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Theory of Finite Nuclei*

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A theory of finite nuclei is formulated, based on the reaction-matrix theory of the nuclear many-body system. The reaction matrix appropriate to the finite nucleus is in the exact theory determined by the solution of coupled Hartree-Fock and reaction-matrix self consistency problems. This formal procedure is extremely difficult to carry out; the finite-nucleus reaction matrix has instead been approximated by the reaction matrix appropriate to the local density, which is a nonlocal coordinate space operator $(\mathbf{r}|K|\mathbf{r}')$. It is shown that this approximation is equivalent to the assumption that a finite nucleus has the same short-range correlation structure as nuclear matter.

The formalism used to determine $(\mathbf{r}|K|\mathbf{r}')$ from the results previously obtained in the study of nuclear matter is derived, and the methods used in explicit evaluation are described. The numerical results discussed are based on the phenomenological two-body potentials of Gammel and Thaler which give an excellent description of all scattering data up to 300 Mev. The operator $(\mathbf{r}|K|\mathbf{r}')$ obtained shows marked nonlocality for r and r' less than 10^{-13} cm. That this is largely associated with the repulsive cores in the potentials is shown by a simple analytic approximation to $(\mathbf{r}|K|\mathbf{r}')$. The nonlocality is further enhanced in the triplet states by the effects of the noncentral forces which lead to marked l dependence in the even states.

The reaction matrix so determined contains a large spin-orbit term. It is shown that this is almost entirely due to the spin-orbit two-body potential and that the tensor forces give only a very small contribution.

Proceeding from the reaction matrix as an effective two-body interaction, the Hartree-Fock problem is formulated taking into account the complicated exchange and nonlocal character of the reaction matrix. A general result is obtained for the single-particle spin-orbit potential which is shown in the case of a local interaction to reduce approximately to the form of the Thomas interaction.

An iteration method is proposed for solving the single-particle eigenvalue problem with a nonlocal potential which reduces the differentio-integral equation characteristic of the theory to an ordinary differential equation. This procedure requires the introduction of a linear derivative term in the differential equation. The method is exact in the limit of convergence of the iteration method or if the nonlocal potential is replaced by a local approximation.

I. INTRODUCTION

IN a series of previous papers[1-20] a theory of the nuclear many-body body problem has been developed and applied to the study of various properties of nuclei. In these applications it has been usually assumed that the nuclei were very large so that the properties determined should be more properly called the properties of "nuclear matter," i.e., the properties of a system of nucleons of sufficient extent so that surface effects can be neglected. To make such a study possible it is also necessary to neglect the Coulomb interaction between the protons. In this approximation various studies have been made of the properties of nuclear matter, particularly a recent detailed numerical study carried out by Brueckner and Gammel[21] based on the phenomenological two-body forces of Gammel, Christian, and Thaler,[22] and of Gammel and Thaler.[23]

In the papers on the theory of the methods used in these calculations, some discussion has been given of the problem of finite nuclei, showing how in principal it is possible to alter the methods used in the nuclear matter problem to allow their applications to finite systems.[1,12,13,20] For reasons to be discussed below, these methods cannot be applied to an actual problem because of their excessive complexity and hence our work has been carried out in an approximation discussed in Sec. II. This approximation is based on the short range of the correlation distances in the nuclear wave functions, and hence the short range over which the nuclear reaction matrix or effective two-body operator differs from the local two-body potential. Once this approximation is made, it is possible to calculate the nonlocal coordinate space operators whose diagonal matrix elements taken with respect to the eigenstates of the finite nucleus give the interaction energies. These

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operators then can be taken to be the basis of a Hartree-Fock calculation for the nuclear "model" state. In Sec. III it is shown how this operator is constructed in detail, proceeding from the results previously obtained in the study of nuclear matter. This operator is of interest, not only as the basis of a Hartree-Fock study, but also since it is the "residual two-body interaction" or effective two-body potential which is the basis of the configuration mixing studies of the shell model.

The Hartree-Fock calculation is formulated in detail in Sec. IV, taking into account the nonlocal character of the reaction matrix and the presence of a spin-orbit term in the reaction matrix. Finally in Sec. V it is shown how the Hartree-Fock equations can be reduced from the differentio-integral equations appearing in the theory to differential equations. The approximation procedure proposed is particularly useful for the nonlocal single-particle potentials characteristic of our theory.

II. APPROXIMATION TO THE FINITE SYSTEM REACTION MATRIX

Our theory of nuclear matter and of finite nuclei is based on the reaction-matrix K which determines the interaction energies and correlation structure of the many-body system. We review here only the necessary properties of K and refer to I and earlier papers for details of the theory.

The reaction matrix K is defined by the integral equation

$$K=v+vGK. \tag{1}$$

To define the Green's function G, we introduce a set of single particle eigenstates φ_i together with the associated eigenvalues E_i. Written in this representation, Eq. (1) becomes

$$K_{ij,kl}=v_{ij,kl}+\sum_{m,n} v_{ij,mn}(E_k+E_l-E_m-E_n)^{-1}K_{mn,kl}, \tag{2}$$

which defines the Green's function in this representation. The sum over m and n in Eq. (2) is to be carried out over empty states only so as to satisfy the Pauli principle. In writing the expression for the energies E_k, we make an approximation similar to one to be made in our use of the Hartree-Fock equation, i.e., we drop terms in E_k which vanish for a large number of particles. These have little effect in large nuclei and become important only for small systems. In this approximation, the single-particle energies are

$$E_i=(p^2/2M)_{ii}+\sum_j (K_{ij,ij}-K_{ij,ji}), \tag{3}$$

where the sum is over all filled states. The coordinate space potential which determines the eigenfunctions φ_i is also determined by the diagonal elements of the K matrix:

$$V(\mathbf{r},\mathbf{r}')=\sum_i \varphi_i^*(\mathbf{r}) \sum_j (K_{ij,ij}-K_{ij,ji})\varphi_i(\mathbf{r}'). \tag{4}$$

In the limit of a weak interaction, K can be replaced by the potential v and the single-particle potential defined by Eq. (4) is just the Hartree-Fock potential. Starting from a given set of eigenfunctions $\varphi_i^{(n)}$ (n meaning, for example, the nth iterate), the new set $\varphi_i^{(n+1)}$ obtained from the single-particle potential $V^{(n)}(\mathbf{r},\mathbf{r}')$ will in general not agree with the input. The problem of obtaining agreement is the self-consistency problem of the Hartree-Fock method. It is usually solved by an iteration-interpolation procedure, starting from a trial guess and improving the wave functions until self-consistency is achieved.

In our problem, a new self-consistency problem arises since a shift in the representation $\varphi_i^{(n)}\rightarrow\varphi_i^{(n+1)}$ not only changes the single-particle potentials but also, through the change in the energy spectrum, changes the Green's function in Eq. (1) and Eq. (2). This shift changes the K matrix which change in turn reacts back on the single-particle potentials and eigenfunctions. Thus a new problem arises of obtaining a self-consistent energy spectrum and reaction matrix. In the study of nuclear matter the usual Hartree-Fock problem does not occur since the eigenstates are known (plane waves). The second self-consistency problem remains, however, and is one of the principal difficulties which have been encountered in the study of nuclear matter.[4,6,21] In a finite system the K matrix and Hartree-Fock self-consistency problems are coupled together and very great computational difficulties arise if an attempt is made to solve the problem exactly. In fact, estimates of the order of magnitude of the computing problem show that it is probably beyond the capacity of presently available computing facilities.

The magnitude of the problem described above has been a severe deterrent to the study of finite nuclei. We believe, however, that a reasonable approximation exists in which the central difficulty is avoided. To show the origin of the approximation, we examine the structure of Eq. (2). We note that the energy differences appearing in the energy denomination are quite large, being the difference between a pair of energies of bound particles and a pair of particles excited above the Fermi surface. These energies are usually quite large, a typical difference being 150 to 250 Mev. Consequently, to determine the Green's function we need only give the large energy differences accurately. These energy differences correspond to quite small wavelengths, the momenta in excited states being of the order of $p\sim1.5p_F$ which, at normal density, corresponds to $\lambda\sim0.5\times10^{-13}$ c.m. If the nuclear density is slowly varying over distances of this size, then we expect that the important values of the excitation energies appearing in the Green's function in the actual finite system can be replaced by those of a spectrum appropriate to a uniform medium at the local density.

An alternative and perhaps clearer way of viewing this approximation is to examine the K matrix in coordinate space. It has already been emphasized in earlier papers[21] that the wave function for relative particle motion very quickly approaches its unperturbed form, the distances involved being about 10^{-13} cm, with marked departures occurring only over somewhat smaller distances. Thus the correlation distances in the wave function are quite small. In terms of the K matrix, this means that K approaches v at distances of the order of 10^{-13} cm. (We shall see in more detail the character of this approach in the following.) Thus we expect the correlation structure in the wave function and the correlation-dependent effects in the K matrix to be determined only by the local density, as long as the density varies slowly over the correlation distance.

We would like to add that the above condition of local density uniformity is certainly a sufficient condition; it may not, however, be necessary. It seems likely to us that a less stringent condition, such as that of linear density variation over the correlation distance, may still leave our approximation quite accurate.

This approximation allows us to compute the K matrix for the finite system directly from the results obtained in the studies of nuclear matter. The K matrix so determined will in general be a nonlocal density-dependent operator in coordinate space. Let $K_{ij,\,kl}(\rho)$ be an element of the K matrix computed in the plane-wave representation at the density ρ. To transform to coordinate space we take the Fourier transform, i.e.,

$$(\mathbf{r}_1,\mathbf{r}_2|K(\rho)|\mathbf{r}_1',\mathbf{r}_2') = \sum_{ij,\,kl} \varphi_i^*(\mathbf{r}_1)\varphi_j^*(\mathbf{r}_2)K_{ij,\,kl}\varphi_k(\mathbf{r}_1')\varphi_l(\mathbf{r}_2'). \quad (5)$$

Our approximation now allows to assume that this is the correct reaction matrix in the finite system, i.e., that Eq. (5) defines that coordinate space operator whose expectation value taken with respect to the eigenstates of the finite nucleus determines the interaction energies. This operator also determines the correlation structure which in our approximation is the same as in nuclear matter at the same local density.

We discuss in the next section the detailed evaluation of Eq. (5).

III. K MATRIX IN COORDINATE SPACE; THEORY

We start from the solutions for the K matrix as determined for a uniform medium as a function of the density, i.e., from the solutions of the equation

$$K_{ij,\,kl} = v_{ij,\,kl} + \sum_{mn} v_{ij,\,mn}(E_k+E_l-E_m-E_n)^{-1}K_{mn,\,kl}. \quad (6)$$

In this equation the density appears through the Fermi momentum $p_F = 1.52/r_0$. The quantum numbers appropriate for the uniform medium problem are the momentum, spin, and isotopic spin. To obtain the K matrix in coordinate space, we shall carry out a Fourier transformation on the *explicit* dependence of K on the momenta but neglect the effects of the change in representation on the intermediate state sum over m and n. The assumptions involved in this approximation have been discussed in the previous section. To carry out this transformation, we start from the definition of the K matrix,

$$K_{ij,\,kl} = (\varphi_{ij}, v\psi_{kl}), \quad (7)$$

where φ_{ij} is the unperturbed wave function and ψ_{kl} is the wave function determined by the solution of the integral equation

$$\psi = \varphi + Gv\psi. \quad (8)$$

This equation is discussed in detail in I; we need only the properties of ψ here and shall not again refer to Eq. (8).

To simplify Eq. (7), we make use of a result obtained in the studies of I which showed that the K matrix is a very slowly varying function of the total momentum $\mathbf{P} = \mathbf{p}_k + \mathbf{p}_l$ and depends strongly only on the relative momentum $\mathbf{k} = \frac{1}{2}(\mathbf{p}_k - \mathbf{p}_l)$. Thus in the following we suppress the dependence of K on $\mathbf{P}$, replacing $\mathbf{P}$ by an average value appropriate to the Fermi gas. This average value we have taken to be $P_{\text{Av}} = p_F$. Then, calling $\frac{1}{2}(\mathbf{p}_i - \mathbf{p}_j) = \mathbf{k}'$, we rewrite Eq. (7) as

$$(\mathbf{k}'|K|\mathbf{k}) = (\varphi_{\mathbf{k}'}, v\psi_{\mathbf{k}}), \quad (9)$$

where we have not yet indicated the spin indices explicitly. We also do not write explicitly the total momentum conservation which is contained in the K matrix. To carry out the transformation to coordinate space, it is convenient to introduce the coordinate space representation of K not by Eq. (5) but by the equivalent defining equation

$$(\mathbf{k}'|K|\mathbf{k}) = \int d\mathbf{r} \int d\mathbf{r}' \varphi_{\mathbf{k}'}^*(r')\chi_s^{m*}(\mathbf{r}'|K|\mathbf{r})\varphi_{\mathbf{k}}(\mathbf{r})\chi_s^m, \quad (10)$$

where we now write the spin functions explicitly, and $\varphi_{\mathbf{k}}(\mathbf{r})$ is a plane wave function for momentum $\mathbf{k}$. We note here that since $(\mathbf{k}'|K|\mathbf{k})$ is diagonal in the total momentum, $(\mathbf{r}'|K|\mathbf{r})$ will be diagonal in the center-of-mass coordinate, i.e., $(\mathbf{r}_{12}|K|\mathbf{r}_{12}')$ will contain a factor $\delta[\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2) - \frac{1}{2}(\mathbf{r}_1'-\mathbf{r}_2')]$. Upon combining Eqs. (7) and (9), it then follows that

$$(\mathbf{r}'|K|\mathbf{r})\chi_s^m = \frac{1}{(2\pi)^3}\int d\mathbf{k}\,\varphi_{\mathbf{k}}^*(\mathbf{r}')v(r)\psi_{\mathbf{k},\,s,\,m}(\mathbf{r}), \quad (11)$$

where we now write the spin indices explicitly. The evaluation of the right-hand side of Eq. (11) can now be carried out by using the angular momentum expansions of φ and ψ. The expansion of $\varphi_{\mathbf{k}}(\mathbf{r}')$ is

$$\varphi_{\mathbf{k}}(\mathbf{r}') = \sum_l [4\pi(2l+1)]^{\frac{1}{2}} j_l(kr') i^l Y_l^0(\mathbf{r}'). \quad (12)$$

For singlet states the expansion of ψ is not complicated by the presence of noncentral forces, and is

$$\psi_{\mathbf{k},\,0,\,0}(\mathbf{r}) = \sum_l [4\pi(2l+1)]^{\frac{1}{2}} u_{l,\,k}^{l0}(r) i^l Y_l^0(\mathbf{r})\chi_0^0, \quad (13)$$

where $u_{l,k}^{l0}(r)$ is the radial function for the singlet state with angular momentum l and relative momentum k. The solution to Eq. (13) has been obtained in I in determining the properties of nuclear matter.

Combining Eqs. (11), (12), and (13), we find for the singlet part of K:

$$(\mathbf{r}'|K|\mathbf{r})_{\text{singlet}}=\frac{4\pi}{(2\pi)^3}\int k^2dk\sum_l(2l+1)j_l(kr')v_{\text{singlet}}(r)\times u_{l,k}^{l0}(r)P_l^0(\mathbf{r},\mathbf{r}'). \quad (14)$$

For the triplet states the presence of noncentral forces results in K being nondiagonal in m. Taking matrix elements of Eq. (11) with respect to spin, we obtain

$$(\mathbf{r}'|K|\mathbf{r})_{m',m}=\frac{1}{(2\pi)^3}\int d\mathbf{k}\varphi_{\mathbf{k}}^*(\mathbf{r}')\chi_s^{m'*}v(r)\psi_{\mathbf{k},s,m}(\mathbf{r}). \quad (15)$$

We now insert the angular momentum expansion of ψ which is [see I, Eq. (43)]

$$\psi_{\mathbf{k},s,m}(\mathbf{r})=\sum_J\sum_l[4\pi(2l+1)]^{\frac{1}{2}}i^lC(ls0m|lsJm)\times\sum_{l'}u_{ll'}^{Js}(r)F_{Jl's}^{m}(\mathbf{r}), \quad (16)$$

where $F_{Jls}^m(\mathbf{r})$ is an eigenfunction of the total angular momentum, $C(ls0m|lsJm)$ is a Clebsch-Gordan coefficient, and $u_{ll'}^{Js}(r)$ is the radial function for total angular momentum J, spin s, angular momentum l', driven by the entrance-channel angular momentum l. We also make use of the equation

$$\int d\Omega_k\,Y_l^0(\mathbf{r}')v(r)F_{Jl's}^m(\mathbf{r})=\sum_{l''}[4\pi/(2l+1)]^{\frac{1}{2}}v_{l'l''}^{Js}(r)F_{Jl''s}^m(\mathbf{r},\mathbf{r}')\delta_{ll'}, \quad (17)$$

where $v_{l'l''}^{Js}$ is defined by the equation

$$v_{l'l''}^{Js}=\int d\Omega\,F_{Jl's}^{m*}vF_{Jl''s}^{m}. \quad (18)$$

We also need the spin matrix element

$$\chi_s^{m'*}F_{Jls}^m(\mathbf{r},\mathbf{r}')=\sum_{m_s}Y_l^{m-m'}(\mathbf{r},\mathbf{r}')C(lsm'\,m-m'|lsJm), \quad (19)$$

which we obtain by using the Clebsch-Gordan expansion of $F_{Jls}^{m_s}$. Collecting these results, we find for K the result

$$(\mathbf{r}'|K|\mathbf{r})_{m',m}=\frac{(4\pi)^{\frac{3}{2}}}{(2\pi)^3}\int k^2dk\sum_{Jll'l''}(-i)^li^{l'}(2l'+1)^{\frac{1}{2}}\times j_l(kr')u_{l'l''}^{Js}(r)v_{l''l}^{Js}(r)C(l's0m|l'sJm)\times C(ls\,m-m'\,m'|lsJm)Y_l^{m-m'}(\mathbf{r},\mathbf{r}'). \quad (20)$$

Equation (20) determines all matrix elements of K. In our Hartree-Fock studies, however, we need only the central and spin-orbit parts of K. We determine these most simply by writing K in the general form[24] for triplet states alone

$$(\mathbf{r}'|k|\mathbf{r})_{\text{triplet}}=A(\mathbf{r},\mathbf{r}')+B(\mathbf{r},\mathbf{r}')i(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\frac{\mathbf{r}'}{r'}\times\frac{\mathbf{r}}{r} \quad (21)$$

$$+C(\mathbf{r},\mathbf{r}')\boldsymbol{\sigma}_1\cdot\left(\frac{\mathbf{r}'}{r'}-\frac{\mathbf{r}}{r}\right)\sigma_2\cdot\left(\frac{\mathbf{r}'}{r'}-\frac{\mathbf{r}}{r}\right)+D(\mathbf{r},\mathbf{r}')\boldsymbol{\sigma}_1\cdot\left(\frac{\mathbf{r}}{r}-\frac{\mathbf{r}'}{r}\right)\times\left(\frac{\mathbf{r}}{r}\times\frac{\mathbf{r}'}{r'}\right)\boldsymbol{\sigma}_2\cdot\left(\frac{\mathbf{r}}{r}-\frac{\mathbf{r}'}{r'}\right)\times\left(\frac{\mathbf{r}}{r}\times\frac{\mathbf{r}'}{r'}\right). \quad (22)$$

The coefficients A and B which interest us are then easily shown to be given by the expressions

$$A(\mathbf{r},\mathbf{r}')=\tfrac{1}{3}\textstyle\sum_m(\mathbf{r}'|K|\mathbf{r})_{m,m},$$
$$B(\mathbf{r},\mathbf{r}')=\tfrac{1}{4}\sqrt{2}[(\mathbf{r}'|K|\mathbf{r})_{-1,0}+(\mathbf{r}'|K|\mathbf{r})_{0,1}]\csc\theta e^{-i\psi}. \quad (23)$$

Using the explicit form for K of Eq. (20), and the formula

$$\sum_m C(l'10m|l'1Jm)C(l10m|l1Jm)=\frac{2J+1}{2l+1}\delta_{l'l}, \quad (24)$$

we obtain, for the central term A,

$$A(\mathbf{r},\mathbf{r}')=\frac{1}{3}\frac{4\pi}{(2\pi)^3}\int k^2dk\sum_{Jll'}(2J+1)j_l(kr')\mu_{ll''}^{Js}(r)\times v_{l''l}^{Js}(r)P_l(\mathbf{r},\mathbf{r}'). \quad (25)$$

We give this explicitly for the states $l=0$ and $l=2$, disregarding the $J-1$, $J+1$ coupling except for the $J=1$ state as was done in the calculations of I. We write v as

$$v(r)=v_c(r)+v_t(r)S_{12}+v_{LS}(r)\mathbf{L}\cdot\mathbf{S}. \quad (26)$$

TABLE I. Parameters of the Gammel-Thaler potentials. The potentials all have the Yukawa form outside of a repulsive core of radius 0.4×10^{-13} cm.

State	Strength (Mev)	Inverse range (10^{+13} cm^{-1})
Triplet central even	−877.39	2.0908
Tensor even	−159.40	1.0494
Spin-orbit even	−5000	3.70
Singlet even	−434.0	1.45
Triplet central odd	−14.0	1.00
Tensor odd	22.0	0.80
Spin-orbit odd	−7315	3.70
Singlet odd	130.0	1.00

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The matrix elements of v are

$$\begin{aligned} v_{00}{}^{11}&=v_c,\\ v_{02}{}^{11}&=v_{20}{}^{11}=v_t/\sqrt{8},\\ v_{22}{}^{11}&=v_c-2v_t-3v_{LS},\\ v_{22}{}^{21}&=v_c+2v_t-v_{LS},\\ v_{22}{}^{31}&=v_c-(4/7)v_t+2v_{LS}. \end{aligned} \tag{27}$$

Inserting these results into Eq. (25), we find

$$\begin{aligned} A(\mathbf{r},\mathbf{r}')=&\frac{1}{3}\frac{4\pi}{(2\pi)^3}\int k^2dk\{3j_0(kr)\\ &\times[u_{00}{}^{11}(r')v_c(r')+u_{02}{}^{11}(r')v_t(r')/\sqrt{8}]\\ &+j_2(kr)P_2(\mathbf{r},\mathbf{r}')[3u_{20}{}^{11}(r')v_t(r')/\sqrt{8}\\ &+3u_{22}{}^{11}(r')(v_c(r')-2v_t(r')-3v_{LS}(r'))\\ &+5u_{22}{}^{21}(r')(v_c(r')+2v_t(r')-v_{LS}(r'))\\ &+7u_{22}{}^{31}(r')(v_c(r')-(4/7)v_t(r')+2v_{LS}(r'))]\}. \end{aligned} \tag{28}$$

As a check, we consider the Born approximation limit where $u_{02}{}^{11}$ and $u_{20}{}^{11}$ vanish, $u_{00}{}^{11}(r')=j_0(kr')$, and $u_{22}{}^{J1}(r')=j_2(kr')$. In this case the coefficient of $v_c(r')$ is just $j_0(kr)j_0(kr')+5j_2(kr)j_2(kr')P_2(\mathbf{r},\mathbf{r}')$ and the coefficients of v_t and v_{LS} vanish, as we expect.

Next we consider the spin-orbit term. Using Eq. (20) and Eq. (23), we find

$$\begin{aligned} B(\mathbf{r},\mathbf{r}')=&\tfrac{1}{4}\sqrt{2}\frac{(4\pi)^{\frac{3}{2}}}{(2\pi)^3}\int k^2dk\\ &\times\{\sum_{Jll'l''}(-i)^l i^{l'}(2l'+1)^{\frac{1}{2}}j_l(kr)u_{l'l''}{}^{Js}(r')v_{l''l}{}^{Js}(r')\\ &\times[C(l'100|l'1J0)C(l11-1|l1J0)\\ &+C(l'101|l'1J1)C(l110|l1J1)]\}\\ &\times Y_l{}^1(\mathbf{r}',\mathbf{r})e^{-i\psi}\csc\theta. \end{aligned} \tag{29}$$

We can bring this to somewhat simpler form by using the relation

$$Y_l{}^1(\cos\theta)e^{-i\psi}\csc\theta=[l(l+1)]^{-\frac{1}{2}}\frac{d}{d\cos\theta}Y_l{}^0(\cos\theta), \tag{30}$$

and also the identity

$$\begin{aligned} \frac{1}{i}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\frac{\mathbf{r}}{r}\times\frac{\mathbf{r}'}{r'}\frac{d}{d\mu}f(r,r',\mu)&=\frac{1}{i}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\mathbf{r}\times\boldsymbol{\nabla}f(r,r',\mu)\\ &=2\mathbf{L}\cdot\mathbf{S}f(r,r',\mu). \end{aligned} \tag{31}$$

Thus the coefficient of $\mathbf{L}\cdot\mathbf{S}$ in the K matrix is

$$\begin{aligned} B'(\mathbf{r},\mathbf{r}')=&\tfrac{1}{2}\sqrt{2}\frac{(4\pi)^{\frac{3}{2}}}{(2\pi)^3}\int k^2dk\\ &\times\sum_{Jll'l''}\{(-i)^l i^{l'}(2l'+1)^{\frac{1}{2}}j_l(kr)Y_l{}^0(\mathbf{r}',\mathbf{r})\\ &\times[l(l+1)]^{-\frac{1}{2}}u_{l'l''}{}^{Js}(r')v_{l''l}{}^{J}(r')\\ &\times[C(l's00|l'sJ0)C(ls1-1|lsJ0)\\ &+C(l's01|l'sJ1)C(ls10|lsJ1)]\}. \end{aligned} \tag{32}$$

Again writing this out explicitly for $l=0$ and 2, we find

$$\begin{aligned} B'(\mathbf{r},\mathbf{r}')=&\frac{1}{12}\frac{4\pi}{(2\pi)^3}\int k^2dk\,j_2(kr)\{-9u_{20}{}^{11}(r')v_t(r')/\sqrt{8}\\ &-9u_{22}{}^{11}(r')[v_c(r')-2v_t(r')-3v_{LS}(r')]\\ &-5u_{22}{}^{21}(r')[v_c(r')+2v_t(r')-v_{LS}(r')]\\ &+14u_{22}{}^{31}(r')[v_c(r')-(4/7)v_t(r')+2v_{LS}(r')]\}\\ &\times P_2(\mathbf{r},\mathbf{r}'). \end{aligned} \tag{33}$$

In Born approximation the terms in v_c and v_t drop out, leaving

$$B'(\mathbf{r},\mathbf{r}')_{\text{Born}}=\frac{4\pi}{(2\pi)^3}\int k^2dk\,j_2(kr)j_2(kr')v_{LS}(r')\times 5P_2(\mathbf{r},\mathbf{r}'), \tag{34}$$

which is just the contribution from $l=2$ to

$$B'(\mathbf{r},\mathbf{r}')_{\text{Born}}=v_{LS}(r)\delta(\mathbf{r}-\mathbf{r}'). \tag{35}$$

IV. *K* MATRIX IN COORDINATE SPACE; EVALUATION

In this section the numerical results we give are all based on the Gammel-Thaler[23] two-body potentials which have also been used in the study of nuclear matter. The parameters of these potentials are given in Table I.

To evaluate the expressions obtained in the previous section, it is first necessary to remove the repulsive core singularity in the potential, which must be treated separately. To do this we consider as an example the singlet state. We rewrite the singlet potential as

$$v_{\text{singlet}}\rightarrow v_{\text{singlet}}+v_{\text{core}}, \tag{36}$$

where by v_{singlet} we now mean the attractive part of the potential. The singlet part of the K matrix then is

$$\begin{aligned} (\mathbf{r}'|K|\mathbf{r})_{\text{singlet}}=&\frac{4\pi}{(2\pi)^3}\sum_l\int k^2dk(2l+1)j_l(kr')\\ &\times[v(r)_{\text{singlet}}+v(r)_{\text{core}}]u_{lk}{}^{l0}(r)P_l(\mathbf{r},\mathbf{r}'). \end{aligned} \tag{37}$$

As in I, we next make the replacement

$$v_{\text{core}}(r)u_{lk}{}^{l0}(r)=\lambda_{lk}{}^{l0}\delta(r-r_c). \tag{38}$$

The constant $\lambda_{lk}{}^{l0}$ is determined by the boundary condition that the wave function vanish at the core radius. This determination is discussed in detail in I [see Eq. (55) of I]. The separation of the core contribution leads to the appearance of a core term in the K matrix, which is

$$\begin{aligned} (\mathbf{r}'|K|\mathbf{r})_{\text{core}}=&\frac{4\pi}{(2\pi)^3}\sum_l\int k^2dk(2l+1)\\ &\times j_l(kr')\lambda_{lk}{}^{l0}P_l(\mathbf{r},\mathbf{r}')\delta(r-r_c). \end{aligned} \tag{39}$$

TABLE II. $2\pi^2(\mathbf{r}|K|\mathbf{r}')$ for singlet $l=0$. The units are Mev $(10^{-13}\text{ cm})^{-3}$. The K matrix for $l=2$ is very close to that for $l=0$ and may be taken as identical in computation. For $r>1.2\times10^{-13}$ cm, $(\mathbf{r}|K|\mathbf{r}')$ can be replaced by the local potential.

r' (10^{-13} cm) \ r (10^{-13} cm)	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00	1.10	1.20
0.45	11 049	10 134	6657	801	−4048													
0.50	8120	8756	6183	1035	−4802	−6384												
0.55	5592	6667	6160	2547	−2758	−4938	−5216											
0.60	2476	4587	5074	3135	−1099	−3331	−4414	−4756										
0.65	1055	2063	3052	2569	166	−1271	−3067	−3807	−3690									
0.70	44	979	1896	2086	1062	−73	−1676	−2616	−3145	−2865								
0.75	183	691	1062	1291	1001	556	−472	−1272	−2045	−2149	−1858							
0.80	515	613	678	721	785	652	240	−284	−1062	−1369	−1523	−1485						
0.85	400	667	536	480	460	230	120	−120	−290	−480	−1127	−1168	−1081					
0.90	474	554	460	370	290	190	90	10	−120	−290	−594	−676	−906	−894				
0.95	0	0	0	0	0	0	0	−35	−80	−130	−240	−300	−660	−691	−641			
1.00	0	0	0	0	0	0	0	0	0	−10	−50	−130	−325	−383	−557	−567		
1.10	0	0	0	0	0	0	0	0	0	0	0	−10	−60	−130	−256	−311	−402	
1.20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	−163	−272

A similar treatment holds for the triplet states; we shall not give the details here but refer to I for further discussion.

The evaluation of the integrals over k such as that appearing in Eq. (39) has been carried out numerically at the computing center of the Los Alamos Scientific Laboratory. The k integration has been cut off at a maximum value of k chosen to insure convergence of the integrals.

One approximation was necessary in carrying this out. In evaluating the Fourier transform of K, we found it desirable to go to very large values of relative momentum to which our previous calculations of I did not extend. These are states far "off-the-energy-shell," in the terminology of I. The K matrix for these states depends somewhat on the initial energy of the interacting pair since this energy appears in the Green's function. The approximation we have adopted is to use in high excited states a mean value of the initial energy which was taken to be the value at the mean Fermi momentum. This approximation affects the small distance or high wave number behavior of K somewhat but is felt to be less important than the over-all inaccuracies inherent in the K matrix evaluation. In carrying out the integrations, the maximum value of k was taken to be $k_{\max}\cong 14p_F$ which corresponds, at normal density, to $\lambda\cong10^{-14}$ cm. This high value of the cutoff was necessary to insure fairly accurate reproduction of the details of K. Although these cannot affect appreciably the expectation values of K in the

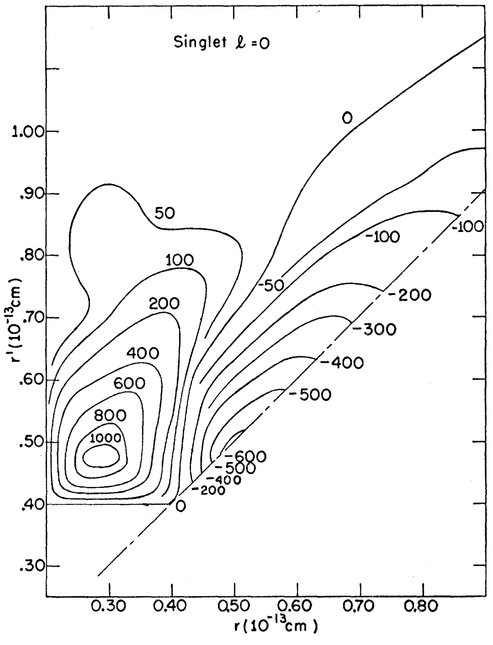

FIG. 1. Contour plot of $2\pi^2(\mathbf{r}|K|\mathbf{r}')$ for $l=0$, singlet. [Since $(\mathbf{r}|K|\mathbf{r}')$ is symmetric in r and r', the function is plotted only for $r<r'$.] The contribution from the core alone [see Eq. (39)] has not been included in this plot; it would occur as a very high repulsive core spike at $r=r'=0.4\times10^{-13}$ cm.

Hartree-Fock problem, they are of importance in exhibiting the structure of K and its approach to the local potential.

One further comment is necessary before we give our results. The K matrix is from its definition symmetric in $\mathbf{r}$ and $\mathbf{r}'$. This is most easily seen from the integral equation for K which, if solved by iteration, gives a manifestly symmetric result. The reason for asymmetry is most easily seen in the core contribution. This contains an explicit $\mathbf{r}$ dependence $\delta(r-r_c)$ but the $\mathbf{r}'$ dependence enters through the k integral

$$\int k^2 dk\, j_l(kr')\lambda_{lk}{}^{l0}. \tag{40}$$

It can be shown that for an infinite cutoff on the k integral, this contains a delta function on $r'-r_c$. Cutting off at finite k, however, replaces the delta function by a spread out function of width $\sim 1/k_{\max}$. Consequently the symmetry of K in this term is lost. For this and other similar reasons, our computed K is slightly asymmetric, the asymmetry extending over distances of $1\text{-}2\times 10^{-14}$ cm. This effect is not physical and further can have no appreciable numerical effect on the Hartree-Fock results; therefore, the results we quote are for the symmetrized K matrix

$$(\mathbf{r}'|K|\mathbf{r})_{\text{sym}}=\tfrac{1}{2}[(\mathbf{r}'|K|\mathbf{r})+(\mathbf{r}|K|\mathbf{r}')]. \tag{41}$$

To exhibit the structure of K clearly, we give contour plots in Figs. 1 and 2 of the central part of K for the singlet and triplet states for $l=0$. These results are also given in tabular form in Tables II, III, and IV. The K matrix shows a rather complicated nonlocal structure for r or r' near the core but quickly approach the local potential for r and r' greater than 10^{-13} cm.

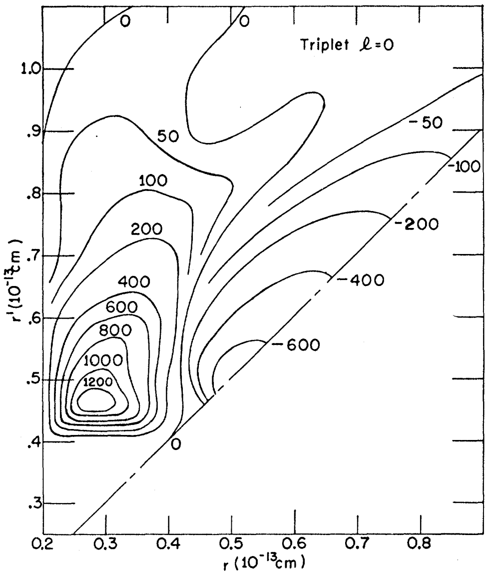

FIG. 2. Contour plot of $2\pi^2(\mathbf{r}|K|\mathbf{r}')$ for $l=0$, triplet. The core contribution is omitted here as in Fig. 1.

TABLE III. $2\pi^2(\mathbf{r}|K|\mathbf{r}')$ for triplet $l=0$. The units are Mev $(10^{-13}\text{ cm})^{-3}$. For $r>1.20\times 10^{-13}$ $(\mathbf{r}|K|\mathbf{r}')$ can be replaced by the $l=0$ part of $f(r)\delta(r-r')$, where $f(r)=-32.53$ Mev, -18.03 Mev, -10.26 Mev, -5.72 Mev at $r=1.4$, 1.6, 1.8, 2.0×10^{-13} cm, respectively. For $r>2.0\times 10^{-13}$ cm $f(r)$ can be taken as equal to the local central potential.

r' (10^{-13} cm) \ r (10^{-13} cm)	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00	1.10	1.20
0.45	13 586	12 928	9018	1955	−804													
0.50	9000	10 829	7943	1773	−5391	−7470												
0.55	6987	8284	7524	3079	−3468	−6264	−6107											
0.60	3757	5678	6061	3475	−2067	−4579	−5623	−5638										
0.65	1755	2939	3834	2821	−456	−2335	−3933	−4552	−4305									
0.70	574	1644	2487	2305	630	−685	−2345	−3200	−3729	−3212								
0.75	573	1170	1538	1535	832	−201	−952	−1648	−2257	−2347	−2067							
0.80	690	926	1027	962	754	478	−80	−622	−1201	−1505	−1643	−1523						
0.85	654	829	767	570	315	252	134	−27	−486	−712	−1068	−1170	−1085					
0.90	492	637	562	298	−37	−52	158	103	−34	−251	−625	−809	−898	−843				
0.95	261	323	347	165	−183	−244	−74	0	3	−62	−381	−419	−590	−667	−614			
1.00	14	138	206	118	−153	−259	−261	−211	−90	−45	−93	−165	−343	−450	−526	−514		
1.10	−102	−68	12	82	163	137	−302	−274	−234	−180	21	54	−24	−44	−275	−298	−339	
1.20	191	−4	−32	−48	90	81	143	121	−35	−40	−78	−66	−12	20	−8	−19	−164	−206

TABLE IV. $2\pi^2(\mathbf{r}|K|\mathbf{r}')\times[5P_2(\mathbf{r},\mathbf{r}')]^{-1}$ for triplet $l=2$. The units are Mev $(10^{-13}\text{ cm})^{-3}$. For $r>1.20\times10^{-13}$ cm $(\mathbf{r}|K|\mathbf{r}')$ can be replaced by the $l=2$ part of $g(r)\delta(\mathbf{r}-\mathbf{r}')$, where $g(r)=-22.31$ Mev, -11.97 Mev, -6.82 Mev, -3.88 Mev at $r=1.4$, 1.6, 1.8, 2.0×10^{-13} cm, respectively. For $r>2.0\times10^{13}$ cm $g(r)$ can be taken as equal to the local central potential.

$r'(10^{-13}\text{ cm})$ \ $r(10^{-13}\text{ cm})$	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00	1.10
0.45	139 326	9393	2048	−5876	−12 045												
0.50	12 353	8292	8293	−5301	−12 833	−13 255											
0.55	5468	6054	6054	2857	−7433	−8506	−7323										
0.60	4973	5286	5286	2116	−5903	−6851	−7486	−7315									
0.65	338	1598	1598	2890	−2152	−2645	−4771	−5091	−4593								
0.70	445	1423	1433	2319	−452	−1024	−3566	−3847	−4149	−3692							
0.75	605	718	719	808	346	239	−1332	−1394	−2316	−2294	−2049						
0.80	555	628	628	644	669	523	−205	−405	−1509	−1557	−1843	−1652					
0.85	755	608	609	138	232	189	411	346	−398	−442	−1091	−1102	−1036				
0.90	650	517	517	111	−130	−133	434	356	−10	−105	−762	−800	−952	−871			
0.95	95	207	207	254	−284	−318	56	0	60	70	248	−237	−537	−568	−571		
1.00	82	174	174	209	−299	−317	−300	−283	−10	12	−38	−55	−376	−414	−553	−527	
1.10	−78	8	8	146	103	+71	−329	−302	−140	−106	56	75	−114	−122	−240	−267	−301

The structure of the K matrix shown in Figs. 1 and 2 can be qualitatively understood rather easily. We return to the definition of the K matrix in Eq. (11) and consider for simplicity the singlet case. As in Eqs. (32), (33), and (34) we eliminate the repulsive core and obtain

$$(\mathbf{r}'|K|\mathbf{r})=(\mathbf{r}'|K|\mathbf{r})_{\text{core}}+(\mathbf{r}'|K|\mathbf{r})_a, \tag{42}$$

where for S states alone

$$(\mathbf{r}'|K|\mathbf{r})_{\text{core}}=\frac{4\pi}{(2\pi)^3}\int k^2dk\, j_0(kr')\delta(r-r_c)\lambda_{0k}{}^{00}, \tag{43}$$

$$(\mathbf{r}'|K|\mathbf{r})_a=\frac{4\pi}{(2\pi)^3}\int k^2dk\, j_0(kr')v_a(r')u_{0k}{}^{00}(r'), \tag{44}$$

the constant $\lambda_{0k}{}^{00}$ is [see Eq. (55) of I]

$$\lambda_{0k}{}^{00}=-\left[j_0(kr_c)+4\pi\int G_0(v_c,r'')v_a(r'')u_{0k}{}^{00}(r'')r''^2dr''\right]$$

$$\times[4\pi r_c{}^2G_0(r_c,r_c)]^{-1}. \tag{45}$$

We now work to first order in the interaction $v_a(r)$ and replace $u_{0k}{}^{00}(r'')$ in Eq. (45) by its first Born approximation value $j_0(kr'')$. In so doing we of course retain only the qualitative features of the K matrix. We then substitute for $\lambda_{0k}{}^{00}$ in Eq. (39). The result is

$$(\mathbf{r}'|K|\mathbf{r})_{\text{core}}=-\frac{4\pi}{(2\pi)^3}\int k^2dk\, j_0(kr')j_0(kr_c)$$

$$\times\frac{\delta(r-r_c)}{4\pi r_c{}^2G_0(r_c,r_c)}-\frac{(4\pi)^2}{(2\pi)^3}\int r''^2\frac{dr''G_0(r_c,r'')}{4\pi r_c{}^2G_0(r_c,r_c)}$$

$$\times v_a(r'')\int k^2dk\, j_0(kr')j_0(kr''). \tag{46}$$

The Green's function is a slowly varying function of k; if we neglect its variation, we can do the integrals over k which give

$$\frac{4\pi}{(2\pi)^3}\int k^2dk\, j_0(kr')j_0(kr_c)=\frac{\delta(r'-r_c)}{4\pi r_c{}^2}, \tag{47}$$

and similarly for the integral with r_c replaced by r''. Thus Eq. (47) becomes

$$(\mathbf{r}'|K|\mathbf{r})_{\text{core}}=-\frac{\delta(r'-r_c)\delta(r-r_c)}{(4\pi r_c{}^2)^2G_0(r_c,r_c)}$$

$$-\frac{G(r_c,r')}{G(r_c,r_c)}v_a(r')\delta(r-r_c). \tag{48}$$

We next consider the term in K resulting from $v_a(r)$, given by Eq. (44). We now retain the first order term in $v_a(r)$ and replace $u_{0k}{}^{00}(r)$ by the second Born approximation

$$u_{0\kappa}^{00}(r)=j_0(kr)+4\pi\int G_0(r,r')v_a(r')j_0(kr')(r')^2dr'. \qquad (49)$$

Substituting Eq. (49) into Eq. (44) and carrying out the k integrals, we obtain

$$(\mathbf{r}'|K|\mathbf{r})_a=\frac{\delta(r-r')}{4\pi r^2}v_a-\delta(r-r_c)v_a(r')\frac{G_0(r',r_c)}{G_0(r_c,r_c)}. \qquad (50)$$

The combined result of $K_{\text{core}}+K_a$ then is

$$(\mathbf{r}'|K|\mathbf{r})=-\frac{\delta(r'-r_c)\delta(r-r_c)}{(4\pi r_c^2)^2G_0(r_c,r_c)} -\left[\delta(r-r_c)v_a(r')\frac{G_0(r',r_c)}{G_0(r_c,r_c)}+(r\leftrightarrow r')\right] +v_a(r)\frac{\delta(r-r')}{4\pi r^2}, \qquad (51)$$

which is now manifestly symmetric in r and r'. We see that the core repulsion not only leads to the term proportional to $\delta(r-r_c)\delta(r'-r_c)$ which has not been included in Figs. 1 and 2 but also to the appearance of repulsive terms lying along the lines $r=r_c$ and $r'=r_c$. These are the origin of the repulsions seen clearly in Figs. 1 and 2. The effects of our finite momentum cutoff are seen in the displacement of roughly 10^{-14} cm of the repulsive peak from the repulsive core line.

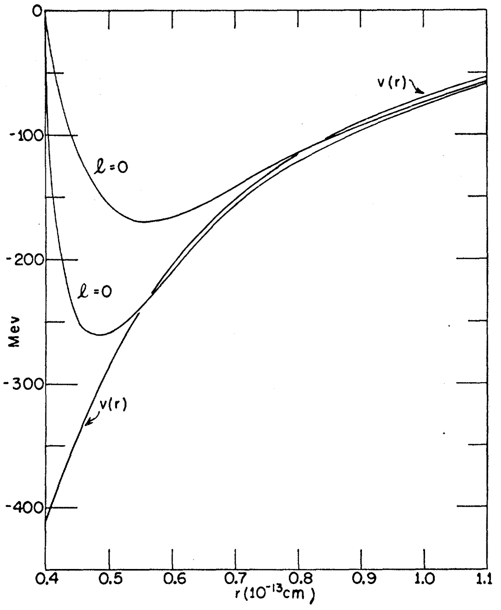

FIG. 3. Integral of $(\mathbf{r}|K|\mathbf{r}')$ normalized to the correct asymptotic behavior, for singlet $l=0$ and $l=2$. Also included is the local singlet potential with parameters shown in Table I.

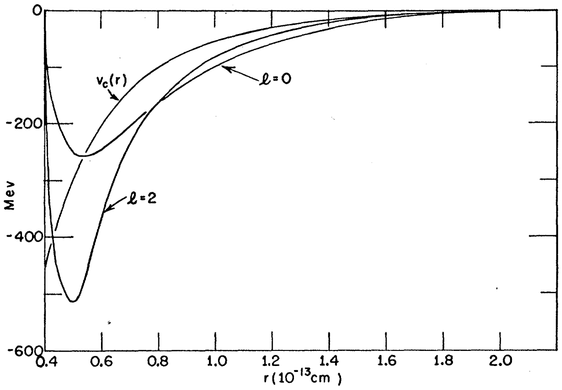

FIG. 4. Integral of $(\mathbf{r}|K|\mathbf{r}')$ for triplet $l=0$ and $l=2$, together with the central part of the triplet even-state potential.

The approach of $(\mathbf{r}|K|\mathbf{r}')$ to the local potential can be seen more readily by considering the function

$$f(r)=\int d\mathbf{r}'(\mathbf{r}|K|\mathbf{r}'), \qquad (52)$$

which approaches the central part of the local potential $v_c(r)$ for large r. The actual point at which $f(r)$ and $v_c(r)$ become equal is a sensitive test of the correlation distance in the wave function since it is this which determines the difference between the reaction matrix K and $v(r)$.

The function $f(r)$ together with $v_c(r)$ is given in Figs. 3 and 4 for the singlet and triplet states. For convenience we have also included with the $l=0$ result the predictions for $l=2$. In the singlet case, for both l values, the departure from the potential is marked only for $r<10^{-13}$ cm, particularly at the core where the integrated K matrix vanishes, in contrast to the behavior of the potential. This difference is, of course, due to the vanishing of the wave function at this point. We also note that the values of r for which K and v are appreciably different coincide approximately with the region where K is markedly nonlocal. This is, of course, an expected result. A further feature clearly shown in the results is the close similarity of the $l=0$ and $l=2$ terms in the singlet K matrix except for r close to the core radius. This is due to the particularly rapid approach of K to v in the singlet case. For the triplet case, the $l=0$ and $l=2$ terms show much greater difference, reflecting the strongly l-dependent effect of the noncentral forces. In Born approximation these do not contribute to the spin-averaged K matrix we consider, as emphasized in the last section. They do have a pronounced effect at distances less than 2×10^{-13} cm where the noncentral terms in the potential strongly perturb the wave function.

We next consider the spin-orbit term in the K matrix as given by Eq. (17). It would be convenient to break this down into two contributions, the first arising from the tensor forces and the second from the spin-orbit and tensor forces combined. It is not possible, however,

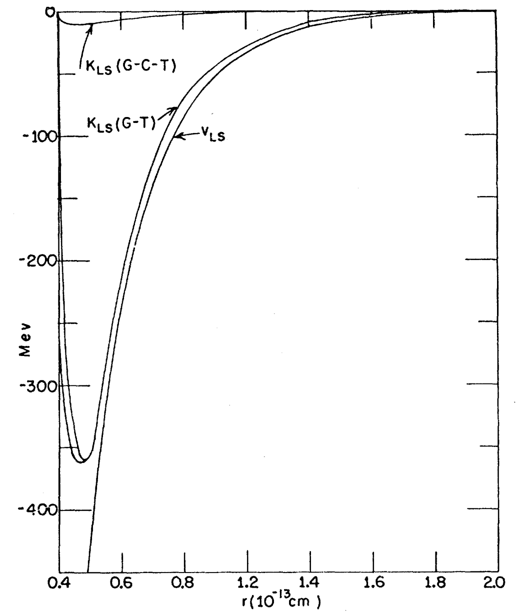

FIG. 5. Integral of $(\mathbf{r}|K|\mathbf{r}')_{LS}$ from tensor forces in Gammel-Christian-Thaler potential compared with the same integral for Gammel-Thaler potential. Also included are the Gammel-Thaler spin-orbit potentials for even and odd-states.

to do this with our present results. Instead we shall quote some results obtained with a previous choice of the even state potentials which contained no spin-orbit force but otherwise fit the scattering data. These were the Gammel-Christian-Thaler potentials considered in I. The parameters of the even-state potentials are tabulated in Table V. For simplicity we give only the K matrix in this state integrated over r', choosing the normalization so that in Born approximation we would obtain the local spin-orbit potential (if such a term were present).

This function is given in Fig. 5. For comparison we give the similar term computed from the present Gammel-Thaler potentials we consider together with the spin-orbit term contained in their even and odd state potentials. It is clear from these results that the even-state tensor term in the two-body potential gives an almost negligible contribution to the spin-orbit term in the K matrix and that this arises almost entirely from the spin-orbit term in the potential. We give in Fig. 6 a contour plot of the $\mathbf{L}\cdot\mathbf{S}$ term in the K matrix and also in Table VI the numerical values.

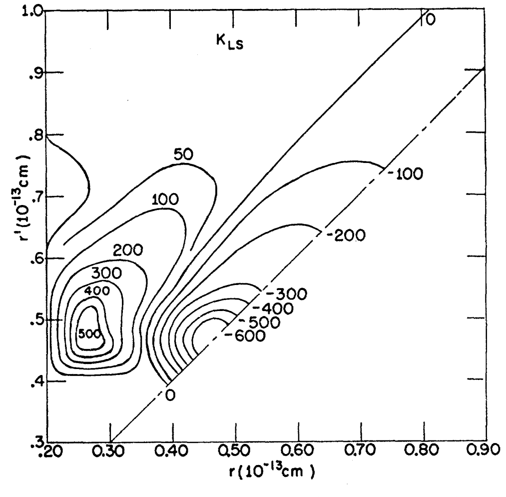

FIG. 6. Contour plot of $(6\pi^2/5)(\mathbf{r}|K|\mathbf{r}')_{LS}/[5P_2(\mathbf{r},\mathbf{r}')]$ for even states.

TABLE V. Parameters of Gammel-Christian-Thaler even-state potentials. The potentials all have the Yukawa form outside a repulsive core of radius 0.5×10^{-13} cm.

State	Strength (Mev)	Inverse range (10^{13} cm^{-1})
Triplet central	−6395	2.936
Triplet tensor	−45	0.73421
Singlet	−905.6	1.70

We finally turn to another important property of the K matrix, its variation with density. This is particularly important since, as we shall see, it determines the saturating character of the interaction. To show the density effect, we consider the integrals over r' of the K matrix for $l=0$ since it is only in this state that appreciable density variation appears. We first consider the contribution from the attractive part of the potential. This is shown in Fig. 7 and Fig. 8 for the singlet and triplet state, at densities corresponding to $r_0=0.80\times10^{-13}$ cm and $r_0=1.07\times10^{-13}$ cm, a density ratio of 2.39. These show a density dependence which is sufficiently weak so that we neglect it in the following. A much more striking effect is seen in the core repulsion computed from Eq. (39). To compare the result at the two densities it is convenient to replace the symmetrized core contribution of Eq. (39) by a function with the same volume integral, of the form $A\delta(r-r_c)\times[\delta(r'-r_c)/4\pi r_c^2]$. Comparing this with Eq. (39) for $l=0$, singlet, leads to

$$A_{\text{singlet},\,l=0}=\frac{(4\pi)^2}{(2\pi)^3}\int\frac{(r')^2}{r_c^2}dr'\int k^2dk\,j_0(kr')\lambda_{0k}^{00}, \qquad (53)$$

together with a similar result for the triplet state. The constant A has the values in these cases (for $l=0$)

$$\left.\begin{aligned}A_{\text{singlet}}&=215\text{ Mev }(10^{-13}\text{ cm}),\ r_0=1.07\times10^{-13}\text{ cm}\\&=301\text{ Mev }(10^{-13}\text{ cm}),\ r_0=0.80\times10^{-13}\text{ cm},\\A_{\text{triplet}}&=257\text{ Mev }(10^{-13}\text{ cm}),\ r_0=1.07\times10^{-13}\text{ cm}\\&=346\text{ Mev }(10^{-13}\text{ cm}),\ r_0=0.80\times10^{-13}\text{ cm},\end{aligned}\right\} \qquad (54)$$

which is an increase in repulsion at the higher density of 39.7% for singlet and 34.7% for triplet. This change is much more pronounced than that of the attractive part of the potential. The rapid increase in the repulsion with increasing density is the principal origin of the saturation of the forces, the pronounced energy

TABLE VI. $(12/5)\pi^2(\mathbf{r}|K|\mathbf{r}')\times[5P_2(r,r')]^{-1}$ for spin orbit, $l=2$. The units are Mev $(10^{-13}\text{ cm})^{-3}$. For $r>1.1\times10^{-13}$ cm, $(\mathbf{r}|K|\mathbf{r}')$ can be replaced by the local potential.

$r'(10^{-13}$ cm) \ $r(10^{-13}$ cm)	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1
0.3	0								
0.4	0	0							
0.5	4064	−3867	−7468						
0.6	2429	1534	−2204	−3454					
0.7	272	1238	366	−1650	−1630				
0.8	87	161	385	96	−569	−662			
0.9	141	−58	−78	368	100	−280	−315		
1.0	31	35	−96	−102	90	41	−122	−161	
1.1	−12	32	51	−168	−53	67	21	−68	−80

minimum in nuclear matter occurring at −15.2 Mev per particle at $r_0=1.02\times10^{-13}$ cm. If the density variation of the K matrix is neglected, the system will not show saturation.

The origin of the different behavior of the attractive and repulsive parts of the K matrix is easily seen. At high densities the attractive part of K approaches closely to the attractive potential except near the core radius; consequently the attraction is only weakly affected by density variations, at least near normal nuclear density. On the other hand, the single core gives a repulsive term in the K matrix which never approaches the Born approximation limit and instead varies with increasing rapidity as the sensity is increased, particularly as $p_F r_c$ starts to approach unity.[25]

To represent the density effect on the repulsive core terms in the K matrix, we shall assume that it has the density dependence

$$K_{\text{core}}\sim(1+b/r_0)^{-1}. \qquad (55)$$

This form of the dependence is given by the theory of a core repulsion alone and is a reasonable approximation for a range of r_0 from 0.8 to 1.6×10^{-13} cm, this corresponding to a density variation from 2.39 to 0.30 times the normal density ($r_0=1.07\times10^{-13}$ cm). From our above results, we find a value for b of -0.488×10^{-13} cm for singlet and -0.459×10^{-13} cm for triplet, which allows us to write

$$\frac{K_{\text{core}}(r_0)}{K_{\text{core}}(1.07\times10^{-13}\text{ cm})} \begin{aligned} &=0.544(1-0.488/r_0)^{-1}, \text{ singlet} \\ &=0.472(1-0.459/r_0)^{-1}, \text{ triplet} \end{aligned} \qquad (56)$$

with r_0 measured in units of 10^{-13} cm. This result we shall use in our actual calculations, together with the predictions for the attractive contributions at $r_0=1.07\times10^{-13}$ cm.

All of the above remarks of the section refer to the even angular momentum states only. To treat the odd angular momentum states, we content ourselves with a much cruder approximation. Before discussing this we wish to summarize some of the features of the odd-state contributions. They arise from considerably weaker interactions than those acting in even states, except for the spin-orbit term. The attraction in the triplet central odd state also tends to be compensated by the singlet odd repulsion. As a consequence of the weakness and opposing signs of these forces, the contribution (from the central forces) to the nuclear binding as evaluated in the nuclear matter studies of I is negligible. The strong-odd state spin-orbit force also has no binding effect since it vanishes on spin-averaging in a spin-uncorrelated medium. This is true only if the force does not appreciably polarize the medium, this however does not occur in the odd angular momentum states.

For these reasons it is sufficiently accurate to treat the odd-state interactions in Born approximation. One complication arises from the repulsive core; we approximate to the effect of this by cutting off the potential at the core radius. This approximate procedure has been checked by numerical evaluation of the energy and found to lead to results in good agreement with the exact calculations of I.

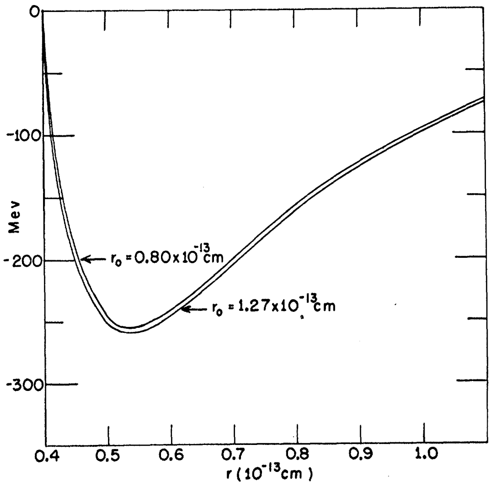

FIG. 7. Integral of $(\mathbf{r}|K|\mathbf{r}')$ for triplet $l=0$, at densities corresponding to $r_0=0.80\times10^{-13}$ cm and $r_0=1.07\times10^{-13}$ cm. The core contribution is omitted.

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[25] H. Bethe and J. Goldstone, Proc. Roy. Soc. (London) A238, 551 (1956). This point is also discussed in I.

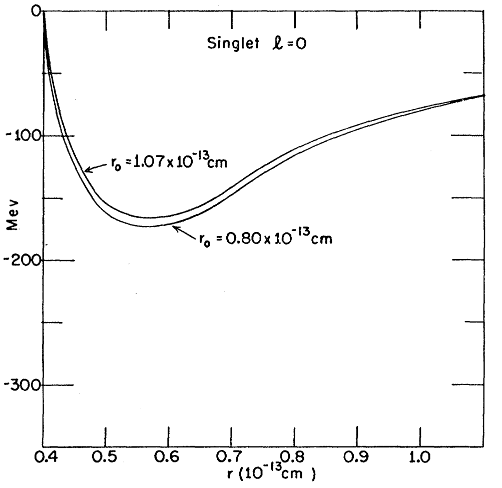

FIG. 8. Integral of $(\mathbf{r}|K|\mathbf{r}')$ for singlet $l=0$, at densities corresponding to $r_0=0.80\times10^{-13}$ cm and $r_0=1.07\times10^{-13}$ cm. The core contribution is omitted.

V. HARTREE-FOCK EQUATIONS

Taking the nonlocal density dependent operator $(\mathbf{r}|K|\mathbf{r}')$ discussed in the previous section as an effective two-particle interaction, the formulation of the Hartree-Fock problem proceeds in the usual way.[26] We simplify the result obtained by dropping terms of the form

$$(ml|K|mn),\quad l\neq n$$
$$\sum_i\left(n\left|\frac{p_i^2}{2N}\right|m\right),\quad n\neq m \tag{57}$$

which vanish for a large system. These considerably simplify the equations to be considered and have only a very small quantitative effect in the systems we shall study. This approximation can be removed in a more exact formulation of the problem. If such terms are dropped, then the Hartree-Fock equation for the single-particle eigenfunctions and eigenvalues becomes

$$(E-H_0)\psi_i(\mathbf{r}_1)=\sum_j\int\psi_j^*(\mathbf{r}_2)[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')\psi_j(\mathbf{r}_2')\psi_i(\mathbf{r}_1')$$
$$-(\mathbf{r}_{12}|K|\mathbf{r}_{12}')\psi_j(\mathbf{r}_1')\psi_i(\mathbf{r}_2')]d\mathbf{r}_1'd\mathbf{r}_2'd\mathbf{r}_2, \tag{58}$$

where the second term arises from the exchange of all particle coordinates. In evaluating the exchange, we shall not use the isotopic spin formalism but instead separate the sum over neutrons and protons. Thus if i and j refer to different charge states, the exchange term does not appear. For identical particles, we separate K into singlet-even and triplet-odd operators, i.e., we write

$$(\mathbf{r}_{12}|K|\mathbf{r}_{12}')=(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,e}\tfrac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)$$
$$+(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,o}\tfrac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2). \tag{59}$$

We also carry out the spin exchange indicated in the exchange term by introducing the spin exchange operator

$$P_\sigma=\tfrac{1}{2}(1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2). \tag{60}$$

We next exchange the variables of integration $\mathbf{r}_1'$, $\mathbf{r}_2'$ in the exchange term, making use of the fact that these are dummy variables in the integration. We then can rewrite that part of the right-hand side of Eq. (54) which comes from like-particle interactions as

$$\sum_j\int d\mathbf{r}_1'd\mathbf{r}_2d\mathbf{r}_2'\psi_j(\mathbf{r}_2)\{(\mathbf{r}_{12}|K|\mathbf{r}_{12}')$$
$$-[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,e}\tfrac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)$$
$$+(\mathbf{r}_{12}|K|-\mathbf{r}_{12}')_{t,o}\tfrac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)]$$
$$\times\tfrac{1}{2}(1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\}\psi_j(\mathbf{r}_2')\psi_i(\mathbf{r}_1'). \tag{61}$$

We next use the results

$$\begin{aligned}\tfrac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\tfrac{1}{2}(1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)&=-\tfrac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2),\\ \tfrac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\tfrac{1}{2}(1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)&=\tfrac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2).\end{aligned} \tag{62}$$

and

$$\begin{aligned}(\mathbf{r}_{12}|K|-\mathbf{r}_{12}')_{s,e}&=(\mathbf{r}_{12}|K|\mathbf{r}_{12}'),\\ (\mathbf{r}_{12}|K|-\mathbf{r}_{12}')_{t,o}&=-(\mathbf{r}_{12}|K|\mathbf{r}_{12}').\end{aligned} \tag{63}$$

Collecting these results, we find that the exchange term is exactly equal to the direct term. Consequently, in evaluating the sum over states j in Eq. (58) and Eq. (61), the exchange effect simply introduces a factor of two for those terms in the sum where the state being summed over is occupied by a particle of the same charge as that for which the single-particle potential is being calculated. It is therefore convenient to break the sum over j in Eq. (58) into contributions coming from like- and unlike-particle interactions. We consider first a neutron; Eq. (58) can then be written

$$(E-H_0)\psi_i(\mathbf{r}_1)=\int V_n(\mathbf{r}_1,\mathbf{r}_1')\psi_i(\mathbf{r}_1')d\mathbf{r}_1', \tag{64}$$

where

$$V_n(\mathbf{r}_1,\mathbf{r}_1')=\tfrac{1}{2}\sum_{j\text{ (neutrons)}}\int\psi_j^*(\mathbf{r}_2)[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,e}$$
$$+3(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,o}]\psi_j(\mathbf{r}_2')d\mathbf{r}_2d\mathbf{r}_2'$$
$$+\tfrac{1}{4}\sum_{j\text{ (protons)}}\int\psi_j^*(\mathbf{r}_2)[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,e}$$
$$+3(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,e}+(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,o}$$
$$+3(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,o}]\psi_j(\mathbf{r}_2')d\mathbf{r}_2d\mathbf{r}_2'. \tag{65}$$

The proton potential $V_p(\mathbf{r}_1,\mathbf{r}_1')$ is similar except that the sums over neutrons and protons are interchanged. For convenience in the following we shall simply write

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[26] See, for example, F. Seitz, *The Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), Chap. VI.

the neutron and proton potential as

$$V_i(\mathbf{r}_1,\mathbf{r}_1') =\sum_j C_{ij}\int \psi_j^*(\mathbf{r}_2)(\mathbf{r}_{12}|K|\mathbf{r}_{12}')\psi_j(\mathbf{r}_2')d\mathbf{r}_2d\mathbf{r}_2', \quad (66)$$

where C_{ij} is the proper statistical factor appearing in Eq. (65).

To carry out the angular momentum reduction of Eqs. (64) and (66), we first consider the expectation of the spin-orbit term

$$\tfrac{1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\mathbf{r}_{12}\times\mathbf{p}_{12}B'(\mathbf{r}_{12},\mathbf{r}_{12}'). \quad (67)$$

We suppose that the state of particle "1" is being considered and is a specified spin state. The expectation value of $\boldsymbol{\sigma}_2$ summed over the spin states of particle 2 then will be taken to be zero if the states are all populated equally with spin up and down. This is not exactly true since a spin-orbit interaction in the single-particle potentials splits the two states with the same orbital motion but opposing spins. This effect appears, however, to second order in the spin-orbit potential strength and we shall drop it, since the spin-orbit potential is weak relative to the central potential. We shall also neglect any possible lack of spin-pairing in unfilled shells. Consequently our results will hold only at and near closed shells. To evaluate the expectation value of $\mathbf{r}_{12}\times\mathbf{p}_{12}$, we first write $\mathbf{L}_{12}$ as

$$\mathbf{r}_{12}\times\mathbf{p}_{12}=\tfrac{1}{2}(\mathbf{r}_1\times\mathbf{p}_1+\mathbf{r}_2\times\mathbf{p}_2-\mathbf{r}_1\times\mathbf{p}_2-\mathbf{r}_2\times\mathbf{p}_1). \quad (68)$$

We then use the relation

$$\mathbf{p}_2B'(\mathbf{r}_{12},\mathbf{r}_{12}')=-\mathbf{p}_1B'(\mathbf{r}_{12},\mathbf{r}_{12}') \quad (69)$$

so that Eq. (68) can be written

$$\mathbf{r}_{12}\times\mathbf{p}_{12}\rightarrow\mathbf{r}_1\times\mathbf{p}_1-\mathbf{r}_2\times\mathbf{p}_1. \quad (70)$$

Consider first the expectation value of the first term. This is

$$\sum_j C_{ij}\int\psi_j^*(r_2)[\mathbf{r}_1\times\mathbf{p}_1B'(\mathbf{r}_{12},\mathbf{r}_{12}')]\psi_j(\mathbf{r}_2')d\mathbf{r}_2d\mathbf{r}_2', \quad (71)$$

where the operator $\mathbf{p}_1$ operates only on $B(\mathbf{r}_{12},\mathbf{r}_{12}')$. We now make use of the delta function on the center-of-mass coordinate which previously has not been explicitly included. Evaluating the integral over $\mathbf{r}_2'$, we then obtain

$$8\sum_j C_{ij}\int\psi_j^*(\mathbf{r}_2)[\mathbf{r}_1\times\mathbf{p}_1B'(\mathbf{r}_{12},\,\mathbf{r}_{12}-2(\mathbf{r}_1-\mathbf{r}_1'))\times\psi_j(\mathbf{r}_2+\mathbf{r}_1-\mathbf{r}_1')]d\mathbf{r}_2. \quad (72)$$

If. B' were a local function and hence contained a delta function on $\mathbf{r}_1-\mathbf{r}_1'$, then $\mathbf{r}_1-\mathbf{r}_1'$ would drop out of $\psi_l(\mathbf{r}_2+\mathbf{r}_1-\mathbf{r}_1')$ and we could remove $\mathbf{r}_1\times\mathbf{p}_1$ from the integral. We shall still proceed to do this, arguing (a) that the nonlocality in B' is of very short range, and (b) that ψ_j is slowly varying relative to B'.

Next we need to evaluate

$$\sum_j C_{ij}\int\psi_j^*(\mathbf{r}_2)\mathbf{r}_2B(\mathbf{r}_{12},\mathbf{r}_{12}')\psi_j(\mathbf{r}_2')d\mathbf{r}_2d\mathbf{r}_2'. \quad (73)$$

This must be proportional to a vector constructed from $\mathbf{r}_1$ and $\mathbf{r}_1'$. If the nonlocality in B is of very short range, it is sufficiently accurate to simply take this vector to be $\mathbf{r}_1$. This approximation is similar to that already made in removing $\mathbf{p}_1$ from the integral of Eq. (71). We therefore retain only the component of $\mathbf{r}_2$ along $\mathbf{r}_1$, i.e., we make the replacement

$$\mathbf{r}_2\rightarrow(\mathbf{r}_1\cdot\mathbf{r}_2)\mathbf{r}_1/r_1^2. \quad (74)$$

This allows us in taking the expectation value of the spin-orbit term to make the replacement

$$\langle\mathbf{r}_{12}\times\mathbf{p}_{12}\rangle\rightarrow\mathbf{r}_1\times\mathbf{p}_1\langle 1-\mathbf{r}_1\cdot\mathbf{r}_2/r_1^2\rangle. \quad (75)$$

This treatment of the spin-orbit term gives for the single-particle potential

$$(\mathbf{r}_1|V_i|\mathbf{r}_1')=(\mathbf{r}_1|V_i^{(c)}|\mathbf{r}_1')+\mathbf{L}_1\cdot\mathbf{S}_1(\mathbf{r}_1|V_i^{(LS)}|\mathbf{r}_1'), \quad (76)$$

where

$$(\mathbf{r}_1|V_i^{(c)}|\mathbf{r}_1')=\sum_j C_{ij}\int d\mathbf{r}_2d\mathbf{r}_2'\psi_j^*(\mathbf{r}_{12})\times(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{\text{central}}\psi_j(\mathbf{r}_2'), \quad (77)$$

and

$$(\mathbf{r}_1|V_i^{(LS)}|\mathbf{r}_1')=\sum_j C_{ij}\int d\mathbf{r}_2d\mathbf{r}_2'\psi_j(\mathbf{r}_2)^*(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{LS}\times(1-\mathbf{r}_1\cdot\mathbf{r}_2/r_1^2)\psi_j(\mathbf{r}_2'). \quad (78)$$

Before going on to the angular momentum reduction of Eq. (58), we note in passing a further simplifying approximation to Eq. (78). Let us for the moment neglect exchange effects and also assume that the $\mathbf{L}\cdot\mathbf{S}$ two-body interaction is local. In Eq. (78) we then replace $(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{LS}$ by $f_{LS}(\mathbf{r}_{12})\delta(\mathbf{r}_{12}-\mathbf{r}_{12}')$. This also allows us to replace the product $\psi_j^*(\mathbf{r}_2)\psi_j(\mathbf{r}_2')$ by $|\psi_j(\mathbf{r}_2)|^2$. Then the sum over j is just the density, i.e.,

$$\textstyle\sum_j|\psi_j(r_2)|^2=\rho(r_2). \quad (79)$$

Making this replacement, Eq. (78) becomes

$$(\mathbf{r}_1|V^{(LS)}|\mathbf{r}_1')=\delta(\mathbf{r}_1-\mathbf{r}_1')\int d\mathbf{r}_2\rho(r_2)\times f_{LS}(r_{12})(1-\mathbf{r}_1\cdot\mathbf{r}_2/r_1^2). \quad (80)$$

We next make the change in variable from $\mathbf{r}_2$ to $\mathbf{r}_1-\mathbf{r}_2=\mathbf{x}$. We also introduce the expansion of $\rho(\mathbf{r}_2)$ about $\mathbf{r}_2=\mathbf{r}_1$,

$$\rho(r_2)=\rho(r_1)+(\mathbf{r}_2-\mathbf{r}_1)\cdot\boldsymbol{\nabla}_1\rho(r_1)+\cdots. \quad (81)$$

We then can rewrite Eq. (78) as

$$(\mathbf{r}_1|V^{LS}|\mathbf{r}_1')=\delta(\mathbf{r}_1-\mathbf{r}_1')\int d\mathbf{x}\times[\rho(r_1)-\mathbf{x}\cdot\nabla_1\rho(r_1)+\cdots]\frac{\mathbf{r}_1\cdot\mathbf{x}}{r_1^2}f_{LS}(x). \quad (82)$$

The term proportional to $\rho(r_1)$ vanishes on angular averaging; the second term gives [now dropping higher derivatives of $\rho(r_1)$]

$$(\mathbf{r}_1|V^{LS}|\mathbf{r}_1')=-\delta(\mathbf{r}_1-\mathbf{r}_1')\left[\frac{4\pi}{3}\int x^4dxf_{LS}(x)\right]\frac{1}{r_1}\frac{d}{dr_1}\rho(r_1), \quad (83)$$

which is just the familiar form of the Thomas $\mathbf{L}\cdot\mathbf{S}$ potential.

It is now convenient to break the sum over j in Eq. (78) down into sums over the principal quantum number n, the total and orbital angular momenta J and l, and the z component of angular momentum m. To do this we separate the angular dependence of the wave function, writing

$$\psi_j(\mathbf{r}_2)=\frac{R_{nlJ}(r_2)}{r_2}F_{Jls}{}^m(\mathbf{r}_2), \quad (84)$$

where $F_{Jls}{}^m(\mathbf{r}_2)$ is an eigenfunction of the total angular momentum. In evaluating the sum over the z component of angular momentum, we shall neglect the possible nonfilling of the state and carry out the sum as if the state were completely filled. Thus the sum over azimuthal quantum numbers gives

$$\sum_m F_{Jls}{}^m(\mathbf{r}_2)^*F_{Jls}{}^m(\mathbf{r}_2')=\left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}}\frac{N_{Jln}}{2J+1}Y_l{}^0(\mathbf{r}_2,\mathbf{r}_2'), \quad (85)$$

where N_{Jln} is the actual number in the state. For a completely occupied shell, N_{Jln} is of course equal to $2J+1$. We carry out the remaining sums over J, n, l and introduce new functions

$$\begin{aligned}H_N(\mathbf{r}_2,\mathbf{r}_2')&=\sum_l H_l{}^N(r_2,r_2')Y_l{}^0(\mathbf{r}_2,\mathbf{r}_2'),\\ H_P(\mathbf{r}_2,\mathbf{r}_2')&=\sum_l H_l{}^P(r_2,r_2')Y_l{}^0(\mathbf{r}_2,\mathbf{r}_2')\end{aligned} \quad (86)$$

by defining equations

$$\begin{aligned}H_l{}^N(\mathbf{r}_2,r_2')&=\sum_{nJ\text{ (neutrons)}}\frac{R_{nJl}(r_2)}{r_2}\frac{R_{nJl}(r_2')}{r_2'}\frac{N_{Jnl}}{2J+1}\left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}},\\ H_l{}^P(r_2,r_2')&=\sum_{nJ\text{ (protons)}}\frac{R_{nJl}(r_2)}{r_2}\frac{R_{nJl}(r_2')}{r_2'}\frac{N_{Jnl}}{2J+1}\left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}}.\end{aligned} \quad (87)$$

The neutron and proton potentials then can be written:

$$\begin{aligned}V_N(\mathbf{r}_1,\mathbf{r}_1')&=V_N{}^{(c)}(\mathbf{r}_1,\mathbf{r}_1')+V_N{}^{(LS)}(\mathbf{r}_1,\mathbf{r}_1')\mathbf{L}_1\cdot\mathbf{S}_1,\\ V_P(\mathbf{r}_1,\mathbf{r}_1')&=V_P{}^{(c)}(\mathbf{r}_1,\mathbf{r}_1')+V_P{}^{(LS)}(\mathbf{r}_1,\mathbf{r}_1')\mathbf{L}_1\cdot\mathbf{S}_1,\end{aligned} \quad (88)$$

where

$$\begin{aligned}V_N{}^{(c)}(\mathbf{r}_1,\mathbf{r}_1')=&\frac{1}{2}\int H_N(\mathbf{r}_2,\mathbf{r}_2')[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,\,e}\\ &+3(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,\,o,\,\text{central}}]d\mathbf{r}_2d\mathbf{r}_2'+\frac{1}{4}\int H_P(\mathbf{r}_2,\mathbf{r}_2')\\ &\times[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,\,e}+3(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,\,e,\,\text{central}}\\ &+(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{s,\,o}+(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,\,o,\,\text{central}}]d\mathbf{r}_2d\mathbf{r}_2',\end{aligned} \quad (89)$$

$$\begin{aligned}V_N{}^{(LS)}(\mathbf{r}_1,\mathbf{r}_1')=&\frac{3}{2}\int H_N(\mathbf{r}_2,\mathbf{r}_2')(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,\,o,\,LS}d\mathbf{r}_2d\mathbf{r}_2'\\ &+\frac{3}{4}\int H_P(\mathbf{r}_2,\mathbf{r}_2')[(\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{t,\,e,\,LS}\\ &+(r_{12}|K|r_{12}')_{t,\,o,\,LS}]d\mathbf{r}_2d\mathbf{r}_2'.\end{aligned} \quad (90)$$

The proton potential is given by the same expressions with H_N and H_P interchanged.

In the approximation described in the previous section, $K_{t,\,e,\,\text{central}}$ is given by $A(\mathbf{r}_{12},\mathbf{r}_{12}')$ as defined in Eq. (28), $K_{t,\,e,\,LS}$ by $B'(\mathbf{r}_{12},\mathbf{r}_{12}')$ in Eq. (33), $K_{s,\,e}$ in Eq. (14), and the odd states in Born approximation.

The final step to be carried out is the angular momentum reduction of the Hartree-Fock equation. Again introducing Eq. (84) for ψ_j, we rewrite Eq. (64) as

$$\frac{1}{r_1}\left\{E+\frac{1}{2M}\left(\frac{d^2}{dr_1^2}+\frac{l(l+1)}{r_1^2}\right)\right\}R_{nJl}(r_1)F_{Jls}{}^m(\mathbf{r}_1)=\int d\mathbf{r}_1'\{(\mathbf{r}_1|V^{(c)}|\mathbf{r}_1')+\mathbf{L}_1\cdot\mathbf{S}_1(\mathbf{r}_1|V^{(LS)}|\mathbf{r}_1')\}\times\frac{R_{nJl}(r_1')}{r_1'}F_{Jls}{}^m(\mathbf{r}_1'). \quad (91)$$

The angular function $F_{Jls}{}^m$ is an eigenfunction of $\mathbf{L}_1\cdot\mathbf{S}_1$; hence, operating to the left with $\mathbf{L}_1\cdot\mathbf{S}_1$, we obtain the eigenvalue $\frac{1}{2}[J(J+1)-l(l+1)-\frac{3}{4}]$. We next introduce the angular momentum expansions of $V^{(c)}$ and $V^{(LS)}$:

$$\begin{aligned}(\mathbf{r}_1|V^{(c)}|\mathbf{r}_1')&=\sum_l(2l+1)V_l{}^{(c)}(r_1,r_1')P_l(\mathbf{r}_1,\mathbf{r}_1'),\\ (\mathbf{r}_1|V^{(LS)}|\mathbf{r}_1')&=\sum_l(2l+1)V_l{}^{(LS)}(r_1,r_1')P_l(\mathbf{r}_1,\mathbf{r}_1').\end{aligned} \quad (92)$$

Multiplying Eq. (91) from the left by $F_{Jls}{}^{m*}(\mathbf{r}_1)$ and integrating over the angles of $\mathbf{r}_1$ and $\mathbf{r}_1'$, we finally obtain

$$\frac{1}{r_1}\left\{E+\frac{1}{2M}\left[\frac{d^2}{dr_1^2}-\frac{l(l+1)}{r_1^2}\right]\right\}R_{nJl}(r_1)=4\pi\int(r_1')^2dr_1'V_{Jl}(r_1,r_1')\frac{R_{nJl}(r_1')}{r_1'}, \quad (93)$$

where

$$V_{Jl}(r_1,r_1')=V_l{}^{(c)}(r_1,r_1')+\tfrac{1}{2}[J(J+1)-l(l+1)-\tfrac{3}{4}]V_l{}^{(LS)}(r_1,r_1'). \quad (94)$$

This completes the angular momentum reduction of the Hartree-Fock equation.

VI. APPROXIMATE REDUCTION OF THE HARTREE-FOCK EQUATION TO A DIFFERENTIAL EQUATION

The Hartree-Fock equation derived in the previous section is a differentio-integral equation due to the nonlocality of the single-particle potential. We shall in this section discuss an approximation to this equation which reduces it to a much simpler form. The approximation we use is useful since it is exact in the limit of convergence of our iteration procedure and also exact if the potential is replaced by a local approximation. This latter feature is particularly useful since the potential $V(\mathbf{r}_1,\mathbf{r}_1')$ is nonlocal over quite small distances.

The equation to be solved is of the form

$$(E-H_0)\frac{R(r)}{r}=4\pi\int r'dr'\ V(r,r')R(r'). \tag{95}$$

This equation can also be rewritten

$$(E-H_0)\frac{R(r)}{r}=\left[4\pi\int r'dr'\ V(r,r')\frac{R(r')R(r)}{D(r)}\right]R(r)+\left[4\pi a^2\int r'dr'\ V(r,r')R(r')\left(\frac{d}{dr}R(r)\right)\Big/D(r)\right]\times\frac{dR(r)}{dr}, \tag{96}$$

where

$$D(r)=R^2(r)+a^2(dR/dr)^2,$$

and a is a constant with dimensions of length. We discuss its choice in the following. Let us now consider the computation of the $(n+1)$st approximation to the solution of Eq. (96), assuming that we know the nth solution. We then approximate to Eq. (96) by

$$(E-H_0)\frac{R^{n+1}(r)}{r}=\left[4\pi\int r'dr'\ V(r,r')\frac{R^n(r')R^n(r)}{D^n(r)}\right]R^{n+1}(r)+\left[4\pi a^2\int r'dr'\ V(r,r')\frac{R^n(r')}{D^n(r)}\frac{dR^n(r)}{dr}\right]\frac{dR^{n+1}(r)}{dr}. \tag{97}$$

This now is an ordinary differential equation for $R^{n+1}(r)$ which differs from the usual Schrödinger equation in the appearance of the first derivative term. If this equation is solved by a convergent iteration-interpolation procedure, then it of course converges to the exact answer.

We note here that the appearance of the gradient term in the equation is necessitated by the nonlocal nature of V. At the zeros of $R(n)$, the integral $\int r'V(r,r')R(r')dr'$ does not in general vanish. Consequently, if we wish to retain this feature, we can do it most simply by adding a derivative term to the ordinary differential equation which automatically will not vanish at the zeros of R. This feature also suggests that a convenient choice for a is a length determined by the nonlocality in V, which we expect to be about 0.5 to 1.0×10^{-13} cm.

This approximation of Eq. (93) still is not quite satisfactory since we have not yet made use of the short range of the nonlocality in V. To see this, we replace V by a local function,

$$V(r,r')\rightarrow\frac{1}{4\pi r^2}f(r)\delta(r-r'), \tag{98}$$

in which case Eq. (97) becomes

$$(E-H_0)\frac{R^{n+1}(r)}{r}=f(r)\frac{\{[R^n(r)]^2R^{n+1}(r)+a^2R^n(r)[dR^n(r)/dr][dR^{n+1}(r)/dr]\}}{[R^n(r)]^2+a^2[dR^n(r)/dr]^2}. \tag{99}$$

The correct equation in this limit is of course

$$(E-H_0)\frac{R^{n+1}(r)}{r}=f(r)R^{n+1}(r), \tag{100}$$

which is approached by Eq. (99) only at convergence.

To remove this difficulty, we have made a further modification of Eq. (99), which is to add an additional term to the right-hand side:

$$4\pi a^2\int r'dr'\frac{V(r,r')}{D^n(r)}\left\{-\frac{dR^n(r')}{dr'}R^n(r)\frac{dR^{n+1}(r)}{dr}+\frac{dR^n(r')}{dr'}\frac{dR^n(r)}{dr}R^{n+1}(r)\right\}. \tag{101}$$

This term vanishes at convergence; in the limit of locality it cancels the last term of Eq. (99) and adds the appropriate term to give the exact result.

Combining Eq. (93) and Eq. (95), we obtain as our final approximation

$$(E-H_0)\frac{R^{n+1}(r)}{r}=F^n(r)R^{n+1}(r)+G^n(r)\frac{dR^{n+1}(r)}{dr}, \tag{102}$$

where

$$\begin{aligned}F^n(r)&=4\pi\int r'dr'\frac{V(r,r')}{D^n(r)}\times\left[R^n(r')R^n(r)+a^2\frac{dR^n(r')}{dr'}\frac{dR^n(r)}{dr}\right],\\ G^n(r)&=4\pi a^2\int r'dr'\frac{V(r,r')}{D^n(r)}\times\left[R^n(r')\frac{dR^n(r)}{dr}-R^n(r)\frac{dR^n(r')}{dr}\right].\end{aligned} \tag{103}$$

These equations are now being solved; the results will be presented in a later paper.