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Density-Matrix Expansion for an Effective Nuclear Hamiltonian*

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An expansion for the nuclear wave-function density matrix in relative and c.m. coordinates is developed such that the leading term is the corresponding nuclear-matter density matrix at the local neutron and proton density. Truncation of all derivatives beyond second order yields an extremely simple form for the energy density which retains all the computational simplicity of the modified δ interaction and the Skyrme force, while maintaining contact with nuclear-matter theory based on a realistic interaction and reproducing the results of more-complicated density-dependent Hartree-Fock calculations.

I. INTRODUCTION

Attempts thus far to approximate the nuclear many-body ground state by a Slater determinant of single-particle wave functions determined self-consistently from the average field created by the other nucleons differ greatly in their computational complexity and the degree to which they retain contact with the phenomenological force between two free nucleons. The purpose of this present work is to relate the extremely simplified effective interaction used in a previous paper[1] to a more fundamental and thus computationally cumbersome theory derived directly from the nucleon-nucleon force.[2]

Because a comprehensive review of various approaches is now available,[3] we shall only briefly review several references of direct relevance to this present work. Several calculations[2,4-6] have now demonstrated that a local-density approximation to the reaction matrix derived from a realistic potential such as the Reid potential[7] yields satisfactory results for the gross properties of finite nuclei. We wish to retain the essential physical ideas of a two-body reaction matrix influenced by the presence of other particles via the Pauli operator and self-consistent energy denominators as discussed in Ref. 2, while eliminating, as much as possible, the complications of successive intermediate definitions of various effective interactions. The final form which is sought is a theory similar to Ref. 1 in which the potential energy density may be simply related to the nuclear density, the gradient of the density, and the kinetic energy density.

As a result of the form of the desired theory, it closely resembles previous work by Skyrme,[8] Köhler,[9] and Moszkowski.[10] Skyrme appears to have been the first to propose truncating an expansion of the forward scattering amplitude, or reaction matrix, in momentum space. He explicitly emphasized that the strength of the scattering changes with density, which was to be accounted for by letting the parameters depend upon

density or by a zero-range three-body force. The same basic philosophy has been used by Köhler,[9] with additional emphasis on attempting to distinguish density dependence and momentum dependence. It is because of the ambiguities involved in parametrizing and approximating the reaction matrix that we have chosen rather to focus on approximating the nuclear density matrix.

In contrast to the approach of Skyrme and Köhler, Moszkowski[10] motivates his modified δ interaction by considering the expansion of the Fourier transform of a short-range local potential. Since the effective reaction matrix of Ref. 2 is essentially local, it is natural to attempt to relate the two theories via a moment expansion. However, since the long-range part of the reaction matrix heals to the bare one-pion-exchange-potential (OPEP) tail, it is evident that integrals of the effective interaction multiplied by higher powers of the relative coordinate cannot be truncated. It was this convergence difficulty which lead us to rearrange the expansion so that the dominant term included the long-range OPEP tail exactly for the nuclear-matter density matrix.

Brueckner and co-workers[11,12] have developed a theory which bears some resemblance to this present work, since it deals with functionals of the density obtained from nuclear-matter calculations. However, it differs significantly from the previously mentioned phenomenological theories and this work in that the kinetic energy density is completely eliminated in terms of the density from the outset.

Although we have chosen to formulate the energy density in a finite nucleus as the exact nuclear-matter energy density arising from an arbitrary reaction matrix plus correction terms, the derivation is considerably simplified if one specializes to the case of an interaction of the form used in Ref. 2. Hence, in Secs. II and III, we derive the density-matrix expansion (DME) and corresponding energy density for this special case. In Sec. IV, it is demonstrated how the theory may be straightforwardly generalized to the case of an arbitrary, nonlocal, energy-dependent reaction matrix, and various correction terms are discussed. The single-particle equations resulting from variation are derived in Sec. V and are shown to be of essentially the same simple form as in Ref. 1. Section VI explains the additional effective interaction approximations used in our preliminary numerical calculations and summarizes the numerical results. Coefficients for a polynomial representation of functions appearing in the energy density are tabulated, and are related to the parameters in Ref. 1. Since this theory essentially reproduces the results of Ref. 2

for finite nuclei, detailed results are not presented and only discrepancies between the theories are discussed.

II. DENSITY-MATRIX EXPANSION

The density matrix may be formally expanded in relative and center-of-mass coordinates $\vec{s}$ and $\vec{R}$ as follows:

$$\rho\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)=\sum_a \phi_a^*\left(\vec{R}+\frac{\vec{s}}{2}\right)\phi_a\left(\vec{R}-\frac{\vec{s}}{2}\right)$$

$$=e^{\vec{s}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)/2}\sum_a \phi_a^*(\vec{R}_1)\phi_a(\vec{R}_2),$$

$$\tag{2.1}$$

where $\vec{\nabla}_1$ acts on $\vec{R}_1$, $\vec{\nabla}_2$ acts on $\vec{R}_2$, and the wave functions are evaluated at $\vec{R}_1=\vec{R}_2=\vec{R}$. If time-reversed orbitals are filled pairwise, the linear term of the exponential expansion vanishes, since

$$(\vec{\nabla}_1-\vec{\nabla}_2)[\phi_m^*(\vec{R}_1)\phi_m(\vec{R}_2)+\phi_m(\vec{R}_1)\phi_m^*(\vec{R}_2)]=0.$$

$$\tag{2.2}$$

Thus, through second-order terms, the angular integral of the square of a density matrix may be replaced by the integral of the square of the angle average of the density matrix. This property is crucial to the following development:

Performing the angular integral over the direction of $\vec{s}$ the expansion becomes

$$\tilde{\rho}\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)$$

$$=\frac{1}{2}\int d\cos\varphi\exp[\cos\varphi\tfrac{1}{2}\vec{s}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)]\rho(\vec{R}_1,\vec{R}_2)$$

$$=\frac{\sinh[\tfrac{1}{2}\vec{s}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)]}{\tfrac{1}{2}\vec{s}\cdot(\vec{\nabla}_1-\vec{\nabla}_2)}\rho(\vec{R}_1,\vec{R}_2).$$

$$\tag{2.3}$$

The physical motivation for our subsequent development is provided by noting that (2.3) involves only even powers and may be rewritten as

$$\tilde{\rho}\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)=F\left(\left(\frac{\vec{\nabla}_1-\vec{\nabla}_2}{2}\right)^2\right)\rho(\vec{R}_1,\vec{R}_2),$$

where

$$F(k^2)=\frac{\sinh(ks)}{ks}\quad k^2>0$$

$$=\frac{\sin(|k|s)}{|k|s}\quad k^2<0.$$

Since the expectation value of $[(\vec{\nabla}_1-\vec{\nabla}_2)/2]^2$ is negative in the nuclear interior, F should be expanded around some average value $-k^2$ rather than

zero.[13] Thus,

$$F\left(\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2}\right)^2\right)$$

$$= F(-k^2) + F'(-k^2)\left[\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2}\right)^2 + k^2\right] + \cdots$$

$$= j_0(ks) + \frac{s}{2k} j_1(ks)\left[\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2}\right)^2 + k^2\right] + \cdots .$$

$$(2.4)$$

For two individual interacting particles, k is obviously the relative momentum, and a natural approximation for the total density matrix in a finite nucleus at some c.m. position $\vec{R}$ is to average both sides of (2.4) over the phase space of nuclear-matter states corresponding to the density $\rho(R)$. The right-hand side then becomes the Slater mixed density plus an infinite sequence of correction terms involving powers of $[(\vec{\nabla}_1 - \vec{\nabla}_2)/2]^2 + k^2$. For the contributions to the density matrix from a small number of levels near the Fermi surface which will be considered in a later section, it is reasonable to choose $k = k_F(\rho(R))$ in (2.4) rather than to average over all relative momenta.

Although (2.4) is a simple way of motivating our intent to build into the DME the average information about the local derivatives of wave functions, the following equivalent expansion turns out to be more convenient. Since an expansion for the density matrix is sought in which the first term is the Slater mixed density, we make use of the following formal Bessel-function expansion:

$$\frac{1}{xy}\sinh(xy) = \frac{1}{x}\sum_{k=0}^{+\infty}(4k+3)j_{2k+1}(x)Q_k(y^2),$$

where Q_k is related to the usual Legendre polynomial by:

$$Q_k(z^2) = \frac{P_{2k+1}(iz)}{iz}$$

$$= \frac{1}{2^{2k+1}}\sum_{l=0}^{k}\frac{(4k+2-2l)!\,z^{2(k-l)}}{l!\,(2k+1-l)!\,(2k+1-2l)!}.$$

In order to obtain the appropriate argument for the Slater mixed density, k_F and $1/k_F$ are grouped with the corresponding terms in (2.3) with the result

$$\hat{\rho}\left(\vec{R}+\frac{\vec{s}}{2}, \vec{R}-\frac{\vec{s}}{2}\right) = \frac{1}{sk_F}\left[\sum_{n=0}^{+\infty}(4n+3)j_{2n+1}(sk_F)\right.$$

$$\left.\times Q_n\left(\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2k_F}\right)^2\right)\right]\rho(\vec{R}_1, \vec{R}_2).$$

$$(2.5)$$

A significant property of the expansion in (2.5) is that each term beyond the first vanishes identically in uniform nuclear matter. Explicitly evaluating the gradient term in nuclear matter,

$$\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2k_F}\right)^{2n}\rho(\vec{R}_1, \vec{R}_2)$$

$$= \frac{1}{(2\pi)^3}\int_0^{k_F}\frac{d^3k}{k_F^{2n}}\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2}\right)^{2n}e^{-i\vec{k}\cdot(\vec{R}_1 - \vec{R}_2)}$$

$$= (-1)^n\left(\frac{3}{2n+3}\right)\rho(\vec{R}, \vec{R}).$$

$$(2.6)$$

Substituting (2.6) in the definition of Q_n and using the orthogonality relation for Legendre polynomials, we obtain:

$$Q_n\left(\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2k_F}\right)^2\right)\rho(\vec{R}_1, \vec{R}_2) = 3\rho(\vec{R}, \vec{R})\left(\frac{1}{2^{2n+1}}\sum_{k=0}^{n}\frac{(-1)^{n-k}(4n+2-2k)!}{k!\,(2n+1-k)!\,(2n+1-2k)!\,(2n-2k+3)}\right)$$

$$= \tfrac{3}{2}(-1)^n\rho(\vec{R}, \vec{R})\int_{-1}^{+1}P_1(x)P_{2n+1}(x)dx$$

$$= \rho(\vec{R}, \vec{R})\delta_{n0}.$$

$$(2.7)$$

Thus, termination of (2.5) at any n yields a result which is exact for nuclear matter.

As will become evident in the subsequent development, a tractable theory results only if derivatives beyond second order are neglected. Thus, the question arises as to how to truncate the expansion for $\hat{\rho}(\vec{R}+\vec{s}/2, \vec{R}-\vec{s}/2)$.

Although the argument preceding equation (2.2) shows that no nonspherical terms contribute

through $n = 1$, it is clear that we have ignored nonspherical contributions in higher orders, and this will be seen quantitatively in Fig. 1. In addition, by retaining only derivatives through second order, there exists infinite freedom to rearrange the series, essentially by adding and subtracting terms of the form $C(4m+3)j_{2m+1}(sk_F)$ $\times Q_1([(\vec{\nabla}_1 - \vec{\nabla}_2)/2k_F]^2)$, grouping the added term with the $n = 1$ term which is retained and the subtracted

term with the $n = m$ term which is truncated. By construction, each truncated term still gives a zero contribution to nuclear matter. Thus, the rearranged expansion will have the function $7j_3(sk_F)/sk_F$ replaced with a power series in $(sk_F)^2$, the first coefficient of which is $\frac{1}{5}$ and with all higher coefficients essentially undetermined. Although undesirable, this lack of uniqueness is not terribly serious, since the unique quadratic term dominates in the region where the nuclear force is strongest.

Since our attempts at obtaining an additional constraint on the higher power of $(sk_F)^2$ by considering analytic expressions for $\rho(\vec{R}_1, \vec{R}_2)$ in a linear surface did not yield useful results, we have instead simply compared the result of using the first two terms of (2.5) with an exact numerical calculation using Hartree-Fock (HF) wave functions for neutrons in ^{208}Pb. Explicitly evaluating

$$Q_1\left(\left(\frac{\vec{\nabla}_1 - \vec{\nabla}_2}{2k_F}\right)^2\right)\rho(\vec{R}_1, \vec{R}_2)$$

in (2.5), the following expression is obtained:

$$\rho\left(\vec{R}+\frac{\vec{s}}{2}, \vec{R}-\frac{\vec{s}}{2}\right) = \rho_{\mathrm{SL}}(sk_F)\rho(\vec{R}) + \frac{35}{2sk_F^{\,3}}\, j_3(sk_F)[\tfrac{1}{4}\nabla^2\rho(\vec{R}) - \tau(\vec{R}) + \tfrac{3}{5}k_F^{\,2}\rho(\vec{R})]$$

$$= [1 - \tfrac{1}{10}(sk_F)^2 + \tfrac{1}{280}(sk_F)^4 - \cdots]\rho(\vec{R}) + \frac{s^2}{6}[1 - \tfrac{1}{18}(sk_F)^2 + \cdots][\tfrac{1}{4}\nabla^2\rho(\vec{R}) - \tau(\vec{R}) + \tfrac{3}{5}k_F^{\,2}\rho(\vec{R})],$$

where

$$\rho(\vec{R}) = \rho(\vec{R}, \vec{R}) = \sum_a |\phi_a(\vec{R})|^2, \qquad \tau(\vec{R}) = \sum_a |\vec{\nabla}\phi_a(\vec{R})|^2, \qquad \rho_{\mathrm{SL}}(sk_F) = \frac{3}{sk_F}\, j_1(sk_F). \tag{2.8}$$

Since the energy density involves $\rho^2(\vec{R}_1, \vec{R}_2)$, the validity of the approximation is demonstrated in Fig. 1 by comparing the exact normalized expression

$$\left[\frac{1}{\rho(\vec{R})}\sum_a \phi_a^*\left(\vec{R}+\frac{s}{2}\hat{e}\right)\phi_a\left(\vec{R}-\frac{s}{2}\hat{e}\right)\right]^2, \tag{2.9}$$

with

$$\rho_{\mathrm{SL}}^{\,2}(sk_F) + \frac{35}{2sk_F^{\,3}}\, j_3(sk_F)\rho_{\mathrm{SL}}(sk_F)\left(\frac{\nabla^2\rho(\vec{R})}{2\rho(\vec{R})} - \frac{2\tau(\vec{R})}{\rho(\vec{R})} + \tfrac{6}{5}k_F^{\,2}\right), \tag{2.10}$$

for various values of R. The exact density matrix (2.9) was computed with the unit vector $\hat{e}$ in both the radial direction, and perpendicular to the radial direction, and these extremal values are denoted by the ends of the error bars in Fig. 1. For comparison, the Slater approximation $\rho_{\mathrm{SL}}^{\,2}(sk_F)$, and the quadratic approximation, obtained by retaining only the terms quadratic in s in the expanded form of equation (2.8) are graphed, as well as the corrected Slater expansion, (2.10). It is evident from Fig. 1 that even at R = 7.5 fm, which is well into the surface, (2.10) yields an excellent approximation for s less than 2 fm. It should be noted in passing, that although this approximation is adequate for the present application, since the correction term containing $j_3(sk_F)/sk_F^{\,3}$ in (2.10) systematically overestimates the discrepancy between the exact result and the Slater approximation, the non-uniqueness in the truncation of (2.5) could be profitably utilized to replace $j_3(sk_F)/sk_F^{\,3}$ by a function with a larger coefficient multiplying $(-s^4)$.

III. APPROXIMATE POTENTIAL ENERGY DENSITY

For notational simplicity in the ensuing formulas, the two-body reaction matrix will be assumed to be local, state-independent, and identical in all partial waves of a specified spin and isospin. The final results may be straightforwardly generalized to include state dependence, the appropriate sums over angular momentum, and integrals over spatial variables for the completely general case. Summing over spin and isospin functions as in Ref. 2, the potential energy may be expressed in terms of the spatial wave functions as follows:

$$\langle V \rangle = \frac{1}{2}\int d^3r_1 d^3r_2 \{[\rho_p(\vec{r}_1)\rho_p(\vec{r}_2) + \rho_n(\vec{r}_1)\rho_n(\vec{r}_2)][\tfrac{1}{4}G^{\,SE}(r_{12}) + \tfrac{3}{4}G^{\,TO}(r_{12})]$$

$$+ 2\rho_p(\vec{r}_1)\rho_n(\vec{r}_2)[\tfrac{3}{8}G^{\,TE}(r_{12}) + \tfrac{1}{8}G^{\,SE}(r_{12}) + \tfrac{3}{8}G^{\,TO}(r_{12}) + \tfrac{1}{8}G^{\,SO}(r_{12})]$$

$$+ [\rho_p^{\,2}(\vec{r}_1, \vec{r}_2) + \rho_n^{\,2}(\vec{r}_1, \vec{r}_2)][\tfrac{1}{4}G^{\,SE}(r_{12}) + \tfrac{3}{4}G^{\,TO}(r_{12})]$$

$$+ 2\rho_p(\vec{r}_1, \vec{r}_2)\rho_n(\vec{r}_1, \vec{r}_2)[\tfrac{3}{8}G^{\,TE}(r_{12}) + \tfrac{1}{8}G^{\,SE}(r_{12}) - \tfrac{3}{8}G^{\,TO}(r_{12}) - \tfrac{1}{8}G^{\,SO}(r_{12})]\}, \tag{3.1}$$

where p and n indicate the proton and neutron densities, respectively. Substitution of (2.8), transformation to relative and c.m. coordinates, and integration over s reduces the exchange terms in (3.1) to the desired form of a one-dimensional integral involving only $\rho(\vec{R})$ and $\tau(\vec{R})$. The direct terms may be similarly reduced by expanding the product $\rho_\alpha(\vec{R}+\vec{s}/2)\rho_\beta(\vec{R}-\vec{s}/2)$ about $\vec{R}$ as in (2.1), with the result being given by (2.5) with $\rho(\vec{R}_1,\vec{R}_2)$ replaced by $\rho_\alpha(\vec{R}_1)\rho_\beta(\vec{R}_2)$. Expanding $\rho_{SL}(sk_F)$ and $j_3(sk_F)$ as in (2.8) the following equation is obtained:

$$\frac{1}{4\pi}\int d\Omega_s\,\rho_\alpha\left(\vec{R}+\frac{\vec{s}}{2}\right)\rho_\beta\left(\vec{R}-\frac{\vec{s}}{2}\right)=[1-\tfrac{1}{10}(sk_F)^2+\tfrac{1}{280}(sk_F)^4-\cdots]\rho_\alpha(\vec{R})\rho_\beta(\vec{R})+\tfrac{1}{6}s^2[1-\tfrac{1}{18}(sk_F)^2+\cdots]$$

$$\times[\tfrac{1}{4}\nabla^2\rho_\alpha(\vec{R})\rho_\beta(\vec{R})+\tfrac{1}{4}\rho_\alpha(\vec{R})\nabla^2\rho_\beta(\vec{R})-\tfrac{1}{2}\vec{\nabla}\rho_\alpha(\vec{R})\cdot\vec{\nabla}\rho_\beta(\vec{R})+\tfrac{3}{5}k_F{}^2\rho_\alpha(\vec{R})\rho_\beta(\vec{R})]+\cdots.$$

$$(3.2)$$

In (3.2), it is evident that the $(sk_F)^2$ coefficient of $\rho_\alpha\rho_\beta$ occurring in the ρ_{SL} expansion exactly cancels the $(sk_F)^2$ coefficient in the j_3 term, and it is straightforward to verify that the sum of the contributions originating from the terms in Q_n involving no derivatives yields $[j_3(sk_F)-1]\rho_\alpha(\vec{R})\rho_\beta(\vec{R})$. Thus, a natural rearrangement and truncation of (2.5) for the direct term in (3.1) is

$$\frac{1}{4\pi}\int d\Omega_s\,\rho_\alpha\left(\vec{R}+\frac{\vec{s}}{2}\right)\rho_\beta\left(\vec{R}-\frac{\vec{s}}{2}\right)=\rho_\alpha(\vec{R})\rho_\beta(\vec{R})+\frac{35}{2sk_F{}^3}j_3(sk_F)[\tfrac{1}{4}\nabla^2\rho_\alpha(\vec{R})\rho_\beta(\vec{R})+\tfrac{1}{4}\rho_\alpha(\vec{R})\nabla^2\rho_\beta(\vec{R})-\tfrac{1}{2}\vec{\nabla}\rho_\alpha(\vec{R})\cdot\vec{\nabla}\rho_\beta(\vec{R})].$$

$$(3.3)$$

For notational convenience, since the same function appears in the quadratic term of the direct and exchange expansion, it is convenient to define

$$g(sk_F)=\frac{35}{2(sk_F)^3}j_3(sk_F)=\tfrac{1}{6}[1-\tfrac{1}{18}(sk_F)^2+\cdots].$$

$$(3.4)$$

We emphasize once again that the coefficients of $(sk_F)^{2n}$ for $n\geq1$ are not unique. The choice of $g(sk_F)$ has already been justified for the exchange term by the results in Fig. 1. For the direct term, it is reason-
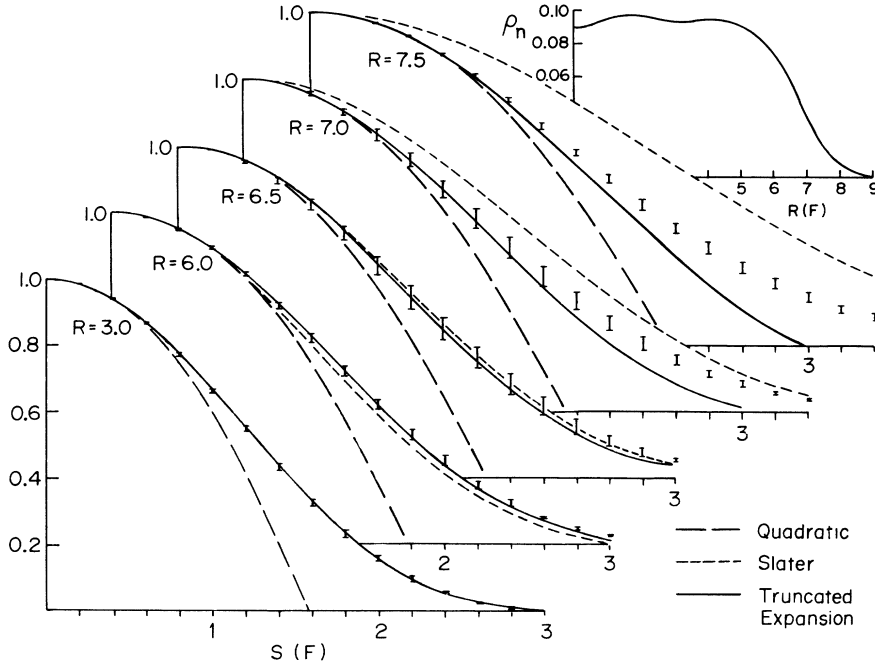

FIG. 1. Comparison of the square of the exact neutron-density matrix in [208]Pb with the truncated expansion. The neutron-density distribution is shown for reference; and for five values of the c.m. coordinate R, the square of the density matrix is plotted as a function of relative coordinate s. The error bars denote the extrema of (2.9) in the radial direction and perpendicular to the radial direction. The long dashes denote the result when only the quadratic terms in (2.8) are retained, the short dashes indicate the Slater approximation, and the solid curves correspond to (2.10).

able that $g(sk_F)$ should cut off at a range of a Fermi wavelength, since k_F governs both the surface thickness and the wavelength of density fluctuations. In Sec. VI we will discuss the actual sensitivity of the structure of finite nuclei to the detailed behavior of $g(sk_F)$ at large s.

Substitution of the above expansions in the direct and exchange terms of (3.1) and transformation to relative and c.m. coordinates yields:

$$\langle V \rangle = \frac{1}{2}\int d^3R \left\{ \rho_p{}^2(\vec{R}) \int d^3s [\tfrac{1}{4}G^{SE}(s) + \tfrac{3}{4}G^{TO}(s)] + \rho_p(\vec{R})\rho_n(\vec{R}) \int d^3s [\tfrac{3}{8}G^{TE}(s) + \tfrac{1}{8}G^{SE}(s) + \tfrac{3}{8}G^{TO}(s) + \tfrac{1}{8}G^{SO}(s)] \right.$$

$$+ \rho_p{}^2(\vec{R}) \int d^3s\, \rho_{SL}{}^2(k_p s)[\tfrac{1}{4}G^{SE}(s) - \tfrac{3}{4}G^{TO}(s)] + \rho_p(\vec{R})\rho_n(\vec{R}) \int d^3s\, \rho_{SL}(k_p s)\rho_{SL}(k_n s)$$

$$\left. \times [\tfrac{3}{8}G^{TE}(s) + \tfrac{1}{8}G^{SE}(s) - \tfrac{3}{8}G^{TO}(s) - \tfrac{1}{8}G^{SO}(s)] + p \to n \right\}$$

$$+ \frac{1}{2}\int d^3R \left\{ [\tfrac{1}{2}\rho_p(\vec{R})\nabla^2\rho_p(\vec{R}) - \tfrac{1}{2}|\nabla\rho_p(\vec{R})|^2] \int d^3s\, s^2 g(sk_p)[\tfrac{1}{4}G^{SE}(s) + \tfrac{3}{4}G^{TO}(s)] \right.$$

$$+ [\tfrac{1}{2}\rho_p(\vec{R})\nabla^2\rho_n(\vec{R}) - \tfrac{1}{2}\nabla\rho_n(\vec{R})\cdot\nabla\rho_p(\vec{R})] \int d^3s\, s^2 g(sk)[\tfrac{3}{8}G^{TE}(s) + \tfrac{1}{8}G^{SE}(s) + \tfrac{3}{8}G^{TO}(s) + \tfrac{1}{8}G^{SO}(s)]$$

$$+ \rho_p(\vec{R})[\tfrac{3}{5}k_p{}^2\rho_p(\vec{R}) - 2\tau_p(\vec{R}) + \tfrac{1}{2}\nabla^2\rho_p(\vec{R})] \int d^3s\, s^2\rho_{SL}(sk_p)g(sk_p)[\tfrac{1}{4}G^{SE}(s) - \tfrac{3}{4}G^{TO}(s)]$$

$$+ \rho_p(\vec{R})[\tfrac{3}{5}k_n{}^2\rho_n(\vec{R}) - 2\tau_n(\vec{R}) + \tfrac{1}{2}\nabla^2\rho_n(\vec{R})] \int d^3s\, s^2$$

$$\left. \times \rho_{SL}(sk_p)g(sk_n)[\tfrac{3}{8}G^{TE}(s) + \tfrac{1}{8}G^{SE}(s) - \tfrac{3}{8}G^{TO}(s) - \tfrac{1}{8}G^{SO}(s)] + p \to n \right\}, \tag{3.5}$$

where $k_p = [3\pi^2\rho_p(\vec{R})]^{1/3}$ and similarly for k_n, $k = \{3\pi^2[\rho_p(\vec{R}) + \rho_n(\vec{R})]/2\}^{1/3}$ and $p \to n$ represents the analogous terms with p and n interchanged. The integrand of the first integral in (3.5) is exactly the potential energy of nuclear matter with neutron and proton densities ρ_n and ρ_p and will be denoted $V_{NM}(\rho_p, \rho_n)$. All of the corrections arising from finite nuclear wave functions are included in the second integral. Note that all of the relative integrals in the second term contain an additional factor of s^2, so that only the long-range components of the nuclear force contribute significantly, and that the second term vanishes identically in uniform nuclear matter. It is convenient to simplify (3.5) by introducing the following notation:

$$\langle V \rangle = \int d^3R \left\{ V_{NM}(\rho_p, \rho_n) + V_D^L(\rho_p)(\rho_p\nabla^2\rho_p - |\vec{\nabla}\rho_p|^2) + V_D^L(\rho_n)(\rho_n\nabla^2\rho_n - |\vec{\nabla}\rho_n|^2) \right.$$

$$+ V_D^U\left(\frac{\rho_n + \rho_p}{2}\right)(\rho_p\nabla^2\rho_n + \rho_n\nabla^2\rho_p - 2\vec{\nabla}\rho_n\cdot\vec{\nabla}\rho_p) + [V_E^L(\rho_p)\rho_p + V_E^U(\rho_n, \rho_p)\rho_n](\tfrac{3}{5}k_p{}^2\rho_p - 2\tau_p + \tfrac{1}{2}\nabla^2\rho_p)$$

$$\left. + [V_E^L(\rho_n)\rho_n + V_E^U(\rho_p, \rho_n)\rho_p](\tfrac{3}{5}k_n{}^2\rho_n - 2\tau_n + \tfrac{1}{2}\nabla^2\rho_n) \right\}, \tag{3.6}$$

where the direct and exchange forces between like and unlike particles are defined as follows:

$$V_D^L(\rho) = \frac{1}{16}\int d^3s\, s^2 g(ks)[G^{SE}(\rho, s) + 3G^{TO}(\rho, s)],$$

$$V_D^U(\rho) = \frac{1}{32}\int d^3s\, s^2 g(ks)[G^{SE}(\rho, s) + 3G^{TE}(\rho, s) + G^{SO}(\rho, s) + 3G^{TO}(\rho, s)],$$

$$V_E^L(\rho) = \frac{1}{8}\int d^3s\, s^2\rho_{SL}(ks)g(ks)[G^{SE}(\rho, s) - 3G^{TO}(\rho, s)], \tag{3.7}$$

$$V_E^U(\rho_\alpha, \rho_\beta) = \frac{1}{16}\int d^3s\, s^2\rho_{SL}(k_\alpha s)g(k_\beta s)\left[G^{SE}\left(\frac{\rho_\alpha + \rho_\beta}{2}, s\right) + 3G^{TE}\left(\frac{\rho_\alpha + \rho_\beta}{2}, s\right) - G^{SO}\left(\frac{\rho_\alpha + \rho_\beta}{2}, s\right) - 3G^{TO}\left(\frac{\rho_\alpha + \rho_\beta}{2}, s\right)\right].$$

Here $k = (3\pi^2\rho)^{1/3}$ and we have explicitly displayed the dependence of the reaction matrix on the density of the interacting particles. For unlike particles, the dependence on the complicated Pauli exclusion operator for unequal Fermi spheres has been approximated by that of two equal spheres excluding the same volume of phase space.

Defining

$$F(\rho_n, \rho_p) = V_D^L(\rho_n)\rho_n + V_D^U[\tfrac{1}{2}(\rho_n + \rho_p)]\rho_p + \tfrac{1}{2}V_E^L(\rho_n)\rho_n + \tfrac{1}{2}V_E^U(\rho_p, \rho_n)\rho_p, \tag{3.8}$$

the $\nabla^2 \rho_n$ terms in (3.6) are integrated by parts:

$$F(\rho_n, \rho_p)\nabla^2\rho_n = -\frac{\partial F(\rho_n, \rho_p)}{\partial \rho_n}|\vec{\nabla}\rho_n|^2 - \frac{\partial F(\rho_n, \rho_p)}{\partial \rho_p}\vec{\nabla}\rho_n \cdot \vec{\nabla}\rho_p. \tag{3.9}$$

Eliminating $\nabla^2\rho_n$ and $\nabla^2\rho_p$ from (3.6) in this way, the following final form of the energy density is obtained:

$$H(\vec{R}) = \frac{\hbar^2}{2m}[\tau_n(\vec{R}) + \tau_p(\vec{R})] + A[\rho_p(\vec{R}), \rho_n(\vec{R})] + B[\rho_p(\vec{R}), \rho_n(\vec{R})]\tau_p(\vec{R}) + B[\rho_n(\vec{R}), \rho_p(\vec{R})]\tau_n(\vec{R})$$

$$+ C[\rho_n(\vec{R}), \rho_p(\vec{R})]|\vec{\nabla}\rho_n(\vec{R})|^2 + C[\rho_p(\vec{R}), \rho_n(\vec{R})]|\vec{\nabla}\rho_p(\vec{R})|^2 + D[\rho_n(\vec{R}), \rho_p(\vec{R})]\vec{\nabla}\rho_n(\vec{R}) \cdot \vec{\nabla}\rho_p(\vec{R}), \tag{3.10}$$

where

$$A(\rho_n, \rho_p) = V_{\text{NM}}(\rho_n, \rho_p) - \tfrac{3}{5}(3\pi^2)^{2/3}[\rho_n^{5/3}B(\rho_n, \rho_p) + \rho_p^{5/3}B(\rho_p, \rho_n)],$$

$$B(\rho_n, \rho_p) = -2[\rho_n V_E^L(\rho_n) + \rho_p V_E^U(\rho_p, \rho_n)],$$

$$C(\rho_n, \rho_p) = -V_D^L(\rho_n) - \frac{\partial F(\rho_n, \rho_p)}{\partial \rho_n},$$

$$D(\rho_n, \rho_p) = -2V_D^U[\tfrac{1}{2}(\rho_n + \rho_p)] - \frac{\partial F}{\partial \rho_p}(\rho_n, \rho_p) - \frac{\partial F}{\partial \rho_n}(\rho_p, \rho_n).$$

Thus, we have obtained an expression for the energy density which depends upon τ, ρ, and $\vec{\nabla}\rho$. Although the nuclear-matter term $V_{\text{NM}}(\rho_n, \rho_p)$ was written in terms of a simplified effective interaction, we will subsequently show that even for a general, nonlocal interaction, the dominant potential energy contribution is the exact nuclear-matter result. Since the correction terms for finite nuclei depend on the long-range part of the reaction matrix, and thus essentially on the long-range part of the bare potential, we expect V_D^L, V_D^U, V_E^L, and V_E^U derived from the effective interaction in Ref. (2) to be applicable for calculation with any realistic two-body interactions. Thus, the functions $B(\rho_n, \rho_p)$, $C(\rho_n, \rho_p)$, and $D(\rho_n, \rho_p)$ presented in this work combined with $V_{\text{NM}}(\rho_n, \rho_p)$ for any interaction should yield the approximate structure of finite nuclei with that interaction.

IV. GENERALIZATION OF THE EXPANSION

The derivation of (3.10) was based on a variety of simplifying assumptions concerning the form of two-body reaction matrix and the presence of spin-saturated shells. We now seek to generalize this result by including correction terms arising from a more realistic reaction matrix and more general configurations.

Extension to Nonlocal Forces

For notational convenience, we will consider only the case of a nucleus with four nucleons in

each state (two neutrons and two protons with opposite spins). The general case may be handled in a similar way, the only difference being that neutron and proton densities have to be written explicitly. The potential energy of a system of $A = 4N$ nucleons interacting via a nonlocal two-body force

$$v(\vec{r}_1, \vec{r}_2|\vec{r}_3, \vec{r}_4) = \delta(\vec{r}_1 + \vec{r}_2 - \vec{r}_3 - \vec{r}_4)V(\vec{r}_1 - \vec{r}_2, \vec{r}_3 - \vec{r}_4) \tag{4.1}$$

may be written as

$$E = \frac{1}{2}\int d^3R d^3s d^3t\, \rho\left(\vec{R} + \frac{\vec{s}}{2}, \vec{R} + \frac{\vec{t}}{2}\right)$$

$$\times \rho\left(\vec{R} - \frac{\vec{s}}{2}, \vec{R} - \frac{\vec{t}}{2}\right)K(\vec{s}, \vec{t}), \tag{4.2}$$

where K in this equation includes the exchange interaction term

$$K(\vec{s}, \vec{t}) = V(\vec{s}, \vec{t}) - V(\vec{s}, -\vec{t}). \tag{4.3}$$

An expansion for the product of the two density matrices in (4.2) may be obtained by first writing

$$\rho\left(\vec{R} \pm \frac{\vec{s}}{2}, \vec{R} \pm \frac{\vec{t}}{2}\right) = \rho\left(\vec{R}^{\pm} \pm \frac{\vec{\Delta}}{2}, \vec{R}^{\pm} \mp \frac{\vec{\Delta}}{2}\right), \tag{4.4}$$

where the vectors appearing in the right-hand side are defined by

$$\vec{R}^{\pm} = \vec{R} \pm \tfrac{1}{2}\vec{\Sigma}, \quad \vec{\Sigma} = \tfrac{1}{2}(\vec{s} + \vec{t}), \quad \vec{\Delta} = \tfrac{1}{2}(\vec{s} - \vec{t}). \tag{4.5}$$

Expression (4.4) is expanded by means of (2.8). Multiplying the formulas corresponding to plus

and minus signs one obtains

$$\rho\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}+\frac{\vec{t}}{2}\right)\rho\left(\vec{R}-\frac{\vec{s}}{2},\vec{R}-\frac{\vec{t}}{2}\right) = \rho_{SL}(\Delta k_F(\vec{R}^+))\rho_{SL}(\Delta k_F(\vec{R}^-))\rho(\vec{R}^+)\rho(\vec{R}^-)$$

$$+\Delta^2\rho_{SL}(\Delta k_F(\vec{R}^+))\rho(\vec{R}^+)g(\Delta k_F(\vec{R}^-))[\tfrac{1}{4}\nabla^2\rho(\vec{R}^-) - \tau(\vec{R}^-) + \tfrac{3}{5}\rho(\vec{R}^-)k_F{}^2(\vec{R}^-)]$$

$$+\Delta^2\rho_{SL}(\Delta k_F(\vec{R}^-))\rho(\vec{R}^-)g(\Delta k_F(\vec{R}^+))[\tfrac{1}{4}\nabla^2\rho(\vec{R}^+) - \tau(\vec{R}^+) + \tfrac{3}{5}\rho(\vec{R}^+)k_F{}^2(\vec{R}^+)].$$

$$(4.6)$$

All terms in the previous formula may be reduced to the form $\alpha[\rho(\vec{R}^+)]\alpha[\rho(\vec{R}^-)]$. Such terms are expanded by means of the following straightforward extension of (3.3):

$$\alpha[\rho(\vec{R}^+)]\alpha[\rho(\vec{R}^-)] = \alpha^2[\rho(\vec{R})] + \tfrac{1}{2}\Sigma^2 g(\Sigma k_F(\vec{R}))(\alpha\nabla^2\alpha - |\vec{\nabla}\alpha|^2). \tag{4.7}$$

Only the lowest-order term in (4.7) contributes to the quadratic part of the product of the two density matrices when expanding the second and third terms in (4.6). Therefore through second order

$$\rho\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}+\frac{\vec{t}}{2}\right)\rho\left(\vec{R}-\frac{\vec{s}}{2},\vec{R}-\frac{\vec{t}}{2}\right) = \alpha^2[\rho(\vec{R})] + \tfrac{1}{2}\Sigma^2 g(\Sigma k_F(\vec{R}))(\alpha\nabla^2\alpha - |\vec{\nabla}\alpha|^2)$$

$$+2\Delta^2\rho_{SL}(\Delta k_F(\vec{R}))\rho(\vec{R})g(\Delta k_F(\vec{R}))[\tfrac{1}{4}\nabla^2\rho(\vec{R}) - \tau(\vec{R}) + \tfrac{3}{5}\rho(\vec{R})k_F{}^2(\vec{R})], \tag{4.8}$$

where the function $\alpha(\rho)$ is defined by

$$\alpha(\rho) = \rho_{SL}(\Delta k_F)\rho = \frac{3}{x}j_1(x)\rho, \quad x = \Delta k_F. \tag{4.9}$$

Rewriting the gradient and Laplacian operators acting on $\alpha[\rho(\vec{R})]$ in (4.8) in terms of $\vec{\nabla}\rho$ and $\nabla^2\rho$ one obtains

$$\alpha\nabla^2\alpha - |\vec{\nabla}\alpha|^2 = \alpha(\rho)\alpha'(\rho)\nabla^2\rho(\vec{R}) + (\alpha\alpha'' - \alpha'^2)|\vec{\nabla}\rho(\vec{R})|^2, \tag{4.10}$$

where the derivatives of α, calculated from (4.9), are

$$\alpha'(\rho) = j_0(\Delta k_F), \quad \alpha''(\rho) = -(\Delta k_F/3\rho)j_1(\Delta k_F). \tag{4.11}$$

Collecting the previous results we obtain

$$\rho\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}+\frac{\vec{t}}{2}\right)\rho\left(\vec{R}-\frac{\vec{s}}{2},\vec{R}-\frac{\vec{t}}{2}\right) = \rho_{SL}{}^2(\Delta k_F)\rho^2(\vec{R}) + \tfrac{1}{2}\Sigma^2 g(\Delta k_F)\{\rho_{SL}(\Delta k_F)j_0(\Delta k_F)\rho(\vec{R})\nabla^2\rho(\vec{R})$$

$$- [j_0{}^2(\Delta k_F) + j_1{}^2(\Delta k_F)]|\vec{\nabla}\rho|^2\}$$

$$+2\Delta^2\rho_{SL}(\Delta k_F)\rho(\vec{R})g(\Delta k_F)[\tfrac{1}{4}\nabla^2\rho(\vec{R}) - \tau(\vec{R}) + \tfrac{3}{5}\rho(\vec{R})k_F{}^2(\vec{R})]. \tag{4.12}$$

This expression allows one to write the energy of the system as an integral of an energy density of the form

$$H(\vec{R}) = A[\rho(\vec{R})] + B[\rho(\vec{R})]\tau(\vec{R}) + C[\rho(\vec{R})]|\nabla\rho(\vec{R})|^2 \tag{4.13}$$

as in the case of a local two-body force. The expression for the functions A and B

$$A(\rho) = \tfrac{1}{2}\rho^2 \int d^3\Delta d^3\Sigma\, K(\vec{\Delta}+\vec{\Sigma},\vec{\Delta}-\vec{\Sigma})\rho_{SL}(\Delta k_F)[\rho_{SL}(\Delta k_F) + \tfrac{6}{5}\Delta^2 g(\Delta k_F)k_F{}^2],$$

$$(4.14)$$

$$B(\rho) = -\rho \int d^3\Delta d^3\Sigma\, K(\vec{\Delta}+\vec{\Sigma},\vec{\Delta}-\vec{\Sigma})\Delta^2\rho_{SL}(\Delta k_F)g(\Delta k_F),$$

can be readily obtained from (4.12). The expression for the function $C(\rho)$ requires an integration by parts, with the result

$$C(\rho) = \frac{1}{4}\int d^3\Delta d^3\Sigma\, K(\vec{\Delta}+\vec{\Sigma},\vec{\Delta}-\vec{\Sigma})\left\{[\Sigma^2 j_0(\Delta k_F) + \Delta^2]\left[\frac{35}{8}\rho_{SL}(\Delta k_F)\frac{j_4(\Sigma k_F)}{(\Sigma k_F)^2} - g(\Sigma k_F)j_0(\Delta k_F)\right] - \Sigma^2 g(\Sigma k_F)j_0{}^2(\Delta k_F)\right\}$$

$$-\frac{1}{4}\int d^3\Delta d^3\Sigma\, \frac{\partial K}{\partial\rho}(\vec{\Delta}+\vec{\Sigma},\vec{\Delta}-\vec{\Sigma})\rho\rho_{SL}(\Delta k_F)g(\Sigma k_F)[\Sigma^2 j_0(\Delta k_F) + \Delta^2]. \tag{4.15}$$

Notice that we have used angle averages over the directions of $\vec{\Delta}$ and $\vec{\Sigma}$ in deriving expansion (4.12). The validity of this approximation is supported by the rotational invariance of the two-body interaction and it is indeed exact for a nonlocal interaction of the form

$$V(\vec{r}, \vec{r}') = F(|\vec{r} + \vec{r}'|)G(|\vec{r} - \vec{r}'|) . \tag{4.16}$$

Notice also that from the construction of (4.12), it contains as a particular case the expansion formulas (2.8) and (3.3) which are appropriate for the case of a local two-body force. For a local interaction the direct term corresponds to $\vec{s} = \vec{t}$ and (4.12) reduces to (3.3). The exchange term is obtained by setting $\vec{s} = -\vec{t}$ and in this case, (4.12) reduces to (2.8).

Extension to Spin-Unsaturated Shells

In the case of spin-unsaturated shells, the density matrix is no longer a scalar in spin space and its vector part $\vec{\rho}(\vec{R}_1, \vec{R}_2)$ defined by

$$\rho(\vec{R}_1, \sigma_1; \vec{R}_2, \sigma_2)$$

$$= \tfrac{1}{2}\rho(\vec{R}_1, \vec{R}_2)\delta_{\sigma_1\sigma_2} + \tfrac{1}{2}(\sigma_2 |\vec{\sigma}| \sigma_1) \cdot \vec{\rho}(\vec{R}_1, \vec{R}_2) \tag{4.17}$$

has to be taken into account explicitly. In (4.17) $\vec{\sigma}$ denotes the Pauli spin matrices, σ the spin coordinate of one nucleon, and $\rho(\vec{R}_1, \vec{R}_2)$ is the scalar part of the density matrix

$$\rho(\vec{R}_1, \vec{R}_2) = \sum_{i,\sigma} \phi_i^*(\vec{R}_1, \sigma)\phi_i(\vec{R}_2, \sigma)$$

for which an expansion formula was already constructed in Sec. II.

Inverting (4.17) the vector part of the density matrix may be written

$$\vec{\rho}(\vec{R}_1, \vec{R}_2) = \sum_{i,\sigma_1,\sigma_2} \phi_i^*(\vec{R}_1, \sigma_1)(\sigma_1 |\vec{\sigma}| \sigma_2)\phi_i(\vec{R}_2, \sigma_2) , \tag{4.18}$$

and from this expression one may readily see that, if the set of occupied states is invariant under time reversal, then $\vec{\rho}$ is an antisymmetric function of $\vec{R}_1$ and $\vec{R}_2$. Denoting by $\bar{i}$ the time-reversed state of the state i, one has

$$\vec{\rho}(\vec{R}_1, \vec{R}_2) = \sum_{i,\sigma_1,\sigma_2} \phi_{\bar{i}}^*(\vec{R}_1, \sigma_1)(\sigma_1 |\vec{\sigma}| \sigma_2)\phi_{\bar{i}}(\vec{R}_2, \sigma_2)$$

$$= \sum_{i,\sigma_1,\sigma_2} \phi_i(\vec{R}_1, \sigma_1)(\sigma_1 |\sigma_y\vec{\sigma}\sigma_y| \sigma_2)\phi_i^*(\vec{R}_2, \sigma_2)$$

$$= -\vec{\rho}(\vec{R}_2, \vec{R}_1) .$$

The short-range behavior of $\vec{\rho}(\vec{R}_1, \vec{R}_2)$ may also be obtained from (4.18) and from the identity

$$(\vec{A} \cdot \vec{B})\vec{C} = \tfrac{1}{3}(\vec{A} \cdot \vec{C})\vec{B} + \tfrac{1}{2}(\vec{A} \times \vec{C}) \times \vec{B}$$

$$- (\tfrac{5}{3})^{1/2}[[\vec{A} \times \vec{C}]^{(2)} \times \vec{B}]^{(1)} .$$

Due to time-reversal invariance only the second term contributes, with the result:

$$\vec{\rho}\left(\vec{R} + \frac{\vec{s}}{2}, \vec{R} - \frac{\vec{s}}{2}\right) = \frac{i}{2}\vec{s} \times \vec{J}(\vec{R}) + \cdots, \tag{4.19}$$

where the spin density $\vec{J}$ is defined by

$$\vec{J}(\vec{R}) = -i \sum_{i,\sigma_1,\sigma_2} \phi_i^*(\vec{R}, \sigma_1)\vec{\nabla}\phi_i(\vec{R}_2, \sigma_2) \times (\sigma_1 |\vec{\sigma}| \sigma_2) .$$

In the case of a spherical nucleus one can show[14] that the vector part of the density matrix is of the form

$$\rho(\vec{R}_1, \vec{R}_2) = i\vec{R}_1 \times \vec{R}_2 \rho_1(\vec{R}_1, \vec{R}_2) , \tag{4.20}$$

where ρ_1 is a real scalar quantity which is symmetric in $\vec{R}_1$ and $\vec{R}_2$. For a single (nlj) shell obtained by filling the orbitals

$$\phi_{nljm}(\vec{r}, \sigma) = \frac{R_{nlj}(r)}{r} \sum_{m_l m_s} (l\tfrac{1}{2}m_l m_s |jm)Y_{lm}(\hat{r})\chi_{m_s}(\sigma) ,$$

the contribution to ρ_1 is[14]

$$\rho_1(\vec{R}_1, \vec{R}_2) = \pm \frac{1}{2\pi r_1^2 r_2^2} R_{nlj}(R_1)R_{nlj}(R_2)P_l'(\cos\alpha)$$

for $j = l \pm \tfrac{1}{2} .$

This expression shows that if both doublets $j = l \pm \tfrac{1}{2}$ are occupied and have identical radial wave functions then $\vec{\rho}(\vec{R}_1, \vec{R}_2)$ vanishes. Contributions to the vector part of the density matrix therefore arise primarily from particles near the Fermi surface, $|\vec{k}| \simeq k_F$, in contrast to the case of the scalar part where all particles with $|\vec{k}| \leq k_F$ contribute. Thus the rearrangement of the short-range expansion carried out in Sec. II is not appropriate to the present case.

Since any rearrangement of the series (4.19) is a tedious procedure, we have used for spin-unsaturated shells the alternative approach discussed in connection with (2.4), which consists of an expansion of the density matrix in momentum space, weighted by the appropriate nuclear-matter phase-space factor.

In this method, the vector part of the density matrix is first written as

$$\vec{\rho}\left(\vec{R} + \frac{\vec{s}}{2}, \vec{R} - \frac{\vec{s}}{2}\right)$$

$$= e^{i\vec{s} \cdot \vec{k}} \sum_{i,\sigma_1,\sigma_2} (\sigma_1 |\vec{\sigma}| \sigma_2)[e^{\vec{s} \cdot [\frac{1}{2}(\vec{\nabla}_1 - \vec{\nabla}_2) - i\vec{k}]}$$

$$\times \phi_i^*(\vec{R}_1, \sigma_1)\phi_i(\vec{R}_2, \sigma_2)]|_{\vec{R}_1 = \vec{R}_2 = \vec{R}}, \tag{4.21}$$

where $\vec{k}$ is an arbitrary vector which may be interpreted as the wave number of one nucleon. Indeed, for a single plane wave the second exponential in (4.21) reduces to unity. Expanding this ex-

ponential in a Taylor series yields

$$\bar{\rho}\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)$$

$$=e^{i\vec{s}\cdot\vec{k}}\sum_{i,\sigma_1,\sigma_2}(\sigma_1|\vec{\sigma}|\sigma_2)\{1+\vec{s}\cdot[\tfrac{1}{2}(\vec{\nabla}_1-\vec{\nabla}_2)-i\vec{k}]+\cdots\}$$

$$\times\phi_i^*(\vec{R}_1,\sigma_1)\phi_i(\vec{R}_2,\sigma_2)|_{\vec{R}_1=\vec{R}_2=\vec{R}}\,.$$

$$(4.22)$$

Since $\vec{\rho}(\vec{R}_1,\vec{R}_2)$ is antisymmetric, the first term in (4.22) vanishes together with the part of the linear term containing no gradient operator. Finally, from (4.19) one obtains

$$\vec{\rho}\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)=\tfrac{1}{2}i\,e^{i\vec{k}\cdot\vec{s}}\,\vec{s}\times\vec{J}(\vec{R})+\cdots\,.$$

Averaging over the orientation of all $|\vec{k}|=k_F$ yields

$$\vec{\rho}\left(\vec{R}+\frac{\vec{s}}{2},\vec{R}-\frac{\vec{s}}{2}\right)=\tfrac{1}{2}i\,j_0(sk_F)\vec{s}\times\vec{J}(\vec{R})+\cdots\,. \quad (4.23)$$

Unfortunately, in contrast to the case of spherical nuclei, we have not succeeded in expressing higher-order terms in a simple closed form.

(i) Case of a central force. To illustrate the previous technique let us first consider a Wigner interaction $v(r_{12})$. In this case the potential energy (including the exchange term) is

$$V=\frac{1}{2}\sum_{ij}\int d^3R_1 d^3R_2\,v(|\vec{R}_1-\vec{R}_2|)\phi_i^*(\vec{R}_1)\phi_j^*(\vec{R}_2)$$

$$\times(1-P_mP_\sigma P_\tau)\phi_i(\vec{R}_1)\phi_j(\vec{R}_2)\,. \quad (4.24)$$

In (4.24) the spinor notation for wave functions has been used for more simplicity. Replacing the spin-exchange operator P_σ by $\frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$ one obtains for the contribution V_1 of spin-unsaturated shells to the potential energy:

$$V_1=\frac{1}{4}\int d^3R_1 d^3R_2\,v(|\vec{R}_1-\vec{R}_2|)$$

$$\times\{[\vec{\rho}_n(\vec{R}_1,\vec{R}_2)]^2+[\vec{\rho}_p(\vec{R}_1,\vec{R}_2)]^2\}\,, \quad (4.25)$$

where the index n (p) in $\vec{\rho}$ indicates that the summation runs over neutron (proton) states only. Inserting expansion (4.23) into this equation, the integration over the angular coordinates of $\vec{s}$ can be carried out and V_1 may be written

$$V_1=\int d^3R\{\varphi[k_n(\vec{R})]J_n^2(\vec{R})+\varphi[k_p(\vec{R})]J_p^2(\vec{R})\}\,,$$

where the function $\varphi(k)$ is given by

$$\varphi(k)=-\tfrac{1}{6}\pi\int_0^{+\infty}v(s)j_0^2(ks)s^4ds\,.$$

From (4.28) and (4.29) one may observe that in the case of an attractive force, the contribution of spin-unsaturated shells to the total energy is repulsive since, because of time-reversal invariance, the spin density $\vec{J}$ is real.

(ii) Case of a tensor force. For a tensor force

$$V_T=v_T(s)\left(\frac{1}{3s^2}(\vec{\sigma}_1\cdot\vec{s})(\vec{\sigma}_2\cdot\vec{s})-\vec{\sigma}_1\cdot\vec{\sigma}_2\right), \quad (4.26)$$

the contribution of the direct term to the potential energy vanishes because $\vec{\rho}(\vec{R}_1,\vec{R}_2)$ is antisymmetric. Since interaction (4.26) acts in triplet spin states only, the spin-exchange operator P_σ may be replaced by 1 in calculating the exchange term as in the previous subsection. Furthermore, due to (4.23), only the second term in (4.26) contributes in lowest order. The contribution of the tensor force to the total energy is therefore

$$V=-\frac{1}{2}\int d^3R_1 d^3R_2\,v_T(|\vec{R}_1-\vec{R}_2|)$$

$$\times\{[\vec{\rho}_n(\vec{R}_1,\vec{R}_2)]^2+[\vec{\rho}_p(\vec{R}_1,\vec{R}_2)]^2\}\,.$$

This equation being identical to (4.25), the derivation of local energy density can be carried out as in the previous subsection by replacing $v(s)$ by $-2v_T(s)$.

(iii) Two-body spin-orbit force. The two-body spin-orbit interaction

$$V_{LS}=-\tfrac{1}{4}i\,v_{LS}(|\vec{R}_1-\vec{R}_2|)(\vec{R}_1-\vec{R}_2)\times(\vec{\nabla}_1-\vec{\nabla}_2)\cdot(\vec{\sigma}_1+\vec{\sigma}_2)$$

$$(4.27)$$

acts also in triplet spin states only, so that in evaluating the exchange term, p_σ may be replaced by 1 as for the tensor force. Since $\vec{\rho}(\vec{R}_1,\vec{R}_2)$ is antisymmetric, terms of the form $\vec{\nabla}_1\times\vec{\sigma}_2$ and $\vec{\nabla}_2\times\vec{\sigma}_1$ do not contribute to the direct term. Also, from the relations

$$\vec{\nabla}\cdot(\vec{A}\times\vec{B})=\vec{B}\cdot\vec{\nabla}\times\vec{A}-\vec{A}\cdot\vec{\nabla}\times\vec{B}\,,$$

$$\vec{\nabla}\times(f\vec{A})=\vec{\nabla}f\times\vec{A}+f\vec{\nabla}\times\vec{A}\,,$$

it may be seen that the terms $\vec{\nabla}_1\times\vec{\sigma}_1$ and $\vec{\nabla}_1\times\vec{\sigma}_2$ in (4.27) give equal contributions to the exchange term. The total potential energy is therefore

$$V=\frac{1}{2}\int d^3R_1 d^3R_2\,v_{LS}(|\vec{R}_1-\vec{R}_2|)$$

$$\times[-\tfrac{1}{2}\rho(\vec{R}_1)\vec{s}\cdot\vec{J}(\vec{R}_2)+i\,\vec{s}\times\vec{\nabla}_2\rho_n(\vec{R}_1,\vec{R}_2)\cdot\vec{\rho}_n(\vec{R}_1,\vec{R}_2)$$

$$+i\,\vec{s}\times\vec{\nabla}_2\rho_p(\vec{R}_1,\vec{R}_2)\cdot\vec{\rho}_p(\vec{R}_1,\vec{R}_2)]\,. \quad (4.28)$$

In (4.28) the first term corresponds to the direct term and the two others to the exchange term. Since in Sec. II we used for the direct term an expansion whose lowest-order term is that of the short-range series, the same procedure will be used here and the first term in (4.28) will be

expanded as

$$\frac{1}{4\pi}\int d\Omega_s\,\rho\left(\vec{R}+\frac{\vec{s}}{2}\right)\vec{s}\cdot\vec{J}\left(\vec{R}-\frac{\vec{s}}{2}\right)$$

$$=\frac{1}{8\pi}\sum_{\mu,\nu}\int d\Omega_s\,s_\mu s_\nu$$

$$\times[\nabla_\mu\rho(\vec{R})J_\nu(\vec{R})-\rho(\vec{R})\partial_\mu J_\nu(\vec{R})]+\cdots$$

$$=\tfrac{1}{6}s^2[\vec{\nabla}\rho(\vec{R})\cdot\vec{J}(\vec{R})-\rho(\vec{R})\vec{\nabla}\cdot J(\vec{R})]+\cdots.$$

Next inserting expansion (2.8) into (4.28) one first obtains

$$\vec{\nabla}_2\rho(\vec{R}_1,\vec{R}_2)=(\tfrac{1}{2}\vec{\nabla}_{\vec{R}}-\vec{\nabla}_{\vec{s}})\left(\frac{3}{sk_F(\vec{R})}\,j_1(sk_F)\rho(\vec{R})+\cdots\right).$$

$$(4.29)$$

Since the gradient operator acting on the relative coordinate in (4.29) gives a result proportional to $\vec{s}$, the vector product in (4.28) reduces to

$$\vec{s}\times\vec{\nabla}_2\rho(\vec{R}_1,\vec{R}_2)=\frac{1}{2}\left(\frac{3}{sk_F}\,j_1(sk_F)-j_2(sk_F)\right)$$

$$\times\vec{s}\times\vec{\nabla}\rho(\vec{R})+\cdots$$

$$=\tfrac{1}{2}j_0(sk_F)\vec{s}\times\vec{\nabla}\rho(\vec{R})+\cdots.$$

Finally, inserting expansion (4.23) into (4.28) the expression for the potential energy may be written

$$V=\frac{1}{2}\int d^3R\,d^3s\,v_{LS}(s)\{\tfrac{1}{12}s^2[\rho(\vec{R})\vec{\nabla}\cdot\vec{J}(\vec{R})-\vec{\nabla}\rho(\vec{R})\cdot\vec{J}(\vec{R})]$$

$$-\tfrac{1}{4}j_0^2[sk_n(\vec{R})](\vec{s}\times\vec{\nabla}\rho_n[\vec{R}])\cdot(\vec{s}\times\vec{J}_n[\vec{R}])$$

$$-\tfrac{1}{4}j_0^2[sk_p(\vec{R})](\vec{s}\times\vec{\nabla}\rho_p[\vec{R}])\cdot(\vec{s}\times\vec{J}_p[\vec{R}])\}.$$

$$(4.30)$$

In (4.30) the integration over the angular variables $\hat{s}$ of $\vec{s}$ can be carried out by means of the relation

$$\int d\hat{s}\,(\vec{A}\times\vec{s})\cdot(\vec{B}\times\vec{s})=\tfrac{8}{3}\pi(\vec{A}\cdot\vec{B}).$$

Furthermore, an integration by parts may be performed in the direct term after integrating over angular variables. The potential energy arising from the two-body spin-orbit force is thus

$$V=\frac{1}{2}\int d^3R\{\varphi(0)\vec{\nabla}\rho(\vec{R})\cdot\vec{J}(\vec{R})$$

$$+\varphi[k_n(\vec{R})]\vec{\nabla}\rho_n(\vec{R})\cdot\vec{J}_n(\vec{R})$$

$$+\varphi[k_p(\vec{R})]\vec{\nabla}\rho_p(\vec{R})\cdot\vec{J}_p(\vec{R})\},\qquad(4.31)$$

where the function $\varphi(k)$ is defined by

$$\varphi(k)=-\frac{2\pi}{3}\int_0^{+\infty}v_{LS}(s)j_0^2(sk)s^4ds.$$

It will be seen later that for a short-range force the previous equations give the Blin-Stoyle formula.[15]

Starting-Energy Dependence

We shall refer to the dependence of the reaction matrix upon the single-particle energies of the two interacting particles as the starting-energy dependence. Although the sum of all orders of perturbation theory is independent of the choice of single-particle energies, since we are attempting to relate the lowest-order energy in finite nuclei to that in nuclear matter, it is necessary to treat single-particle energies consistently in the two systems.

The primary difficulty in relating starting energies in finite nuclei to those in nuclear matter is that in finite nuclei, the "natural" definition of the single-particle energy is the eigenvalue $E_i=T_i+V_i+\Delta V_i$, where ΔV_i denotes the $\partial V/\partial\rho$ contributions; whereas in nuclear matter, it is most convenient to use the HF energy, $\epsilon_i=T_i+V_i$. It was the mixing of these two different definitions of energies in Ref. 2, which lead to the apparently anomalous low saturation density of nuclear matter at $k_F=1.31$ F^{-1}. If one asks the proper question of how nuclear matter saturates using the effective interaction of Ref. 2 with energy denominators defined in nuclear matter in the same way as in finite nuclei, a simple perturbation argument shows that the saturation density is increased to a reasonable value and the binding energy is increased to about 16.6 MeV in agreement with the semiempirical estimate of Baym and Pethick.[16]

In nuclear matter, the change in potential arising from changing the HF single-particle energies of particles i and j from the average nuclear-matter value $\bar{\epsilon}_{NM}$ to ϵ_i and ϵ_j is

$$\Delta v_{ij}\approx(2\bar{\epsilon}_{NM}-\epsilon_i-\epsilon_j)\left\langle ij\left|\frac{\partial G}{\partial e}\right|ij-ji\right\rangle$$

$$=(2\bar{\epsilon}_{NM}-\epsilon_i-\epsilon_j)K,\qquad(4.32)$$

where K is the integral of the defect wave function. Neglecting the difference between the $\partial V/\partial\rho$ rearrangement terms in finite nuclei and nuclear matter, (4.32) is rewritten in terms of the eigenvalues

$$\Delta v_{ij}=(2\bar{E}_{NM}-\bar{E}_i-\bar{E}_j)K,\qquad(4.33)$$

where at most, we make an error of order K^2 with a small coefficient. Since K arises predominantly from the $^3S_1$-$^3D_1$ tensor force, it is necessary to separate contributions from like and unlike particles. Thus the correction for the potential energy

of the ith neutron may be written

$$\Delta U_i = \sum_{j=\text{neutron}} \left\langle ij \left| \frac{\partial G_{nn}}{\partial e} [2\bar{E}^n_{\text{NM}}(\rho_n, \rho_p) - E_i - E_j] \right| ij - ji \right\rangle$$

$$+ \sum_{j=\text{proton}} \left\langle ij \left| \frac{\partial G_{np}}{\partial e} [\bar{E}^n_{\text{NM}}(\rho_n, \rho_p) + \bar{E}^p_{\text{NM}}(\rho_p, \rho_n) - E_i - E_j] \right| ij - ji \right\rangle. \tag{4.34}$$

Defining K locally in terms of the average nuclear-matter defect function, (4.34) may be rewritten

$$\Delta U_i = \int u_i^2(r) \left\{ K_{nn}(\rho_n, \rho_p) \left[2\bar{E}^n_{\text{NM}}(\rho_n, \rho_p) - E_i - \sum_{j=\text{neutron}} \frac{(2j+1)u_j^2(r)}{4\pi r^2 \rho_n(r)} E_j \right] \right.$$

$$\left. + K_{np}(\rho_n, \rho_p) \left[\bar{E}^n_{\text{NM}}(\rho_n, \rho_p) + \bar{E}^p_{\text{NM}}(\rho_p, \rho_n) - E_i - \sum_{j=\text{proton}} \frac{(2j+1)u_j^2(r)}{4\pi r^2 \rho_p(r)} E_j \right] \right\} \tag{4.35}$$

and the analogous expression for protons is obtained by interchanging n and p.

As discussed in Ref. 2, the Coulomb energy should not be included in the single-particle energies comprising the starting energy, so for protons, E_j represents the eigenvalue minus the Coulomb energy for the jth orbital.

For this calculation, $K_{nn}(\rho_n, \rho_p)$ and $K_{np}(\rho_n, \rho_p)$ are approximated by the following simple polynomials, which are fitted to the wound integrals given by Siemens[17] for symmetric nuclear matter and for a single particle embedded in a sea of unlike particles:

$$K_{nn}(\rho_n, \rho_p) = \rho_n(0.445 - 1.08\rho_n - 0.69\rho_p),$$

$$K_{np}(\rho_n, \rho_p) = \rho_p[3.19 - 10.80(\rho_n + \rho_p)]. \tag{4.36}$$

Finally, $\bar{E}_{\text{NM}}(\rho_n, \rho_p)$ is obtained by retaining the terms in ρ and τ from (3.10) which are nonzero in nuclear matter, varying each wave function ϕ_i^*, summing the integrals of ϕ_i^* times the integrand of $\delta\phi_i^*$, and dividing by the total density, with the result:

$$\bar{E}^n_{\text{NM}}(\rho_n, \rho_p) = \frac{\hbar^2}{2m} \frac{\tau_n}{\rho_n} + \frac{\partial A(\rho_n, \rho_p)}{\partial \rho_n} + \frac{\partial B(\rho_p, \rho_n)}{\partial \rho_n} \tau_p + \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_n} \tau_n + B(\rho_n, \rho_p) \frac{\tau_n}{\rho_n},$$

$$\bar{E}^p_{\text{NM}}(\rho_p, \rho_n) = \frac{\hbar^2}{2m} \frac{\tau_p}{\rho_p} + \frac{\partial A(\rho_n, \rho_p)}{\partial \rho_p} + \frac{\partial B(\rho_p, \rho_n)}{\partial \rho_p} \tau_p + \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_p} \tau_n + B(\rho_p, \rho_n) \frac{\tau_p}{\rho_p}. \tag{4.37}$$

Pauli Corrections

It is straightforward in principle to include first-order perturbation-theory corrections for the difference between the nuclear-matter and finite-nucleus Pauli operators analogous to the starting-energy corrections discussed in the previous section. If the reaction matrices, Pauli operator, and energy denominators in nuclear matter and finite nuclei are distinguished by the subscript N and F, respectively, then the operators are related by the following equation[18]:

$$G_F - G_N^\dagger = G_N^\dagger \left(\frac{Q_N}{e_N} - \frac{Q_F}{e_F} \right) G_F. \tag{4.38}$$

Assuming the energy corrections of the preceding section have already been performed and that G_N and G_F only differ slightly, we obtain

$$\Delta G \approx G_N \left(\frac{Q_N - Q_F}{e_N} \right) G_N. \tag{4.39}$$

Since this correction is not simply related to the nuclear-matter defect function as the energy correction was, we have not actually computed this effect and shall merely indicate schematically how such a calculation should be approached. Momentum space provides the most convenient representation, since G is readily calculated and Q_N is completely trivial. It is advantageous to rewrite (4.39) as

$$\Delta G = G_N \left[\frac{(1 - Q_F) - (1 - Q_N)}{e_N} \right] G_N, \tag{4.40}$$

where $1 - Q$ requires that at least one of the two intermediate states must be an occupied level. Noting that

antisymmetrized matrix elements may be written with only one of the two states antisymmetrized, and inserting a complete set of states,

$$\langle ab | \Delta G | ab - ba \rangle = \tfrac{1}{2} \sum_{k_1 k_2 k_3 k_4} \langle ab - ba | G | k_1 k_2 \rangle \left\langle k_1 k_2 \left| \frac{(1 - Q_F) - (1 - Q_N)}{e_N} \right| k_3 k_4 \right\rangle \langle k_3 k_4 | G | ab - ba \rangle . \tag{4.41}$$

Defining the overlap functions with the normally occupied states as follows:

$$P_F(k, k') = \sum_{n \text{ occupied}} \langle k | \psi_n \rangle \langle \psi_n | k' \rangle ,$$

$$P_N(k, k') = \sum_{k'' < k_F} \langle k | k'' \rangle \langle k'' | k' \rangle = \delta(k - k') \theta(|k_F| - |k|) ;$$

the following result is obtained

$$\langle ab | \Delta G | ab - ba \rangle = \sum_{k_1 k_2 k_4} \frac{1}{e_N} \langle ab - ba | G | k_1 k_2 \rangle \langle k_1 k_4 | G | ab - ba \rangle [P_F(k_2, k_4) - P_N(k_2, k_4)]$$

$$+ \sum_{k_1 k_2 k_3 k_4} [P_F(k_1, k_3) P_F(k_2, k_4) - P_N(k_1, k_3) P_N(k_2, k_4)] \frac{\langle ab - ba | G | k_1 k_2 \rangle \langle k_3 k_4 | G | ab - ba \rangle}{2 e_N} . \tag{4.42}$$

Since the differences in overlap functions are nonzero only in a restricted region of momentum space, evaluation of (4.42) poses no unmanageable computational difficulties.

V. VARIATION

Since the energy density for closed shells in (3.10) is written as a function of

$$\rho_n = \sum_{i = \text{neutron}} \phi_i^* \phi_i , \quad \nabla \rho_n , \quad \tau_n = \sum_{i = \text{neutron}} \vec{\nabla} \phi_i^* \cdot \vec{\nabla} \phi_i ,$$

and corresponding proton terms, it is straightforward to write the variation with respect to a single wave function. Varying a particular neutron wave function, ϕ_n, integrating by parts when necessary, and simplifying, the following single-particle equation is obtained:

$$\left[-\vec{\nabla} \cdot \left(\frac{\hbar^2}{2m} + B(\rho_n, \rho_p) \right) \vec{\nabla} + V_n - E \right] \phi_n = 0 ,$$

$$V_n = \frac{\partial A(\rho_n, \rho_p)}{\partial \rho_n} + \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_n} \tau_n + \frac{\partial B(\rho_p, \rho_n)}{\partial \rho_n} \tau_p + \frac{\partial C(\rho_p, \rho_n)}{\partial \rho_n} | \nabla \rho_p |^2$$

$$- \frac{\partial C(\rho_p, \rho_n)}{\partial \rho_n} | \nabla \rho_n |^2 - \frac{2 \partial C(\rho_n, \rho_p)}{\partial \rho_p} \vec{\nabla} \rho_n \cdot \vec{\nabla} \rho_p - 2 C(\rho_n, \rho_p) \nabla^2 \rho_n - \frac{\partial D(\rho_n, \rho_p)}{\partial \rho_p} | \nabla \rho_p |^2 - D(\rho_n, \rho_p) \nabla^2 \rho_p . \tag{5.1}$$

Thus, a Schrödinger equation is obtained containing a position-dependent effective mass,

$$m^*(r) = \frac{m}{1 + (2m / \hbar^2) B[\rho_n(r), \rho_p(r)]} . \tag{5.2}$$

Specializing to the case of a spherical nucleus, in which $\phi_n = r^{-1} u_n(r) \mathcal{Y}_{ljm}(\Omega)$, the effective mass term may be rewritten as

$$-\vec{\nabla} \cdot B(r) \vec{\nabla} \frac{u_n(r)}{r} \mathcal{Y}_{ljm}(\Omega) = -\frac{\partial B}{\partial r} \frac{\partial}{\partial r} \left(\frac{u_n(r)}{r} \right) \mathcal{Y}_{ljm}(\Omega) - B(r) \nabla^2 \frac{u_n(r)}{r} \mathcal{Y}_{ljm}(\Omega) , \tag{5.3}$$

giving rise to the following radial equation:

$$-\left(\frac{\hbar^2}{2m} + B(\rho_n, \rho_p) \right) u_n''(r) - \left(\rho_n'(r) \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_n} + \rho_p'(r) \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_p} \right) u_n'(r)$$

$$+ \left[\left(\frac{\hbar^2}{2m} + B(\rho_n, \rho_p) \right) \frac{l_n(l_n + 1)}{r^2} + \frac{\rho_n'(r)}{r} \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_n} + \frac{\rho_p'(r)}{r} \frac{\partial B(\rho_n, \rho_p)}{\partial \rho_p} + V_n \right] u_n(r) = E_n u_n(r) . \tag{5.4}$$

The potential energy arising from the tensor force and from spin-unsaturated shells via the central force is

$$V = \int d^3R \{ \varphi[k_n(\vec{R})] J_n{}^2(\vec{R}) + \varphi[k_p(\vec{R})] J_p{}^2(\vec{R}) \},$$

(5.5)

where

$$\varphi(k) = \tfrac{1}{6}\pi \int_0^{+\infty} [2v_T(s) - v(s)] j_0{}^2(ks) s^4 ds.$$

Varying (5.5), one finds that the corresponding contribution to the average nuclear field is the sum of a central and a one-body spin-orbit potential. For a neutron state it is

$$U_n = \frac{k_n}{3\rho_n} \varphi'[k_n(\vec{R})] J_n{}^2(\vec{R}) + 2\varphi(k_n) \vec{J}_n(\vec{R}) \cdot (-i)\vec{\nabla} \times \vec{\sigma},$$

(5.6)

and for a proton state the corresponding formula may be obtained by interchanging indices n and p in (5.6). For a spherical nucleus the spin density is proportional to $\vec{R}$ and the second term in (5.6) therefore reduces to the usual form $f(r)\vec{l}\cdot\vec{\sigma}$.

In the case of a two-body spin-orbit interaction one also finds a central and a spin-orbit term. The result of the variation of (4.31) may be written

$$U_n = -\tfrac{1}{2}\varphi(0)[\vec{\nabla}\cdot\vec{J} - \vec{\nabla}\rho\cdot(-i)(\vec{\nabla}\times\vec{\sigma})]$$
$$- \tfrac{1}{2}\varphi(k_n)[\vec{\nabla}\cdot\vec{J}_n - \vec{\nabla}\rho_n\cdot(-i)(\vec{\nabla}\times\vec{\sigma})]. \qquad (5.7)$$

It is thus evident that the effect of an attractive Wigner force is to decrease the spin-orbit splittings produced by the LS force because potential (5.6) lowers $j = l - \tfrac{1}{2}$ levels. Also, since $v_T(s)$ is positive for both OPEP and Reid's potential, the tensor force gives rise to the same effect. These conclusions are in agreement with those of more elaborated investigations[19, 20] which, unfortunately, tend to yield splittings smaller than observed experimentally.

For a short-range two-body LS force and a spherical $N = Z$ nucleus, one can easily check that the one-body potential (5.7) reduces to

$$\frac{c}{r}\frac{d\rho(r)}{dr}\vec{l}\cdot\vec{\sigma},$$

where

$$c = -\tfrac{1}{2}\pi \int_0^{+\infty} v_{LS}(s) s^4 ds.$$

This result is identical to Blin-Stoyle's formula.[15]

VI. NUMERICAL CALCULATIONS FOR THE LOCAL DENSITY-DEPENDENT EFFECTIVE INTERACTION

Although the theory has been developed quite generally in Sec. IV, our initial computations have dealt with the special case of the local effective in-

teraction derived in Ref. 2. This choice provides us with what we believe to be the simplest final result which still embodies the essential physical effect of the self-consistent structure of finite nuclei. It also provides the opportunity of understanding the quantitative effect of the approximations we have introduced into the density matrix, since the results may be directly compared with the solutions in Ref. 2 which were obtained from solving the nonlocal Schrödinger equation constructed from the finite-range interaction and the exact density matrix.

Calculational Details

The dominant contribution to the ground-state expectation value of H is the nuclear potential energy from closed l shells obtained by using the effective reaction matrix from Ref. 2 in (3.1). Although from Sec. IV it is straightforward to include the contributions from spin-unsaturated shells to the same accuracy, since these shells contribute a relatively small fraction of the total energy, we have introduced the following approximations. The contribution of the central component of the reaction matrix from a j shell is approximated by $(2j+1)/2(2l+1)$ times the contribution from a fully closed l shell. In addition, the contribution from spin-unsaturated shells of the off-diagonal part of the tensor force is neglected.

The spin-orbit force is treated by including the following term in the energy density, as in Ref. 1:

$$H_{so} = \tfrac{1}{2}W_0[\vec{\nabla}(\rho_n + \rho_p)\cdot(\vec{J}_n + \vec{J}_p) + \vec{\nabla}\rho_n\cdot\vec{J}_n + \vec{\nabla}\rho_p\cdot\vec{J}_p]$$
$$= -\tfrac{1}{2}W_0[(\rho_n + \rho_p)\vec{\nabla}\cdot(\vec{J}_n + \vec{J}_p) + \rho_n\vec{\nabla}\cdot\vec{J}_n + \rho_p\vec{\nabla}\cdot\vec{J}_p].$$

(6.1)

For closed j shells in a spherical nucleus,

$$\vec{J}_n = \frac{\vec{r}}{r^4} \sum_{i = \text{neutron}} [j_i(j_i + 1) - l_i(l_i + 1) - \tfrac{3}{4}] u_i{}^2(r).$$

(6.2)

Variation of the nth neutron wave function in a closed j-shell nucleus gives rise to two contributions: a central potential

$$V_n^{so}(r) = -\tfrac{1}{2}W_0\frac{1}{r^2}\frac{\partial}{\partial r}\{r^2[2J_n(r) + J_p(r)]\}, \quad (6.3)$$

and an $\vec{l}\cdot\vec{s}$ potential of the usual Thomas form,

$$V_n^{\vec{l}\cdot\vec{s}}(r) = W_0\frac{1}{r}\frac{d}{dr}(2\rho_n + \rho_p)\vec{l}\cdot\vec{s}. \quad (6.4)$$

Although (6.3) and (6.4) are essentially of the same form as the leading spin-orbit terms derived in Sec. IV, the coefficient $W_0 = 120$ was taken from Ref. 1 and has not been related directly to the two-body effective interaction. However, in

Ref. 2 the spin-orbit coefficient was adjusted to agree with the splittings calculated in ^{40}Ca using the effective reaction matrix, yielding a value only 10% smaller than the value of W_0 we have used, so our present choice is at least roughly consistent with the strength of the spin-orbit component of the reaction matrix.

Due to the range of the Coulomb interaction, the direct term is written

$$H_{\mathrm{CD}} = \frac{1}{2} \iint \rho_p(\vec{R}_1) \rho_p(\vec{R}_2) \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} d^3R_1 \, d^3R_2 , \tag{6.5}$$

giving rise to the only integral expression in the potential for the radial equation. Although the $j_3(sk_F)$ correction terms in (2.8) could straightforwardly be evaluated for the exchange Coulomb contribution, since the exchange correction is already quite small, only the Slater term has been retained. Thus, the exchange Coulomb term is

$$H_{\mathrm{CE}} = -\frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3} e^2 \rho_p^{\,4/3} . \tag{6.6}$$

Center-of-mass corrections have been calculated according to the method of Ref. 2 rather than Ref. 1. The main difference is the fact that dropping the exchange term $\sum_{i \neq j} \vec{p}_i \cdot \vec{p}_j$ in Ref. 1 yields a substantial over-correction for harmonic-oscillator functions, the only case which can be computed unambiguously. In ^{16}O, for example, the energy correction is overestimated by 50%. However, we should emphasize that in any nucleus light enough to have significant c.m. corrections, the cumulative error of our sequence of essentially large nucleus approximations is certainly larger than the ambiguities associated with c.m. corrections, and one should not attach unrealistic significance to the fine details of these corrections. The effect of c.m. motion on the charge density is included with the proton-size correction as in Ref. 2 by folding the point proton distribution with an exponential function of rms radius

$$\langle r^{\mathrm{eff}} \rangle_{\mathrm{rms}} = (0.64 - \tfrac{3}{2} b^2/A)^{1/2} . \tag{6.7}$$

Higher-Order Corrections

Thus far, we have considered a series of approximations to the binding energy in a finite nucleus from the two-body reaction matrix obtained from the Reid potential. We must now consider the most appropriate means of including the effect of all the other contributions besides the two-body ladder diagram. Considerable effort has been expended in investigating these contributions in nuclear matter, and the present situation is reviewed in detail in Ref. 3. For our present purposes, it suffices to note that the most important contribu-

tions appear to be from three- and four-body diagrams and three-body forces, and that these roughly account for the discrepancy between the 11.1-MeV nuclear-matter binding obtained from two-body diagrams with the Reid potential and the value of approximately 16 MeV expected from the semiempirical mass formula.

Since we have already separated the energy density in a finite nucleus into the energy density of nuclear-matter-plus-correction terms, it appears most sensible to include the effect of higher-order corrections directly in the nuclear-matter term. This is essentially equivalent to the short-range assumption made in Ref. 2, and the only remaining question is how to parametrize these corrections, which have only been partially investigated for equal numbers of neutrons and protons near the nuclear-matter density. Since the largest contributions to three- and four-body diagrams, as well as three-body forces arise from the $^3S_1$-$^3D_1$ tensor force, we have chosen to increase the attraction of the short-range part of the triplet even effective interaction. This adjustment is parametrized by a short-range force, the strength of which is a linear function of density, and the two free parameters may be chosen to be the binding energy and saturation density of nuclear matter.

Since the questions of arbitrariness of our choice of the Reid potential and the uncertainty of higher-order corrections are clearly the most serious objections which may be raised against this work, it is important to emphasize what we believe has been achieved by including all uncertainties in the nuclear-matter potential energy contributions. At the very least, since the uncertainties are essentially short range and the finite-nucleus corrections depend only on the noncontroversial long-range components of the nuclear force, one can determine what the nuclear-matter potential energy surface must be in order to obtain the proper bulk properties of finite nuclei, and thereby learn what the true interaction and all corrections must yield in nuclear matter. Thus, the complicated details of off-energy-shell behavior and higher-order corrections are not important to gross nuclear properties, and only the average contributions, in a nuclear-matter sense, need be considered. If one is willing to agree that the major corrections arise from the triplet even states, then one obtains the further result that potential energy for like particles is accurately described by the two-body reaction matrix. Thus neutron-matter calculations near nuclear density are expected to be reliable, and the enhancement in nuclear matter should be applied only to unlike particles thereby increasing the symmetry energy. Since the adjustment in Ref. 2 was applied to both

TABLE I. Expansion coefficients for the energy-density functions appearing in (3.10). Each function is expanded in the form $F(\rho_\alpha, \rho_\beta) = \sum_{IJ} F_{IJ} \rho_\alpha^I \rho_\beta^J$. Since D and V^{NM} are symmetric, redundant off-diagonal elements are omitted. The first four sets of coefficients include higher-order corrections and V^{Reid} reproduces the unadjusted saturation curve of Ref. 17.

	0	1	2	3	4	5	6	7
D^{IJ}								
0	$5.613\,03\times10^{2}$	$-8.451\,42\times10^{3}$	$9.782\,15\times10^{4}$	$-6.626\,99\times10^{3}$	$3.984\,32\times10^{6}$	$-2.696\,82\times10^{7}$	$8.327\,12\times10^{7}$	
1		$1.487\,70\times10^{5}$	$-7.833\,58\times10^{5}$	$-4.559\,55\times10^{5}$	$1.526\,85\times10^{7}$	$3.454\,63\times10^{8}$	$-1.196\,19\times10^{9}$	
2			$-5.281\,76\times10^{6}$	$1.219\,91\times10^{8}$	$-7.680\,96\times10^{8}$	$4.957\,25\times10^{9}$	$-2.928\,41\times10^{10}$	
3				$-6.473\,91\times10^{6}$	$-3.586\,35\times10^{9}$	$-1.048\,75\times10^{10}$	$1.388\,46\times10^{11}$	
4					$-3.609\,42\times10^{9}$	$1.990\,33\times10^{11}$	$1.503\,94\times10^{12}$	
5						$-1.213\,51\times10^{12}$	$-1.633\,19\times10^{13}$	
6							$8.592\,69\times10^{13}$	
V^{NM}_{IJ}								
0	0.0							
1	$-9.887\,16\times10^{-1}$	$-1.341\,41\times10^{3}$						
2	$-1.553\,14\times10^{2}$	$4.937\,75\times10^{3}$	$2.346\,45\times10^{4}$					
3	$-2.914\,48\times10^{2}$	$-2.533\,74\times10^{4}$	$-1.343\,43\times10^{4}$	$2.167\,22\times10^{6}$				
4	$1.257\,08\times10^{4}$	$2.642\,63\times10^{5}$	$-4.376\,52\times10^{6}$	$5.044\,54\times10^{6}$	$-5.153\,04\times10^{7}$			
5	$-9.008\,26\times10^{4}$	$-3.648\,12\times10^{5}$	$9.332\,57\times10^{6}$	$-1.792\,38\times10^{7}$	$1.177\,50\times10^{9}$	$-6.998\,42\times10^{9}$		
6	$2.231\,74\times10^{5}$	$-3.644\,08\times10^{6}$	$8.971\,75\times10^{7}$	$-8.672\,49\times10^{8}$	$2.664\,81\times10^{9}$	$-3.800\,07\times10^{10}$	$3.136\,85\times10^{11}$	
B_{IJ}								
0	0.0	$3.182\,56\times10^{2}$	$-5.805\,13\times10^{3}$	$7.239\,59\times10^{4}$	$-5.127\,80\times10^{5}$	$2.948\,16\times10^{6}$	$-1.573\,74\times10^{7}$	$3.975\,92\times10^{7}$
1	$1.217\,35\times10^{2}$	$-2.184\,24\times10^{3}$	$6.928\,49\times10^{4}$	$-2.125\,27\times10^{5}$	$-6.031\,81\times10^{6}$	$2.000\,51\times10^{7}$	$1.974\,85\times10^{8}$	$-6.607\,97\times10^{8}$
2	$-4.138\,99\times10^{3}$	$1.512\,87\times10^{4}$	$-8.001\,44\times10^{5}$	$-2.092\,23\times10^{6}$	$1.035\,33\times10^{8}$	$-3.425\,14\times10^{8}$	$1.038\,33\times10^{9}$	$-1.278\,50\times10^{10}$
3	$7.625\,47\times10^{4}$	$-3.011\,56\times10^{5}$	$1.056\,65\times10^{7}$	$-4.977\,05\times10^{6}$	$6.840\,39\times10^{6}$	$-2.127\,38\times10^{9}$	$-1.658\,59\times10^{10}$	$1.749\,36\times10^{11}$
4	$-3.770\,66\times10^{5}$	$5.007\,00\times10^{6}$	$-7.495\,36\times10^{7}$	$-3.826\,83\times10^{8}$	$-9.271\,17\times10^{8}$	$-1.443\,77\times10^{9}$	$1.185\,44\times10^{11}$	$1.339\,94\times10^{11}$
5	$-4.494\,04\times10^{6}$	$-3.563\,94\times10^{7}$	$2.005\,03\times10^{8}$	$4.532\,99\times10^{9}$	$1.439\,14\times10^{10}$	$1.697\,32\times10^{10}$	$-4.045\,03\times10^{11}$	$-7.430\,17\times10^{12}$
6	$5.497\,80\times10^{7}$	$8.878\,14\times10^{7}$	$-7.959\,87\times10^{7}$	$-9.213\,86\times10^{9}$	$-1.672\,92\times10^{11}$	$1.015\,56\times10^{12}$	$-2.219\,40\times10^{12}$	$2.455\,05\times10^{13}$
7	$-1.593\,17\times10^{8}$	$0.$	$0.$	$0.$	$0.$	$0.$	$0.$	$0.$
C_{IJ}								
0	$1.309\,34\times10^{2}$	$-1.546\,62\times10^{3}$	$3.056\,87\times10^{4}$	$-8.511\,61\times10^{4}$	$-1.984\,27\times10^{6}$	$8.083\,39\times10^{6}$	$4.426\,96\times10^{7}$	$-1.651\,99\times10^{8}$
1	$-4.740\,89\times10^{3}$	$2.081\,18\times10^{4}$	$-4.640\,41\times10^{5}$	$-1.581\,97\times10^{6}$	$5.669\,79\times10^{7}$	$-1.818\,85\times10^{8}$	$5.191\,67\times10^{8}$	$-6.392\,50\times10^{9}$
2	$1.046\,48\times10^{5}$	$-2.578\,51\times10^{5}$	$6.495\,23\times10^{6}$	$3.664\,25\times10^{6}$	$-9.161\,13\times10^{5}$	$-1.595\,54\times10^{9}$	$-1.243\,94\times10^{10}$	$1.312\,02\times10^{11}$
3	$-5.667\,75\times10^{5}$	$4.530\,68\times10^{6}$	$-6.262\,52\times10^{7}$	$-4.039\,40\times10^{8}$	$-9.271\,17\times10^{8}$	$-1.443\,77\times10^{9}$	$1.185\,44\times10^{11}$	$1.339\,94\times10^{11}$
4	$-1.078\,15\times10^{7}$	$-4.146\,71\times10^{7}$	$2.251\,21\times10^{8}$	$5.666\,24\times10^{9}$	$1.798\,92\times10^{10}$	$2.121\,65\times10^{10}$	$-5.056\,29\times10^{11}$	$-9.287\,71\times10^{12}$
5	$1.447\,28\times10^{8}$	$1.280\,70\times10^{8}$	$-1.193\,98\times10^{8}$	$-1.382\,08\times10^{10}$	$-2.509\,38\times10^{11}$	$1.523\,34\times10^{12}$	$-3.329\,10\times10^{12}$	$3.682\,58\times10^{13}$
6	$-4.750\,56\times10^{8}$	$0.$	$0.$	$0.$	$0.$	$0.$	$0.$	$0.$
V^{Reid}_{IJ}								
0	0.0							
1	$-1.051\,26\times10^{0}$	$-9.900\,74\times10^{2}$						
2	$-1.346\,84\times10^{2}$	$3.108\,91\times10^{3}$	$-5.934\,79\times10^{3}$					
3	$-7.436\,23\times10^{2}$	$1.473\,96\times10^{4}$	$8.216\,93\times10^{4}$	$-2.192\,14\times10^{6}$				
4	$1.668\,27\times10^{4}$	$-2.534\,50\times10^{5}$	$-7.702\,77\times10^{5}$	$-3.353\,15\times10^{6}$	$1.597\,96\times10^{8}$			
5	$-1.102\,19\times10^{5}$	$1.386\,72\times10^{6}$	$1.796\,89\times10^{6}$	$4.828\,51\times10^{7}$	$4.017\,43\times10^{8}$	$-1.091\,38\times10^{10}$		
6	$2.567\,16\times10^{5}$	$-3.105\,56\times10^{6}$	$1.848\,15\times10^{7}$	$-4.953\,84\times10^{8}$	$2.770\,46\times10^{9}$	$-1.953\,76\times10^{10}$	$2.438\,88\times10^{11}$	

the like and unlike interactions, the new restriction of the enhancement to the unlike interaction in this work will lead to slight systematic changes from the previous results which will be discussed in connection with Table III.

Evaluation of the Energy Density Functions

Although the functions $V_{NM}(\rho_\alpha, \rho_\beta)$, $V_D^L(\rho)$, $V_D^U(\rho)$, $V_F^L(\rho)$, and $V_F^U(\rho_\alpha, \rho_\beta)$ appearing in the approximate energy density are completely specified by (3.7) and the preceding definitions, it is still necessary to adopt some practical curve-fitting procedure to parametrize these functions. In spite of the fact that these functions should properly be expanded in powers of k_F, we have found it most practical to fit them to polynomials in ρ in the region of densities encountered in nuclei. Sixth-degree polynomials were found to be adequate, and each of the five functions is thus expressed in the form

$$F(\rho_\alpha, \rho_\beta) = \sum_{IJ=0}^{7} F_{IJ}\, \rho_\alpha^I \rho_\beta^J$$

or   (6.8)

$$F(\rho) = \sum_{I=0}^{7} F_I \rho^I \, .$$

Each of the functions $F(\rho_n, \rho_p)$ was evaluated on a two-dimensional 16×16 mesh of points evenly spaced in steps of 0.01 F^{-3}, and the coefficients F_{IJ} were obtained by a least-squares fit weighted to insure particularly accurate agreement in the region $\rho_n \sim \rho_p \sim 0.08$ F^{-3}. The functions of one variable were least-squares-fitted analogously on a 16 point mesh with the same spacing. Polynomial coefficients for $B(\rho_\alpha, \rho_\beta)$, $C(\rho_\alpha, \rho_\beta)$, and $D(\rho_\alpha, \rho_\beta)$ are obtained straight-forwardly from (3.8) and (3.11). The coefficients for V^{NM}, B, C, and D obtained with the effective interaction adjusted to give a nuclear-matter binding energy of 16.6 MeV per particle at $k_F = 1.34$ F^{-1} are tabulated in Table I. For comparison, we have also tabulated the coefficients V_{IJ}^{NM} for the unadjusted effective interaction which yields 11 MeV at $k_F = 1.44$ F^{-1}.

Comparison with Skyrme's Interaction

Since HF calculations made with Skyrme's interaction in Ref. 1 yield results very similar to those obtained in the local-density approximation, it is interesting to compare the Hamiltonian density derived in Sec. III with that obtained from Skyrme's force, which in our notation is given by:

$$A(\rho_n, \rho_p) = \tfrac{1}{2}t_0[(1 + \tfrac{1}{2}x_0)\rho^2 - (x_0 + \tfrac{1}{2})(\rho_n^2 + \rho_p^2)]$$
$$+ \tfrac{1}{4}t_3\rho_n\rho_p\rho \, ,$$
$$B(\rho_n, \rho_p) = \tfrac{1}{4}(t_1 + t_2)\rho + \tfrac{1}{8}(t_2 - t_1)\rho_n \, ,$$
$$C(\rho_n, \rho_p) = \tfrac{3}{32}(t_1 - t_2) \, ,$$ (6.9)
$$D(\rho_n, \rho_p) = \tfrac{1}{8}(t_2 - 3t_1) \, ,$$

where t_0, t_1, t_2, t_3, and x_0 denote the parameters of the Skyrme force. Of course, the previous expression cannot reproduce identically the Hamiltonian density (3.10) for all values of ρ_n and ρ_p. However, for the purpose of making HF calculations, values of the quantities A, B, C, and D near the equilibrium nuclear-matter density are most important and therefore one may attempt to construct an equivalent Skyrme interaction by identifying (3.10) and (6.9) in the neighborhood of $\rho_n = \rho_p = \rho_{NM}/2$. The coefficients t_0, t_1, t_2, and t_3 are then determined by requiring

$$A + B\tau + (C + \tfrac{1}{2}D)|\nabla\rho|^2$$
$$\equiv \tfrac{3}{8}t_0\rho^2 + \tfrac{1}{16}t_3\rho^3 + \tfrac{1}{16}(3t_1 + 5t_2)\rho\tau + \tfrac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 \, ,$$ (6.10)

and the parameter x_0 may be obtained from values of A off the diagonal $\rho_n = \rho_p$, e.g.,

$$A(\tfrac{1}{2}(\rho + \delta\rho), \tfrac{1}{2}(\rho - \delta\rho))$$
$$\simeq A(\tfrac{1}{2}\rho, \tfrac{1}{2}\rho) - \tfrac{1}{4}t_0(x_0 + \tfrac{1}{2})\delta\rho^2 - \tfrac{1}{16}t_3\rho\delta\rho^2 \, .$$ (6.11)

This procedure gives explicitly:

$$t_0 = (8/3\rho^2)(3A - \rho A'), \quad t_1 = \tfrac{1}{3}(8C + 4D + 4B/\rho) \, ,$$ (6.12)

$$t_2 = \tfrac{1}{5}(12B/\rho - 8C - 4D), \quad t_3 = (16/\rho^3)(\rho A' - 2A) \, ,$$

TABLE II. Equivalent parameters of the Skyrme interaction defined by (6.12)–(6.14) compared with Sets I and II of Ref. 1.

Parameter Set	ρ_n (F^{-3})	ρ_p (F^{-3})	B.E./A (MeV)	k_F (F^{-1})	t_0 (MeV F^3)	t_1 (MeV F^5)	t_2 (MeV F^5)	t_3 (MeV F^6)	x_0
I			16	1.32	−1057.3	235.9	−100.	14463.	0.56
II			16	1.30	−1169.9	585.6	−27.1	9331.	0.34
1	0.080	0.080	16.6	1.34	−1248.0	381.1	15.1	14542.	0.50
2	0.093	0.064	16.6	1.34	−1233.1	391.9	8.3	13974.	0.49
3	0.080	0.080	11.0	1.44	−993.9	379.	16.1	8691.2	0.36
4	0.093	0.064	11.0	1.44	−987.3	389.7	9.4	8438.6	0.35

where

$$A' = \frac{1}{2}\left(\frac{\partial A}{\partial \rho_n} + \frac{\partial A}{\partial \rho_p}\right) .$$

The parameters obtained in this way for $\rho_n = \rho_p$ = 0.8 with the adjusted force are tabulated as Set 1 in Table II. Comparison with the parameters for forces I and II of Ref. 1, which are also tabulated for reference, shows that the strength t_3 of the density-dependent force turns out to be rather close to that of force I, whereas nonlocality effects, which depend essentially on the parameter combination $3t_1 + 5t_2$, should be expected to be similar to those obtained from force II.

To investigate how well the Hamiltonian density (3.10) can be reproduced from Skyrme's interaction, we have graphed in Fig. 2 the variation, as a function of the density ρ, of the parameters t_0, t_1, t_2, t_3, and x_0, calculated from (6.11), (6.12) at $\rho_n = \rho_p$ = $\rho/2$ and normalized to their nuclear-matter values. Whereas the parameters t_0, t_3, and x_0 stay rather close to their nuclear-matter values, significant deviations occur for the coefficients t_1 and t_2 of the velocity-dependent δ forces. One should note, however, that since the P-wave component of the force is quite small at nuclear-matter density, the deviation of t_2 does not correspond in fact to an important over-all change in the nucleon-nucleon effective interaction. One can also notice in Fig. 2 that for a density slightly smaller than nuclear-matter density, one gets a somewhat stronger repulsion from the t_1 and t_3 terms, together with a nearly constant value t_0 of the attractive component of the force.

An alternative derivation of Skyrme's parameters can be made by calculating the Hamiltonian density in the neighborhood of values of ρ_n and ρ_p corresponding to the interior of the real nucleus ^{208}Pb rather than to nuclear matter. Identifying A and it's two partial derivatives with the expressions obtained from (6.9) one obtains

$$t_0 = \frac{8}{3\rho^2(1+\alpha)}[3a(1+\alpha) - \rho\Sigma] ,$$

$$t_3 = \frac{16}{\rho^3(1+3\alpha)}(\rho\Sigma - 2a) , \qquad (6.13)$$

$$x_0 = -\frac{1}{t_0}\left(\frac{\Delta}{\delta\rho} + \frac{t_0}{2} + \frac{t_3}{4}\rho\right) ,$$

where

$$\rho = \rho_n + \rho_p , \qquad \delta\rho = \rho_n - \rho_p ,$$

$$\alpha = \frac{1}{3}\left(\frac{\delta\rho}{\rho}\right)^2 , \qquad \Sigma = \frac{1}{2}\left(\frac{\partial A}{\partial \rho_n} + \frac{\partial A}{\partial \rho_p}\right) ,$$

$$\Delta = \frac{\partial A}{\partial \rho_n} - \frac{\partial A}{\partial \rho_p} , \qquad a = A - \frac{1}{4}\Delta\delta\rho .$$

The parameters t_1 and t_2 cannot be defined uniquely, since one cannot reproduce even locally the variations of the six functions $B(\rho_n, \rho_p)$, $B(\rho_p, \rho_n)$, $C(\rho_n, \rho_p), \ldots, D(\rho_p, \rho_n)$, with only two parameters. The choice we have made has been to describe the function B alone which is important to reproduce nonlocality effects. We have required

$$B(\rho_n, \rho_p)\tau_n + B(\rho_p, \rho_n)\tau_p$$

$$= \frac{1}{4}(t_1 + t_2)\rho\tau + \frac{1}{8}(t_2 - t_1)(\rho_n\tau_n + \rho_p\tau_p) ,$$

which yields

$$t_1 = 2\alpha/\rho - 5\beta/\delta\rho , \qquad t_2 = 2\alpha/\rho + \beta/\delta\rho , \qquad (6.14)$$

where α and β denote the quantities $\frac{1}{2}[B(\rho_n, \rho_p) + B(\rho_p, \rho_n)]$ and $B(\rho_n, \rho_p) - B(\rho_p, \rho_n)$, respectively. This way of deriving t_1 and t_2 is different from the one we used before, where the coefficients of τ and $(\nabla\rho)^2$ were identified for $\rho_n = \rho_p$. Therefore comparing the values calculated from (6.12) and (6.14) tabulated as 1 and 2 in Table II yields another criterion for the validity of a Skyrme-type parametrization for the Hamiltonian density.

In order to relate the adjustment of the force to the Skyrme parameters, we have also tabulated the analogous parameters obtained without the adjustment as Sets 3 and 4 in Table II. The dominant effects are simply those expected from the difference in nuclear-matter saturation: Lack of binding of the unadjusted force is reflected in the smaller magnitude of t_0 and the higher saturation density is reflected in a smaller density dependence t_3.

The over-all agreement of our derived parameters and the phenomenological parameters of Ref. 1 is gratifying and suggests that this theory should
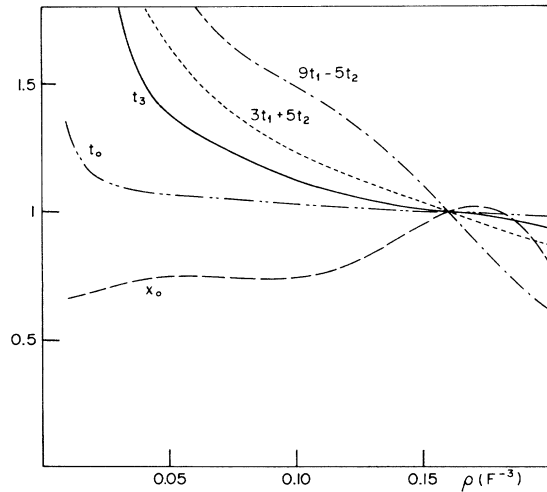

FIG. 2. The equivalent Skyrme parameters at equal neutron and proton densities, normalized to unity at ρ =0.16 F^{-3}. The absolute values are tabulated in Table II.

account for the systematic behavior of gross properties of nuclei. In addition, although on the basis of binding energies and densities, the phenomenological theory was unable to distinguish the nonlocality of the interaction, essentially allowing any effective mass between 0.6 and 1, this present work shows that the effective mass near nuclear density must be approximately 0.6, which is the value required to obtain agreement with experimental 0s proton-knockout energies.

Numerical Results

Self-consistent calculations have been performed using the DME and the approximations discussed above for the spherical nuclei ^{16}O, ^{40}Ca, ^{90}Zr, and ^{208}Pb. The radial equations, (5.4) were solved using Runge-Kutta integration and iterated to self-consistency. The self-consistent wave functions were used to evaluate the point particle distributions, charge distributions, and binding energies, including the starting energy corrections. The binding energies and rms radii are tabulated in Table III and the density distributions are graphed in Fig. 3. The single-particle energies agree quite closely with the density-dependent Hartree-Fock (DDHF) results of Ref. 2 and are therefore not presented.

The most significant result is that the approximations introduced to obtain a simple form for the local energy density in the DME yield only minor changes in the calculated properties of finite nuclei compared with the DDHF results.[21] In order to clarify the physical origin of the various discrep-

ancies, it is worthwhile to discuss them individually in some detail.

The binding-energy systematics of the DME results differ primarily because of the differences in the treatment of the starting energy corrections and the adjustment of the nuclear-matter saturation curve to account for higher-order corrections. As explained in Sec. IV, our improved treatment of starting energy dependence which treats energy denominators equivalently in nuclear matter and finite nuclei necessarily requires a redefinition of the nuclear-matter saturation curve. In addition, the new restriction of the enhancement to triplet even states also inhibits the direct comparison of energies calculated for nuclei with the two different theories.

For these reasons, the adjustment of the two free parameters of the triplet even force was performed simply to obtain the proper charge radius and binding energy in ^{208}Pb and is totally unrelated to parameters obtained in the DDHF theory. The fact that we deliberately overbound Pb by 0.2 MeV unfortunately makes the energies in Table III slightly confusing, but is useful, since the starting-energy correction is 0.2 MeV in Pb, and we have thereby built this small starting-energy effect directly into the effective Hamiltonian, eliminating the need to explicitly evaluate starting-energy corrections for many applications in this region. If one compensates by removing roughly 0.2 MeV from each of the DME values in Table III, one observes extremely good systematic agreement, which in our opinion is at least partially fortuitous given the approximations contained in the theory.

Although density distributions will be considered qualitatively in connection with Fig. 3, one obtains

TABLE III. Binding energies and rms radii obtained with the present density-matrix expansion (DME) and the finite-range, nonlocal density-dependent Hartree-Fock theory (DDHF).

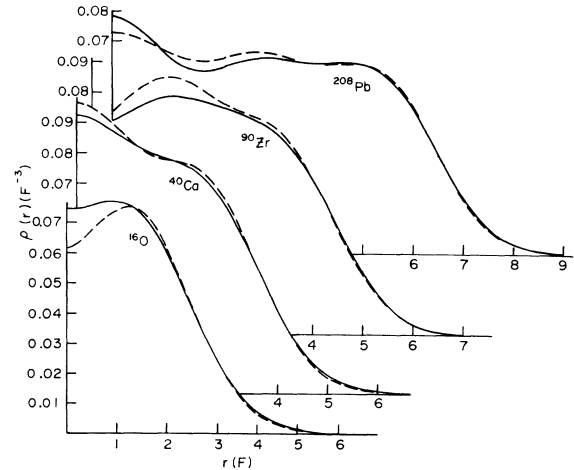|	^{16}O	^{40}Ca	^{90}Zr	^{208}Pb
B.E./A (MeV)				
Expt	7.98	8.55	8.71	7.87
DME	7.99	8.82	8.97	8.08
DDHF	7.59	7.99	8.33	7.83
$\langle r^2\rangle_{charge}^{1/2}$ (F)				
"Expt"	2.73	3.48	4.24	5.50
DME	2.79	3.50	4.29	5.49
DDHF	2.75	3.46	4.23	5.49
$\langle r^2\rangle_{p}^{1/2}$ (F)				
DME	2.75	3.45	4.24	5.45
DDHF	2.71	3.41	4.18	5.45
$\langle r^2\rangle_{n}^{1/2}$ (F)				
DME	2.72	3.40	4.31	5.65
DDHF	2.69	3.37	4.30	5.68

FIG. 3. Point proton density distributions calculated with the density-matrix expansion (solid curves) and with the finite-range, nonlocal DDHF theory (dashed lines).

an instructive quantitative comparison from the rms radii tabulated in Table III. The "experimental" charge radii are obtained from phenomenological fits to elastic scattering,[22] and although they are therefore subject to an undetermined admixture of theoretical prejudice, they provide a useful comparison for our present purposes. Given that the DME and DDHF theories were essentially adjusted to agree in ^{208}Pb, one observes that they have extremely similar systematic behavior, with the DME producing slightly larger radii in light nuclei. Since even small errors in the energy density in the surface of a light nucleus could easily propagate into a large discrepancy in the self-consistent radius, we view these small differences as a strong indication of the validity of the DME. In examining the differences between proton and neutron radii, one observes the fact that whereas the differences are comparable in the two theories for symmetric nuclei, the difference between the neutron and proton radius is diminished by the DME for nuclei with a neutron excess. This is not likely to be due to approximations in the derivation of the DME, but rather to arise from our choice of enhancing the triplet even interaction, thereby increasing the symmetry energy and tending to make neutrons and protons correlate more strongly.

The salient features of the differences between density distributions calculated with the DME and DDHF theories are exhibited by the point proton distributions graphed in Fig. 3. One observes both from the slightly broader surfaces of all the nuclei and from the interior oscillations of the symmetric nuclei that the total mass density tends to be slightly smoother in the completely local DME theory than in the DDHF theory which still incorporates the finite range of the nuclear force. Although there is no obvious reason forcing it to do so, it is certainly true that a local theory has more freedom to let the potential respond to sharp shell-model oscillations in the density in such a way as to damp them out, than a finite-range theory which is forced to generate a rather smooth potential because of the range of the force. We should point out that the systematic trend for the surface discrepancy to disappear in heavy nuclei is simply due to increasing influence of the Coulomb potential which begins to dominate the proton potential in the surface.

In principle, information concerning the behavior of wave functions further away from the center of mass of two interacting particles could be included by carrying higher derivatives in the expansion for the direct and exchange terms in Sec. III. This immediately suggests that the nonunique terms beyond order s^2 in (2.8) or (3.3) might also be exploited for the same purpose. Since the range of

the exchange contribution is essentially cut off by the presence of the factor $\rho_{SL}(sk_F)$ in (2.10), numerical results are extremely insensitive to changes in the fourth-order term in the expansion. However, changing the coefficient of s^4 in the derivative correction term in (3.3) effectively increases or decreases the response of the potential to fluctuations in the density. A convenient means of parametrizing the s^4 term in the direct expansion is to multiply the integrands of V_D^L and V_D^U in (3.7) by the factor $1 + \alpha(sk_F)^2$. One then finds that $\alpha \approx -0.03$ significantly improves agreement with the DDHF theory. At present, we have no physical argument to motivate doing this, and, consequently, it has not been included in any of the results reported in this work.

An additional effect in the case of ^{208}Pb, which has a large neutron excess, is evident in Fig. 3. One observes that the fluctuations in the proton densities are enhanced compared to those occurring in the DDHF theory. The neutron density, which is not shown, has equally large, compensating fluctuations such that the mass density is again extremely smooth. This behavior is related to that discussed for symmetric nuclei, but differs in that it is sensitive to the response of the neutron potential to fluctuations in the proton density and vice versa. Since the force between unlike particles has the strongest and longest range components, it is not surprising that these fluctuations should be slightly misreproduced by the theory. Again, this behavior may be remedied by introducing a fudge factor of the form discussed above. The value $\alpha = -0.03$ helps significantly, and one can doubtless do even better by taking separate values of α for V_D^L and V_D^U. We should emphasize that the fluctuations are totally insignificant in determining the gross properties of nuclei, and since the whole purpose of this theory has been to remove as much superfluous detailed wave-function information as possible from the density matrix, it goes against the spirit of the work to focus undue attention on the details of the shell-model fluctuations arising from the last few wave functions in the nucleus.

VII. DISCUSSION

We have shown that the energy density in a finite nucleus for a general two-body reaction matrix may be separated into the exact contribution of that reaction matrix in nuclear-matter-plus-correction terms, which depend essentially on the well-established long-range components of the nuclear force. The validity of the extremely simple energy expression thus obtained has been established by explicitly writing ρ and τ in terms of single-particle wave functions and comparing the result-

ing calculations with the DDHF results.

It should be emphasized that this is a completely variational theory and does not correspond precisely to the lowest-order Goldstone diagram in an expansion in terms of reaction matrices. However, we would suggest that our effective Hamiltonian defines an ideal basis in which to systematically calculate corrections to a specified order in the exact reaction matrix. Since the evaluation of the contributions of one-body operators to diagrams is extremely easy, the advantages of having the proper zero-order energy and density more than compensate the loss of the otherwise convenient diagramatic cancellations brought about by defining the basis in terms of various on-energy-shell mass operators.

One important accomplishment of the theory is that higher-order corrections have been completely absorbed into the nuclear-matter potential energy term. Thus one may incorporate the effect of many complicated contributions which at present are not understood, such as off-energy-shell behavior, many-body diagrams, three-body forces, and various clustering phenomena, without being forced to become involved in inessential details of these contributions. In this way, the theory results in a nuclear-matter potential energy surface which must be reproduced by a nuclear force if it is to produce the required properties of finite nuclei.

One of the main advantages of this theory, which have not been made use of in this work, is that the energy density is expressed in terms of only two functions, ρ and τ. In principle, if one succeeded in formulating the constraint between ρ and τ, one would have a variational theory in terms of two functions which represents a tremendous simplification compared with the N functions required in

HF theory. Because the statistical approximation relating τ to $\rho^{5/3}$ is extremely inaccurate in the surface, and such errors are greatly amplified upon variation, it is evident that this theory cannot be reduced to a Thomas-Fermi theory. Although some progress can be made by relating ρ and τ via sums of WKB wave functions, we are, at present, unable to formulate the constraint satisfactorily and hence are forced to reintroduce the explicit wave functions.

Because of the simplicity of the final expression for the energy density, many applications are possible which are impractical with more complicated theories. Deformation, collective motion, and fission are all amenable to calculation with this theory, and it would be even more desirable to express these phenomena directly in terms of ρ and τ. Calculations involving large numbers of nucleons, such as clustering phenomena in neutron-star matter are also practical and are presently being pursued. Unfortunately, although calculations of superheavy nuclei would be very easy, they would not be meaningful, since the crucial question of the single-particle eigenvalue spectrum is not dealt with adequately, because we have thus far not explicitly evaluated the contributions of spin-unsaturated shells derived in Sec. IV. Finally, we believe that the expansion for the density matrix is sufficiently simple that it could easily be used in phenomenological analyses of nucleon optical potentials to properly include the exchange contribution which is presently ignored in deference to the inviting simplicity of the direct term.

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Sufficient Conditions for Saturation of Nuclear Forces

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Conditions are given and proven that are sufficient to insure the saturation property of nuclear binding energies. Interactions mediated by two-body local static potentials are considered. For some classes of potentials these sufficient conditions are also necessary for saturation.

1. INTRODUCTION

Recently, a rigorous approach to the old problem[1,2] of the saturation property of nuclear binding energies has been revived, and necessary conditions for saturation have been given, i.e., inequalities that the nuclear interaction must satisfy to be consistent with asymptotic saturation.[3] These rigorous conditions can be used to demonstrate that a given model of the nuclear force is inconsistent with saturation, or to pinpoint which features of a possibly saturating nuclear interaction are essential to bring about saturation. A remarkable outcome of these investigations is the observation that current models of the nuclear force do not comply with the requirements of saturation in an entirely satisfactory manner.[3] Moreover, these results indicate that it is unlikely that the empirical saturation displayed by the nuclear binding energies could be reconciled with a nuclear interaction whose static part, considered by itself, does not saturate. This conclusion, coupled with the remark that the more usual and simple non-static interactions (e.g., a local spin-orbit force) are essentially incompatible with saturation,[3(c)-3(e)] focuses attention on the static part of the nuclear

force, and thus justifies the fact that our consideration is hereafter limited to a nuclear interaction mediated by a two-body static (local) potential.

Two basic features can be responsible for saturation: the exchange character of the nuclear force, and its predominantly repulsive nature at short range. While either one of these features can produce saturation, it is presumably a combination of them that is operative in the nuclear case. It is, nonetheless, quite interesting, to the extent that it is feasible, to elucidate the role that each feature is playing; this can to some extent be done, for a given model of the nuclear force, by modifying it so as to emphasize one or the other feature, and then testing whether saturation is, or is not, achieved. As noted above, a useful instrument to carry out this program is (necessary) conditions that the nuclear force must satisfy in order to be consistent with saturation[3]; obviously no less useful is the complementary tool consisting of (sufficient) conditions such that if the nuclear interaction satisfies them, saturation is guaranteed. It is the purpose of this paper to report such conditions,[4] together with their proofs.

Clearly sufficient conditions for saturation provide, moreover, an important tool to facilitate