Exchange potentials in relativistic Hartree-Fock theory of closed-shell nuclei*

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The relativistic Hartree formalism for nuclei is extended to include the exchange potentials which result from various kinds of one-boson-exchange interactions. A numerical simplification is presented which uncouples the relativistic Hartree-Fock equations and enables local (though state-dependent) single-particle potentials to be defined for the exchange interactions. Calculations are presented for a vector-scalar nucleon-nucleon force model. Comparison of these calculations with Hartree calculations (using the same model) indicates that the exchange terms contribute a net attraction of about 1.5 MeV per particle in light nuclei, while rms radii are reduced by about 0.03 fm. A study is also made of the exchange potentials resulting from the pseudoscalar part (one-pion-exchange) of the nucleon-nucleon interaction. These terms appear to be important, although self-consistent calculations are not possible in the present framework due to numerical instabilities induced by the pseudoscalar term. The instabilities appear to be related to an incorrect enhancement of the effects of virtual N-$\bar{N}$ pair creation which is present in the coordinate space relativistic one-pion-exchange potential.

[NUCLEAR STRUCTURE ^{16}O, ^{40}Ca, ^{48}Ca; calculated binding energies, eigenvalues, charge radii, exchange potentials. Relativistic Hartree-Fock method, spherical nuclei.]

I. INTRODUCTION

It has recently been shown[1] that a relativistic nucleon-nucleon (N-N) interaction, consisting of potentials obtained from single exchange of vector and scalar mesons, can reproduce the total binding energies, rms charge radii, and single-particle eigenvalue spectra of doubly magic nuclei when used in a relativistic Hartree approximation. The most important characteristic of this N-N model was the large strengths of the resultant vector and scalar potentials. In a nonrelativistic reduction the vector and scalar contributions to the static central potential are of opposite sign, whereas the contributions to the spin-orbit potential, the velocity-dependent potential, etc. are of the same sign. This fact enables the static central (nonrelativistic) potential to be weak (through cancellations between vector and scalar interactions), while the relativistic corrections (spin-orbit etc.) become much stronger than would be expected from an analogy with the electromagnetic interaction. It was, indeed, shown[2] that the good nuclear saturation properties of the calculations presented in Ref. 1 were due to large relativistic corrections to the single-particle kinetic energy expectation values. The strengths of the vector and scalar interactions had completely invalidated the nonrelativistic form for the kinetic energy operator.

Relativistic corrections to the binding energy of nuclear matter have recently been calculated by Brown, Jackson, and Kuo,[3] by Bhakar,[4] and by Richards, Haftel, and Tabakin.[5] The authors of Ref. 3 obtain the relativistic corrections by using a modified form of the Reid soft-core[6] potential which reproduces the experimental N-N phase shifts when used in the Blankenbecler-Sugar[7] equation. The scattering amplitude so obtained obeys a relativistic elastic unitarity relation. These authors note that the relativistic equation for the scattering amplitude is equivalent to the Lippmann-Schwinger equation with an energy-dependent potential. They obtain the relativistic corrections by calculating the binding energy of nuclear matter with the modified energy-dependent potential and comparing it to the result obtained with the nonrelativistic form of the Reid potential. This prescription yields an attractive relativistic correction of 0.5 MeV/A to the binding energy of nuclear matter. The author of Ref. 4 calculated in first-order perturbation theory the expectation value of the Galilean noninvariant potential which, when added to the Tabakin[8] potential, produces a potential which transforms as a relativistic scalar to order $(v/c)^2$. This potential expectation value was then added to the expectation value of the relativistic correction to the kinetic energy operator to obtain the relativistic correction to the binding energy of nuclear matter. This alternate prescription produces a correction of 0.5 MeV/A but of opposite sign to the correction of Ref. 3. The authors of Ref. 5 performed a similar calculation to that of Ref. 3 with the exception that a

different off-shell convention for the modified potential was imposed by including retardation effects in the generalized Yukawa terms. This prescription results in a relativistic correction of 1.4 MeV/A and of opposite sign to that of Ref. 3.

While these calculations reached no firm consensus regarding the sign and size of the relativistic corrections to nuclear-matter binding, they all may be characterized as what is referred to as "minimal" relativistic corrections. Each work starts with a nonrelativistic model of the N-N potential and adds to it a minimal correction which makes the modified interaction satisfy some relativistic property such as Lorentz covariance, relativistic elastic unitarity, or retardation. The relativistic effects for finite nuclei investigated in Refs. 1 and 2 and in the present work are clearly in a different category, which might be characterized as "maximal" relativity inasmuch as the relativistic effects are largely enhanced by building large cancellations between the central static interaction terms.

The strengths of the vector and scalar interactions of Ref. 1 were chosen specifically to produce good nuclear saturation properties. Nevertheless, such cancellations would have to be judged problematical were it not for the fact that they are qualitatively consistent with the vector and scalar interaction strengths found in recent one-boson-exchange analyses[9-13] of the nucleon-nucleon experimental phase shifts.[14,15] It is thus plausible that these relativistic effects play a significant role in determining the saturation properties of nuclei.

The possible importance of relativistic effects (other than spin-orbit) for nuclear physics has been suggested many times before.[16-22] Such suggestions have not been followed up for the nuclear many-body problem because of interest in the effects of two-body and higher-order correlations in nuclei. Still, the inclusion of two-body correlations in many-body calculations has not produced agreement with the experimental saturation properties of nuclei except when at least partly phenomenological effective interactions have been used.[23]

There is no compelling reason to believe that the use of highly relativistic interactions will remove the need for including two-body and possibly higher-order correlations in nuclear many-body calculations. Nevertheless, the complete absence of a computationally practical relativistic many-body theory leads us to consider the Hartree and Hartree-Fock approximations to a relativistic many-body problem. The Hartree approximation was the subject of Ref. 1. There it was shown that only scalar and vector meson exchange could contribute to the relativistic self-consistent interactions. In the present work the formalism is extended to include the Fock or exchange parts of the self-consistent interactions. A numerical simplification of the exchange terms is presented which allows a complete decoupling of the relativistic Hartree-Fock equations. This simplification, which is analogous to a method used by Brueckner and coworkers[24-26] for nonlocal potentials, allows local (though state-dependent) single-particle exchange potentials to be defined corresponding to each type of relativistic two-body interaction. The relativistic situation differs from the nonrelativistic analog in that no momentum-dependent effective potential occurs. The arbitrary length which was interpreted as the range of nonlocality in Refs. 24–26 is thus not present. This formalism is then used to perform relativistic Hartree-Fock calculations for the doubly magic nuclei ^{16}O, ^{40}Ca, and ^{48}Ca using the vector-scalar model of Ref. 1 for the N-N interaction. Comparison of the results with those of Ref. 1 yields an exchange contribution of about 1.5 MeV/A to the total binding energy and about a 0.03 fm reduction in the rms charge radii of these nuclei. Thus, while the vector and scalar exchange contributions are important, they do not drastically alter the saturation properties of these nuclei.

Of perhaps more interest than the vector and scalar exchange terms, are the effects of the pseudoscalar (one-pion-exchange) interaction. This interaction does not contribute at all to the direct potentials for these nuclei. One thus has no prior expectations as to what order of magnitude the exchange terms will be. Preliminary numerical estimates quoted in Ref. 1, which indicated that these terms were small, were erroneous. Perturbation calculations will be presented in this work which show that the one-pion-exchange contribution to the Fock exchange terms might be quite large. Unfortunately, we are not able to go beyond first-order perturbation calculations for these terms in the present formalism. The relativistic Hartree-Fock equations become unstable in the presence of the pseudoscalar terms so that self-consistency is never achieved. The problem is that the coordinate space form (Yukawa function) of the one-pion-exchange potential is not an appropriate form for the interaction between a positive energy and a negative energy plane-wave spinor. Such terms are, however, important for the pseudoscalar interaction because the γ^5 matrix is odd.

II. RELATIVISTIC HARTREE-FOCK THEORY OF NUCLEI

The time-favored metric tensor ($ab = a_0 b_0 - \vec{a}\cdot\vec{b}$) is adopted along with the following representations

for Dirac matrices:

$$\beta=\gamma^0=\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix};\ \vec{\gamma}=\begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix};\quad \vec{\alpha}=\gamma^0\vec{\gamma};$$

$$\gamma^5=\gamma^0\gamma^1\gamma^2\gamma^3=-i\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}. \tag{1}$$

The Dirac γ matrices appropriate to spherical coordinates will also be used. These will be introduced as tensor transformations upon the representation shown in Eq. (1).

The basis of the present work, as in Ref. 1, is the static, relativistic, coordinate-space form of the one-boson-exchange potentials for scalar, vector, and pseudoscalar mesons,

$$V_s=-(\vec{\tau}_1\cdot\vec{\tau}_2)^{I_s}\gamma_1^0\gamma_2^0 J_s(|\vec{r}_1-\vec{r}_2|), \tag{2}$$

$$V_v=(\vec{\tau}_1\cdot\vec{\tau}_2)^{I_v}\gamma_1^0\gamma_2^0\gamma_1^\mu\gamma_{2\mu}J_v(|\vec{r}_1-\vec{r}_2|), \tag{3}$$

$$V_{ps}=(\vec{\tau}_1\cdot\vec{\tau}_2)^{I_{ps}}\gamma_1^0\gamma_2^0\gamma_1^5\gamma_2^5 J_{ps}(|\vec{r}_1-\vec{r}_2|). \tag{4}$$

The factor $(\vec{\tau}_1\cdot\vec{\tau}_2)^I$ establishes the isospin dependence of the interaction for isovector ($I=1$) and isoscalar ($I=0$) mesons. The subscripts 1 and 2 denote the two interacting particles.

The functions $J(|\vec{r}_1-\vec{r}_2|)$ may be thought of as Yukawa functions,

$$J(r)=e^{-\mu r}/r, \tag{5}$$

where the quantity μ is the meson mass in units of inverse length ($\mu=mc/\hbar$). In practice the following form will be used for J:

$$J(r)=[\Lambda^2/(\Lambda^2-\mu^2)]^2(e^{-\mu r}/r-e^{-\Lambda r}$$

$$\times\{1+[(\Lambda^2-\mu^2)/2\Lambda]r\}/r). \tag{6}$$

This form results from including a meson-nucleon form factor,[9,27] of the form:

$$F(q^2)=\Lambda^2/(\Lambda^2-q^2). \tag{7}$$

In nonrelativistic one-boson-exchange calculations the form factor serves the function of removing r^{-3} singularities in the tensor and spin-orbit forces. No such singularities arise in the present formalism; however, the form factors are retained since nucleons appear to have a definite spatial extension.

The model N-N interaction consists of the sum of terms like those of Eqs. (2)–(4), weighted by the meson-nucleon coupling constants of the model,

$$V(|\vec{r}_1-\vec{r}_2|)=\sum_s g_s^2\hbar c V_s+\sum_v g_v^2\hbar c V_v+\sum_{ps} g_{ps}^2\hbar c V_{ps}. \tag{8}$$

The relativistic Hartree-Fock equations for a set of occupied nucleon states $\{\phi_i\}$, may be written in terms of the N-N interaction,

$$(c\vec{\alpha}\cdot\vec{p}+\beta Mc^2)\phi_i(\vec{r}_1)+\sum_{j=1}^{A}\int\phi_j^\dagger(\vec{r}_2)V(|\vec{r}_1-\vec{r}_2|)\phi_j(\vec{r}_2)d^3r_2\phi_i(\vec{r}_1)$$

$$-\sum_{j=1}^{A}\int\phi_j^\dagger(\vec{r}_2)V(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2\phi_j(\vec{r}_1)=E_i\phi_i(\vec{r}_1). \tag{9}$$

It was shown in Ref. 1 that only the scalar and the zeroth component of the vector interactions contribute to the direct potential in Eq. (9) when closed-shell nuclei are considered. Our present interest is with the exchange terms which were not calculated in Ref. 1. The nonlocal exchange potential can be converted to local form (for the purposes of Hartree-Fock iteration) by multiplying and dividing by $\phi_i^\dagger(\vec{r}_1)\phi_i(\vec{r}_1)$,

$$U_{ex}^i(\vec{r}_1)=-\sum_{j=1}^{A}\int\phi_j^\dagger(\vec{r}_2)V(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2\{\phi_j(\vec{r}_1)\phi_i^\dagger(\vec{r}_1)\}/\phi_i^\dagger(\vec{r}_1)\phi_i(\vec{r}_1). \tag{10}$$

This potential, although local, appears to depend upon all the quantum numbers of the state i. If, however, we are restricted to closed-shell nuclei, the dependence upon the magnetic quantum number is illusory. Such dependence would violate the spherical symmetry which holds for the Hartree-Fock solutions for closed-shell nuclei. One can thus sum independently both the numerator and denominator of the right-hand

side of Eq. (10) over m_i to obtain

$$U^i_{ex}(\vec{r}_1) = -\frac{\sum_{m_i}\sum_{j=1}^{A}\int \phi_j^\dagger(\vec{r}_2)V(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2\{\phi_j(\vec{r}_1)\phi_i^\dagger(\vec{r}_1)\}}{\sum_{m_i}\phi_i^\dagger(\vec{r}_1)\phi_i(\vec{r}_1)}. \tag{11}$$

One notes that the term $\{\phi_j(\vec{r}_1)\phi_i^\dagger(\vec{r}_1)\}$ in Eqs. (10) and (11) is a 4×4 matrix. To handle this term we note the general expansion

$$M=\frac{1}{4}\sum_A \mathrm{Tr}(M\gamma_A)\gamma^A, \tag{12}$$

and obtain

$$\{\phi_j(\vec{r}_1)\phi_i^\dagger(\vec{r}_1)\}=\frac{1}{4}\sum_A [\phi_i^\dagger(\vec{r}_1)\gamma_A\phi_j(\vec{r}_1)]\gamma^A. \tag{13}$$

The matrices γ^A are the 16 linearly independent matrices formed from products of the four Dirac matrices γ^μ. These matrices can be grouped into five categories; scalar (I), vector (γ^μ), pseudoscalar ($\gamma^5=\gamma^0\gamma^1\gamma^2\gamma^3$), pseudovector ($\gamma^5\gamma^\mu$), and tensor $[\sigma^{\mu\nu}=(1/2i)(\gamma^\mu\gamma^\nu-\gamma^\nu\gamma^\mu)]$. The names of the categories signify the tensor transformation properties of the various current densities that can be formed from these matrices.

Using these properties for the exchange potentials, one obtains the most general local single-particle Dirac equation for the relativistic Hartree-Fock equation,

$$\{c\vec{\alpha}\cdot\vec{p}+\beta[Mc^2+U_s(\vec{r})+g_{\mu\nu}\gamma^\mu U_v^\nu(\vec{r})+\gamma^5 U_{ps}(\vec{r}) + g_{\mu\nu}\gamma^5\gamma^\mu U_a^\nu(\vec{r})+g_{\alpha\beta}g_{\gamma\delta}\sigma^{\alpha\gamma}U_t^{\beta\delta}(\vec{r})]\}\phi_i(\vec{r}) = E_i'\phi_i(\vec{r}). \tag{14}$$

The functions $U_s(\vec{r})$, $U_v^\mu(\vec{r})$, $U_{ps}(\vec{r})$, $U_a^\mu(\vec{r})$, and $U_t^{\mu\nu}(\vec{r})$ are referred to as the scalar, vector, pseudoscalar, pseudovector, and tensor relativistic single-particle potentials, respectively, for the Dirac equation. Before going on to the specific expressions for these potentials, it is instructive to consider the simplifications resulting from the restriction to closed-shell nuclei. For this case, the single-particle nucleon states are states of good total angular momentum and parity. The relativistic single-particle potential must then commute with the total angular momentum and parity operators,

$$[U(\vec{r}),\vec{J}]=[U(\vec{r}),P]=0, \tag{15}$$

where U is the total relativistic single-particle potential,

$$U(\vec{r})=\beta[U_s(\vec{r})+g_{\mu\nu}\gamma^\mu U_v^\nu(\vec{r})+\gamma^5 U_{ps}(\vec{r}) + g_{\mu\nu}\gamma^5\gamma^\mu U_a^\nu(\vec{r})+g_{\alpha\beta}g_{\gamma\delta}\sigma^{\alpha\gamma}U_t^{\beta\delta}(\vec{r})], \tag{16}$$

and $\vec{J}$ and P are the usual relativistic single-particle total angular momentum and parity operators

$$\vec{J}=\vec{r}\times\vec{p}+\frac{\hbar}{2}\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}, \tag{17}$$

and

$$P=\beta P_0$$

(P_0 is the nonrelativistic parity operator). It is well known that the vanishing of the commutators in Eq. (15) requires the scalar and the zeroth component of the vector potentials to be angle-independent,

$$U_s(\vec{r})=U_s(r),\qquad U_v^0(\vec{r})=U_v^0(r). \tag{18}$$

These equations also require the pseudoscalar and pseudovector single-particle potentials to vanish; however, radial components of the two 3-vectors, $U_v^j(\vec{r})$ and $U_t^{0j}(r)$, $j=1, 2, 3$, may still contribute. These radial components are denoted $U_v^r(r)$ and $U_t^r(r)$ for the vector and tensor potentials respectively.

The single-particle relativistic potential thus has the form,

$$U(r)=\beta[U_s(r)+\gamma^0U_v^0(r)-\gamma^rU_v^r(r)-\gamma^0\gamma^rU_t^r(r)]. \tag{19}$$

The symbol γ^r is the radial Dirac γ matrix and has the expected form

$$\gamma^r=\begin{pmatrix}0 & \sigma_r\\ -\sigma_r & 0\end{pmatrix}. \tag{20}$$

A Dirac wave function with good J^2, J_z, and parity as well as time reversal symmetry has the fol-

lowing form:

$$\phi(\vec{r})=\frac{1}{r}\begin{pmatrix} F_J^{\tilde{\omega}}(r)\mathcal{Y}_{Jm}^{\tilde{\omega}}(\theta,\phi) \\ iG_J^{\tilde{\omega}}(r)\mathcal{Y}_{Jm}^{-\tilde{\omega}}(\theta,\phi)\end{pmatrix}, \tag{21}$$

where $F(r)$ and $G(r)$ are the large and small component radial wave functions, respectively. These are real functions. The $\mathcal{Y}_{Jm}^{\tilde{\omega}}$ are functions of spin and angular variables,

$$\mathcal{Y}_{Jm}^{\tilde{\omega}}(\theta,\phi)=\left\langle J+\frac{\tilde{\omega}}{2},\tfrac{1}{2},m-\tfrac{1}{2},\tfrac{1}{2}\middle|Jm\right\rangle \mathcal{Y}_{J+\frac{\omega}{2}\,m-1/2}(\theta,\phi)\begin{pmatrix}1\\0\end{pmatrix}+\left\langle J+\frac{\tilde{\omega}}{2},\tfrac{1}{2},m+\tfrac{1}{2},-\tfrac{1}{2}\middle|Jm\right\rangle \mathcal{Y}_{J+\frac{\omega}{2}\,m+1/2}(\theta,\phi)\begin{pmatrix}0\\1\end{pmatrix}. \tag{22}$$

The quantum number $\tilde{\omega}$ takes the values ±1 and is related to the parity quantum number of ϕ as follows,

$$P=(-1)^{J+\tilde{\omega}/2}. \tag{23}$$

Note that $\tilde{\omega}$ has the opposite sign for the small component spin-angular function. This angular function thus has opposite parity from the spin-angular function of the large component as is required for the relativistic parity, defined by Eq. (17), to be conserved. For discrete single-particle states the nodal quantum number (plus one) of the large component radial wave function $[F(r)]$ may be used to further specify the state. Thus the set of quantum numbers $(n\tilde{\omega}Jm\tau_3)$ completely specify the single-particle nucleon states in the relativistic Hartree-Fock self-consistent potentials. The relativistic spectral notation for single-nucleon states can thus be made completely analogous to the nonrelativistic notation for single-particle states when a spin-orbit potential is present. It must be remembered, however, that this notation rigorously represents only the large component of the relativistic wave function.

Using the wave function of Eq. (21) and an eigenvalue appropriate to a positive energy solution ($E'=Mc^2+E$), the Dirac equation appropriate to rotational, parity, and time reversal invariances can be reduced to radial form:

$$\frac{dG(r)}{dr}=\left\{\frac{i[U_v^\tau(r)+U_t^\tau(r)]}{\hbar c}+\frac{\tilde{\omega}(J+\frac{1}{2})}{r}\right\}G(r)+\left[\frac{U_s(r)+U_v^0(r)-E_i}{\hbar c}\right]F(r), \tag{24}$$

and

$$\frac{dF(r)}{dr}=\left\{\frac{i[U_v^\tau(r)-U_t^\tau(r)]}{\hbar c}-\frac{\tilde{\omega}(J+\frac{1}{2})}{r}\right\}F(r)+\left[\frac{2Mc^2+U_s(r)-U_v^0(r)+E_i}{\hbar c}\right]G(r). \tag{25}$$

Eqs. (24) and (25) are the basis for numerical solutions to the Dirac equation. One immediately notices in Eqs. (24) and (25) the imaginary unit (i) multiplying the potentials U_v^τ and U_t^τ. This is no cause for concern because it will later be shown that the potentials U_v^τ and U_t^τ are pure imaginary. In fact, one can infer that U_v^τ and U_t^τ are imaginary by requiring the single-particle potential, Eq. (19), to commute with the time reversal operator.

At this point one may note a very unusual property of the potential U_v^τ. If the potentials in Eq. (19) are not state-dependent, then a requirement that $U(r)$ be Hermitian would imply that U_v^τ is real, in contradiction to the requirements of time reversal invariance. Of course, the HF potentials are always state-dependent in such a way that hermiticity is restored even when U_v^τ is purely imaginary. One is left, however, with the curious fact that the state dependence of U_v^τ is absolutely necessary for U_v^τ to represent a physically valid interaction and not just an unfortunate aspect of our Hartree-Fock Method. It is really this curious property of U_v^τ which enables one to replace the nonlocal exchange potential by an equivalent local (state-dependent but momentum-independent) form. Such replacements are not possible in nonrelativistic quantum mechanics. A paper devoted to analyzing these curious properties of U_v^τ and their possible physical consequences is in preparation.[28]

III. REDUCTION OF LOCAL EXCHANGE POTENTIALS

The general form for the local exchange potential resulting from a particular two-body interaction term $[V(|\vec{r}_1-\vec{r}_2|)]$ is given in Eq. (11). One may now reduce this general equation to radial form and obtain the radial single-particle potentials which will actually be used in numerical computations. As the full reduction of these potentials is tedious, the reduction appropriate to

the scalar two-body potential [Eq. (2)] will be sketched and the final results will then be given. The local exchange potentials appropriate for the electrostatic interaction in atomic relativistic Hartree-Fock theory have already been published.[29]

Suppressing the isospin factor for the moment, one finds the following expression for the local exchange potential resulting from the scalar two-body interaction:

$$U_{\rm ex}^{i}(\vec{r}_1)=\frac{1}{4}\Big[\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)\Big]^{-1}\sum_{j=1}^{A}\sum_{m_j}\int\phi_j^{\dagger}(\vec{r}_2)\gamma_2^0 J_s(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2\,\gamma_1^0\sum_{A=1}^{16}[\phi_i^{\dagger}(\vec{r}_1)\gamma_A\phi_j(\vec{r}_1)]\gamma_1^A. \tag{26}$$

The fact that only four terms of the A sum contribute to Eq. (26) when the spherical representation of the γ^A is used is an important simplication. Comparing Eq. (26) with Eq. (19), one finds the following four contributions to the radial potentials:

$$U_{\rm s}^{i}(r_1)=\frac{1}{4}\Big[\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)\Big]^{-1}\sum_{j=1}^{A}\sum_{m_j}\int\phi_j^{\dagger}(\vec{r}_2)\gamma^0 J_s(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2[\phi_i^{\dagger}(\vec{r}_1)\phi_j(\vec{r}_1)], \tag{27}$$

$$U_{\rm v}^{0i}(r_1)=\frac{1}{4}\Big[\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)\Big]^{-1}\sum_{j=1}^{A}\sum_{m_j}\int\phi_j^{\dagger}(\vec{r}_2)\gamma^0 J_s(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2[\phi_i^{\dagger}(\vec{r}_1)\gamma_0\phi_j(\vec{r}_1)], \tag{28}$$

$$-U_{\rm v}^{ri}(r_1)=\frac{1}{4}\Big[\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)\Big]^{-1}\sum_{j=1}^{A}\sum_{m_j}\int\phi_j^{\dagger}(\vec{r}_2)\gamma^0 J_s(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2[\phi_i^{\dagger}(\vec{r}_1)\gamma_r\phi_j(\vec{r}_1)], \tag{29}$$

and

$$-U_{\rm t}^{ri}(r_1)=\frac{1}{4}\Big[\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)\Big]^{-1}\sum_{j=1}^{A}\sum_{m_j}\int\phi_j^{\dagger}(\vec{r}_2)\gamma^0 J_s(|\vec{r}_1-\vec{r}_2|)\phi_i(\vec{r}_2)d^3r_2[\phi_i^{\dagger}(\vec{r}_1)\gamma_r\gamma_0\phi_j(\vec{r}_1)]. \tag{30}$$

The term $\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)$ is common to all four single-particle potentials and reduces to the following angle-independent form:

$$\sum_{m_i}\phi_i^{\dagger}(\vec{r}_1)\phi_i(\vec{r}_1)=(2J_i+1)/4\pi r_1^2[F_i^2(r_1)+G_i^2(r_1)]. \tag{31}$$

Further simplication of Eqs. (27)–(30) is accomplished by utilizing the following theorem which has been given in slightly different form by Rose, Biedenharn, and Arfken[30]:

$$\mathcal{Y}_{Jm}^{\tilde{\omega}\dagger}(\theta,\phi)\mathcal{Y}_{J'm'}^{\tilde{\omega}'}(\theta,\phi)=(4\pi)^{-1/2}\sum_{L}(-)^{J+J'+1/2[l+3l'+3L+6m'+1]}\begin{pmatrix}J & J' & L\\ -m & m' & m-m'\end{pmatrix}Z(lJl'J';\tfrac{1}{2}L)\mathcal{Y}_{Lm'-m}(\theta,\phi), \tag{32}$$

where

$$l=J+\tilde{\omega}/2. \tag{33}$$

The primed quantities l', J', and $\tilde{\omega}'$ are related similarly. The left-hand side of Eq. (32) is just the contraction of two general central field spinors of the type defined in Eq. (22). The right-hand side is just the expansion of this contraction in ordinary spherical harmonics. The symbol Z is the Z coefficient of Blatt and Biedenharn.[31] The phase convention for the Z coefficient used in this work is that of Messiah.[32]

Another useful relation for simplifying the exchange potentials is the expansion of the Yukawa function in spherical harmonics:

$$\frac{e^{-\mu|\vec{r}_1-\vec{r}_2|}}{|\vec{r}_1-\vec{r}_2|}=\sum_{r=0}^{\infty}\sum_{s=-r}^{r}4\pi f_r(r_1r_2)\mathcal{Y}_{rs}^{*}(\theta_1\phi_1)\mathcal{Y}_{rs}(\theta_2\phi_2), \tag{34}$$

where

$$f_\nu(r_1 r_2) = (r_1 r_2)^{-1/2} K_{\nu+1/2}(\mu r_>) I_{\nu+1/2}(\mu r_<) . \quad (35)$$

The I and K are the modified spherical Bessel functions of the first and third kind, respectively. The symbols $r_<$ and $r_>$ are the lesser and greater respectively of the radial variables r_1 and r_2.

So far the isospin dependence of the two-body interaction has been ignored. Actually our intent is that the single-nucleon wave functions ϕ_i are not only four-component Dirac spinors but also two-component isospinors which indicate whether the state i is a neutron or proton orbital. Suppose the scalar meson exchanged is isoscalar. Then the interaction used in Eq. (26) is the appropriate one, however, the spinor contractions in Eqs. (27)–(30) represent isospin contractions as well. It is clear that these contractions give zero unless both states ϕ_i and ϕ_j have the same third component of isospin. The sum over the states j in Eqs. (27)–(30) should thus be restricted to states with the same isospin as the state i for which the potentials are being calculated.

For the case of charged scalar meson exchange, the interaction of Eq. (26) should be modified to include the isospin factor $\vec{\tau}_1 \cdot \vec{\tau}_2$. The effect of this factor upon the single-particle exchange potentials is best observed by expressing the factor in the form:

$$\vec{\tau}_1 \cdot \vec{\tau}_2 = \tau_{1z} \tau_{2z} + 2(\tau_{1+} \tau_{2-} + \tau_{1-} \tau_{2+}) , \quad (36)$$

where $\tau_{\alpha+}$ and $\tau_{\alpha-}$ are the isospin raising and lowering operators, respectively, for the nucleon state with the space coordinates $\vec{r}_\alpha$. Consider first the $\tau_{1z} \tau_{2z}$ part of this operator. Here the j sums in Eqs. (27)–(30) are restricted in exactly the same way as they were for the isoscalar scalar meson. This term represents the contribution to exchange diagrams mediated by the uncharged member of the isovector triplet of scalar mesons and hence can only occur when both states i and j have the same third component of isospin. In contrast, the remaining terms in Eq. (36) (involving only raising and lowering operators) contribute only when the j sums of Eqs. (27)-(30) run over states whose third components of isospin are different from that of state i for which the potentials are being calculated. These terms represent exchange diagrams mediated by the two charged members of the isovector triplet of scalar mesons. Note that this sum carries the factor of 2, since for any two states i and j the isospin matrix elements for only one of the two operators $\tau_{1+} \tau_{2-}$ and $\tau_{1-} \tau_{2+}$ will be nonzero.

After properly restricting the summations to account for the isospin of the meson exchanged, one can multiply Eqs. (27)–(30) by the factor $g_s^2 \hbar c$ and sum over the scalar mesons of the model [as in Eq. (8)] to obtain the total Hartree-Fock exchange potential resulting from the scalar mesons.

The Hartree-Fock exchange potentials resulting from other terms in the two-body interaction may be obtained by straightforward application of the methods that have been used for the scalar case. To facilitate the expression of the results for these interaction terms, one may introduce a notation whereby all of the single-particle exchange potentials U_s^i, U_v^{0i}, U_v^{ri}, and U_t^{ri} are four-component objects

$$\underline{U}^i = \begin{bmatrix} \text{scalar} & U^i \\ \text{time vector} & U^i \\ R \text{ vector} & U^i \\ \text{pseudoscalar} & U^i \end{bmatrix} . \quad (37)$$

The upper (scalar) component represents the case of scalar meson exchange which has just been discussed [Eqs. (27)–(30)]. The two middle components represent contributions from vector meson exchange. The time-vector component represents the term in the sum $\gamma_1^\mu \gamma_{2\mu}$ where μ is zero. The R-vector term represents the term in the sum whereby μ is the r index of Eqs. (19) and (20). This obviously implies the sum $\gamma_1^\mu \gamma_{2\mu}$ is to be evaluated in spherical coordinates:

$$\gamma_1^\mu \gamma_{2\mu} = \gamma_1^0 \gamma_{20} + \gamma_1^r \gamma_{2r} + \gamma_1^\theta \gamma_{2\theta} + \gamma_1^\phi \gamma_{2\phi} . \quad (38)$$

Straightforward application of the tensor transformation properties of 4-vector densities under transformation to spherical coordinates yields:

$$\gamma^\theta = -\frac{1}{r^2} \gamma_\theta = \frac{1}{r} \begin{pmatrix} 0 & \sigma_\theta \\ -\sigma_\theta & 0 \end{pmatrix} , \quad (39)$$

and

$$\gamma^\phi = \frac{-1}{r^2 \sin^2\theta} \gamma_\phi = \frac{1}{r \sin\theta} \begin{pmatrix} 0 & \sigma_\phi \\ -\sigma_\phi & 0 \end{pmatrix} . \quad (40)$$

Our claim of simplicity for the remaining terms of the two-body interaction does not apply to the terms involving γ^θ and γ^ϕ in Eq. (38). These terms are thus excluded from the vector representation of Eq. (37). The difficulty with these latter terms will be discussed at the end of this section. Finally, the last component (pseudoscalar) of Eq. (37) represents the exchange potentials resulting from pseudoscalar mesons.

Using the notation introduced in Eq. (37), the

single-particle exchange potentials are:

$$\underline{U}_s^i(\vec{r}_1)=\frac{1}{4}\begin{bmatrix}+\\-\\-\\-\end{bmatrix}\{(2J_i+1)[F_i^2(r_1)+G_i^2(r_1)]\}^{-1}\sum_{J_j\omega_j l}\left\{\begin{bmatrix}Z(l_iJ_il_jJ_j;\frac{1}{2}l)F_i(r_1)F_j(r_1)\\-Z(l_iJ_il_jJ_j;\frac{1}{2}l)F_i(r_1)F_j(r_1)\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)F_i(r_1)G_j(r_1)\\Z(l_iJ_il_j'J_j;\frac{1}{2}l)F_i(r_1)G_j(r_1)\end{bmatrix}\right.$$

$$+(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix}Z(l_i'J_il_j'J_j;\frac{1}{2}l)G_i(r_1)G_j(r_1)\\Z(l_i'J_il_j'J_j;\frac{1}{2}l)G_i(r_1)G_j(r_1)\\Z(l_i'J_il_j'J_j;\frac{1}{2}l)F_i(r_1)G_j(r_1)\\Z(l_i'J_il_jJ_j;\frac{1}{2}l)F_i(r_1)G_j(r_1)\end{bmatrix}\Bigg\}\Bigg\{\begin{bmatrix}Z(l_iJ_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)\,f_i(r_1r_2)dr_2\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)\,f_i(r_1r_2)dr_2\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)\,f_i(r_1r_2)dr_2\\Z(l_iJ_il_j'J_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)\,f_i(r_1r_2)dr_2\end{bmatrix}$$

$$-(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix}Z(l_i'J_il_j'J_j;\frac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_i(r_1r_2)dr_2\\-Z(l_i'J_il_j'J_j;\frac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_i(r_1r_2)dr_2\\Z(l_i'J_il_j'J_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)f_i(r_1r_2)dr_2\\Z(l_i'J_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)f_i(r_1r_2)dr_2\end{bmatrix}\Bigg\}, \tag{41}$$

$$\underline{U}_v^{0i}(r_1)=\frac{1}{4}\begin{bmatrix}+\\-\\-\\-\end{bmatrix}\{2J_i+1)[F_i^2(r_1)+G_i^2(r_1)]\}^{-1}\sum_{J_j\tilde{\omega}_j l}\left\{\begin{bmatrix}Z(l_iJ_il_jJ_j;\frac{1}{2}l)F_i(r_1)F_j(r_1)\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)F_i(r_1)F_j(r_1)\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)F_i(r_1)G_j(r_1)\\Z(l_iJ_il_j'J_j;\frac{1}{2}l)F_i(r_1)G_j(r_1)\end{bmatrix}\right.$$

$$-(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix}Z(l_i'J_il_j'J_j;\frac{1}{2}l)G_i(r_1)G_j(r_1)\\-Z(l_i'J_il_j'J_j;\frac{1}{2}l)G_i(r_1)G_j(r_1)\\Z(l_i'J_il_j'J_j;\frac{1}{2}l)G_i(r_1)F_j(r_1)\\Z(l_i'J_il_jJ_j;\frac{1}{2}l)G_i(r_1)F_j(r_1)\end{bmatrix}\Bigg\}\Bigg\{\begin{bmatrix}Z(l_iJ_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)\,f_i(r_1r_2)dr_2\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)\,f_i(r_1r_2)dr_2\\Z(l_iJ_il_jJ_j;\frac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)\,f_i(r_1r_2)dr_2\\Z(l_iJ_il_j'J_j;\frac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)\,f_i(r_1r_2)dr_2\end{bmatrix}$$

$$-(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix} Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \\ -Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i' J_i\, l_j J_j;\tfrac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)f_l(r_1r_2)dr_2 \end{bmatrix}\Bigg\}, \tag{42}$$

$$\underline{U}_v^{rt}(r_1) = -\frac{i}{4}\begin{bmatrix}+\\+\\-\\+\end{bmatrix}\{(2J_i+1)[F_i^2(r_1)+G_i^2(r_1)]\}^{-1}\sum_{J_j\,\omega_j\,l}\left\{\begin{bmatrix} Z(l_i J_i\, l_j J_j;\tfrac{1}{2}l)F_i(r_1)G_j(r_1) \\ Z(l_i J_i\, l_j J_j;\tfrac{1}{2}l)F_i(r_1)G_j(r_1) \\ Z(l_i J_i\, l_j J_j;\tfrac{1}{2}l)F_i(r_1)F_j(r_1) \\ Z(l_i J_i\, l_j' J_j;\tfrac{1}{2}l)F_i(r_1)F_j(r_1) \end{bmatrix}\right.$$

$$+(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix} Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)G_i(r_1)F_j(r_1) \\ -Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)G_i(r_1)F_j(r_1) \\ Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)G_i(r_1)G_j(r_1) \\ Z(l_i' J_i\, l_j J_j;\tfrac{1}{2}l)G_i(r_1)G_j(r_1) \end{bmatrix}\Bigg\}\left\{\begin{bmatrix} Z(l_i J_i\, l_j J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i J_i\, l_j J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i J_i\, l_j J_j;\tfrac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \end{bmatrix}\right.$$

$$-(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix} Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \\ -Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i' J_i\, l_j' J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2 \\ Z(l_i' J_i\, l_j J_j;\tfrac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)f_l(r_1r_2)dr_2 \end{bmatrix}\Bigg\}, \tag{43}$$

and

$$\underline{U}\,{}^{i}_{i}(r_1) = \frac{i}{4}\begin{bmatrix}+\\+\\-\\+\end{bmatrix}\{(2J_i+1)[F_i^2(r_1)+G_i^2(r_1)]\}^{-1}\sum_{J_j\tilde{\omega}_j l}\left\{\begin{bmatrix}Z(l_iJ_il_jJ_j;\tfrac{1}{2}l)F_i(r_1)G_j(r_1)\\Z(l_iJ_il_jJ_j;\tfrac{1}{2}l)F_i(r_1)G_j(r_1)\\Z(l_iJ_il_jJ_j;\tfrac{1}{2}l)F_i(r_1)F_j(r_1)\\Z(l_iJ_il_j'J_j;\tfrac{1}{2}l)F_i(r_1)F_j(r_1)\end{bmatrix}\right.$$

$$-(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix}Z(l_i'J_il_j'J_j;\tfrac{1}{2}l)G_i(r_1)F_j(r_1)\\-Z(l_i'J_il_j'J_j;\tfrac{1}{2}l)G_i(r_1)F_j(r_1)\\Z(l_i'J_il_j'J_j;\tfrac{1}{2}l)G_i(r_1)G_j(r_1)\\Z(l_i'J_il_jJ_j;\tfrac{1}{2}l)G_i(r_1)G_j(r_1)\end{bmatrix}\Bigg\}\Bigg\{\begin{bmatrix}Z(l_iJ_il_jJ_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)f_l(r_1r_2)dr_2\\Z(l_iJ_il_jJ_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)F_j(r_2)f_l(r_1r_2)dr_2\\Z(l_iJ_il_jJ_j;\tfrac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)f_l(r_1r_2)dr_2\\Z(l_iJ_il_j'J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2\end{bmatrix}$$

$$-(-)^{(\tilde{\omega}_i-\tilde{\omega}_j)/2}\begin{bmatrix}Z(l_i'J_il_j'J_j;\tfrac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2\\-Z(l_i'J_il_j'J_j;\tfrac{1}{2}l)\int_0^\infty G_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2\\Z(l_i'J_il_j'J_j;\tfrac{1}{2}l)\int_0^\infty F_i(r_2)G_j(r_2)f_l(r_1r_2)dr_2\\Z(l_i'J_il_jJ_j;\tfrac{1}{2}l)\int_0^\infty F_j(r_2)G_i(r_2)f_l(r_1r_2)dr_2\end{bmatrix}\Bigg\}\,, \tag{44}$$

where products of two of the four-component objects appearing in Eqs. (41)–(44) are to be computed as follows:

$$\begin{bmatrix}a_1\\a_2\\a_3\\a_4\end{bmatrix}\begin{bmatrix}b_1\\b_2\\b_3\\b_4\end{bmatrix} = \begin{bmatrix}a_1b_1\\a_2b_2\\a_3b_3\\a_4b_4\end{bmatrix} \tag{45}$$

These equations form the basis of the numerical calculation of the relativistic Hartree-Fock exchange potentials. They are, to be sure, quite complicated, particularly because they have to be calculated separately for each $J\tilde{\omega}$-subshell.

Nevertheless, if one demands exact solutions of the relativistic Hartree-Fock problem, one is forced to either confront the complications of Eqs. (41)–(44) or else solve the Dirac equation with the nonlocal form of the potentials.

The θ and ϕ contributions to the vector meson sum are not so easy to include because the operators σ_θ and σ_ϕ have very complicated representations in the space of central field spinors $\mathcal{Y}^{\tilde{\omega}}_{jm}(\theta,\phi)$. A more convenient representation of the Pauli spin matrices for this problem is the representation introduced by Biedenharn in his study of two-component forms of the Dirac equation[33]:

$$n_1 = \sigma_r, \quad n_2 = \frac{\vec{\sigma}\cdot\vec{\mathbf{L}}+1}{J+\frac{1}{2}}, \quad n_3 = -i\,n_1n_2\,. \tag{46}$$

The matrices n_1, n_2, and n_3 form a representation of the Pauli spin matrices on any subspace of Hilbert space characterized by good J and parity. Their representation matrices in the space of the central field spinors are simple as shown by the following relations:

$$n_1 \mathcal{Y}^{\omega}_{Jm} = -\mathcal{Y}^{-\omega}_{Jm}, \quad n_2 \mathcal{Y}^{\omega}_{Jm} = -\tilde{\omega}\mathcal{Y}^{\omega}_{Jm}, \quad n_3 \mathcal{Y}^{\omega}_{Jm} = -i\tilde{\omega}\mathcal{Y}^{-\omega}_{Jm}. \tag{47}$$

By use of these operators, it is possible that one could represent the remaining contributions of the vector meson sum to the Hartree-Fock exchange potentials in as simple a form as the terms already represented in Eqs. (41)–(44). This possibility is not pursued further in the present context because of numerical instabilities that are induced by two-body interactions mediated by odd Dirac operators. The use of both the R vector and the pseudoscalar terms in the exchange potentials is questionable.

IV. NUMERICAL METHODS

As was pointed out previously, the radial Dirac equations [Eqs. (24) and (25)] and the radial form of the exchange potentials [Eqs. (41)–(44)] along with the radial equations for the direct potentials [Eqs. (16), (17), (31), (32), and (33) of Ref. 1] form the basis for the numerical solutions of the relativistic Hartree-Fock equations. The numerical integration of Eqs. (24) and (25) is performed by utilizing the Runge-Kutta method appropriate for coupled linear first-order differential equations. The integration was performed with 250 equally spaced mesh points. Mesh sizes of 0.04 and 0.05 fm were used for the ^{16}O and ^{40,48}Ca calculations, respectively. The single-particle eigenvalues were determined by matching the radial wave functions resulting from both outward and inward integrations. Agreement between the wave functions of better than 5 parts in 10 000 was required in the eigenvalue search. The outward integrations were started from analytic expansions of the wave functions about $r = 0$. Sufficient terms were retained to insure that the expansions were as accurate as can be represented in single precision on the Univac 1108 machine. The inward integrations were started from analytic solutions of the differential equations in the region where the potentials were assumed to be zero (beyond 200 mesh points) for the neutron states and from asymptotic (semiconvergent) series which were the only forms of solutions found for the wave functions in the region where only the Coulomb ($1/r$) potential remained for the proton states.

The integrals involved in calculating the potentials, which are indefinite due to the presence of $r_>$ and $r_<$ in Eq. (35), were obtained by using a variant of Simpson's rule. Instead of fitting nonoverlapping parabolas through successive triplets of consecutive points and integrating, this rule consists of averaging the two overlapping parabolas formed by fitting the two triplets of successive points in any four successive points. This averaged parabola is integrated between the two interior points of the four-point group and the process is continued until the entire region of integration (except for the two end-point intervals) has been covered. The two end-point intervals are integrated with the only possible parabolas spanning these points as in Simpson's rule. This rather complicated sounding procedure results in a simple integration rule:

$$\int_a^b y(x)dx = \Delta[\tfrac{3}{8}y(1) + \tfrac{7}{6}y(2) + \tfrac{23}{24}y(3) + y(4) + \cdots + y(n-3) + \tfrac{23}{24}y(n-2) + \tfrac{7}{6}y(n-1) + \tfrac{3}{8}y(n)], \tag{48}$$

where $y(1) = y(a)$, $y(n) = y(b)$, and $\Delta = (b-a)/n$. This result, which resembles the trapezoidal rule (only end-point corrections) more than Simpson's rule, does not require an odd number of grid points (unlike Simpson's rule) and is thus well suited for performing integrals of the type that occur in coordinate space Hartree-Fock calculations.

As well as the potentials, the wave functions, and the single-particle eigenvalues, the total binding energy of a system is also calculated in a Hartree-Fock calculation. The total binding energy is calculated in the present work by a straightforward summation of the terms in the Hartree-Fock binding-energy expression:

$$E = \sum_{i=1}^{A} \langle i|T|i\rangle + \tfrac{1}{2}\sum_{i,j=1}^{A} (\langle ij|V|ij\rangle - \langle ij|V|ji\rangle). \tag{49}$$

The center-of-mass contribution to this energy was approximately removed from Eq. (49) by the same method that was used in Ref. 1.

In Eq. (49) the operator T is the relativistic kinetic energy operator (discussed in Ref. 2) for positive energy states:

$$T = c\vec{\alpha}\cdot\vec{p} + \beta Mc^2 - Mc^2. \tag{50}$$

The states $|i\rangle$ are the occupied positive-energy single-particle states in the Hartree-Fock potentials. The Operator V is, of course, the sum of the two-body interactions given in Eq. (8). The kinetic energy expectation value for a state i may

be shown to be:

$$\langle i|T|i\rangle = \int_0^\infty [E_i - U_s^i(r) - U_v^{0i}(r)]F_i^2(r)\,dr + \int_0^\infty [U_s^i(r) - U_v^{0i}(r) + E_i]G_i^2(r)\,dr - i\int_0^\infty 2U_t^{ri}(r)F_i(r)G_i(r)\,dr, \tag{51}$$

where E_i, F_i, and G_i are the eigenvalue and large and small component radial wave functions, respectively, of state $|i\rangle$; and U_s^i, U_v^{0i}, and U_t^{ri} are the scalar, zeroth component of the vector, and second rank tensor potentials of the state $|i\rangle$. The summation over the direct two-body potential matrix elements may be written in radial form as single-particle matrix elements of the direct single-particle potentials:

$$\sum_{ij}\langle ij|V|ij\rangle = \sum_i (2J_i+1)\{\int_0^\infty [F_i^2(r) - G_i^2(r)]U_s(r)\,dr + \int_0^\infty [F_i^2(r) + G_i^2(r)]U_v^0(r)\,dr\}, \tag{52}$$

where U_s and U_v^0 are the (state-independent) direct scalar and vector potentials.

The summation of the exchange two-body matrix elements in Eq. (49) may also be given as radial single-particle matrix elements of the exchange potentials:

$$\sum_{ij}\langle ij|V|ji\rangle = \sum_i (2J_i+1) \times \int_0^\infty [F_i^2(r) + G_i^2(r)]4U_v^0(r)_{ex}^i\,dr. \tag{53}$$

Here $U_v^0(r)_{ex}^i$ is the exchange part only of the zeroth component of the vector potential for the state $|i\rangle$. The factor of 4 in Eq. (53) is needed to compensate for the factor of $\frac{1}{4}$ in Eq. (42). It is necessary to calculate the single-particle matrix elements in Eqs. (51), (52), and (53) with wave functions from the same iteration that was used to calculate the Hartree-Fock potentials if one is to avoid using a mixed basis for the calculation of E. The total binding energy was calculated for each Hartree-Fock iteration and convergence was defined as the point beyond which the variation in E was less than 1 part in 5000 for two successive iterations. The eigenvalues, wave functions, and potentials were printed out on each iteration and it was observed that fluctuations in these quantities were usually in the neighborhood of 1 part in 1000 at convergence.

A basis of wave functions for starting the Hartree-Fock iteration procedure was obtained by first obtaining the self-consistent Hartree solutions for each nucleus. Normally between 10 and 15 Hartree-Fock iterations (beyond the Hartree calculations) were required to satisfy the convergence criterion. This iteration scheme has been tested for stability by performing calculations with different mesh sizes and by using different starting bases for the iteration scheme. Within the accuracy of the convergence criterion, it was found to be stable.

TABLE I. N-N model parameters of Ref. 1.

Meson	T	J^P	Mass	g^2
ω	0	1^-	782.8	17.0
ϵ	0	0^+	782.8	17.0
σ	0	0^+	277.4	0.646
ρ	1	1^-	763.0	1.74

V. CALCULATIONS

The phenomenological N-N force model which was used in the Hartree calculations of Ref. 1 is shown in Table I. This model consists of two vector mesons (ρ and ω) and two scalar mesons. The Coulomb interaction was treated by introducing a third vector meson with a very small mass (0.002 MeV). The absence of the pion in this model reflects the fact that the one-pion-exchange potential does not contribute to the Hartree potential for spherical nuclei. In the Hartree approximation the parameters of this model were adjusted to give good agreement with experimental binding energies, rms charge radii, and single-particle separation energies for doubly magic nuclei over the range ^{16}O–^{208}Pb. In Table II a comparison is made for binding energies and rms radii between the Hartree (Ref. 1) and Hartree-Fock (present) results for ^{16}O, ^{40}Ca, and ^{48}Ca. The exchange contributions of the scalar, time-vector, and R-vector components of Eqs. (41)–(44) are included.

TABLE II. Comparison between relativistic Hartree (Ref. 1) and Hartree-Fock (present) calculations.

	−binding energy/A (MeV)		rms charge radii (fm)	
	Ref. 1	Present	Ref. 1	Present
^{16}O	7.35	8.60	2.70	2.67
^{40}Ca	8.25	9.68	3.49	3.47
^{48}Ca	8.55	10.29	3.49	3.46

TABLE III. Single-particle eigenvalues for Hartree and Hartree-Fock calculations.

	^{16}O				^{40}Ca				^{48}Ca			
	Neutron		Proton		Neutron		Proton		Neutron		Proton	
State	Ref. 1	Present	Ref. 1	Present	Ref. 1	Present	Ref. 1	Present	Ref. 1	Present	Ref. 1	Present
$1s_{1/2}$	44.12	44.42	39.93	40.21	56.09	55.10	48.05	47.13	56.64	55.87	55.25	55.51
$1p_{3/2}$	23.96	24.68	20.03	20.69	41.23	41.25	33.48	33.49	42.13	42.27	42.28	43.40
$1p_{1/2}$	14.67	13.67	10.83	9.80	35.68	35.47	27.90	27.67	37.98	37.55	37.77	38.52
$1d_{5/2}$					25.68	26.15	18.24	18.64	26.73	27.31	27.48	28.92
$1d_{3/2}$					16.37	15.95	8.99	8.51	18.34	17.67	18.70	19.08
$2s_{1/2}$					14.95	12.59	7.71	5.46	16.28	13.19	14.24	12.19
$1f_{7/2}$									11.51	12.21		

One notices in Table II that the exchange contribution to the binding energy is attractive and adds about 1.5 MeV per particle to the binding. It is a little surprising that the contribution is attractive because in atomic Hartree-Fock calculations the exchange energy of an interaction has the opposite sign to the direct energy of that interaction. The same is true here; however, the near cancellation between vector and scalar two-body matrix elements is responsible for the present situation. The direct energy results from a large cancellation between scalar (attractive) and vector (repulsive) matrix elements in which the scalar matrix elements are slightly larger in magnitude than the vector. The exchange energy arises from a similar cancellation; however, the vector matrix elements are slightly larger than the scalar in this case.

Note that the exchange contributions to the binding energies are proportionately larger than the contributions to the rms radii. The exchange potentials then have a relatively small effect upon the self-consistent wave functions even though the contributions to the binding energy are significant. Further evidence of this is shown in Table III where the self-consistent single-particle eigenvalues are compared for the Hartree and Hartree-Fock calculations. The eigenvalue changes are quite small with the exception of a few states near the fermi surface.

The exchange contributions to the total binding energy of the scalar, time-vector, and R-vector components of the meson model are shown for the single-particle shells of ^{40}Ca in Table IV. Each entry represents the exchange energy of a shell interacting with all other occupied shells through a particular component of the two-body interaction [a single term in the summation on the right-hand side of Eq. (53)]. One notes that the R-vector contribution is much smaller in magnitude than the scalar and time-vector contributions. It is, however, a significant contribution to the total exchange energy due to the cancellation between the vector and scalar contributions. By adding the R-vector contributions in Table IV, one finds a contribution of 0.18 MeV per particle as compared with a total exchange contribution of 1.43 MeV per particle. This gives us an order of magnitude estimate of the relative importance of the θ and ϕ exchange contributions of the vector mesons which are excluded in the present formalism. In the last line of Table IV, the state dependence of the exchange energy per particle is displayed. Note that the contributions of the $j=l-\frac{1}{2}$ states are considerably larger than the $j=l+\frac{1}{2}$ state contributions. Within each of these two categories, one notes an increase of the exchange contribution per particle with increasing j. The results for the $1s_{1/2}$ and $2s_{1/2}$ states indicate that the exchange energy per particle may de-

TABLE IV. Major shell exchange contributions to binding energy of ^{40}Ca. Direct matrix elements and kinetic energies from all nucleons contribute −318.68 MeV. Total with exchange is −369.46.

	$1s_{1/2}$		$1p_{3/2}$		$1p_{1/2}$		$1d_{5/2}$		$1d_{3/2}$		$2s_{1/2}$	
	p	n	p	n	p	n	p	n	p	n	p	n
Scalar	93.28	95.64	160.72	164.20	79.66	81.56	193.30	197.98	118.01	122.38	44.74	48.25
Time vector	−93.18	−95.46	−163.37	−166.93	−82.32	−84.32	−199.43	−204.21	−126.82	−131.76	−45.89	−49.56
R vector	−0.72	−0.73	−0.41	−0.39	−1.11	−1.16	−0.14	−0.12	−2.21	−2.35	1.11	1.19
Sum	−0.62	−0.55	−3.06	−3.12	−3.77	−3.92	−6.27	−6.55	−11.02	−11.73	−0.04	−0.12
Sum per particle	−0.32	−0.27	−0.76	−0.78	−1.88	−1.96	−1.04	−1.09	−2.75	−2.98	−0.02	−0.06

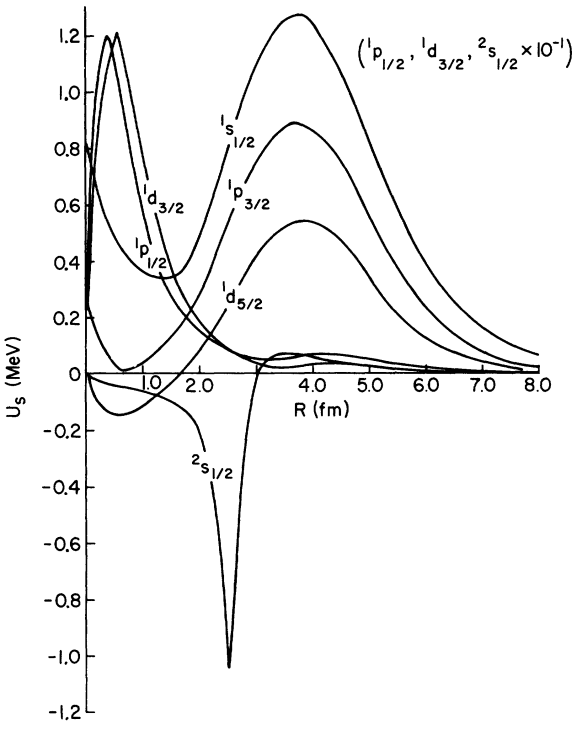

FIG. 1. Exchange contribution to the scalar (U_s) single-particle potentials of states in ^{40}Ca. The N-N interaction is the vector-scalar meson model of Ref. 1.

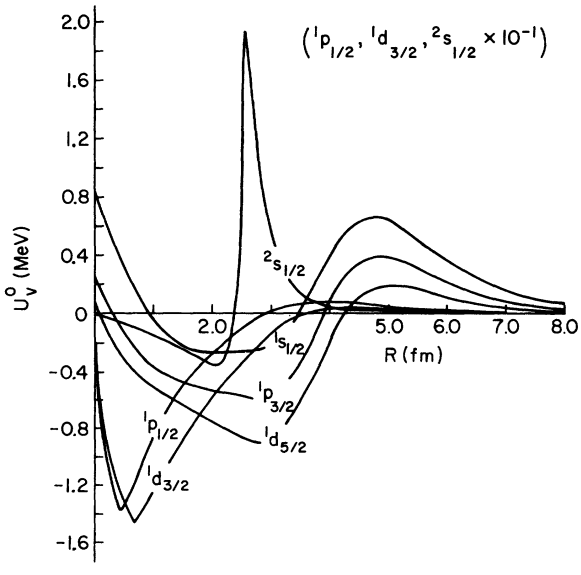

FIG. 2. Exchange contributions to the time-like vector (U_V^0) single-particle potentials of states in ^{40}Ca. The N-N interaction is the vector-scalar meson model of Ref. 1.

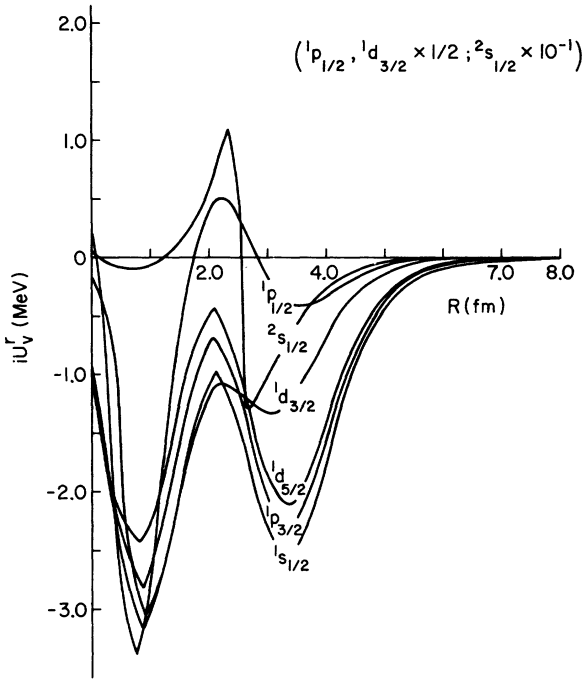

FIG. 3. Exchange contributions to the space-like vector (iU_V^r) single-particle potentials of states in ^{40}Ca. The N-N interaction is the vector-scalar meson model of Ref. 1.

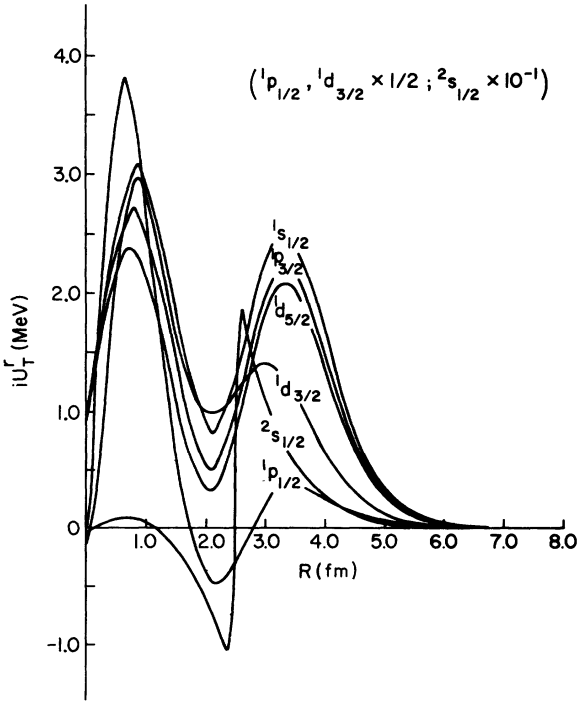

FIG. 4. Exchange contributions to the tensor (U_t^r) single-particle potentials of states in ^{40}Ca. The N-N interaction is the vector-scalar meson model of Ref. 1.

crease significantly with increasing nodal quantum number.

In Figs. 1–4 the total exchange contributions to the single particle potentials U_s, U_v^0, iU_v^r, and iU_t^r, respectively, are shown for the single-particle states of ^{40}Ca. These potentials are much smaller than the direct potentials (U_s and U_v^0) which are shown for ^{40}Ca in Fig. 5. Due to the similarity between neutron and proton potentials, only potentials for neutrons are shown in Figs. 1–5. In Figs. 1–4 one notes the considerable state dependence of the exchange potentials. In Figs. 1 and 2 the scale for the $1p_{1/2}$, $1d_{3/2}$, and $2s_{1/2}$ potentials is multiplied by the factor 10^{-1} to make the curves comparable to the $1s_{1/2}$, $1p_{3/2}$, and $1d_{5/2}$ curves. In Figs. 3 and 4 the $1p_{1/2}$ and $1d_{3/2}$ scales are multiplied by 2^{-1} while the $2s_{1/2}$ scale is multiplied by 10^{-1}. Note in all cases the general similarity between the potentials for the $1s_{1/2}$, $1p_{3/2}$, and $1d_{5/2}$ ($j=l+\frac{1}{2}$) states and between the $1p_{1/2}$ and $1d_{3/2}$ ($j=l-\frac{1}{2}$) states. The potentials for the $2s_{1/2}$ state are all characterized by a rapid fluctuation near 2.5 fm. This structure is caused by a node in the large component of the $2s_{1/2}$ wave function near 2.5 fm. A nonrelativistic analog of these local exchange potentials which did not include the momentum-dependent term of Brueckner *et al.*[24-26] would have a true singularity at the nodal point of the radial wave function. The relativistic exchange potentials are large but finite at the nodal points because of the presence of the nonvanishing small component of the wave function in the denominator of Eqs. 41–44.

At this point one may conclude that the exchange contributions of vector and scalar mesons are not large enough to invalidate the qualitative conclusions obtained from the Hartree calculations of Ref. 1, although their effect is large enough to necessitate a slight readjustment of the model parameters if quantitative agreement with the experimental quantities (particularly binding energies) is to be recovered. Such a parameter readjustment within the vector-scalar model is not of much interest at present because the exchange formalism provides a mechanism whereby one may study the more interesting question of the contributions of the one-pion-exchange potential to the relativistic Hartree-Fock problem for nuclei.

In Figs. 6–8 the single-particle exchange potentials resulting from one-pion-exchange [Eq. (4)] are shown for the $1s_{1/2}$, $1p_{3/2}$, and $1p_{1/2}$ states, respectively, of ^{16}O. The ^{16}O single-particle states are not self-consistent, but are generated from a scalar (U_s) Woods-Saxon well of depth 60 MeV, radius 3.0 fm, and diffuseness 0.66 fm via the Dirac equation. The Coulomb interaction was neglected. The potentials in Figs. 6–8 may be viewed as first-order perturbation calculations of the exchange potentials. The pion-nucleon coupling constant was chosen to be 14 and a pion mass of 138.7 MeV was used. No vertex renormalization

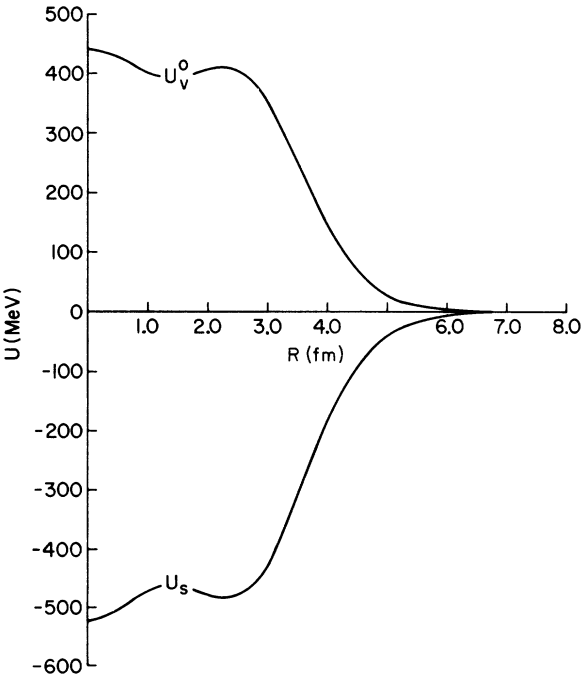

FIG. 5. Hartree contribution to the scalar (U_s) and time-like vector (U_v^0) single-particle potential for ^{40}Ca. The N-N interaction is the vector-scalar meson model of Ref. 1.

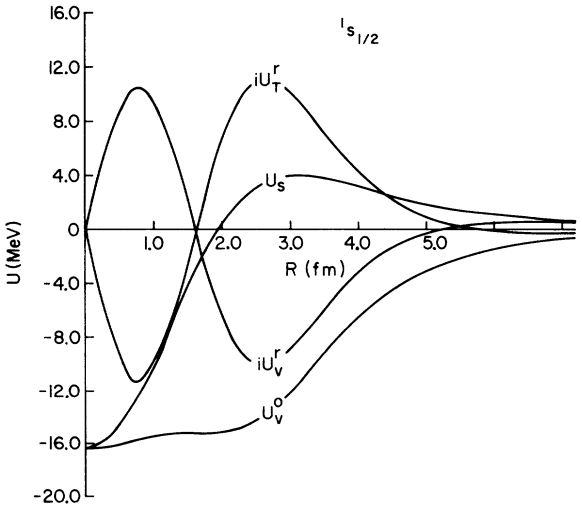

FIG. 6. Exchange potential contribution of the one-pion-exchange interaction to the $1s_{1/2}$ state of ^{16}O.

[Eq. (6)] was included in this calculation. One notes from Figs. 6 and 7 that the potentials for the $1s_{1/2}$ and $1p_{3/2}$ states are very similar in shape as was the case for the potentials in Figs. 1–4. The pion potentials in Figs. 6–8 differ significantly in shape and magnitude from the scalar and vector meson exchange potentials of Figs. 1–4. The pion contribution to the $1p_{1/2}$ state exchange potentials (Fig. 7) is extremely large at short distances. This is surprising because the basis that is used has only a 0.22-MeV spin-orbit splitting between the $1p_{3/2}$ and $1p_{1/2}$ states. This difference in quantum numbers, however, leads to a difference of two orders of magnitude in the size of the $1p_{1/2}$ and $1p_{3/2}$ exchange potentials.

The matrix elements for the total binding energy contribution have also been calculated in the Woods-Saxon basis. The total contribution from the one-pion-exchange potential in this basis is attractive and amounts to 378 MeV. This is quite a sizable contribution, leading to a binding energy for ^{16}O of about 100 MeV since the kinetic energy amounts to 278 MeV. The binding energy contributions per particle for the one-pion-exchange interaction are 29.2, 15.8, and 33.8 MeV for the $1s_{1/2}$, $1p_{3/2}$, and $1p_{1/2}$ shells, respectively, interacting with all the occupied states.

This represents a contribution of 23.6 MeV/A for the one-pion-exchange contribution to the ^{16}O binding energy. While this number is comparable to the 25 MeV/A contribution to the binding energy of nuclear matter from the one-pion-exchange potential in the $^3S_1$-$^3D_1$ channel found by Haftel, Tabakin, and Richards,[34] it is still suspiciously large in view of the fact that the present calculation is for a finite nucleus and is made only in first order (V-matrix element instead of G matrix element).

This simple perturbation calculation of one-pion-exchange contributions to a finite nucleus binding energy suggests that the one-pion-exchange contribution is very important for a fundamental understanding of the properties of finite nuclei. This conclusion is not surprising in view of the known importance of the tensor force contribution to nonrelativistic Hartree-Fock calculations (even in first order). One also concludes that the addition of the one-pion-exchange potential to the meson force model of Table I would lead to overbinding by at least 20 MeV/A in relativistic Hartree-Fock solutions for the ground states of nuclei.

The next obvious step in an orderly investigation of relativistic Hartree-Fock calculations for nuclei is to go beyond the purely phenomenological N-N force models which have been studied up to now and investigate more realistic models of the N-N force which incorporate the important one-pion-exchange interaction. The one-boson-exchange potential models which have attempted to incorporate relativistic effects[12,13,22,35] are of relevance for this study. There are two major difficulties retarding progress in this direction at

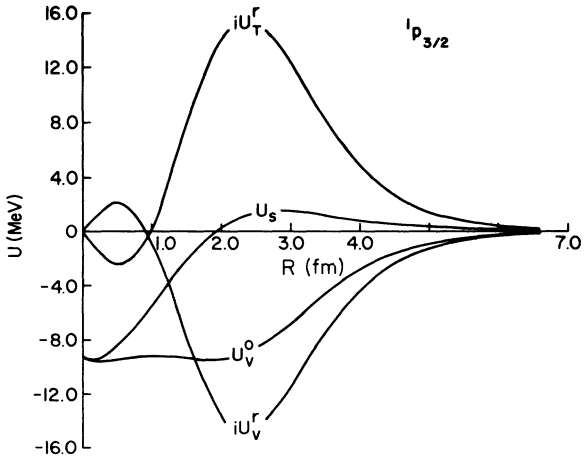

FIG. 7. Exchange potential contribution of the one-pion-exchange interaction to the $1p_{3/2}$ state of ^{16}O.

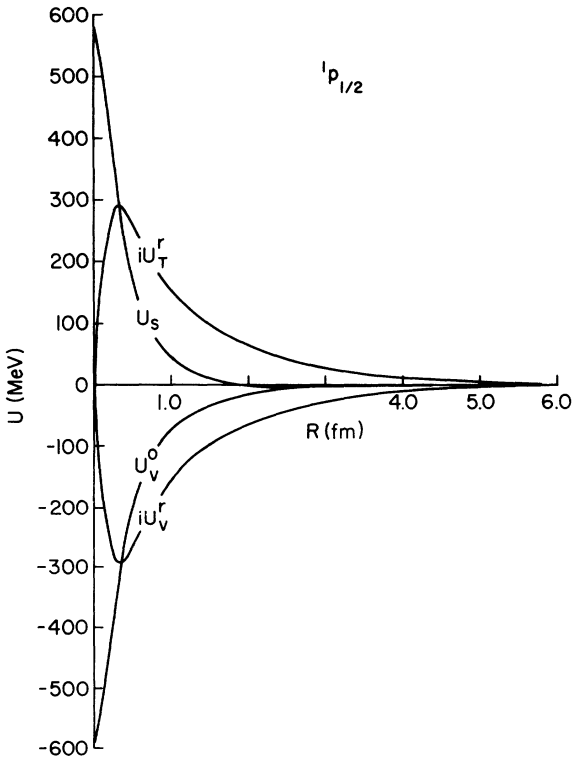

FIG. 8. Exchange potential contribution of the one-pion-exchange interaction to the $1p_{1/2}$ state of ^{16}O.

present. One difficulty is that the formalism, as presented in the present work, is not appropriate for meson-nucleon field theories resulting from derivative coupling. This deficiency prevents a realistic study of the ρ-meson contributions and also prevents an investigation of the differences between pseudoscalar and pseudovector coupling for the pion. The derivative coupling formalism for the Hartree or direct potentials for vector mesons has been developed[36]; however, the formalism for the exchange potentials is still lacking. The isovector nature of the ρ meson leads to considerable cancellation between neutron and proton contributions to the direct potential. The cancellation does not occur for the exchange potentials, leading one to believe that it is the exchange potentials which are the most important contributions of this meson.

The other difficulty is that the relativistic one-pion-exchange interaction [Eq. (4)] leads to numerical instabilities when used in relativistic Hartree-Fock calculations. All attempts to perform further Hartree-Fock iterations with the one-pion-exchange contributions reported above have led to collapsed states of the nucleus in which the small components of the single-particle wave functions have become larger and larger.

VI. SUMMARY AND CONCLUSION

A formalism for treating the Hartree-Fock exchange potentials is developed and applied to relativistic Hartree-Fock calculations for ^{16}O, ^{40}Ca, and ^{48}Ca. It is found that the exchange terms, while numerically important, do not change the qualitative results for scalar and vector meson models of the N-N force. The state dependence of the exchange potentials and binding energy contributions are investigated. The contributions for spin-orbit states with $J<l$ are found to be significantly larger than for states with $J>l$.

The exchange contributions for a coordinate-space one-pion-exchange potential are also investigated and found to be large. Such terms are too important to be considered as a mere perturbation upon the previous Hartree calculations. In fact, the first-order one-pion-exchange contribution to the binding energy of ^{16}O seems to be sufficient to bind the nucleus, although the resulting Hartree-Fock potentials would probably not bind all the single-particle states in ^{16}O. The coordinate space form of the interaction [Eq. (4)] and the potentials and energies resulting from the first-order perturbation calculation are suspect, however, since the one-pion-exchange terms cause the nucleus to collapse when further Hartree-Fock iterations are performed. Field theoretic considerations suggest that retardation effects [neglected in Eq. (4)] are important for exchange processes involving one-pion-exchange interactions. Neglect of retardation in relativistic Hartree-Fock calculations of exchange potentials appears to greatly enhance the contributions of virtual pair creation and annihilation for odd vertex operators. One may speculate then that it is the neglect of retardation which is responsible for the collapse induced by the one-pion-exchange potential of Eq. (4).

While the present perturbation calculations of one-pion-exchange effects in finite nuclei are suspect, the magnitude of the results suggest that one-pion-exchange may be very important for understanding the structure of finite nuclei. The problem of finding a form of the one-pion-exchange interaction, which is appropriate for use in relativistic Hartree-Fock calculations, must be solved before one can go on to the more fundamental problems of going beyond Hartree-Fock approximation in the relativistic many-body problem and determining whether the highly relativistic interactions studied in the present work are physically reasonable.

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