

Nonsymmetric nonlocal potentials and Hartree-Fock scattering formalisms

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(Received 15 November 1976)

Scattering formalisms that take antisymmetrization into account may result in nonsymmetric nonlocal potentials for the effective interaction. Furthermore, when the incident particle state is antisymmetrized with respect to single-particle states of the target, these states appear as redundant states in the scattering spectrum. This requires the Fredholm determinant associated with the kernel of the integral equation for the physical wave function to be zero for all wave numbers of the incident particle. Under these circumstances, a scattering solution may not exist. The conditions for existence are examined, and a consistency condition is established. Evidence is presented that the nonlocal potential in the full Hartree-Fock equation including target excitations is not symmetric, and thus that the equation will not exhibit a scattering solution unless certain consistency requirements are met in its construction. Since the scattering solution must be orthogonal to each of the single-particle states of the target, the standard procedure in Hartree-Fock scattering formalisms is to drop all terms in the potential which project onto these states. This results in the reduced Hartree-Fock equation usually considered. It is demonstrated that constructing the reduced equation without reference to the full equation may result in a failure of the solution of the reduced equation to meet the consistency condition required for it to be a solution of the full equation.

[NUCLEAR REACTIONS Antisymmetrization, scattering by a nonlocal potential,]
[nonsymmetric nonlocal potentials, Hartree-Fock scattering, redundant states.]

I. INTRODUCTION

This paper examines procedures discussed in the literature for obtaining single-particle wave functions which describe the scattering of a particle from an A -particle target. In particular, we consider the consequences of antisymmetrization of the incident particle with respect to particles identical to it in the scattering center, and the effects of antisymmetrization on the single-particle scattering wave function.

As has been demonstrated by Feshbach,^{1,2} the effective single-particle potential which acts on a nucleon incident upon an A -particle nucleus is nonlocal due to exchange effects and to the possibility of excitation of the target nucleus. Excitation of the target as incorporated into the effective single-particle potential is usually spoken of in the literature as target polarization. In the formalism of Feshbach it is more natural to discuss excitation of the target nucleus in terms of the prompt and time-delayed physical process which take place.² Exclusion of the effects of excitation of the target nucleus is often referred to as the no-polarization approximation. This approximation is discussed in detail in Refs. 3–5.

Based upon Feshbach's results, we have previously examined some of the consequences of antisymmetrization as they relate to the scattering process.⁶ The derivation presented in Ref. 6 is restricted to energies below the inelastic threshold,

but formally takes into account all target excitation and antisymmetrization effects. It is important to note that, below the inelastic threshold, the effective potential is real.⁷

An important example of a nonlocal potential incorporating antisymmetrization, which has been widely used in the literature in scattering investigations, is the Hartree-Fock potential. In addition to introducing antisymmetrization in terms of an $(A+1)$ -particle Slater determinant of the incident particle and ground state target wave function, the Hartree-Fock potential usually neglects target excitation. However, the results obtained here point out the importance of considering excitation of the target nucleus as an essential feature of the effective potential. The designation Hartree-Fock will be used in this paper to refer to the more generalized potential obtained when neglecting dynamical correlations (as opposed to Pauli correlations) but including the effects of target excitation. Indeed, much of the discussion will center on the necessity of this more complete potential.

One of the basic tenets of all Hartree-Fock scattering formalisms is that once the Hartree-Fock equation has been established there exists a scattering solution to this equation. Furthermore, since the desired scattering solution must be orthogonal to each of the single-particle states of the target nucleus, the standard procedure is to drop all terms in the potential which project onto these states and thus give zero when operating on the

scattering solution. One can then easily demonstrate that the scattering solution of the Schrödinger equation with this "reduced" potential exists, satisfies the full Hartree-Fock equation, and is automatically orthogonal to the wave functions of the occupied states.⁸

The purpose of this paper is to present evidence that the full Hartree-Fock equation will not, in general, exhibit a scattering solution unless certain specific requirements are met in its construction. These can be expressed in terms of a consistency condition which will be satisfied only if effects of target excitation have been properly incorporated. Once this constraint has been met, the assertions in the preceding paragraph follow. That is, a scattering solution to the full Hartree-Fock equation exists which is orthogonal to the wave functions of the occupied states, and this scattering solution is the unique solution of the reduced equation.

An immediate consequence of expressing antisymmetrization of the incident particle state with respect to A single-particle states $|\xi_i\rangle$ of the target is the existence of the states $|\xi_i\rangle$ as redundant states^{9,10} in the spectrum of solutions of the single-particle scattering equation. It is this feature of the Hartree-Fock formulation of the scattering problem which leads to the necessity of a consistency requirement in constructing the Hartree-Fock equations. When the Hartree-Fock integro-differential scattering equation is expressed as an integral equation for the physical solution $|\Psi^+\rangle$, the redundant states $|\xi_i\rangle$ are the solutions of the associated homogeneous integral equation. Once the presence of redundant solutions has been formulated in this way, the conditions which must be met in order that the inhomogeneous integral equation possess a scattering solution $|\Psi^+\rangle$ are specified by the Fredholm theory of integral equations with compact kernels.¹¹ The full Hartree-Fock equation must satisfy these conditions in order that a scattering solution to this equation exist.

For any symmetric nonlocal potential the question of the existence of a scattering solution has been settled. It is proved in Ref. 12 that the inhomogeneous integral equation for scattering with a symmetric, nonlocal potential always has a scattering solution $|\Psi^+\rangle$ even when the associated homogeneous integral equation has solutions. On the other hand, as will be demonstrated in Sec. III, when the nonlocal potential is nonsymmetric and the associated homogeneous integral equation has a solution, the inhomogeneous equation can be expected to exhibit a scattering solution only when certain special requirements have been met.

Formalisms that take antisymmetrization into

account in the derivation of an effective interaction may result in nonsymmetric nonlocal potentials. This is exemplified by the post-prior paradox which occurs in the description of Bates, Fundamitsky, and Massey.¹³ The question has been further investigated by Schenter and Thaler,¹⁴ with specific reference to the Hartree-Fock nonpolarization approximation as a special case. It has been demonstrated in Ref. 6 that this lack of symmetry exists even when target excitations are taken into account when constructing the single-particle equation. Thus, before a solution of the Hartree-Fock scattering equation is undertaken it is necessary to investigate specifically the existence of a scattering solution to that equation.

It is important to note that Hartree-Fock calculations reported in the literature do not use the full Hartree-Fock equation, but rather the reduced equation referred to earlier. Since the reduced Hartree-Fock equation will not exhibit redundant solutions, this equation will always have a scattering solution. However, unless the consistency condition for a scattering solution of the full equation has been met, the reduced equation may not be appropriate for the original physical problem. This can lead to errors in the calculation and interpretation of results, as will be demonstrated in Sec. VI in terms of examples. Furthermore, it will be shown that information about the effects of target excitation arises directly from application of the necessary consistency condition.

The conclusions of this paper depend upon the expressions for the effective potential derived in Ref. 6. These expressions will be summarized in Sec. IV. Sections II and III are devoted to a discussion of the connection between antisymmetrization and redundant states and a derivation of the conditions under which a nonsymmetric nonlocal potential has a scattering solution simultaneously with a redundant state solution. In presenting this proof, the nonlocal potential is assumed to be real. As mentioned earlier, this is consistent with the restriction imposed in Ref. 6 that energies be below the inelastic threshold.

II. ANTISYMMETRIZATION AND REDUNDANT STATES

The condition that the single-particle Schrödinger equation

$$(\epsilon - T_0)|u\rangle = u|u\rangle \quad (1)$$

have redundant solutions $|\xi_i\rangle$ can be expressed by the statement that, if at any energy the state $|u\rangle$ is a solution of Eq. (1), the equation will have redundant solutions $|\xi_i\rangle$ if and only if at that energy the state $|u'\rangle$, defined by

$$|\mu'\rangle = |\mu\rangle + \sum_{i=1}^A a_i |\xi_i\rangle \quad (2)$$

is also a solution of Eq. (1) for any values of the constants a_i . The integral equation for the physical solution $|\Psi^+\rangle$ of Eq. (1) is

$$|\Psi^+\rangle = |\Phi\rangle + \mathcal{G}^+ \mathcal{U} |\Psi^+\rangle, \quad (3)$$

where $|\Phi\rangle$ is the incident state and \mathcal{G}^+ is the Green's function which yields outgoing, spherical waves at infinity. The homogeneous integral equation associated with Eq. (3) is

$$|\Psi_h^+\rangle = \mathcal{G}^+ \mathcal{U} |\Psi_h^+\rangle. \quad (4)$$

The redundant states $|\xi_i\rangle$ will be solutions only of Eq. (4), the homogeneous integral equation, and not of Eq. (3), the inhomogeneous integral equation. However, the condition expressed in terms of Eq. (2) for the presence of redundant states remains correct for the inhomogeneous integral equation.

It is clear from the above discussion that the existence of redundancies in the single-particle scattering solution makes this solution nonunique. This unusual feature results from incorporating antisymmetrization of the incident particle with respect to particles in the target nucleus via an $(A+1)$ -particle Slater determinant. However, the Pauli principle requires a single-particle scattering wave function from which all components of states in the target filled by particles identical to the projectile are excluded. It is this wave function which is the wave function of physical significance. One of the major considerations of this paper is to examine the procedures involved in obtaining such a wave function which correctly takes the Pauli principle into account.

The theory of integral equations¹¹ states that a homogeneous integral equation such as Eq. (4) has a nontrivial solution if and only if the Fredholm determinant associated with the kernel $\mathcal{G}^+ \mathcal{U}$ is zero. We shall refer to this Fredholm determinant as $D^+(k)$. Thus the condition that Eq. (1), and therefore Eq. (3), exhibit redundant solutions requires that $D^+(k)$ be zero for all wave numbers k of the incident particle.

III. EXISTENCE OF SCATTERING SOLUTIONS FOR NONSYMMETRIC POTENTIALS

The question of whether or not an inhomogeneous integral equation has a solution when the Fredholm determinant associated with its kernel is zero requires a careful examination of the existence conditions.¹¹ We discuss first the general form of these conditions and then apply them to the integral equations which describe the scattering problem. For convenience, we consider the case

when the homogeneous integral equation has a single solution. In the case of multiple solutions of the homogeneous equation each solution must meet the conditions given for a single solution.

The radial integral equations associated with the Schrödinger equation with a nonlocal potential are of the form

$$\chi(r) = F(r) + \int_0^\infty K(r|s)\chi(s)ds. \quad (5)$$

The homogeneous equation associated with Eq. (5),

$$\chi_h(r) = \int_0^\infty K(r|s)\chi_h(s)ds, \quad (6)$$

has a nontrivial solution if and only if the Fredholm determinant associated with the kernel $K(r|s)$ is zero. The inhomogeneous equation (5) then has a solution if and only if the inhomogeneous term $F(r)$ is orthogonal to the solution $\bar{\chi}_h(r)$ of the transposed homogeneous equation

$$\bar{\chi}_h(r) = \int_0^\infty K(s|r)\bar{\chi}_h(s)ds. \quad (7)$$

Thus the existence condition for $\chi(r)$ when the Fredholm determinant is zero is the orthogonality of the inhomogeneous term $F(r)$ and the solution $\bar{\chi}_h(r)$ of the transposed homogeneous equation associated with Eq. (5). This result is known as Fredholm's third theorem.

The radial equation associated with Eq. (1) will be considered only in the $l=0$ partial wave. The extension to higher partial waves is straightforward, but cumbersome. The $l=0$ radial equation can be written as

$$u(k, r)'' + k^2 u(k, r) = \int_0^\infty \mathcal{V}(r, s) u(k, s) ds. \quad (8)$$

The physical solution $\psi^+(k, r)$ of Eq. (8) satisfies the integral equation

$$\begin{aligned} \psi^+(k, r) = \text{sink}r + \int_0^\infty \int_0^\infty G^+(k, r, r') \mathcal{V}(r', s) \\ \times \psi^+(k, s) ds dr', \end{aligned} \quad (9)$$

where

$$G^+(k, r, r') = -k^{-1} e^{ikr} > \text{sink}r <. \quad (10)$$

The homogeneous equation associated with Eq. (9) is

$$\begin{aligned} \psi_h^+(k, r) = \int_0^\infty \int_0^\infty G^+(k, r, r') \mathcal{V}(r', s) \\ \times \psi_h^+(k, s) ds dr'. \end{aligned} \quad (11)$$

The transposed equation associated with Eq. (9) can be written in the form

$$\bar{\psi}^+(k, r) = \text{sink}r + \int_0^\infty \int_0^\infty \bar{v}(r, r') G^+(k, r', s) \times \bar{\psi}^+(k, s) ds dr', \quad (12)$$

where

$$\bar{v}(r, r') = v(r', r) \quad (13)$$

and use has been made of the fact that

$$G^+(k, s, r') = G^+(k, r', s). \quad (14)$$

The transposed homogeneous equation is

$$\bar{\psi}_h^+(k, r) = \int_0^\infty \int_0^\infty \bar{v}(r, r') G^+(k, r', s) \bar{\psi}_h^+(k, s) ds dr'. \quad (15)$$

The necessary and sufficient condition for the existence of a solution of Eq. (11) is that

$$D^+(k) = 0. \quad (16)$$

Condition (16) is also sufficient to insure the existence of a solution of Eq. (15).¹⁵ As discussed earlier, when $D^+(k) = 0$ a solution of Eq. (9) will exist if and only if the orthogonality condition

$$\int_0^\infty \text{sink}r \bar{\psi}_h^+(k, r) dr = 0 \quad (17)$$

is satisfied.

Equation (17) can be cast in a more useful form by considering the adjoint of Eq. (8), given by¹⁶

$$\bar{u}(k, r)'' + k^2 \bar{u}(k, r) = \int_0^\infty \bar{v}(r, s) \bar{u}(k, s) ds, \quad (18)$$

where $\bar{v}(r, s)$ is defined by Eq. (13). The adjoint physical solution $\bar{\psi}^+(k, r)$ is defined by the integral equation

$$\bar{\psi}^+(k, r) = \text{sink}r + \int_0^\infty \int_0^\infty G^+(k, r, r') \bar{v}(r', s) \bar{\psi}^+(k, s) ds dr' \quad (19)$$

with $G^+(k, r, r')$ given by Eq. (10). The homogeneous equation associated with Eq. (19) is

$$\bar{\psi}_h^+(k, r) = \int_0^\infty \int_0^\infty G^+(k, r, r') \bar{v}(r', s) \bar{\psi}_h^+(k, s) ds dr'. \quad (20)$$

As pointed out in Ref. 16, the solution $\bar{\psi}_h^+(k, r)$ of Eq. (20) is not the same as the solution $\bar{\psi}_h^+(k, r)$ of Eq. (15). The relationship between these solutions can be obtained by multiplying Eq. (20) by \bar{v} and integrating over r . This yields

$$\int_0^\infty \bar{v}(r, s) \bar{\psi}_h^+(k, s) ds = \int_0^\infty \int_0^\infty \bar{v}(r, s) G^+(k, s, r') \times \int_0^\infty \bar{v}(r', s') \bar{\psi}_h^+(k, s') ds' dr' ds. \quad (21)$$

Comparison of Eqs. (15) and (21) shows that

$$\bar{\psi}_h^+(k, r) \propto \int_0^\infty \bar{v}(r, s) \bar{\psi}_h^+(k, s) ds. \quad (22)$$

Thus the necessary and sufficient condition stated in Eq. (17) for the existence of a solution of Eq. (9) can be written in the alternate form

$$\int_0^\infty \int_0^\infty \text{sink}r \bar{v}(r, s) \bar{\psi}_h^+(k, s) ds dr = 0. \quad (23)$$

The result given in Eq. (23) goes over onto that for a symmetric nonlocal potential [Ref. 12, Eq. (61)] under the condition $\bar{v} = v$, in which case it follows that $\bar{\psi}_h^+ = \psi_h^+$. Although Eq. (23) provides a specific test for the existence of a solution of Eq. (9), the essential difference between the existence of a solution of Eq. (9) for a symmetric and for a nonsymmetric nonlocal potential requires further consideration.

For this purpose it is convenient to consider the Jost solution of Eq. (8) defined by

$$f^+(k, r) = e^{ikr} - \int_r^\infty \int_0^\infty G(k, r, r') v(r', s) f^+(k, s) ds dr', \quad (24)$$

where

$$G(k, r, r') = k^{-1} \text{sink}(r - r'). \quad (25)$$

The homogeneous equation associated with Eq. (24) is

$$f_h^+(k, r) = - \int_r^\infty \int_0^\infty G(k, r, r') v(r', s) f_h^+(k, s) ds dr'. \quad (26)$$

The adjoint equation associated with Eq. (24) can be written in the form

$$\bar{f}^-(k, r) = e^{ikr} - \int_r^\infty \int_0^\infty G(k, r, r') \bar{v}(r', s) \bar{f}^-(k, s) ds dr'. \quad (27)$$

The homogeneous equation associated with Eq. (27) is

$$\bar{f}_h^-(k, r) = - \int_r^\infty \int_0^\infty G(k, r, r') \bar{v}(r', s) \bar{f}_h^-(k, s) ds dr'. \quad (28)$$

Using the Green's function identity

$$- \int_r^\infty G(k, r, r') h(r') dr' = \int_0^\infty G^+(k, r, r') h(r') dr' + k^{-1} e^{ikr} \int_0^\infty \text{sink}r' h(r') dr', \quad (29)$$

valid for arbitrary $h(r)$, Eq. (28) can be rewritten

in the form

$$\begin{aligned} \tilde{f}_h^+(k, r) = & \int_0^\infty \int_0^\infty G^+(k, r, r') \tilde{v}(r', s) \tilde{f}_h^+(k, s) ds dr' \\ & + k^{-1} e^{ikr} \int_0^\infty \int_0^\infty \text{sink} r' \tilde{v}(r', s) \tilde{f}_h^+(k, s) ds dr'. \end{aligned} \quad (30)$$

An expression dependent upon the integral in Eq. (23) and which provides a basis for discussing the existence of a scattering solution for a nonlocal potential with a redundant solution can be obtained by comparing expressions derived using Eqs. (20) and (30). Multiplying Eq. (20) by \tilde{v} and integrating gives

$$\int_0^\infty \tilde{v}(r, s) \tilde{\psi}_h^+(k, s) ds = \int_0^\infty \int_0^\infty \int_0^\infty \tilde{v}(r, s') G^+(k, s', r') \tilde{v}(r', s) \tilde{\psi}_h^+(k, s) ds dr' ds', \quad (31)$$

which can be rewritten using Eq. (13) and the symmetry of G^+ as

$$\int_0^\infty \tilde{v}(r, s) \tilde{\psi}_h^+(k, s) ds = \int_0^\infty \int_0^\infty \int_0^\infty \tilde{\psi}_h^+(k, s) \tilde{v}(s, r') G^+(k, r', s') \tilde{v}(s', r) ds' dr' ds. \quad (32)$$

Multiplying Eq. (32) with $\tilde{f}_h^+(k, r)$ and integrating over r yields

$$\int_0^\infty \int_0^\infty \tilde{\psi}_h^+(k, s) \tilde{v}(s, r) \tilde{f}_h^+(k, r) dr ds = \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \tilde{\psi}_h^+(k, s) \tilde{v}(s, r') G^+(k, r', s') \tilde{v}(s', r) \tilde{f}_h^+(k, r) dr ds' dr' ds. \quad (33)$$

Multiplying Eq. (30) by $\int_0^\infty \tilde{\psi}_h^+(k, s) \tilde{v}(s, r) ds$ and integrating over r gives

$$\begin{aligned} & \int_0^\infty \int_0^\infty \tilde{\psi}_h^+(k, s) \tilde{v}(s, r) \tilde{f}_h^+(k, r) dr ds \\ & = \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \tilde{\psi}_h^+(k, s) \tilde{v}(s, r') G^+(k, r', s') \tilde{v}(s', r) \tilde{f}_h^+(k, r) dr ds' dr' ds \\ & \quad + k^{-1} \int_0^\infty \int_0^\infty e^{ikr} \tilde{v}(r, s) \tilde{\psi}_h^+(k, s) ds dr \int_0^\infty \int_0^\infty \text{sink} r' \tilde{v}(r', s') \tilde{f}_h^+(k, s') ds' dr'. \end{aligned} \quad (34)$$

Subtracting Eq. (32) from Eq. (34) yields

$$\begin{aligned} & \int_0^\infty \int_0^\infty \tilde{\psi}_h^+(k, s) [\tilde{v}(s, r) - \tilde{v}(s, r')] \tilde{f}_h^+(k, r) dr ds \\ & = k^{-1} \int_0^\infty \int_0^\infty e^{ikr} \tilde{v}(r, s) \tilde{\psi}_h^+(k, s) ds dr \int_0^\infty \int_0^\infty \text{sink} r' \tilde{v}(r', s') \tilde{f}_h^+(k, s') ds' dr'. \end{aligned} \quad (35)$$

Equation (35) is the desired relationship. If the potential \tilde{v} is symmetric, then the left hand side of Eq. (35) becomes identically zero for all values of k . From this, it follows [Ref. 12, p. 2138] that $\tilde{f}_h^+(k, r) = \tilde{\psi}_h^+(k, r)$, that condition (23) holds for every energy of the incident particle, and that a scattering solution exists at every energy. Thus, for a real symmetric nonlocal potential which produces redundant states the existence of a scattering solution is automatic. For a nonsymmetric nonlocal potential the left hand side of Eq. (35) would not in general be zero. Existence of a scattering solution for a nonsymmetric nonlocal potential with a redundant state relies, rather, upon the condition that the potential depend upon the wave number k in such a way as to satisfy condition (23) explicitly at every energy.

In the next section we discuss the Hartree-Fock potential which results from incorporating excitations of the target nucleus, including as an ex-

ample an explicit calculation of the potential for a two-particle Slater determinant target. The non-symmetry of the potential is apparent in this discussion. A study of the full and reduced equations associated with potentials such as the Hartree-Fock potential which exhibit redundant states is presented in Sec. V. Examples of solutions of the full and reduced equations for potentials which produce redundant states are given in Sec. VI, with emphasis upon the compatibility conditions for the existence of a scattering solution of the full equation.

IV. HARTREE-FOCK POTENTIAL

The potential \mathfrak{u} referred to in Eq. (1) is the full nonlocal potential in the Schrödinger equation for the single-particle scattering state $|\mu\rangle$. In Ref. 6 we showed that, by introducing only the restric-

tion that the target nucleus be represented by a Slater determinant of A single-particle states, the potential \mathfrak{u} in Eq. (1) for the scattering of an incident nucleon from the nucleus can be put into the form

$$\mathfrak{u} = (\epsilon - T_0) \sum_{i=1}^A |\xi_i\rangle\langle\xi_i| + \mathfrak{u}_2, \quad (36)$$

where the potential \mathfrak{u}_2 is given in configuration space by

$$\begin{aligned} \langle \tilde{\mathbf{r}}_0 | \mathfrak{u}_2 | \mathfrak{u} \rangle = & \int \left[\int \cdots \int \varphi_0(\tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \cdots \tilde{\mathbf{r}}_A) \langle \tilde{\mathbf{r}}_0 \tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \cdots \tilde{\mathbf{r}}_A | V_0 + \mathfrak{R} | \tilde{\mathbf{r}}'_0 \tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2 \cdots \tilde{\mathbf{r}}'_A \rangle \right. \\ & \times \varphi_0(\tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2 \cdots \tilde{\mathbf{r}}'_A) d\tilde{\mathbf{r}}_1 d\tilde{\mathbf{r}}_2 \cdots d\tilde{\mathbf{r}}_A d\tilde{\mathbf{r}}'_1 d\tilde{\mathbf{r}}'_2 \cdots d\tilde{\mathbf{r}}'_A \left. \right] u(\tilde{\mathbf{r}}'_0) d\tilde{\mathbf{r}}'_0 \\ & - \int A \left[\int \cdots \int \varphi_0(\tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \cdots \tilde{\mathbf{r}}_A) \langle \tilde{\mathbf{r}}_0 \tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \cdots \tilde{\mathbf{r}}_A | V_0 + \mathfrak{R} | \tilde{\mathbf{r}}'_0 \tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2 \cdots \tilde{\mathbf{r}}'_A \rangle \right. \\ & \times \varphi_0(\tilde{\mathbf{r}}'_0 \tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2 \cdots \tilde{\mathbf{r}}'_A) d\tilde{\mathbf{r}}_1 d\tilde{\mathbf{r}}_2 \cdots d\tilde{\mathbf{r}}_A d\tilde{\mathbf{r}}'_0 d\tilde{\mathbf{r}}'_1 d\tilde{\mathbf{r}}'_2 \cdots d\tilde{\mathbf{r}}'_A \left. \right] u(\tilde{\mathbf{r}}'_1) d\tilde{\mathbf{r}}'_1, \end{aligned} \quad (37)$$

φ_0 is the ground state wave function of the target nucleus,

$$V_0 = \sum_{i=1}^A V_{0i} \quad (38)$$

is the local or nonlocal nucleon-nucleon potential acting between the incident and target nucleons, and the nonlocal operator \mathfrak{R} takes into account excitation of the target nucleus.

It was demonstrated in Ref. 6 that the potential \mathfrak{u}_2 satisfies the condition

$$\mathfrak{u}_2 |\xi_i\rangle = 0. \quad (39)$$

That is, we found that the effective potential \mathfrak{u} divides naturally into terms containing projection operators onto the subspace spanned by the states $|\xi_i\rangle$ and the subspace orthogonal to these states. The first term on the right hand side of Eq. (36) contains explicitly the projection operator

$$\Omega = \sum_{i=1}^A |\xi_i\rangle\langle\xi_i| \quad (40)$$

onto the subspace spanned by the states $|\xi_i\rangle$. That the associated projection operator

$$\Lambda = 1 - \Omega \quad (41)$$

is implicit in the term \mathfrak{u}_2 follows from Eq. (39). That is,

$$\mathfrak{u}_2 \equiv \mathfrak{u}_2 \Lambda. \quad (42)$$

Equation (1) with the potential of Eq. (36) can be written in the form

$$\left[(\epsilon - T_0) - (\epsilon - T_0) \sum_{i=1}^A |\xi_i\rangle\langle\xi_i| \right] |\mathfrak{u}\rangle = \mathfrak{u}_2 |\mathfrak{u}\rangle \quad (43a)$$

or

$$(\epsilon - T_0) \Lambda |\mathfrak{u}\rangle = \mathfrak{u}_2 \Lambda |\mathfrak{u}\rangle. \quad (43b)$$

The term $(\epsilon - T_0) \sum_{i=1}^A |\xi_i\rangle\langle\xi_i|$ is responsible for

the redundant states which arise from the potential \mathfrak{u} . This follows immediately from substituting for $|\mathfrak{u}\rangle$ in Eq. (43a) or (43b) the state $|\xi_j\rangle$. Because of Eq. (39), for $|\mathfrak{u}\rangle = |\xi_j\rangle$ each side of Eq. (43a) is *separately* zero. Said another way, the term $\mathfrak{u}_2 |\xi_j\rangle$ drops out, leaving only the identity $(\epsilon - T_0) |\xi_j\rangle - (\epsilon - T_0) |\xi_j\rangle = 0$. This verifies that $|\xi_j\rangle$ is, indeed, a redundant solution to Eq. (1) with the potential given by Eq. (36).

That the structure of the full Hartree-Fock potential is somewhat complicated becomes clear when the potential is written out in terms of a special case. Consider, for example, $A = 2$, in which case the Slater determinant for the ground state target wave function is

$$\varphi_0(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) = (2)^{-1/2} [\xi_1(\tilde{\mathbf{r}}_1) \xi_2(\tilde{\mathbf{r}}_2) - \xi_1(\tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_1)]. \quad (44)$$

We introduce the simplifying assumption that the matrix elements of $V_0 + \mathfrak{R}$ be local, namely,

$$\begin{aligned} \langle \tilde{\mathbf{r}}_0 \tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 | V_0 + \mathfrak{R} | \tilde{\mathbf{r}}'_0 \tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2 \rangle = & \delta(\tilde{\mathbf{r}}_0 - \tilde{\mathbf{r}}'_0) \delta(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_1) \\ & \times \delta(\tilde{\mathbf{r}}_2 - \tilde{\mathbf{r}}'_2) \mathcal{T}(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2). \end{aligned} \quad (45)$$

In terms of the local interaction \mathcal{T} the expression for \mathfrak{u}_2 given in Eq. (37) becomes

$$\begin{aligned} \int \mathfrak{u}_2(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) u(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 = & \mathfrak{w}_1(\tilde{\mathbf{r}}_0) u(\tilde{\mathbf{r}}_0) \\ & + \int \mathfrak{w}_2(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) u(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1, \end{aligned} \quad (46)$$

where

$$\mathfrak{w}_1(\tilde{\mathbf{r}}_0) = \int \int \varphi_0^*(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) \mathcal{T}(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) \varphi_0(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_1 d\tilde{\mathbf{r}}_2 \quad (47)$$

and

$$\mathcal{W}_2(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) = -A \int \varphi_0^*(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) \mathcal{T}(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) \varphi_0(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2. \quad (48)$$

We further assume that \mathcal{T} can be expressed as a sum of two-body interactions, and write it in the form

$$\mathcal{T}(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2) = \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) + \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2). \quad (49)$$

Substituting Eqs. (44) and (49) into Eq. (47) yields

$$\begin{aligned} \mathcal{W}_1(\tilde{\mathbf{r}}_0) &= \int \xi_1^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \xi_1(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 \\ &+ \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2. \end{aligned} \quad (50)$$

Similarly, we find that

$$\begin{aligned} \mathcal{W}_2(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) &= -\xi_1^*(\tilde{\mathbf{r}}_1) \xi_1(\tilde{\mathbf{r}}_0) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) - \xi_2^*(\tilde{\mathbf{r}}_1) \xi_2(\tilde{\mathbf{r}}_0) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \\ &- \xi_1^*(\tilde{\mathbf{r}}_1) \xi_1(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 - \xi_2^*(\tilde{\mathbf{r}}_1) \xi_2(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_1(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 \\ &+ \xi_2^*(\tilde{\mathbf{r}}_1) \xi_1(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 + \xi_1^*(\tilde{\mathbf{r}}_1) \xi_2(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_1(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2. \end{aligned} \quad (51)$$

Equation (46) for the term \mathfrak{u}_2 in the Hartree-Fock potential in the case $A = 2$ and under the assumptions stated thus assumes the form

$$\begin{aligned} \int \mathfrak{u}_2(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 &= \mathfrak{u}(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \xi_1(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 + \mathfrak{u}(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 \\ &- \xi_1(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 - \xi_2(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 \\ &- \xi_1(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 \\ &- \xi_2(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 \int \xi_1^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_1(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 \\ &+ \xi_1(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 \int \xi_1^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 \\ &+ \xi_2(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_1(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2. \end{aligned} \quad (52)$$

It follows by straightforward substitution into Eq. (52) that $\mathfrak{u}_2|\xi_1\rangle = \mathfrak{u}_2|\xi_2\rangle = 0$. All of the terms in Eq. (52) are necessary in effecting this orthogonality. But, as pointed out earlier in this section, elimination of the term $(\epsilon - T_0) \sum_{i=1,2} |\xi_i\rangle \langle \xi_i|$ from \mathfrak{u} eliminates redundant states from the solution of Eq. (1). Thus the potential \mathfrak{u}_2 can be considered the effective potential in the reduced equation. On the other hand, we have already stated and will prove in the next section that solutions to this reduced equation are orthogonal to the states $|\xi_1\rangle$ and $|\xi_2\rangle$. Thus once it is known that the full equation has a scattering solution $|\Psi^+\rangle$ and the term $(\epsilon - T_0) \sum_{i=1,2} |\xi_i\rangle \langle \xi_i|$ has been removed, there is no loss in generality in removing from \mathfrak{u}_2 in Eq. (52) all portions which project onto the states $|\xi_1\rangle$ and $|\xi_2\rangle$. When this is done the potential \mathfrak{v} in the reduced Hartree-Fock equation assumes the further reduced form

$$\begin{aligned} \int \mathfrak{v}(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 &= \mathfrak{u}(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \xi_1(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 + \mathfrak{u}(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_2) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_2) \xi_2(\tilde{\mathbf{r}}_2) d\tilde{\mathbf{r}}_2 \\ &- \xi_1(\tilde{\mathbf{r}}_0) \int \xi_1^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1 - \xi_2(\tilde{\mathbf{r}}_0) \int \xi_2^*(\tilde{\mathbf{r}}_1) \tau(\tilde{\mathbf{r}}_0, \tilde{\mathbf{r}}_1) \mathfrak{u}(\tilde{\mathbf{r}}_1) d\tilde{\mathbf{r}}_1. \end{aligned} \quad (53)$$

It is interesting to note that the potential \mathfrak{v} is symmetric, whereas the potential \mathfrak{u}_2 is not. However, once the term $(\epsilon - T_0) \sum_{i=1,2} |\xi_i\rangle \langle \xi_i|$, and thus the redundant solutions, has been removed from the Hartree-Fock equation, it is known that a scattering solution to the equation will exist whether or not the potential is symmetric.

V. SOLUTIONS OF FULL AND REDUCED EQUATIONS

By making use of the explicit structure given in Eq. (36) for the Hartree-Fock potential, it is possible to discuss the relationship between solutions of the full and reduced Hartree-Fock equations. This relationship is examined in this section for

the case of a single redundant state $|\xi\rangle$. The extension to more than one redundant state is straightforward.

As stated in Sec. III, Fredholm's third theorem implies that for a nonsymmetric potential which produces redundant states a scattering solution is not possible unless the orthogonality condition of Eq. (17) or Eq. (23) holds. This, in effect, imposes a consistency condition upon the potential \mathfrak{u}_2 . For a single redundant state this condition can be expressed most easily in terms of a variable strength parameter λ associated with \mathfrak{u}_2 . For more than one redundant state, additional parameters associated with \mathfrak{u}_2 must be considered.

For a single redundant state $|\xi\rangle$ the scattering solution $|\Psi^+\rangle$ of Eq. (1) with the potential of Eq. (36) with a variable strength parameter λ is

$$|\Psi^+\rangle = |\Phi\rangle + |\xi\rangle\langle\xi|\Psi^+\rangle + (\epsilon - T_0)^{-1}\lambda\mathfrak{u}_2|\Psi^+\rangle. \quad (54)$$

The transposed homogeneous equation associated with Eq. (54) is

$$|\bar{\Psi}_h^+\rangle = |\xi\rangle\langle\xi|\bar{\Psi}_h^+\rangle + \lambda\bar{\mathfrak{u}}_2(\epsilon - T_0)^{-1}|\bar{\Psi}_h^+\rangle. \quad (55)$$

The three-dimensional equivalent of orthogonality condition (17) assumes the form

$$\langle\Phi|\bar{\Psi}_h^+\rangle = 0. \quad (56)$$

Imposing this condition upon Eq. (55) yields

$$\langle\Phi|\xi\rangle\langle\xi|\bar{\Psi}_h^+\rangle = -\langle\Phi|\lambda\bar{\mathfrak{u}}_2(\epsilon - T_0)^{-1}|\bar{\Psi}_h^+\rangle. \quad (57)$$

Although $|\bar{\Psi}_h^+\rangle$ itself is dependent upon the potential strength λ , the consistency condition expressed in Eq. (57) indicates that if a scattering solution $|\Psi^+\rangle$ is to exist for a given functional form for $\mathfrak{u}_2(\mathbf{r}, \mathbf{r}')$, it will do so only for a unique potential strength. That is, if one fixes the strength of \mathfrak{u}_2 by the condition

$$\lambda = -\frac{\langle\Phi|\xi\rangle\langle\xi|\bar{\Psi}_h^+\rangle}{\langle\Phi|\mathfrak{u}_2(\epsilon - T_0)^{-1}|\bar{\Psi}_h^+\rangle}, \quad (58)$$

then the scattering state $|\Psi^+\rangle$ satisfying Eq. (54) exists. That the correct choice of a potential depth is in fact both necessary and sufficient to insure a scattering solution for a nonsymmetric nonlocal potential with redundant solutions will be demonstrated by explicit examples in Sec. VI.

Consider now the class of potentials given by Eq. (36) producing one redundant state and with \mathfrak{u}_2 specified not by Eq. (37) but only by the condition

$$\mathfrak{u}_2|\xi\rangle = 0. \quad (59)$$

We assume that the consistency condition expressed in Eq. (58) is fulfilled, assuring that Eq. (1) has a solution. If one then considers the state $|U\rangle$ which satisfies the Schrödinger equation with the potential \mathfrak{u}_2 , namely,

$$(\epsilon - T_0)|U\rangle = \mathfrak{u}_2|U\rangle, \quad (60)$$

it is possible to demonstrate that

$$\langle\xi|U\rangle = 0. \quad (61)$$

That is, Eq. (60) does not have redundant solutions and $|U\rangle$ is orthogonal to the state $|\xi\rangle$. It then follows from Eqs. (60) and (61) that the most general solution $|\mu\rangle$ to Eq. (1) is

$$|\mu\rangle = a|\xi\rangle + |U\rangle, \quad (62)$$

where the constant a is arbitrary.

The proof that Eqs. (61) and (62) follow from Eq. (60) hinges upon the fact that there exists a solution $|\chi\rangle$ to Eq. (60) such that $\langle\xi|\chi\rangle = 0$. Such a solution can be constructed from any solution $|\mu\rangle$ of Eq. (1) with the potential of Eq. (36) as follows:

$$|\chi\rangle = |\mu\rangle - \langle\xi|\mu\rangle|\xi\rangle. \quad (63)$$

Solving Eq. (63) for $|\mu\rangle$ and substituting into Eq. (1) gives as the equation for $|\chi\rangle$

$$(\epsilon - T_0)|\chi\rangle = \mathfrak{u}_2|\chi\rangle. \quad (64)$$

Thus $|\chi\rangle$ as defined in Eq. (63) satisfies both Eq. (60) for $|U\rangle$ and the condition $\langle\xi|\chi\rangle = 0$. Because of condition (59), it is not possible to form a solution $|U\rangle = |\chi\rangle + b|\xi\rangle$ which satisfies Eq. (60) unless $b \equiv 0$. That is, substituting $|U\rangle = |\chi\rangle + b|\xi\rangle$ into Eq. (60) gives, after using Eq. (64), $(\epsilon - T_0)b|\xi\rangle = 0$. Thus the most general solution $|U\rangle$ of Eq. (60) cannot differ from $|\chi\rangle$ by any amount of the state $|\xi\rangle$, and must satisfy Eq. (61). That Eq. (62) is the most general solution of Eq. (1) then follows from substituting Eq. (62) into Eq. (1), which gives

$$(\epsilon - T_0)|U\rangle = (\epsilon - T_0)|\xi\rangle\langle\xi|U\rangle + \mathfrak{u}_2|U\rangle. \quad (65)$$

The fact that the most general solution of Eq. (1) is given by Eq. (62) demonstrates that the only result of replacing the potential \mathfrak{u} by the potential \mathfrak{u}_2 in Eq. (1) is to remove redundant states from the spectrum of solutions of Eq. (1). It follows that for all other features of the interaction the potential \mathfrak{u}_2 can be considered as the effective potential. However, both the condition that Eq. (62) give the general solution to Eq. (1) and the condition that $|U\rangle$ be orthogonal to the state $|\xi\rangle$ depend upon the existence of a solution to Eq. (1).

This establishes that if a solution of Eq. (1) exists then the solution orthogonal to the redundant state can be obtained from a reduced equation. The implication is, however, that this reduced equation can be found only after the full equation has been obtained and the consistency requirements applied to that equation which guarantee the existence of a scattering solution. On the other hand, the simplicity of the reduced potential makes it a more natural starting point in generating a scattering

wave function, and the question arises as to whether one can actually start with the reduced equation and apply the consistency condition directly to it. We therefore discuss the possibility of starting with a reduced equation, that is, an equation of the form of Eq. (60), and obtaining a solution which will satisfy Eq. (1) and the orthogonality condition (61). The integral equation for the scattering state $|U^+\rangle$ associated with Eq. (60) is

$$|U^+\rangle = |\Phi\rangle + (\epsilon - T_0)^{-1} \lambda' \mathfrak{u}_2 |U^+\rangle. \quad (66)$$

The insertion of λ' into Eq. (66) emphasizes that Eq. (66) is meant to be the reduced equation associated with the full equation (54) only for the specific choice $\lambda' = \lambda$. Equation (66) will not have redundant states, and the scattering solution $|U^+\rangle$ will exist for any choice of λ' .

Even if one starts with an equation like Eq. (60) which does not produce redundant states, it should be possible to obtain a solution to the original problem. To demonstrate this, we treat Eq. (66) as if it were written down without reference to the full equation, Eq. (54), and question the conditions under which a solution of Eq. (66) nevertheless will be a solution of Eq. (54). The consistency condition as derived earlier will not apply, but we will show that a condition sufficient to insure that the solution to Eq. (66) be a solution to the full equation, Eq. (54), is

$$\langle \xi | U^+ \rangle = 0. \quad (67)$$

Imposing condition (67) on Eq. (66) gives

$$\lambda' = - \frac{\langle \xi | \Phi \rangle}{\langle \xi | (\epsilon - T_0)^{-1} \mathfrak{u}_2 | U^+ \rangle}. \quad (68)$$

Assuming that Eq. (68) holds, we now show that this value of λ' is the value λ given by Eq. (58) and that this value insures the existence of a solution of Eq. (54). From Eq. (67) it follows that Eq. (66) can be rewritten as

$$|U^+\rangle = |\Phi\rangle + |\xi\rangle \langle \xi | U^+ \rangle + (\epsilon - T_0)^{-1} \lambda' \mathfrak{u}_2 |U^+\rangle. \quad (69)$$

Equation (69) is known to have the redundant solution $|\xi\rangle$ for any value of λ' , and by comparison with Eq. (54) it follows that Eq. (69) will have a scattering solution $|U^+\rangle$ only if $\lambda = \lambda'$. That is, Eqs. (69) and (54) differ only in the symbol used for the solution, and the conditions imposed on $|\Psi^+\rangle$ following Eq. (54) must also be imposed on Eq. (69) to insure that it have a solution.

In summary, the full equation (54) possesses a scattering solution only for certain values of λ . This scattering solution is not unique, but is arbitrary with respect to the addition of any amount of the redundant state $|\xi\rangle$. Because of this arbitrariness, it is possible to choose a solution $|U^+\rangle$

of Eq. (54) which is orthogonal to $|\xi\rangle$. The state $|U^+\rangle$ will be the solution of the reduced equation, Eq. (60). The reduced equation has a scattering solution for essentially all λ' . However, only for the strength $\lambda' = \lambda$ will the solution to the reduced equation be orthogonal to the redundant solutions and satisfy the full equation. One way to insure that the reduced equation will produce the desired orthogonal solution is to use a reduced equation which has been obtained from the correct full equation. Another way to impose the consistency condition is to solve the reduced equation for arbitrary λ' and fix λ' by making the scattering solution orthogonal to the redundant state.

This latter procedure remains valid even if terms containing the projection operator onto $|\xi\rangle$ are eliminated from the potential. That is, since the potential \mathfrak{u}_2 satisfies condition (59), it follows that it can be written in the form

$$\mathfrak{u}_2 = \mathfrak{u} \Lambda, \quad (70)$$

where

$$\Lambda = 1 - |\xi\rangle \langle \xi|. \quad (71)$$

Although the solution of the equation

$$|\chi^+\rangle = |\Phi\rangle + (\epsilon - T_0)^{-1} \lambda' \mathfrak{u} |\chi^+\rangle \quad (72)$$

may differ from the solution of Eq. (66), imposing on $|\chi^+\rangle$ the condition

$$\langle \xi | \chi^+ \rangle = 0 \quad (73)$$

clearly leads to $\lambda' = \lambda$ and thus to $|\chi^+\rangle = |U^+\rangle$.

VI. EXAMPLES

In order to clarify this discussion, we consider two examples. The first is chosen for its simplicity, the second for its direct connection with the Hartree-Fock potential.

Example 1

In this example we assume that the $l=0$ radial wave equation has a single redundant solution given by

$$\xi(r) = 2\alpha^{3/2} r e^{-\alpha r}. \quad (74)$$

We also choose the potential \mathfrak{u}_2 to be given by

$$\langle r | \mathfrak{u}_2 | s \rangle = \int_0^\infty \frac{\hbar^2}{2m} \lambda e^{-\beta r} e^{-\beta r'} \langle r' | \Lambda | s \rangle dr', \quad (75)$$

where

$$\langle r' | \Lambda | s \rangle = \delta(r' - s) - 4\alpha^3 r' e^{-\alpha r'} s e^{-\alpha s}. \quad (76)$$

These choices make possible an analytic solution to the radial wave equation. This equation, which follows from Eqs. (1), (36), (74), and (75), is

$$\left(\frac{d^2}{dr^2} + k^2\right)u(r) = 2\alpha^{3/2}\langle\xi|u\rangle[-2\alpha e^{-\alpha r} + (\alpha^2 + k^2)r e^{-\alpha r}] + \lambda e^{-\beta r}[A - 2\alpha^{3/2}\langle\xi|u\rangle/(\alpha + \beta)^2], \quad (77)$$

where

$$k^2 = 2m\epsilon/\hbar^2 \quad (78)$$

and

$$A = \int_0^\infty e^{-\beta r} u(r) dr. \quad (79)$$

As discussed in Sec. V, at a given energy Eq. (77) has no solution except the redundant solution $\xi(r)$ unless λ assumes a particular value at that energy. This consistency condition specifies λ as a function of k .

Equation (77) can be treated as an inhomogeneous differential equation, for which the solution will be of the form

$$u(r) = \sin kr + ar e^{-\alpha r} + b(\cos kr - e^{-\beta r}), \quad (80)$$

where the normalization of the free-particle solution has been chosen as unity. Substituting this solution into Eq. (77) yields

$$\begin{aligned} -2a\alpha e^{-\alpha r} + a(\alpha^2 + k^2)r e^{-\alpha r} - b(\beta^2 + k^2)e^{-\beta r} \\ = 2\alpha^{3/2}\langle\xi|u\rangle[-2\alpha e^{-\alpha r} + (\alpha^2 + k^2)r e^{-\alpha r}] \\ + \lambda e^{-\beta r}[A - 2\alpha^{3/2}\langle\xi|u\rangle/(\alpha + \beta)^2]. \end{aligned} \quad (81)$$

Comparing the coefficients of $e^{-\alpha r}$ and $r e^{-\alpha r}$ gives, in each case, the condition

$$a = 2\alpha^{3/2}\langle\xi|u\rangle. \quad (82)$$

Comparing the coefficients of $e^{-\beta r}$ yields the condition

$$b = -\frac{\lambda}{(\beta^2 + k^2)} \left[A - 2\alpha^{3/2} \frac{\langle\xi|u\rangle}{(\alpha + \beta)^2} \right]. \quad (83)$$

$$c = \frac{\lambda' \left[\frac{8\alpha^4 k(\beta^2 + k^2)}{(\alpha^2 + k^2)^2(\alpha + \beta)^2} - k \right]}{(\beta^2 + k^2)^2 - \lambda'(\beta^2 + k^2) \left[\frac{1}{2\beta} - \frac{\beta}{\beta^2 + k^2} - \frac{4\alpha^3}{(\alpha + \beta)^4} + \frac{4\alpha^3(\alpha^2 - k^2)}{(\alpha^2 + k^2)^2(\alpha + \beta)^2} \right]}. \quad (90)$$

It follows that the reduced equation has a solution for any value of λ' [except, perhaps, for that value of k for which the denominator of Eq. (90) goes to zero]. The solution is not, in general, orthogonal to the redundant state. Imposing condition (88) yields

$$\lambda' = \lambda \quad (91)$$

and

$$c = b, \quad (92)$$

We substitute $u(r)$ into $\langle\xi|u\rangle$ in Eqs. (82) and (83) and find that the two equations hold for any choice of a , and are mutually consistent only if

$$\lambda = -\frac{2\alpha\beta(\beta^2 + k^2)(\alpha + \beta)^2}{\beta(\alpha^2 + k^2) - \alpha(\alpha^2 - \beta^2)}, \quad (84)$$

in which case

$$b = 2\alpha k \left[\frac{(\alpha^2 + k^2)^2}{(\alpha + \beta)^2} - (\alpha^2 - k^2) \right]^{-1}. \quad (85)$$

This demonstrates that the existence of a scattering solution is not automatic. Rather, it depends upon an overall consistency between the term $(\epsilon - T_0)|\xi\rangle\langle\xi|$ responsible for the redundant state and the term \mathfrak{U}_2 . Straightforward calculation of the term $\langle\xi|u\rangle$ shows that the expression for b given by Eq. (85) is precisely the condition required for the scattering solution of Eq. (77) to be orthogonal to the redundant solution $\xi(r)$. That is, from Eqs. (84) and (85) it follows that a solution $u(r)$ of Eq. (77) exists and has $\xi(r)$ as a redundant state. The solution $U(r)$ orthogonal to the redundant state is easily constructed by choosing $a = 0$, in which case

$$U(r) = \sin kr + b(\cos kr - e^{-\beta r}). \quad (86)$$

As discussed in Sec. V, the solution $U(r)$ may be obtained from the reduced radial equation

$$\left(\frac{d^2}{dr^2} + k^2\right)\chi(r) = \lambda' e^{-\beta r} [A - 2\alpha^{3/2}\langle\xi|\chi\rangle/(\alpha + \beta)^2], \quad (87)$$

where A is defined in Eq. (79) [with $u(r)$ replaced by $\chi(r)$], by imposing the orthogonality condition

$$\langle\chi|\xi\rangle = 0. \quad (88)$$

The solution of Eq. (87) is

$$\chi(r) = \sin kr + c(\cos kr - e^{-\beta r}) \quad (89)$$

with c given by

where λ and b are given by Eqs. (84) and (85), respectively. Thus if and only if the orthogonality condition is imposed will $\chi(r)$ be a solution of the full equation, Eq. (77), as well as of the reduced equation, Eq. (87).

The potential in Eq. (87) contains a term which projects onto the state $|\xi\rangle$. Eliminating this term leads to the further reduced equation

$$\left(\frac{d^2}{dr^2} + k^2\right)\chi(r) = \lambda' A e^{-\beta r}. \quad (93)$$

The solution of Eq. (93) will not in general be a solution of Eq. (87), nor will the solution of Eq. (87) in general be a solution of Eq. (93). However, for $\lambda' = \lambda$ the solutions of Eqs. (87) and (93) are each equal to $U(r)$, the solution of Eq. (77) which is orthogonal to $\xi(r)$. Thus the solution $U(r)$ can be obtained either from the full equation or from Eq. (87) or (93) with the particular value $\lambda' = \lambda$.

This example started with the full equation, Eq. (77), with the redundant solution $\xi(r)$. Because this equation has no scattering solution unless λ assumes the particular value given in Eq. (84), the redundancy-free solution $U(r)$ of Eq. (77) is unambiguous. In going to the fully reduced equation, Eq. (93), information has been lost. This information can be retrieved by solving Eq. (93) in conjunction with the orthogonality condition of Eq. (88). The orthogonality condition is not automatic. It holds only if λ' is properly chosen. Equivalently, this consistency condition could be satisfied if one had prior knowledge of the value λ which λ' must assume in order for Eq. (93) to yield the solution $U(r)$.

Example 2

We now consider an example more closely related to the Hartree-Fock potential. As in example

$$\left(\frac{d^2}{dr^2} + k^2 + B e^{-\beta r}\right) u(r) = \left(\frac{d^2}{dr^2} + k^2 + B e^{-\beta r}\right) \xi(r) \langle \xi | u \rangle + \lambda e^{-\beta r} \xi(r) \int_0^\infty \xi(r') e^{-\beta r'} \xi(r') dr' \langle \xi | u \rangle - \lambda e^{-\beta r} \xi(r) \int_0^\infty \xi(r') e^{-\beta r'} u(r') dr', \quad (96)$$

where

$$B = -\lambda \int_0^\infty \xi(r') e^{-\beta r'} \xi(r') dr'. \quad (97)$$

In Eq. (96) the last two terms on the right hand side form a potential which acts upon $u(r)$ and which gives zero for $u(r) = \xi(r)$. Equation (96) is no more easily solved than is Eq. (95). We therefore replace it by the equation obtained by setting $B = 0$, namely,

$$\left(\frac{d^2}{dr^2} + k^2\right) u(r) = \left(\frac{d^2}{dr^2} + k^2\right) \xi(r) \langle \xi | u \rangle + \lambda e^{-\beta r} \xi(r) \left[\int_0^\infty \xi(r') e^{-\beta r'} \xi(r') dr' \langle \xi | u \rangle - \int_0^\infty \xi(r') e^{-\beta r'} u(r') dr' \right]. \quad (98)$$

Equation (98) has essentially the same mathematical structure as Eq. (95). It still has $\xi(r)$ as a redundant state, but the potential contains no local terms. The principal virtue of Eqs. (98) is that its solution can be obtained in compact analytic form.

The solution of Eq. (98) is of the form

$$u(r) = \sin kr + Cr e^{-\alpha r} + Dr e^{-(\alpha + \beta)r} + E \cos kr - E e^{-(\alpha + \beta)r}. \quad (99)$$

1, we assume that the $l=0$ radial wave equation has a single redundant solution given by Eq. (74). We construct the potential u_2 using Eq. (52). For a single redundant solution, Eq. (52) leads to a direct term and to an exchange term. Assuming for $\tau(\vec{r}, \vec{r}')$ the form

$$\tau(\vec{r}, \vec{r}') = \lambda \left(\frac{\hbar^2}{2m} \right) e^{-\beta r} e^{-\beta r'} \quad (94)$$

yields the $l=0$ radial equation

$$\left(\frac{d^2}{dr^2} + k^2\right) u(r) = \left(\frac{d^2}{dr^2} + k^2\right) \xi(r) \langle \xi | u \rangle + \lambda e^{-\beta r} u(r) \int_0^\infty \xi(r') e^{-\beta r'} \xi(r') dr' - \lambda e^{-\beta r} \xi(r) \int_0^\infty \xi(r') e^{-\beta r'} u(r') dr'. \quad (95)$$

The effective potential acting on $u(r)$ in Eq. (95) contains the term $(d^2/dr^2 + k^2) \xi(r) \langle \xi | u \rangle$ necessary for generating the redundant state $\xi(r)$. As required, the remainder of the potential is orthogonal to $\xi(r)$. Algebraic solution of Eq. (95) is difficult because of the presence of the direct term, the second term on the right hand side. Therefore, instead of considering Eq. (95), we solve a modified equation.

Equation (95) can be rewritten in the form

Substituting $u(r)$ into Eq. (98) does not yield a solution unless

$$\lambda = - \frac{(\alpha + \beta)^3 (2\alpha + \beta)^3 [(\alpha + \beta)^2 + k^2]^4}{8\alpha^2 (\alpha + \beta)^4 M + N}, \quad (100)$$

where

$$M = (\alpha^2 - k^2)(\alpha + \beta)(2\alpha + \beta)^3 - (\alpha^2 + k^2)^2 [(\alpha + \beta)^2 + k^2] - (\alpha^2 + k^2)^2 (\alpha + \beta)(2\alpha + \beta) \quad (101)$$

and

$$N = \alpha^3(2\alpha + \beta)^3[(\alpha + \beta)^2 + k^2]^3 \\ - 2\alpha^3(2\alpha + \beta)^3(\alpha + \beta)^2\{4(\alpha + \beta)^2[(\alpha + \beta)^2 - k^2] \\ - [(\alpha + \beta)^2 + k^2]^2\} \quad (102)$$

For this value of λ ,

$$C = 2\alpha^{3/2} \langle \xi | u \rangle, \quad (103)$$

$$D = \alpha k(2\alpha + \beta)^3[(\alpha + \beta)^2 + k^2]/M, \quad (104)$$

and

$$E = -2\alpha k(\alpha + \beta)(2\alpha + \beta)^3/M. \quad (105)$$

Thus a scattering solution of Eq. (98) is possible only for the value of λ imposed by the consistency condition. Calculation of the term $\langle \xi | u \rangle$ verifies that the expressions for D and E given in Eqs. (104) and (105) are those required for the scattering solution of Eq. (98) to be orthogonal to the redundant solution $\xi(r)$. Equation (103) shows that C is arbitrary. The solution $U(r)$, orthogonal to the redundant solution, is given by Eq. (99) with $C = 0$ and is

$$U(r) = \sin kr + Dr e^{-(\alpha + \beta)r} + E \cos kr - E e^{-(\alpha + \beta)r}. \quad (106)$$

The solution $U(r)$ also may be obtained from the fully reduced radial equation

$$\left(\frac{d^2}{dr^2} + k^2\right) \chi(r) = -\lambda' e^{-\beta r} \xi(r) \int_0^\infty \xi(r') e^{-\beta r'} \chi(r') dr'. \quad (107)$$

The most general solution of Eq. (107) is of the form

$$\chi(r) = \sin kr + Hr e^{-(\alpha + \beta)r} \\ + I [\cos kr - e^{-(\alpha + \beta)r}]. \quad (108)$$

Substituting this expression for $\chi(r)$ into Eq. (107) yields

$$H = -8\lambda' \alpha^3 k(\alpha + \beta)^4[(\alpha + \beta)^2 + k^2]/J \quad (109)$$

and

$$I = 16\lambda' \alpha^3 k(\alpha + \beta)^5/J, \quad (110)$$

where

$$J = \lambda' L + (\alpha + \beta)^3[(\alpha + \beta)^2 + k^2]^4 \quad (111)$$

with

$$L = \alpha^3[(\alpha + \beta)^2 + k^2]^3 + 2\alpha^3(\alpha + \beta)^2[(\alpha + \beta)^2 + k^2]^2 \\ - 8\alpha^3(\alpha + \beta)^4[(\alpha + \beta)^2 - k^2]. \quad (112)$$

This solution exists for any value of λ' for which J is not zero. Direct calculation shows that $\chi(r)$ is not orthogonal to $\xi(r)$ unless $\lambda' = \lambda$, where λ is

given by Eq. (100).

These examples demonstrate that it is not possible to obtain a scattering solution to an equation with a nonsymmetric nonlocal potential which produces redundant states unless the consistency condition is fulfilled. On the other hand, an equation which does not exhibit redundant solutions will always have a scattering solution. Thus a reduced equation must be accompanied by appropriate constraints if it is to yield a solution of the original equation.

VII. SYMMETRIC POTENTIAL WITH REDUNDANT STATES

It is possible to construct a nonlocal potential which is symmetric and exhibits redundant states. As discussed earlier, if the potential is symmetric it is not necessary to impose a consistency condition in order to assure a scattering solution.¹² However, the physical interpretation of such a potential is open to question, since Eqs. (36) and (37) show nonsymmetry to be an inherent characteristic of a single-particle effective potential which includes the Pauli principle. Thus, while a symmetric potential has the advantage that a consistency condition is not necessary for a solution to exist, such potential cannot describe completely the Hartree-Fock scattering formalism.

A symmetric potential with redundant states suggested by Saito¹⁷ has been employed^{18,19} in describing scattering with antisymmetrization. Saito's potential follows from considering the equation

$$\Lambda(\epsilon - T_0 - V)\Lambda|u\rangle = 0, \quad (113)$$

where Λ is defined in Eq. (41). Writing out Λ explicitly gives

$$(\epsilon - T_0)|u\rangle = [V + (\epsilon - T_0 - V)\Omega + \Omega(\epsilon - T_0 - V) \\ - \Omega(\epsilon - T_0 - V)\Omega]|u\rangle, \quad (114)$$

where Ω projects onto the redundant states and is defined in Eq. (40). The effective potential in Eq. (114) produces redundant states and is symmetric.

The procedure given by Saito for removing redundant solutions from the spectrum of Eq. (114) is discussed in Ref. 6. Dropping from Eq. (114) all terms which project onto the redundant states gives the reduced equation

$$(\epsilon - T_0)|\chi\rangle = [V - \Omega(T_0 + V)]|\chi\rangle. \quad (115)$$

The solutions of Eq. (115) are orthogonal to the redundant states $|\xi_i\rangle$ and satisfy the full equation, Eq. (114). Because the original nonlocal potential in Eq. (114) is symmetric, this orthogonality will hold for any choice of V . The potential in Eq. (115) is not symmetric. However, since the equation

does not have redundant solutions, the question of the existence of a scattering solution does not arise.

Due to the nonsymmetry of the potential, the full Hartree-Fock equation appears somewhat more complicated than the full Saito equation. On the other hand, the potential in the fully reduced equation due to Saito is not symmetric, whereas the potential in the fully reduced Hartree-Fock equation is. Physically, the nonsymmetry of the full Hartree-Fock potential can be viewed as imposing on that Hartree-Fock equation the restriction that no scattering solution can exist unless it is compatible with the Pauli principle. The consistency condition is then assured for the resulting reduced Hartree-Fock equation.

VIII. CONCLUSION

Accurate single-particle scattering wave functions are needed for a variety of calculations. For example, their importance in direct interaction calculations is well known,^{20,21} since the distorted wave transition amplitude is proportional to the single-particle wave functions in the entrance and exit channels. Thus the behavior of the wave function in the interior region where the projectile and target are strongly interacting becomes a matter of critical concern. Austern²² has emphasized that appropriate antisymmetrization procedures to remove redundant solutions should be incorporated in obtaining the single-particle wave functions.

In studying procedures for obtaining the scattering wave functions, our primary focus has been on the Hartree-Fock technique. In particular, we have shown the importance of considering the full Hartree-Fock single-particle equation. Some examples from the literature are now examined in this context.

The fully reduced Hartree-Fock equation for nucleon-nucleus scattering has been considered by Vautherin and Veneroni,²³ Coz, MacKellar, and Arnold,²⁴ and MacKellar, Reading, and Kerman.⁵ References 5 and 23 solve this equation directly for the scattering phase shifts. Reference 24 investigates the local potential equivalent to this nonlocal Hartree-Fock potential.

The reduced Hartree-Fock potential used in these calculations is obtained from many-body theories.²⁵⁻²⁹ However, as Coz, MacKellar, and Arnold³⁰ have pointed out, potentials produced by many-body theories are far from being exact. Many Hartree-Fock single-particle operators are found in the literature corresponding either to different methods of calculation or to different two-body interactions.

From the considerations of the present paper it

follows that unless the full Hartree-Fock equation is considered, the consistency condition discussed here may fail to be imposed upon the reduced Hartree-Fock potential. This consistency condition can be used in choosing between or modifying nucleon-nucleon matrix elements [for example, the matrix element τ of Eq. (49)]. In fact, if a functional form of the matrix element is assumed, the consistency condition can be used to obtain values for parameters of that matrix element. In the absence of the consistency condition, different reduced Hartree-Fock potentials will result in scattering wave functions which are orthogonal to different nuclear target states.

The importance of those terms present in the full Hartree-Fock equation but not in the fully reduced equation has been discussed also by Schenter and Thaler,¹⁴ Schenter,^{3,4} and Schenter and MacKellar.³¹ These calculations employ a dynamically correlated wave function for the ground state of the target. In Ref. 14 the single-particle scattering equation is examined in the limit in which only the Pauli correlations survive. In this limit, the potential differs from the potential u given by Eqs. (36) and (37) only in that the term \mathcal{R} is not present. Initially, therefore, their result retains the basic structure associated with the potential of Eq. (36). Thus in this limit (which is the Hartree-Fock limit of their calculations) their equation can be put into the form of the Schrödinger equation (1) with a potential u which satisfies Eqs. (36) and (39) and exhibits redundant states. As such, it is a full Hartree-Fock equation.

Margolis³² has pointed out that the $(\epsilon - T_0)$ term in the potential cannot contribute to the scattering amplitude. This is consistent with our identification of this term as that responsible for the redundant solutions. Schenter and Thaler assume that the remaining terms in the full Hartree-Fock equation which are expected to give zero when acting on the scattering wavefunction can be eliminated also. However, this presupposes that the consistency condition discussed in the present paper has been fulfilled. If this is not the case, the solution of the reduced equation will not satisfy the full equation and the terms eliminated will not give zero when acting on this scattering wave function.

Schenter and MacKellar³¹ compare the relative effects of the eliminated terms on the damping of the nucleon-nucleus scattering wave function. Based on Schenter's calculations showing only a very small dependence on the form of the correlation function^{33,34} they conclude that in adding two-body correlations to the ground-state target wave function these terms have a significant effect on the damping. The conclusion is correct only if

the terms eliminated in obtaining the reduced Hartree-Fock equation are, in fact, zero. This will be the case only if the consistency condition has been fulfilled. If the consistency condition has not been incorporated, conclusions regarding the importance of the eliminated terms are open to ques-

tion.

We thank L. G. Arnold, B. Bagchi, and B. C. Clark for helpful discussions. In addition, B. C. Clark read the final version of the manuscript and made many useful suggestions.

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