} U_{0}(im_{\omega}, r_{\langle}, r_{\rangle}) \left[G_{a_{1}}^{2}(r_{1}) + F_{a_{1}}^{2}(r_{1}) \right] \left[G_{a_{2}}^{2}(r_{2}) + F_{a_{2}}^{2}(r_{2}) \right].$$
(A17)

Furthermore, we obtain for the remaining exchange terms $(k = \rho, \omega)$

$$\begin{split} \langle \overline{V}_{k}^{E} \rangle &= -(2\,T_{k}+1)\frac{g_{k}^{2}}{4\pi}\sum_{a_{1}}\sum_{a_{2}}\sum_{\substack{I_{1}+I_{2}+L\\ \text{even}}}M_{a_{1},a_{2}}^{k}\hat{j}_{1}\hat{j}_{2}\hat{j}_{2}\hat{L}^{2} \begin{pmatrix} j_{1} & j_{2} & L\\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} \\ & \times \int dr_{1}dr_{2}U_{L}(iM_{a_{1},a_{2}}^{k},r_{<},r_{>})[G_{a_{1}}(r_{1})G_{a_{2}}(r_{1})+F_{a_{1}}(r_{1})F_{a_{2}}(r_{1})] \\ & \times [G_{a_{1}}(r_{2})G_{a_{2}}(r_{2})+F_{a_{1}}(r_{2})F_{a_{2}}(r_{2})], \\ & \overline{\langle \overline{V}_{k}^{E} \rangle} = 2 \cdot (2T_{k}+1)\frac{g_{k}^{2}}{4\pi}\sum_{a_{1}}\sum_{a_{2}}\sum_{\substack{I_{1}+I_{2}+L}}M_{a_{1},a_{2}}^{k}\hat{j}_{1}\hat{j}_{2}\hat{j}_{2}\hat{L}^{2} \end{split}$$

APPENDIX B: INGREDIENTS OF THE HARTREE-FOCK EQUATIONS

The expressions appearing in Eqs. (44) and (45) are given by

$$\tilde{Y}_{a_{1}}^{\pi}(r_{1}) = -6m_{\pi}\hat{j}_{1}^{2} \sum_{L \text{ odd}} \hat{L}^{2} \begin{pmatrix} j_{1} & j_{1} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \int dr_{2} U_{L}(im_{\pi}, r_{\zeta}, r_{>}) G_{a_{1}}(r_{2}) F_{a_{1}}(r_{2}) , \qquad (B1)$$

$$\tilde{Y}_{a_{1}}^{k}(r_{1}) = -2(2T_{k}+1)m_{k}\hat{j}_{1}^{2} \sum_{L \text{ odd}} \hat{L}^{2} \begin{pmatrix} l_{1} & L & \lambda_{1} \\ 0 & 0 & 0 \end{pmatrix}^{2} \int dr_{2}U_{L}(im_{k}, r_{\zeta}, r_{\gamma})G_{a_{1}}(r_{2})F_{a_{1}}(r_{2}) \quad (k=\omega, \rho) , \quad (B2)$$

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$$W_{a_{1}}^{k} \begin{pmatrix} G_{a_{1}}, r_{1} \\ F_{a_{1}} \end{pmatrix} = \mp (2T_{k} + 1) \sum_{a_{2}}' \sum_{\substack{I_{1}+I_{2}+L \\ \text{even}}} M_{a_{1},a_{2}}^{k} \hat{j}_{2}^{2} \hat{L}^{2} \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} \\ \times \frac{G_{a_{2}} (r_{1})}{F_{a_{2}} (r_{1})} \int dr_{2} U_{L} (iM_{a_{1},a_{2}}^{k}, r_{\leq}, r_{>}) [G_{a_{1}}(r_{2})G_{a_{2}}(r_{2}) \mp F_{a_{1}}(r_{2})F_{a_{2}}(r_{2})] \\ (k = \sigma, \omega, \rho). \quad (B3)$$

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The minus sign is referred to as the σ meson. The prime on the summation sign denotes that the summation over a_2 excludes the value a_1 :

$$\begin{split} W_{a_{1}}^{\pi} \begin{pmatrix} G_{a_{1}} & , r_{1} \\ F_{a_{1}} \end{pmatrix} &= -3 \sum_{a_{2}}^{\prime} \sum_{\substack{i_{1}+i_{2}+L \\ i_{0} dd}} M_{a_{1},a_{2}}^{\pi} \hat{j}_{2}^{2} \hat{L}^{2} \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} \\ & \times \begin{pmatrix} G_{a_{2}} & (r_{1}) \\ F_{a_{2}} & (r_{1}) \end{pmatrix} \int dr_{2} U_{L} (iM_{a_{1},a_{2}}^{\pi}, r_{\zeta}, r_{\zeta}) [G_{a_{2}}(r_{2})F_{a_{1}}(r_{2}) + F_{a_{2}}(r_{2})G_{a_{1}}(r_{2})] , \quad (B4) \\ \\ \tilde{W}_{a_{1}}^{k} (F_{a_{1}}, r_{1}) &= -(2T_{k} + 1) \sum_{a_{2}}^{\prime} \sum_{\substack{l \\ i_{1} \neq i_{2} \neq L \\ odd}} M_{a_{1},a_{2}}^{k} j_{2}^{2} L^{2} F_{a_{2}}(r_{1}) \\ & \times \left\{ \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} \int dr_{2} U_{L} (iM_{a_{1},a_{2}}^{k}, r_{\zeta}, r_{\zeta}) F_{a_{1}}(r_{2}) G_{a_{2}}(r_{2}) \\ & + \left[2 \begin{pmatrix} l_{1} & L & \lambda_{2} \\ 0 & 0 & 0 \end{pmatrix}^{2} - \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \right] \right] \\ & \times \int dr_{2} U_{L} (iM_{a_{1},a_{2}}^{k}, r_{\zeta}, r_{\zeta}) F_{a_{2}}(r_{2}) G_{a_{2}}(r_{2}) \\ & (k = \omega, \rho) , \quad (B5) \end{split}$$

$$\begin{split} V_{a_{1}}^{k}(G_{a_{1}},r_{1}) &= -(2T_{k}+1) \sum_{a_{2}} '\sum_{\substack{l \\ l_{1}+l_{2}+L \\ \text{odd}}} M_{a_{1},a_{2}}^{k} j_{2}^{2}L^{2}G_{a_{2}}(r_{1}) \\ & \times \left\{ \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} \int dr_{2}U_{L}(iM_{a_{1},a_{2}}^{k},r_{2},r_{2})G_{a_{1}}(r_{2})F_{a_{2}}(r_{2}) \\ & + \left[2 \begin{pmatrix} l_{2} & L & \lambda_{1} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} - \begin{pmatrix} j_{1} & j_{2} & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^{2} \right] \\ & \times \int dr_{2}U_{L}(iM_{a_{1},a_{2}}^{k},r_{2},r_{2})F_{a_{1}}(r_{2})G_{a_{2}}(r_{2}) \right\} \quad (k = \omega, \rho) \,. \end{split}$$
(B6)

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APPENDIX C: NUMERICAL SOLUTION OF THE RELATIVISTIC HARTREE EQUATIONS

In order to solve the Hartree Eqs. (51) and (52) we have to use trial wave functions as a starting point. "Woods-Saxon spinors" have been chosen for that purpose. They are the solution of the fol-

lowing Dirac equation

$$\frac{dF_{a}(r_{1})}{dr_{1}} + G_{a}(r_{1}) \left[-M - V_{WS}(r_{1}) + E_{a} \right] - \frac{\kappa}{r_{1}} F_{a}(r_{1}) = 0, \quad (C1)$$

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$$\frac{-dG_{a}(r_{1})}{dr_{1}} + F_{a}(r_{1})[M + V_{WS}(r_{1}) + E_{a}] - \frac{\kappa}{r_{1}}G_{a}(r_{1}) = 0, \quad (C2)$$

where we have written to the mass a Woods-Saxon potential:

$$V_{\rm WS}(r) = V_0 \left[1 + \exp\left(\frac{r-c}{t}\right) \right]^{-1} . \tag{C3}$$

Here c is the root mean square radius of the atomic nucleus, while t is the skin thickness of the nucleus and V_0 denotes the strength of the potential. The following parameters of the Woods-Saxon potential for ¹⁶O and ⁴⁰Ca (in parentheses) are taken:

$$V_0 = -60 \text{ MeV} (-85 \text{ MeV}), c = 3 \text{ fm} (4.41 \text{ fm}),$$

t = 0.66 fm (0.6 fm). (C4)

We shall now describe the numerical procedure used to solve Eqs. (C1) and (C2). For this we introduce the following abbreviations:

$$F'(r) = H(r)G(r) + \frac{\kappa}{r} F(r) , \qquad (C5)$$

$$G'(r) = D(r)F(r) - \frac{\kappa}{r} G(r) , \qquad (C6)$$

with

$$H(r) = M - E_a + V_{\rm WS}(r) , \qquad (C7)$$

$$D(\boldsymbol{r}) = M + E_a + V_{WS}(\boldsymbol{r}). \tag{C8}$$

The two differential equations of first order are equivalent to one differential equation of second order,

$$G''(r) = \frac{D'(r)}{D(r)} G'(r) + \left[-\frac{D'(r)}{D(r)} \frac{\kappa}{r} - D(r)H(r) - \frac{l(l+1)}{r^2} \right] G(r) = 0.$$
(C9)

In order to eliminate the first derivative of G(r), we transform

$$G(r) \equiv [D(r)]^{1/2}g(r)$$
 (C10)

and obtain the following differential equation for g(r):

$$g''(r) = \left[-\frac{D''(r)}{2D(r)} + \frac{3}{4} \frac{D'^{2}(r)}{D^{2}(r)} + \frac{D'(r)}{D(r)} \frac{\kappa}{r} + D(r)H(r) + \frac{l(l+1)}{r^{2}} \right] g(r) .$$
(C11)

This differential equation has been solved with the method of Noumerov.⁹ From g(r) we obtain the solutions of the Dirac equation by the following

transformations:

$$G(r) = [D(r)]^{1/2}g(r) ,$$

$$F(r) = \frac{G'(r) + (\kappa/r)G(r)}{D(r)}$$

With the Woods-Saxon parameters (C4) the following single-particle energies for 16 O were obtained:

$$\epsilon_{1s(1/2)} = -36.0 \text{ MeV},$$

 $\epsilon_{1p(3/2)} = -19.7 \text{ MeV},$ (C12)
 $\epsilon_{1p(1/2)} = -19.4 \text{ MeV}.$

The small spin-orbit splitting is of pure relativistic origin.

At first the solution of the Hartree equations requires a calculation of the Hartree potentials $W^{\sigma_1,\rho_1}\omega(r)$ with "Woods-Saxon spinors" as trial functions. $W^{\sigma_1,\rho_1}\omega(r)$ are integral functions of the general form

$$Y(x) = Y(x_0) + \int_{x_0}^{x} Y(\xi) d\xi.$$
 (C13)

They have to be calculated at the equally spaced points $x = x_n = x_0 + nh$ $(n = 1, 2 \cdot \cdot \cdot N)$. The calculation of the integral functions at the positions x_n for n = 2, ..., N is performed at best by using the Simpson rule. At the position x_1 the Simpson rule is not applicable. Here a combination of the $\frac{3}{8}$ rule and the Simpson rule is suitable¹⁰:

$$Y(x_1) = Y(x_0) + \frac{h}{48} \left[17y(x_0) + 42y(x_1) - 16y(x_2) + 6y(x_3) - y(x_4) \right].$$
 (C14)

Now we introduce the following abbreviations:

$$U_{a}^{(\pm)} = W_{a}^{\sigma} \pm (W_{a}^{\omega} + W_{a}^{\rho}).$$
 (C15)

If the potentials $U_a^{(*)}$ and $U_a^{(-)}$ are calculated, we can solve the Hartree equations (51) and (52) with the same method that we used for the solution of the Dirac equation with Woods-Saxon potential. There is only one difference in the definition of the quantities H(r) and D(r). For the solution of the Hartree equations we define

$$H(r) = M - E + U^{(+)}(r) ,$$

$$D(r) = M + E + U^{(-)}(r)$$
(C16)

instead of

$$H(r) = M - E + V_{WS}(r) ,$$

$$D(r) = M + E + V_{WS'}(r)$$
(C17)

as we defined for calculating the solution of the Dirac equation with Woods-Saxon potential. Then the Hartree equations (51) and (52) are solved with the method of Noumerov in successive steps.

This procedure converges in about ten iterations.

Then the difference between the sums of the singleparticle energies for successive iterations is smaller than 0.01 MeV for ¹⁶O and 0.1 MeV for ⁴⁰Ca, respectively. Furthermore, it is noted that the results of the Hartree calculations are independent of the trial wave functions. This was tested by first taking "Woods-Saxon spinors" for ¹⁶O as trial wave functions. Another time the $1s(\frac{1}{2})$. $1p(\frac{3}{2})$, and $1p(\frac{1}{2})$ "Woods-Saxon spinors" for ⁴⁰Ca were taken as trail functions. In both cases we obtained the same results for the Hartree equations. Furthermore, we mention that it has been possible to test the complicated program for the numerical solution of the Hartree equations, since there exists a relativistic Hartree calculation of Miller.³ Miller has fitted the coupling constants and partly the masses of the mesons in order to reproduce the binding energies per nucleon, the

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root mean square radii, and the single-particle energies of several nuclei as well as possible. He solved the relativistic Hartree equations with the procedure of Runge-Kutta while in this work the method of Noumerov was used. Moreover, the integral functions

$$Y(x) = Y(x_0) + \int_{x_0}^{x} Y(\xi) d\xi$$
 (C18)

were calculated with different methods. Nevertheless Miller's results have been reproduced with the methods described in this work. This supports the correctness of both numerical procedures and both computer programs.

Finally it is mentioned that the described numerical method can be easily generalized to provide a procedure to solve the Hartree-Fock equations. This will be discussed in a forthcoming paper.

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