Unitary-Model-Operator Approach to Nuclear-Structure Physics. I*

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(Received 14 April 1967)

A discussion of the unitary-model-operator approach to the correlation problem in nuclei is presented and some calculational detials are discussed. The renormalization of the tensor force is carried out in second-order perturbation theory after the introduction of a set of correlated basis functions. It is indicated that the application of the Hartree-Fock method to the resulting effective Hamiltonian extends the range of application of the theory for which a degree of self-consistency in the calculations may be achieved.

I. INTRODUCTION

IT is well known that the approximation in which one considers nuclear particles moving in some potential field and interacting with a weak residual interaction is highly successful in the study of nuclear properties. In order to understand the nature of the effective interaction to be used in nuclear-structure problems it is necessary first to distinguish between two effects which can lead to an "effective interaction." The distinction between these effects is somewhat arbitrary but is of importance. Even if the fundamental nucleon-nucleon force were nonsingular, a shell-model calculation represents an approximation in that one usually treats the effects of only a few shells. Neglected shells serve to renormalize the interaction in the space of the shells considered in one's calculation. This is a well-known problem and not the major concern of the present work. The second effect, which is of central interest here, is the renormalization of the effective interaction due to the admixture of very-high-energy orbitals into the nuclear wave function. This results from the strongly repulsive nature of the nuclear force at short distances and also from specific characteristics of the tensor force. It is not possible to treat these high-energy admixtures by a variational principle; however, definite prescriptions can be given for these admixtures which lead to the definition of an effective Hamiltonian. As will be seen, this is accomplished by making a unitary substitution of correlated basis functions for the usual uncorrelated functions. This procedure, properly carried through, leads to an effective Hamiltonian defined in the space of the orbitals that one usually considers in shell theory.[1] Once one has arrived at an effective Hamiltonian one may proceed to study various aspects of nuclear physics. In particular, the theory finds application in the calculation of nuclear binding energies,[2,3] spin-orbit splittings,[2,3] transition rates,[4] and spectra.[5] Of particular importance is the fact that the theory provides some foundation for the application of generalized Hartree-Fock methods even when the fundamental nucleon-nucleon interaction is singular.[3] Particular emphasis is placed on this latter point since most nuclear-structure calculations have as their basis the concepts of the independent-particle model. This work serves to aid in resolving the paradox arising from the success of independent-particle concepts for finite nuclei and the singular character of the fundamental nucleon-nucleon interaction which one infers from nucleon-nucleon scattering experiments.

Discussions of a unitary-model-operator approach have been given by Villars[6] and Mittelstaedt,[7] who have also noted the usefulness of this method in justifying the introduction of nonlocal nucleon-nucleon effective interactions. These authors also indicate that by using various possible definitions of the model operator, one can relate this method to the Brueckner-Bethe-Goldstone approach and to the Moszkowski-Scott separation method.

In this work an attempt has been made to avoid solving the full Brueckner-Bethe-Goldstone equation for finite systems. A perturbative scheme has been developed using a basis of correlated functions. Details of the evaluation of the matrix elements are discussed and some results are presented for the Yale potential.[8]

* This work was supported in part through funds provided by the U. S. Atomic Energy Commission under Contract No. AT(30-1)-2098 at M.I.T. and under Contract No. AT(30-1)-1807 at Yale University, and by the U. S. Army Research Office, Durham, at Yale University.

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II. CORRELATED BASIS FUNCTIONS

Consider a general nuclear Hamiltonian

$$H=\sum_{\alpha\beta}(\alpha|t|\beta)a_\alpha^\dagger a_\beta+\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}a_\alpha^\dagger a_\beta^\dagger(\alpha\beta|V_{12}|\gamma\delta)a_\delta a_\gamma, \quad (1)$$

where allowance is made for the possibility that V_{12} may have a hard core. Thus, if the states $|\alpha\beta)$ are uncorrelated, the matrix elements of V_{12} are infinite. This problem can be avoided by taking matrix elements of the Hamiltonian between many-body states that are correlated such that the wave function is zero when any two particles are within the range of the hard core. In the Jastrow theory[9] one introduces states of the form

$$\prod_{i,j}[1+f(|\mathbf{r}_i-\mathbf{r}_j|)]\Phi(\mathbf{r}_1,\cdots,\mathbf{r}_n),$$

where the function $[1+f(|\mathbf{r}_i-\mathbf{r}_j|)]$ is required to vanish when particles i and j are within the core range. Theories of nuclear structure based on the Jastrow approach have not had much success. Particularly, attempts to determine the correlation function variationally do not hold much promise for the nucleon-nucleon potentials of current interest.[8,10] In particular, the presence of strong tensor forces excludes the application of Jastrow theory in its simplest form.

In this work correlations will be introduced into the wave function via a unitary-model operator e^{iS}, such that if the long-range properties of the wave function are specified by a function $\Phi(\mathbf{r}_1,\cdots,\mathbf{r}_n)$, the corresponding correlated state is

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_n)=e^{iS}\Phi(\mathbf{r}_1,\cdots,\mathbf{r}_n). \quad (2)$$

As discussed in some detail previously,[1] it is useful to define an effective Hamiltonian in the space of the uncorrelated functions,

$$H_{\text{eff}}=e^{-iS}He^{iS}. \quad (3)$$

Further, one carries through a cluster expansion[1] of this Hamiltonian,

$$\begin{aligned}H_{\text{eff}}&=H^{(1)}+H^{(2)}+H^{(3)}+\cdots\\&=\sum_{\alpha\beta}(\alpha|t|\beta)a_\alpha^\dagger a_\beta\\&\quad+\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}a_\alpha^\dagger a_\beta^\dagger(\alpha\beta|e^{-iS_{12}}(t_1+t_2+V_{12})e^{iS_{12}}\\&\qquad-(t_1+t_2)|\gamma\delta)a_\delta a_\gamma+\cdots, \quad (4)\end{aligned}$$

where $e^{iS_{12}}$ defines the action of e^{iS} in the space of two-particle wave functions. Here $H^{(n)}$ is an n-body operator. Now if the correlations induced by e^{iS} are of sufficiently short range it can be inferred that the higher-order terms in this expansion which involve effective n-body ($n>2$) forces are small (see Appendix A). Further, extensive use is made of the fact that via the Moshinsky transformation[11] the problem of two particles interacting via a two-body force and moving in a harmonic-oscillator potential can be solved. It is useful therefore to add to H_{eff} a term representing the dispersive effects of the medium:

$$\begin{aligned}&\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}a_\alpha^\dagger a_\beta^\dagger(\alpha\beta|e^{-iS_{12}}(U_1+U_2)e^{iS_{12}}\\&\qquad-(U_1+U_2)|\gamma\delta)a_\delta a_\gamma, \quad (5)\end{aligned}$$

where U_1 and U_2 are one-body harmonic-oscillator potentials: $U_1=\frac{1}{2}kr_1^2$, $U_2=\frac{1}{2}kr_2^2$. Again it may be shown that for the short-range correlations in mind the added term has only a small effect on the matrix elements of H_{eff}. The use of harmonic-oscillator potentials to describe the dispersive effetcs of the medium represents an approximation to the actual nonlocal potential which would affect the motion of nucleons in finite nuclei.

One is led to the following procedure. The undetermined orbitals, say $\psi_\alpha(r)$, are expanded in terms of harmonic-oscillator orbitals,

$$\psi_\alpha(r)=\sum_i C_i^\alpha\phi_i(r)=\sum_i C_i^\alpha|i). \quad (6)$$

In this basis, H_{eff} now reads

$$\begin{aligned}H_{\text{eff}}&=\sum_{i,j}(i|t|j)a_i^\dagger a_j+\tfrac{1}{2}\sum_{i,j,k,l}a_i^\dagger a_j^\dagger a_l a_k\\&\quad\times[(\Psi_{ij}|(t_1+t_2+U_1+U_2+V_{12})|\Psi_{kl})\\&\qquad-(ij|(t_1+t_2+U_1+U_2)|kl)], \quad (7)\end{aligned}$$

where the definition

$$e^{iS_{12}}|ij)=|\Psi_{ij}) \quad (8)$$

has been used. This last equation specifies the unitary substitution of the correlated pair states $|\Psi_{ij})$ for the uncorrelated states $|ij)$ of the harmonic-oscillator basis.

Further, it is useful to write the nucleon-nucleon force as follows:

$$\begin{aligned}V_{12}&=\sum_{l,J,S=0,1}\mathcal{Y}^{lSJ}(\Omega_r)v^{lSJ}(\mathbf{r})(\mathcal{Y}^{lSJ})^\dagger(\Omega_r)\\&\quad+\sum_{l,J\,l';\,l'\neq l}\mathcal{Y}^{l'1J}(\Omega_r)v_T(\mathbf{r})(\mathcal{Y}^{l1J})^\dagger(\Omega_r), \quad (9)\end{aligned}$$

$$r=|\mathbf{r}_1-\mathbf{r}_2|.$$

The force is separated in (9) into those parts that are diagonal in the relative orbital angular momentum and those that are not. Clearly, the second term receives contributions only from the tensor force. The first term contains all other parts of the force as well as the parts of the tensor force that are diagonal in l. [The $\mathcal{Y}^{lSJ}(\Omega_r)$

[9] J. W. Clark and P. Westhaus, Phys. Rev. **141**, 833 (1966), and references given in this work.

[10] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 383 (1962).

[11] M. Moshinsky and T. A. Brody, *Tables of Transformation Brackets* (Monografias del Instituto de Fisica, Mexico City, Mexico, 1960).

are generalized spherical harmonics which include the spin variables.]

In the following v_{12} will be used to refer to the part of the force diagonal in l and $v_T^{\rm OD}$ to refer to the part of the force off-diagonal in l, i.e., $V_{12}=v_{12}+v_T^{\rm OD}$. The separation is made in this way because one is interested in separating the force into a short- and a long-range part such that the short-range part produces no energy shift in the pair state. This is a natural extension to finite nuclei of the zero-phase-shift condition of Moszkowski and Scott[12] for nuclear-matter calculations. In the presence of $v_T^{\rm OD}$ such a separation is not easily made. While the main effect of $v_T^{\rm OD}$ is to admix high-momentum orbitals into the wave function, this admixture is not readily treated by the separation method used for v_{12}. Therefore within the context of this approach the specifically tensor correlations must be treated on a different footing than the correlations due to the short-range part of v_{12}. Thus, leaving $v_T^{\rm OD}$ aside for the moment, write $v_{12}=v_{12}^s+v_{12}^l$ and define the separation into short- and long-range parts so that

$$(t_1+t_2+U_1+U_2+v_{12}^s)|\Psi_{kl})=(\epsilon_k+\epsilon_l)|\Psi_{kl}),$$

where

$$(t_1+U_1)|i)=\epsilon_i|i); \tag{10}$$

that is, the pair state $|\Psi_{kl}\rangle$ has no energy shift relative to the state $|kl\rangle$.[12] In some cases it is necessary to include a short-range pseudopotential to carry out this separation procedure. In that case

$$v_{12}=(v_{12}^s+VP)+(v_{12}^l-VP), \tag{11}$$

and one requires that

$$(t_1+t_2+U_1+U_2+v_{12}^s+VP)|\Psi_{kl})=(\epsilon_k+\epsilon_l)|\Psi_{kl}). \tag{12}$$

In general, therefore, one has

$$H_{\rm eff}=\sum_{ij}(i|t|j)a_i^\dagger a_j+\tfrac{1}{2}\sum_{ijkl}a_i^\dagger a_j^\dagger a_k a_l \times(\Psi_{ij}|(v_{12}^l-VP+v_T^{\rm OD})|\Psi_{kl}). \tag{13}$$

If the shell-model or Hartree-Fock calculations are limited to orbitals having only fairly low momentum components, almost all of the contribution of $v_T^{\rm OD}$ to the binding energy and to the effective interaction will be missed. Most of the contribution of $v_T^{\rm OD}$ may be taken into account by renormalizing the effective Hamiltonian in the independent-pair approximation[13]:

$$H_{\rm eff}=\sum_{ij}(i|t|j)a_i^\dagger a_j+\tfrac{1}{2}\sum_{ijkl}a_i^\dagger a_j^\dagger a_l a_k \times(\Psi_{ij}|v_{12}^l-VP+v_T^{\rm OD}+v_T^{\rm OD}(Q/e)v_T^{\rm OD}|\Psi_{kl}), \tag{14}$$

where Q is a Pauli-principle operator which projects out of the space which is treated explicitly in these calculations. The energy denominator e will be discussed in Sec. IV; however, at this point it is noted that the intermediate energies which contribute to the evaluation of $v_T^{\rm OD}(Q/e)v_T^{\rm OD}$ are quite high and therefore fairly simple approximations to the form of e and to the wave functions used for the intermediate states in the evaluation of $v_T^{\rm OD}(Q/e)v_T^{\rm OD}$ should yield fairly accurate results. If this were not the case the inclusion of the second-order terms in Eq. (14) would be exceedingly complicated at this stage. A simple parametrization of the operator Q and the energy denominator e will be used. The deviation of the simple expressions from the correct expressions should be small (for an appropriate choice of the parametrization) and may be treated via perturbation theory at the end of the calculations.

The inclusion of these second-order terms is extremely important since they contribute about -150 MeV to the potential energy of O^{16}.[3] Inclusion of these terms in Eq. (14) allows one to include their major effects at an early stage of the calculation and avoids the need for extremely large renormalizations at a later stage.

Finally, we note that Eq. (14) provides an expression for an effective Hamiltonian in an arbitrary basis. (In practice, this is the basis provided by harmonic-oscillator wave functions.) If one wishes to improve upon the choice of the orbital functions one may apply the Hartree-Fock method to $H_{\rm eff}$ of Eq. (14). Clearly, once one has introduced an *effective* Hamiltonian, the application of Hartree-Fock methods does not provide a bound on the binding energy. In the context of the effective-interaction method the use of the Hartree-Fock equations may be understood as a procedure for eliminating corrections to the ground state of the one-particle, one-hole type. Application of the Hartree-Fock method using the effective interaction derived here will be given in a subsequent publication.

III. CALCULATION OF MATRIX ELEMENTS

In this section some of the details involved in the determination of the correlated basis functions are discussed.

The harmonic-oscillator functions are specified by the usual quantum numbers n, l, j, m_j, where n is taken equal to zero for the states with no nodes.

It is useful to transform the two-particle states to the L-S representation,

$$|(l,\tfrac{1}{2})j_1(l_2,\tfrac{1}{2})j_2JM,TT_z\rangle =\sum_{\lambda,S}[(2\lambda+1)(2S+1)(2j_1+1)(2j_2+1)]^{1/2} \times\begin{Bmatrix} l_1 & l_2 & \lambda \\ \tfrac{1}{2} & \tfrac{1}{2} & S \\ j_1 & j_2 & J \end{Bmatrix}|(l_1l_2)\lambda(\tfrac{1}{2}\tfrac{1}{2})S,JM,TT_z\rangle. \tag{15}$$

[12] S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) **11**, 65 (1960).
[13] T. T. S. Kuo and G. E. Brown, Phys. Letters **18**, 54 (1965).

Further, the Moshinsky transformation is used to write

$$|n_1l_1n_2l_2,\lambda\rangle=\sum_{nlNL}\langle nlNL\lambda|n_1l_1n_2l_2\lambda\rangle|nlNL,\lambda\rangle, \quad (16)$$

where the $\langle nlNL\lambda|n_1l_1n_2l_2\lambda\rangle$ are the usual Moshinsky brackets.[11] The quantum numbers nl, NL specify the relative motion of the two particles and the motion of the center-of-mass of the pair. The angular momentum λ is the result of the coupling of l and L.

A simple recoupling procedure yields

$$|nlNL\lambda(\tfrac{1}{2}\tfrac{1}{2})S,JM\rangle = (-)^{J+S+\lambda}\sum_{J'}[(2\lambda+1)(2J+1)]^{1/2}\begin{Bmatrix} L & l & \lambda \\ S & J & J' \end{Bmatrix} \times|NL,(nl,S')J',JM\rangle. \quad (17)$$

The fundamental matrix elements of the effective interaction between antisymmetrized, normalized states is (neglecting the second-order terms)

$$\langle(l_1\tfrac{1}{2})j_1(l_2\tfrac{1}{2})j_2JMTT_z|V_{\text{eff}}|(l_3\tfrac{1}{2})j_3(l_4\tfrac{1}{2})j_4JMTT_z\rangle$$
$$=\frac{1}{(1+\delta_{n_1n_2}\delta_{l_1l_2}\delta_{j_1j_2})^{1/2}}\frac{1}{(1+\delta_{n_3n_4}\delta_{l_3l_4}\delta_{j_3j_4})^{1/2}}\sum_{\lambda,\lambda',J',n,n',l',l,N,L}(-)^{\lambda+\lambda'}(2J'+1)(2\lambda+1)(2\lambda'+1)(2S+1)$$
$$\times[(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)]^{1/2}\langle n_1l_1n_2l_2\lambda|nlNL\lambda\rangle\langle n_3l_3n_4l_4\lambda'|n'l'NL\lambda'\rangle$$
$$\times\begin{Bmatrix} l_1 & l_2 & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_1 & j_2 & J \end{Bmatrix}\begin{Bmatrix} l_3 & l_4 & \lambda' \\ \frac{1}{2} & \frac{1}{2} & S \\ j_3 & j_4 & J \end{Bmatrix}\begin{Bmatrix} L & l' & \lambda' \\ S & J & J' \end{Bmatrix}\begin{Bmatrix} L & l & \lambda \\ S & J & J' \end{Bmatrix}[1-(-)^{l+S+T}]\langle(nl,S)J'|V_{\text{eff}}|(n'l',S)J'\rangle, \quad (18)$$

where the curly braces represent the usual 6-j and 9-j symbols, and

$$V_{\text{eff}}=e^{-iS}(t_1+t_2+U_1+U_2+v_{12}+v_T{}^{\text{OD}})e^{iS} -(t_1+t_2+U_1+U_2). \quad (19)$$

The operator e^{iS} is taken to act only on the wave functions of relative motion, i.e.,

$$e^{iS}|(nl,S)J\rangle=|(nl,S)J\rangle_c, \quad (20)$$

where the subscript c indicates a correlated wave. Only that part of $(t_1+t_2+U_1+U_2)$ that depends on the coordinates of the relative motion need be kept; thus, using the Moshinsky transformation,

$$\mathbf{r}=(\mathbf{r}_1-\mathbf{r}_2)/\sqrt{2}, \qquad \mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/\sqrt{2}, \quad (21)$$

one may write

$$(t_1+t_2+U_1+U_2)=(t_r+t_R+U(\mathbf{r})+U(\mathbf{R})), \quad (22)$$

where

$$U(\mathbf{r})=\tfrac{1}{2}kr^2, \quad U(\mathbf{R})=\tfrac{1}{2}kR^2, \quad \text{etc.}$$

Thus

$$\langle(nl,S)J'|V_{\text{eff}}|(n'l',S)J'\rangle = {}_c\langle(nl,S)J'|t_r+U(\mathbf{r})+v_{12}+v_T{}^{\text{OD}}|(n'l',S)J'\rangle_c -\langle(nl,S)J'|t_r+U(\mathbf{r})|(n'l',S)J'\rangle. \quad (23)$$

Again one puts

$$v_{12}=(v_{12}{}^s+VP)+(v_{12}{}^l-VP) \quad (24)$$

and writes

$$\langle(nl,S)J'|V_{\text{eff}}|(n'l',S)J'\rangle = {}_c\langle(nl,S)J'|(v_{12}{}^l-VP)|(n'l,S)J'\rangle_c\delta_{l,l'} +{}_c\langle(nl,1)J'|v_T{}^{\text{OD}}|(nl',1)J'\rangle_c\delta_{l,l'\pm2} +{}_c\langle(nl,S)J'|(t_r+U(\mathbf{r})+v_{12}{}^s+VP)|(nl,S)J'\rangle_c -\langle(nl,S)J'|(t_r+U(\mathbf{r}))|(nl,S)J'\rangle. \quad (25)$$

Now one has

$$[t_r+U(\mathbf{r})]|(nl,S)J'\rangle=\hbar\omega(2n+l+\tfrac{3}{2})|(nl,S)J'\rangle \quad (26)$$

and requires $(v_{12}{}^s+VP)$ to be defined such that

$$(t_r+U(\mathbf{r})+v_{12}{}^s+VP]|(nl,S)J'\rangle_c =\hbar\omega(2n+l+\tfrac{3}{2})|(nl,S)J'\rangle_c. \quad (27)$$

With these definitions the last two terms in Eq. (25) cancel so that, to first order in $v_T{}^{\text{OD}}$,

$$\langle(nl,S)J'|V_{\text{eff}}|(n'l',S)J'\rangle = {}_c\langle(nl,S)J'|(v_{12}{}^l-VP)|(n'l,S)J'\rangle_c\delta_{l,l'} +{}_c\langle(nl,1)J'|v_T{}^{\text{OD}}|(nl',1)J'\rangle_c\delta_{l,l'\pm2}. \quad (28)$$

To avoid confusion, it is noted that the division of v_{12} into $v_{12}{}^s+v_{12}{}^l$ and the possible addition of a pseudopotential term presents a different problem for each set of the quantum numbers of relative motion, l, S, J'. (The value of the isobaric spin T is specified once l and S are given.)

While the effective interaction of Eq. (19) is Hermitian the introduction of the pseudopotential VP leads to a non-Hermitian effective interaction. This is due to the fact that if one requires the healing distance to be the same for all n in Eq. (27) it is found that VP depends

TABLE I. Healing distances and pseudopotentials for the $^1S_0$ state of the Yale potential. $b=(\hbar/M\omega)^{1/2}$.

n \ b	Pseudopotential (MeV) 1.50	1.76	2.09	2.17	2.40
0	−5.0	0.0	0.0	0.0	0.0
1	−26.3	−16.3	−10.0	−7.5	−5.0
2	−53.8	−33.8	−20.0	−17.5	−13.7
3	−86.3	−53.8	−32.5	−27.5	−20.0
4	−126.0	−75.0	−45.0	−40.0	−31.2
5	−181.0	−103.7	−61.25	−53.8	−41.3
6	−255.0	−135.0	−76.56	−68.8	−50.0
Healing distance (F)	1.09	1.09	1.09	1.09	1.09

on n. In particular, as n is increased, VP must be made more attractive to maintain a healing of the correlated state at a fixed distance from the core. In the evaluation of the first term on the right of Eq. (28) there is therefore the question of which pseudopotential to use. In practice an average of the pseudopotential appropriate to the state with n' nodes and the state with n nodes has been used in evaluating the off-diagonal terms in Eq. (28). This problem of the non-Hermitian character of the effective interaction also arises if one does not introduce a pseudopotential to obtain healing. In the latter case the effective interaction becomes non-Hermitian due to the dependence of the separation distance on the quantum number n.

The following suggestion for overcoming this difficulty is proposed: One may choose some maximum value for n and determine a set of n correlated functions as defined by Eq. (27). These functions may then be orthonormalized by a standard procedure. The operator e^{iS} may then be defined as in Eq. (20) except that the correlated wave indicated in Eq. (20) would be a member of an orthonormal set. With this definition of e^{iS}, the evaluation of the matrix elements of V_{eff} given by Eq. (19) would lead to a Hermitian effective interaction. [Since the correlated states would now be linear combinations of the states defined by Eq. (27), the latter equation would be useful in the evaluation of the matrix elements of V_{eff}.] This suggestion for obtaining a Hermitian effective interaction has not been applied in this work where the calculational procedure has been limited to using the average value of VP in evaluating the matrix elements appearing in Eq. (28).

TABLE II. Pseudopotentials for central $^3S_1$ Yale potential. Healing distance=1.13 F.

n \ b	VP (MeV) 1.50	1.76	2.09	2.17	2.40
0	−95	−90	−85	−85	−85
1	−115	−105	−95	−95	−90
2	−145	−120	−110	−105	−100
3	−180	−146	−120	−115	−110
4	−225	−170	−135	−130	−120
5	−290	−200	−150	−145	−130
6	−372	−235	−170	−160	−140

TABLE III. P- and D-state pseudopotentials and healing distances for the Yale potential.

State	VP (MeV)	Healing distances (F) ($n=0$, $b=1.76$ F)
$^1P_1$	−687.0	0.99
$^3P_0$	−254.0	0.99
$^3P_1$	−262.0	0.99
$^3P_2$	0.0	0.87
$^3D_1$	−50.0	0.80
$^3D_2$	−200.0	0.96
$^3D_3$	−200.0	0.98
$^1D_2$	0.0	0.94

The method outlined above has been used in connection with the Yale potential.[8] The pseudopotential was taken to be a square well extending from the edge of the core out to about 1 F. For the $^1S_0$ states, the state with $n=0$ was usually allowed to "heal" without the introduction of a pseudopotential. For the states with $n>0$ a pseudopotential was found that gave healing at the healing distance of the $n=0$ state. The pseudopotentials used are given in Table I for various values of n and of b, the oscillator size parameter $[b=(h/M\omega)^{1/2}]$. The healing distances obtained are also given in Table I. In Fig. 1 is shown the correlated wave function and the uncorrelated wave function calculated for the $^1S_0$ Yale potential with $b=1.76$ F and $n=0$.

The $^3S_1$ central potential was forced to heal at 1.13 F by the introduction of pseudopotentials. The pseudopotentials used are given in Table II. Unlike the $^1S_0$ case, a pseudopotential was needed to heal the $n=0$ wave. The coupling of the $^3D_1$ state to the $^3S_1$ state via the tensor force is discussed in Sec. IV, where a perturbative method is described.

For the P and D states of the Yale potential the variation of VP with the number of nodes was found to be unimportant. In Table III are listed the pseudopotentials and healing distances for these states. The healing distances are given for $n=0$, $b=1.76$ F, but the variation with n and b of this quantity is quite small.

In the next section the important second-order terms due to the tensor force are discussed, and also the question of the convergence of the perturbation $(v_{12}{}^l-VP)$ is considered by evaluating second-order corrections in this quantity. While it may be shown that the second-order terms in $v_{12}{}^l$ are quite small, some of the pseudopotentials introduced are large and can contribute significantly in second order.

IV. THE TREATMENT OF THE SECOND-ORDER TERMS

In the previous discussion it was shown how one may introduce correlated wave functions which deviate from the harmonic-oscillator wave functions over only a small region. Thus far, however, only central correlations have

been introduced. It is known from nuclear-matter calculations that while the second-order terms in the perturbation expansion for the energy are small for central forces, they are quite large for the tensor force.

In Eq. (9) a separation was made of the two-body force into those parts that were diagonal in the orbital angular momentum of the relative motion and a part which was nondiagonal in that quantity. The important second-order terms will arise from the latter part. This effect may be understood by noting that if the relative motion of a pair of particles in a $^3S_1$ state is considered and some admixture of a $^3D_1$ wave is allowed in their *relative* wave function, there will be a significant gain in energy due to the large tensor force which acts between these states.

The treatment of the second-order terms given below is somewhat lacking in precision and is therefore not completely satisfactory. However, the results obtained yield reasonable agreement between theory and experiment for various quantities and also provide important insight into the role of the tensor interaction in nuclei. The various treatments of this problem—those due to MacKellar,[14] Kuo and Brown,[13] and others,[15] and the one presented here—are in basic agreement as to the over-all size of the $^3S_1$ matrix elements. This general agreement is encouraging. None of the calculational procedures is free from criticism and it will be of interest to understand which is most accurate.

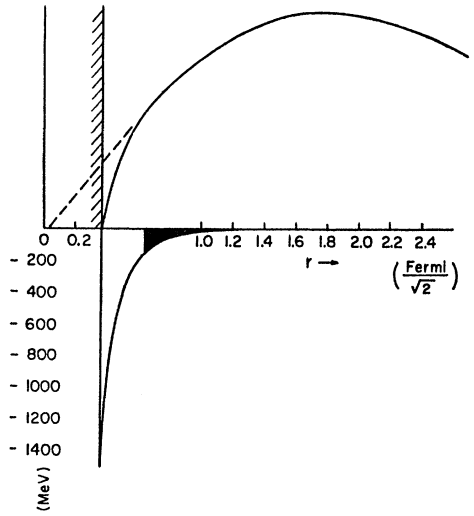
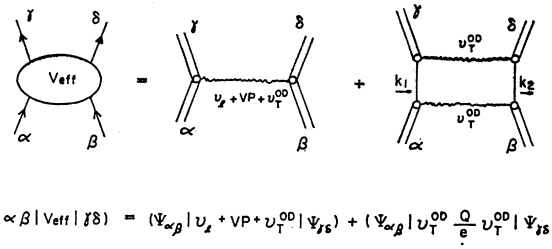


FIG. 1. Correlated and uncorrelated wave function (dashed line) for the $^1S_0$-Yale potential. Here, $b=1.76$ F and $n=0$. The $^1S_0$ potential is shown and the vertical scale indicates its strength. The horizontal scale is in Moshinsky units which may be converted to fermis by multiplying by $\sqrt{2}$. The shaded portion of the potential is the "long-range" part as determined by the separation procedure.



$$(\alpha\beta\,|\,V_{\rm eff}\,|\,\gamma\delta) = (\Psi_{\alpha\beta}\,|\,v_t + VP + v_T^{\rm OD}\,|\,\Psi_{\gamma\delta}) + (\Psi_{\alpha\beta}\,|\,v_T^{\rm OD}\,\frac{Q}{e}\,v_T^{\rm OD}\,|\,\Psi_{\gamma\delta})$$

FIG. 2. Schematic representation of the effective interaction used in this work. Double lines are meant to indicate the use of correlated pair states. Plane-wave states are used for the intermediate states in the second-order terms.

The approximation used in this work for the effective interaction may be specified diagrammatically. In Fig. 2 a double line is used to indicate that correlated *pair* states have been introduced (which have central correlations only). In the basis of correlated states (v^l-VP) is taken to first order and $v_T{}^{\rm OD}$ to first and second order. Some discussion of the second-order terms in (v^l-VP) will be given at the end of this section and in a following work where their contribution to the binding energy will be estimated. The second-order terms in $v_T{}^{\rm OD}$ have been extensively calculated only for the $^3S_1$ state of relative motion. For the treatment of the intermediate states the same approximation is used as Kuo and Brown[13] for their discussion of this problem—plane-wave intermediate states and an angle averaged operator to take account of the Pauli principle in the intermediate states. However, unlike these authors, there is no attempt to make a division of the tensor force into a short- and a long-range part. Since the correlated basis functions have been introduced, one is able to calculate the matrix elements of $v_T{}^{\rm OD}$ in that basis. It still seems to be an open question as to whether there exists a useful separation method dividing the tensor force into short- and long-range parts.

The calculation of the second-order terms in the $^3S_1$ state is carried through as follows. One evaluates

$$M_{nl,n'l'}{}^{NL} = \langle NL,(\tilde{n}l,S)JM\,|\,v_T{}^{\rm OD}\frac{Q}{e}v_T{}^{\rm OD}\,|\,NL,(\tilde{n}'l,S)JM\rangle, \quad (29)$$

with $l=0$, $S=1$, $J=1$. The notation $\tilde{n}'l$ and $\tilde{n}l$ refers to the use of correlated states of relative motion. With Kuo and Brown,[13] intermediate plane-wave states of momenta $\mathbf{k}_1$ and $\mathbf{k}_2$ are introduced. The transformation

$$\mathbf{k}=(\mathbf{k}_1-\mathbf{k}_2)/2, \qquad \mathbf{K}=(\mathbf{k}_1+\mathbf{k}_2) \quad (30)$$

[14] A. D. MacKellar, Ph.D. thesis, Texas A & M University, 1966 (unpublished); A. D. MacKellar and R. L. Becker, Phys. Letters 18, 308 (1965).

[15] A. Kallio, Ann. Acad. Sci. Fennicae, Ser. A, No. 163 (1964); A. Kallio and K. Kolltviet, Nucl. Phys. 53, 87 (1964); 59, 211 (1964); J. F. Dawson, I. Talmi, and J. D. Walecka, Ann. Phys. (N. Y.) 18, 339 (1962); J. F. Dawson and J. D. Walecka, *ibid.* 22, 133 (1963); R. K. Bhaduri and E. L. Tomusiak (unpublished); T. T. S. Kuo and G. E. Brown (unpublished); Y. E. Kim (unpublished).

is made and the operator Q is specified as

$$Q(k,K,k_F)=0 \quad \text{for} \quad k^2+K^2/4<k_F^2,$$
$$=1 \quad \text{for} \quad k-K/2>k_F,$$
$$=(k^2+K^2/4-k_F^2)/kK \text{ otherwise.} \quad (31)$$

Further, one writes

$$e=\frac{\hbar^2}{2m}(k_1^2+k_2^2)+\Delta=\frac{\hbar^2}{m}(k^2+\tfrac{1}{4}K^2)+\Delta, \quad (32)$$

where Δ is a measure of the binding of the interacting pair in the nucleus.[13]

Some rather straightforward angular-momentum algebra yields

$$M_{nl,n'l}{}^{NL}=\frac{4}{\pi^2}\int K^2dK\int k^2dk\frac{Q(k,K,k_F)}{e(k,K,\Delta)}$$
$$\times|\langle(l,1)J|S_{12}|(l+2,1)J\rangle|^2$$
$$\times F_{NL}{}^2(K)I_{nl}(k)I_{n'l}(k), \quad (33)$$

with

$$F_{NL}(K)=\int_0^\infty j_L\left(\frac{KR}{\sqrt{2}}\right)\varphi_{NL}(R)R^2dR,$$

$$I_{nl}(k)=\int_0^\infty j_l(\sqrt{2}kr)V_T(r)\tilde{\varphi}_{nl}(r)r^2dr,$$

$$\langle(l,1)J|S_{12}|(l+2,1)J\rangle=\frac{6[J(J+1)]^{1/2}}{2J+1}.$$

The tensor interaction is denoted as $V_T(r)S_{12}$ with the usual definition of S_{12}. [This S_{12} should not be confused with the S_{12} of Eq. (4).] Further, $\tilde{\phi}_{nl}(r)$ is a correlated state of relative motion, j_l is a spherical Bessel function, $\phi_{NL}(R)$ is a harmonic-oscillator function, and R and r are Moshinsky coordinates for the center-of-mass and relative motions, respectively. For the $^3S_1$ state one has $\langle(0,1)1|S_{12}|(2,1)1\rangle=2\sqrt{2}$, so that

$$M_{n0,n'0}{}^{NL}=\int_0^\infty f(k)dk, \quad (34)$$

with

$$f(k)=\frac{32}{\pi^2}k^2\int K^2dK\frac{Q(k,K,k_F)}{e(k,K,\Delta)}$$
$$\times F_{NL}{}^2(K)I_{n0}(k)I_{n'0}(k). \quad (35)$$

In Fig. 3 is plotted the function $f(k)$ for the case $b=1.50$ F, $\Delta=20$ MeV, $n=l=N=L=0$, and $k_F=1.4$ F^{-1}. The upper limit on the K integral was taken as $2k_F$. As pointed out by Kuo and Brown, the values of k contributing to the integration in Eq. (34) are quite large. This result implies that the uncertainty in the specification of Δ appearing in Eq. (32) is not a serious source of error. In the present calculations $\Delta=20$ MeV has been used. This value is reasonable for the least tightly bound orbitals where one usually applies shell theory. The error made in using the same Δ for the more tightly bound orbitals is not large. One may consider the specification of k_F and Δ to provide a parametrization of the second-order terms. At some later stage of this work it is possible to estimate the errors introduced via this simple parametrization (see Appendix B).

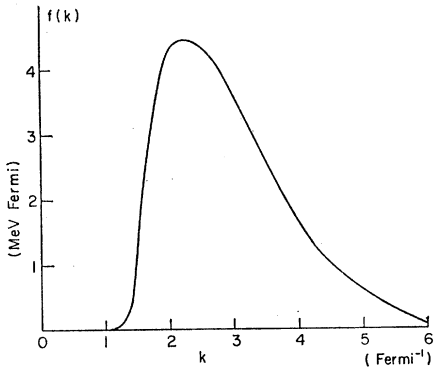


FIG. 3. The function $f(k)$ [Eq. (35)] plotted as a function of k for the case $b=1.50$ F, $\Delta=20$ MeV, $k_F=1.4$ F^{-1}, and $n=l=N=L=0$.

A sample of some first- and second-order matrix elements for the Yale potential is given in Table IV. The size of the second-order tensor terms does not imply nonconvergence, as might appear, since the study of Dahlblom *et al.*[16] shows that the second-order contribution of the tensor force is anomalously large. They estimate the third order to be less than 20% of the second, and the fourth order to be smaller. The convergence in the quantity $(v_{12}{}^l-VP)$ is estimated by calculating the second-order terms in a manner quite analogous to the second-order tensor calculation. The results are given in Table IV, where it may be seen that in most cases the convergence is reasonably good. It is possible that the use of plane-wave intermediate states overestimates the size of these terms somewhat. It was also found that small variations of the healing distance; i.e., equivalently, the use of different pseudopotentials in the various states did not change the sum of the first- and second-order terms appreciably.

Studies have also been made of the dependence of the second-order tensor matrix elements on the choice on k_F and Δ and on the values of N and L, the center-of-mass quantum numbers. At $b=1.76$ F ($\Delta=20$ MeV) increasing k_F to 1.50 F^{-1} decreases the second-order tensor elements by about 0.3 MeV, while decreasing k_F to 1.30 F^{-1} increases that element by about 0.3 MeV. (This represents about a 4% change in the matrix element.) Also at $b=1.76$ F, $k=1.4$ F^{-1}, an increase of Δ by about 20 MeV yields about a 5% decrease in the second-order matrix element. For a Δ appropriate to the more deeply

[16] T. Dahlblom, K.-G. Fögel, B. Quist, and A. Törn, Nucl. Phys. **56**, 177 (1964).

TABLE IV. First- and second-order matrix elements for the Yale potential. Pseudopotentials and healing distances as in Tables I–III. ($b=1.76$ F.)

State	nl	NL	First order (V_l-VP)	Second order $V_T^{OD}(Q/e)V_T^{OD}$	Second order $(V_l-VP)(Q/e)(V_l-VP)$
$^3S_1$	00	00	0.631	−8.59	−0.61
$^3S_1$	10	00	3.19	−9.59	−0.95
$^1S_0$	00	00	−5.96	···	−0.14
$^1S_0$	10	00	−3.91	···	−0.14
$^1P_1$	01	00	2.49	···	−1.39
$^3P_0$	01	00	−2.17	···	−0.23
$^3P_1$	01	00	2.62	···	−0.33
$^3P_2$	01	00	−0.84	···	···
$^1D_2$	02	00	−0.58	···	···
$^3D_1$	02	00	1.09	···	···
$^3D_2$	02	00	−2.01	···	···
$^3D_3$	02	00	0.06	···	···

bound orbits ($\Delta\sim 80$ MeV) the second-order tensor matrix elements are decreased by about 15%. Further, it is found that the neglect of the dependence of the second-order terms on the variable N and L leads to about a 10% uncertainty in the value of these terms. To keep the calculation within bounds, the second-order terms were extensively evaluated for $N=0$, $L=0$, $k_F=1.4$ F^{-1}, $\Delta=20$ MeV only. Tables of the effective-interaction matrix elements for these parameters will be presented in a subsequent paper for several values of b.

V. DISCUSSION

In this work an attempt has been made to investigate the usefulness of the unitary-model-operator approach for the discussion of the effective interaction in nuclei. The importance of the second-order tensor terms has been stressed and some questions of convergence have been discussed. The use of the pseudopotentials to produce healing of the correlated states appears as a useful procedure which is reasonably convergent. The treatment of the second-order tensor terms is reasonably simple and yields results in good agreement with other approximations. Generally, the methods presented provide a reasonable approximation for calculating the effective-interaction matrix elements in finite nuclei. In a subsequent paper extensive tables of matrix elements calculated by the procedure outlined here will be presented as well as the results of Hartree-Fock calculations based on the effective Hamiltonian which has been constructed in this work.

ACKNOWLEDGMENTS

The authors would like to thank Professor F. Villars, Professor A. K. Kerman, and Professor S. A. Moszkowski for discussions and suggestions.

APPENDIX A

Recently, Bethe and Moszkowski have discussed the contribution of higher clusters in the Brueckner-Bethe-Goldstone theory of nuclear matter.[17,18] Bethe has pointed out that in order to obtain reasonable convergence in that theory one must consider an expansion of the energy in terms of the density, the relevant parameter being the correlation volume divided by the average volume per particle. In practice this means that one must consider the entire class of diagrams which have three hole lines if one wishes to discuss the question of three-body clusters. Moszkowski has suggested that the consideration of Jastrow-like correlations are appropriate for the discussion of the size of the three-body clusters and that the contribution from these terms is quite small.

It is possible to make some comparisons of the approach of this paper to the method of correlated basis functions based on the Jastrow idea. A more general version of the Jastrow correlation method is presented by using the method of second quantization. (A recent discussion of Jastrow-type wave functions is given in Ref. 9.)

A correlation factor of the Jastrow type may be written as

$$F=\prod_{ij}(1+f_{ij}), \tag{A1}$$

where f_{ij} is a function of the distance between particles i and j; more generally, one can allow f_{ij} to be a general two-body operator which acts upon the wave functions of particles i and j. If the operator F is a many-body operator, it is useful to write

$$F=1+\sum_{n=2}^{N}F^{(n)}, \tag{A2}$$

where $F^{(n)}$ is an n-body operator and N is the number of particles in the system. It may readily be demonstrated that

$$F^{(2)}=\frac{1}{2!}\sum a_\alpha^\dagger a_\beta^\dagger(\alpha\beta|f_{12}|\gamma\delta)a_\delta a_\gamma, \tag{A3}$$

$$F^{(3)}=\frac{1}{3!}\sum a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger(\alpha\beta\gamma|f_{12}f_{13}+f_{13}f_{23}+f_{12}f_{23}+f_{12}f_{23}f_{13}|\rho\eta\phi)a_\phi a_\eta a_\rho, \tag{A4}$$

etc.

Consider the expectation value of an operator between wave functions of the Jastrow type. For example, if one is interested in the expectation value of the Hamiltonian it is useful to consider a cluster expansion:

$$\tilde{H}=F^\dagger HF=\tilde{H}^{(1)}+\tilde{H}^{(2)}+\tilde{H}^{(3)}+\cdots, \tag{A5}$$

where $\tilde{H}^{(n)}$ is the n-body part of $\tilde{H}$. One finds

$$\tilde{H}^{(1)}=T=\sum a_\alpha^\dagger a_\beta(\alpha|t|\beta), \tag{A6}$$

$$\tilde{H}^{(2)}=\tfrac{1}{2}\sum a_\alpha^\dagger a_\beta^\dagger(\alpha\beta|(1+f_{12}^\dagger)(t_1+t_2+v_{12})\times(1+f_{12})-(t_1+t_2)|\gamma\delta)a_\delta a_\gamma, \tag{A7}$$

and if one considers the term in $H^{(3)}$ arising from the

[17] H. A. Bethe, Compt. Rend. Congr. Internat. Phys. Nucl., Paris (1964) 1, 101 (1965); H. A. Bethe, Phys. Rev. 138, 804 (1965).
[18] S. A. Moszkowski, Phys. Rev. 140, 283 (1965).

potential energy there results

$$\tilde{V}^{(3)}=\frac{1}{3!}\sum a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger(\alpha\beta\gamma|\,(1+f_{12}^\dagger)(1+f_{13}^\dagger)(1+f_{23}^\dagger)$$
$$\times(v_{12}+v_{23}+v_{13})(1+f_{12})(1+f_{23})(1+f_{13})$$
$$-(1+f_{12}^\dagger)v_{12}(1+f_{12})-(1+f_{13}^\dagger)v_{13}(1+f_{13})$$
$$-(1+f_{23}^\dagger)v_{23}(1+f_{23})|\rho\eta\varphi)a_\varphi a_\eta a_\rho. \quad \text{(A8)}$$

The Jastrow form has some advantage in that one can in principle calculate all the higher cluster terms; however, the calculation of matrix elements of various operators, and the normalization of the states becomes very complicated largely because the basis loses the property of orthonormality on the application of the correlation operator F. In the present calculation, therefore, a unitary-model operator e^{iS} has been employed. The price for this is that one cannot be as explicit in the calculation of the higher-order terms in the cluster expansion. This is due to the fact that the behavior of e^{iS} in the space of three-body wave functions is difficult to specify although one may attempt some simple approximations. To the extent that $e^{iS_{12}}\varphi(r_{12})\approx(1+f_{12})\varphi(r_{12})$ for some uncorrelated state $\varphi(r_{12})$, there is a reasonably close analogy between the two approaches. (It must be remembered, however, that the approach taken here in determining the short-range correlation structure is nonvariational.)

For example, in the unitary-model-operator approach the correlation correction to the potential energy appears as

$$V^{(3)}=\frac{1}{3!}\sum a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger(\alpha\beta\gamma|\,e^{-i(S_{12}+S_{23}+S_{13})}(v_{12}+v_{23}+v_{13})$$
$$\times e^{i(S_{12}+S_{23}+S_{13})}-e^{-iS_{12}}v_{12}e^{iS_{12}}-e^{-iS_{23}}v_{23}e^{iS_{23}}$$
$$-e^{-iS_{13}}v_{13}e^{iS_{13}}|\rho\eta\varphi)a_\varphi a_\eta a_\rho. \quad \text{(A9)}$$

If it is assumed that to a reasonable approximation

$$e^{i(S_{12}+S_{23}+S_{13})}\approx(1+f_{12})(1+f_{23})(1+f_{13}),$$
$$e^{iS_{12}}\approx(1+f_{12}), \quad \text{(A10)}$$

etc., it can explicitly be shown that the three-body terms are small with the exception of those terms which may be understood as giving rise to dispersive corrections in the two-body matrix elements.[1] For example, consider the contribution of the v_{13} term in (A8). Assume that particles 2 and 3 are not close together so that $f_{23}\approx 0$. Then there remains a term of the form

$$(1+f_{12}^\dagger)(1+f_{13}^\dagger)v_{13}(1+f_{13})(1+f_{12})$$
$$-(1+f_{13}^\dagger)v_{13}(1+f_{13}) \quad \text{(A11)}$$

in Eq. (A8). Defining a

$$v_{13}^{\text{eff}}=(1+f_{13}^\dagger)v_{13}(1+f_{13}),$$

one obtains from (A11)

$$(1+f_{12}^\dagger)v_{13}^{\text{eff}}(1+f_{12})-v_{13}^{\text{eff}}.$$

Terms of this type give rise to dispersive effects[1] on the motion of particles 1 and 2. (Since one is only using central correlations in our cluster expansion the dispersive effects of the tensor force are not apparent in this approach.)

In the present work, harmonic-oscillator potentials have been used to represent the dispersive effects of the medium [Eq. (5)]. The actual importance of the dispersive effects in nuclear matter depends strongly on the size and nature of the core.[12,19] It is possible that the use of soft-core potentials will give matrix elements quite similar to those obtained in this work and having, at the same time, very small dispersion corrections.[20]

APPENDIX B

In this Appendix the advantages of the present treatment of the second-order terms in allowing the achievement of a more rapid convergence for the energy of the system than would be possible otherwise are indicated.

Assume that one applies the Hartree-Fock method to the effective Hamiltonian of Eq. (13). In this way one would obtain a set of single-particle orbitals and an estimate of the binding energy of the system. The next step would involve the calculation of the corrections in second order, the most important of which would involve $v_T^{\text{OD}}(Q_{\text{HF}}/e_{\text{HF}})v_T^{\text{OD}}$, where Q_{HF} would be a projection operator which would eliminate the occupied Hartree-Fock states as intermediate states, and e_{HF} would refer to the difference in Hartree-Fock energies for the intermediate states and the occupied states. As mentioned previously, this would be a very large correction.

Now if one applies the Hartree-Fock procedure to the Hamiltonian of Eq. (14) one could again estimate the magnitude of the correction terms. As before, the most important would be $v_T^{\text{OD}}(Q_{\text{HF}}/e_{\text{HF}})v_T^{\text{OD}}$; however, a term $v_T^{\text{OD}}(Q(k,K,k_F)/e(k,K,\Delta))v_T^{\text{OD}}$ has been added to the interaction. Thus the correction to the calculation would involve the *difference* between the second-order term and the term which is added, i.e.,

$$v_T^{\text{OD}}\left[\frac{Q_{\text{HF}}}{e_{\text{HF}}}-\frac{Q(k,K,k_F)}{e(k,K,\Delta)}\right]v_T^{\text{OD}}. \quad \text{(B1)}$$

With a good choice for k_F and Δ the correction to the Hartree-Fock calculation for the binding energy from these second-order terms may be about 1 MeV per particle rather than about 8 MeV per particle.

[19] H. S. Köhler and Y. R. Waghmare, Nucl. Phys. **66**, 261 (1965).
[20] S. A. Moszkowski (private communication).