INELASTIC SCATTERING FORM FACTORS USING PROJECTED HARTREE-FOCK WAVE FUNCTIONS

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ABSTRACT

The theory of inelastic scattering is formulated, using detailed nuclear wave functions which are obtained from nuclear structure calculations. The inelastic scattering is assumed to proceed through a "direct" reaction, and nuclear states are obtained by projecting states of good \( (I^P, J_z) \) from a variational Hartree-Fock wave function. General expressions for transition amplitudes and the nuclear form factors are derived, and the form factors for inelastic proton scattering are presented. These form factors are compared with those based on the shell model and macroscopic collective model. It is concluded that the restrictions imposed in the Hartree-Fock model must be relaxed if the model is to give the correct order of magnitude for reaction cross sections.

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SUMMARY

The theory of inelastic scattering is formulated by use of detailed nuclear wave functions which are obtained from nuclear structure calculations. The inelastic scattering is assumed to proceed through a "direct" reaction, and nuclear states are obtained by projecting states of good \((J^z, J_\pi)\) from a variational Hartree-Fock wave function.

General expressions for transition amplitudes and the nuclear form factors are derived, and the form factors for inelastic proton scattering are presented. These form factors are compared with those based on the shell model and macroscopic collective model. It is concluded that the restrictions imposed in the Hartree-Fock model must be relaxed if the model used here is to give the correct order of magnitude for reaction cross sections.

INTRODUCTION

The success of the distorted wave method in direct reactions, coupled with the availability of more accurate data, makes possible detailed studies of the effects of nuclear structure in nuclear reactions. In the past, however, only relatively simple nuclear wave functions have been used in such studies, namely, those based on the spherical-shell model or the macroscopic collective model. The use of these models in reaction studies has been discussed exhaustively in the literature (refs. 1 to 3). Although the results so obtained have been fairly successful, it is well known that such primitive nuclear wave functions are inadequate for nuclear structure calculations. This raises considerable doubt as to their reliability for the scattering calculations. The point has been emphasized by Glendenning and Veneroni, who, in a recent study of inelastic proton scattering from the even nickel isotopes, found that inelastic scattering is rather sensitive to the details of a microscopic description of the target (ref. 4). Satchler (ref. 5) has given a discussion of inelastic scattering based on the shell-model description of nuclei situated
near closed shells. Reaction studies (ref. 6) which were done after Satchler's work, namely, $A(\text{pp'})A^*$ and $A(p,n)B$, indicate that a more detailed description of the nuclear form factor is required.

In reaction theory, efforts to use detailed descriptions of states of a collective nature have been minimal (ref. 7). Furthermore, it is well known that the spherical shell model does not produce collective effects. Detailed descriptions of the inelastic scattering of $\alpha$-particles and deuterons through collective excitation are generally limited to vibrational states in the region of spherical nuclei. At the present stage of development, reaction studies which make use of the collective model provide only the deformation parameter and multipolarity of the transition. In nucleon inelastic scattering, if such a model is used, there is no provision for the study of spin exchange or particle exchange, and the absence of spin-dependent forces prohibits the study of unnatural parity states which may be excited via spin-flip. More complex projectiles, such as $\alpha$-particles, may require the use of coupled-channel methods to study parity states.

When the macroscopic model is used in distorted wave Born approximation (DWBA) reaction calculations, it is assumed that the inelastic processes result from nonspherical components in the optical potential. A Taylor expansion of the optical potential, in terms of the deformation parameter, is made, and the first order term in the expansion is retained as the interaction which gives rise to inelastic scattering. In the microscopic description, the choice of effective interaction is not this simple. A sum of effective two-body forces between the projectile and the target nucleon will be assumed in this paper. The justification of such a choice will only be apparent after the results of detailed calculations are compared with experiment. As Satchler has suggested (ref. 5), the use of such an effective interaction assumes that multiple scattering is not important; however, if one uses phenomenological optical potentials to describe the distorted waves, then multiple scattering is neglected only in the off-diagonal parts of the scattering matrix. There is little that can be said about the analytic form of the effective interaction because it cannot, as yet, be calculated. The nucleon-nucleon interaction may be chosen to be either the two-nucleon t-matrix or a spin-dependent phenomenological interaction. The nucleon-alpha or nucleon-deuteron t-matrix may be chosen in a similar fashion. It is suggested, however, that for the case of nucleon-nucleon scattering the phenomenological projectile-target nucleon interaction (for intermediate energies, 10 to 50 MeV) should not be radically different from the residual two-body force in the structure problem because the interaction occurs in the field of nuclear matter.

In recent years, the Hartree-Fock (HF) theory (ref. 8) has received considerable attention in nuclear structure studies in the $(p, s-d)$ shell nuclei. Recently Bouten, et al., using HF methods, were quite successful in a structure study of carbon 12 (ref. 9). Structure calculations for other nuclei (refs. 10 and 11) in the $(1, s-d)$ shell have been
equally successful. The self-consistent HF method provides a microscopic model which may be used to study systems of many bound nucleons. A particularly attractive feature of this model is the inclusion of residual two-body forces between the nucleons in the system. The self-consistency requirement coupled with the use of residual two-body forces in the Hamiltonian for the nucleus gives rise to deformed orbits, if the angular HF method is used. If a static (time independent) HF calculation is performed, one obtains an intrinsic wave function for a statically deformed nucleus, and it is possible to project from the intrinsic wave function states of good J and M which exhibit a rotational character. The extension of these methods to a time dependent formalism may be used to describe vibrational states (ref. 12), although these states are not discussed in any detail herein.

The major objective of this paper is to formulate a microscopic theory of inelastic scattering from deformed nuclei. The nuclear wave functions for the target and residual nucleus are obtained by projecting states of good J and M from the intrinsic HF state. These wave functions are then used to calculate nuclear form factors for reaction studies. Furthermore, a recent study of the exchange term in the transition amplitude for inelastic nucleon scattering indicates that the exchange term is not negligible (ref. 3); these effects will be included in the reaction formalism to be presented herein.

The transition amplitude is discussed in detail, and nuclear form factors are defined; detailed expressions are given for the nuclear form factors for the case in which the nuclear states are described by projected HF wave functions. A comparison of the HF form factors with those obtained from use of projected shell model states and the macroscopic collective model is also presented.

**SYMBOLS**

\[
\begin{align*}
A(B) & \quad \text{refers to (A-1), particle systems} \\
A_{jm}, B_{jm} & \quad \text{irreducible tensors of rank } j \\
a, b, \ldots & \quad \text{quantum numbers for particular single-particle states} \\
a_s & \quad \text{diffuseness of Wood-Saxon well} \\
B & \quad \text{N} \times \text{N matrix} \\
B_{\lambda\mu} & \quad \text{element of matrix } B \\
C_J & \quad \text{normalization factor for macroscopic form factor} \\
C_{jm} & \quad \text{expansion coefficients for Hartree-Fock orbits}
\end{align*}
\]
\( \mathbf{D}^{J}_{MK}(\Omega) \)  
rotation matrix

\( e_{\lambda} \)  
Hartree-Fock single-particle energy

\( f_{LS}^{ab}(r_0) \)  
single-particle form factors

\( h \)  
Hartree-Fock Hamiltonian

\( i(f) \)  
incident (outgoing) channel

\( (J, M) \)  
total angular momentum transfer and its projection onto z-axis

\( (J_i, M_i) \)  
total angular momentum and projection for nucleus in channel i

\( (j_a m_a) \)  
total angular momentum and projection for single-particle

\( \langle j_1 m_1, j_2 m_2 |JM \rangle \)  
Clebsch-Gordan coefficient

\( K \)  
projection of J onto z-axis of the body-fixed system

\( k_i \)  
wave number of the projectile in channel i

\( (LM_L) \)  
orbital angular momentum transfer and projection

\( (l_a, m_a) \)  
single-particle orbital angular momentum and projection

\( \{l_1 s_1 j_1\} \)  
symmetric 9-j coefficient

\( m \)  
reduced mass of the projectile

\( \mathcal{N} \)  
normalization factor

\( P_L(r_0, r_1) \)  
Legendre polynomial with argument which is cosine of angle between \( r_0 \) and \( r_1 \)

\( P^{J}_{MK} \)  
angular momentum projection operator

\( P_{SE} \)  
projection operator for singlet-odd states

\( P_{TE} \)  
projection operator for triplet-even states

\( P_{H} \)  
Heisenberg exchange operator

\( R_S \)  
radius of Wood-Saxon well

\( S^J_J \)  
spectroscopic factor for angular momentum transfer J

\( S^n_J \)  
neutron part of spectroscopic factor

4
$S^p_J$  
proton part of spectroscopic factor

$(S, \mu_S)$  
spin angular momentum and projection

$(S_0, \mu)$  
projectile spin and projection onto z-axis

$T_{ab}$  
single-particle transition amplitude

$T_{if}$  
direct-reaction transition amplitude

$T_{JM}$  
coupled form of transition amplitude

$T_{qr}$  

coupled form of $T_{qr}(0)$

$T_{qrLJM}$  
transition amplitude for transfer of definite $L$ and $S$

$t_{qr}(0)$  
effective single-particle interaction

$t_{JM}(0)$  
coupled form of $t_{qr}(0)$

$t(0, 1)$  
projectile-nucleon interaction

$U(j_1j_2 J j_4; j_3 J')$  
$\left[(2j_3 + 1)(2J' + 1)\right]^{1/2} W(j_1j_2 J j_4; j_3 J')$

$U_0$  
strength of real part of optical potential

$V_{op}(r_0)$  
optical potential

$v(i, j)$  
two-particle interaction used in structure calculations

$W(j_1j_2 J j_4; j_3 J')$  
Racah coefficient

$Y_{LM}^{(r_0)}$  
spherical harmonic with argument denoted by unit vector $\hat{r}_0$

$Y_{LSJ}^{M}$  
spin-angle tensor

$\beta_J$  
deformation parameter

$\eta_a, \eta^\dagger_a$  
destruction and creation operators for single-particle states

$\lambda$  
Hartree-Fock single-particle orbits

$\vec{\sigma}_S$  
spin tensor operator

$\frac{d\sigma}{d\Omega}$  
differential cross section

$\tau$  
isospin

$\Phi$ or $\Phi_K$  
determinantal wave function for A-particle system
Under the assumption that the projectile-target interaction can be written as a sum of two-body interactions, the DWBA transition amplitude for inelastic scattering from a target containing \( A \) nucleons is

\[
T_{if} = A \langle \psi_f^- (0) \psi_f (1 \ldots A) | t(0, 1) | \psi_i^+ (0) \psi_i (1 \ldots A) \rangle
\]

The initial and final nuclear states are represented by \( \psi_i \) and \( \psi_f \), and the initial and final projectile states by the distorted waves \( \psi_i^+ \) and \( \psi_f^- \). We assume that integration over the internal coordinates of the projectile has already been carried out, so that 0 stands for the spin, isospin, and center-of-mass coordinates of the projectile. The projectile-nucleon interaction is represented by \( t(0, 1) \); it may be the \( t \)-matrix, for instance, or a phenomenological pseudopotential. For nucleon-nucleus scattering, the major exchange term (ref. 3) may be included simply by writing

\[
t(0, 1) \left( 1 - P_{01}^H \right)
\]

in place of \( t(0, 1) \), where \( P_{01}^H \) is the (Heisenberg) operator which exchanges all the coordinates of particles 0 and 1.
Because of the assumption that the projectile-target interaction is two body in character, it is possible to express the transition amplitude in terms of single-particle transition amplitudes. We begin by expanding the initial and final nuclear states in a complete set \( \{ \varphi_{jm} \} \) of single-particle wave functions, where \( j \) stands for all the quantum numbers \((nlj\tau)\) except for the \( z \)-component of angular momentum, which is denoted by \( m_0 \). (Often, however, \( a \) will be written for the set \( j_\alpha m_\alpha \), the set \( j_\alpha \), or even the set \( n_\alpha l_\alpha \tau_\alpha \), when no confusion will result.) Thus,

\[
\Psi_i(1 \ldots A) = A^{-1/2} \sum_a \varphi_a(1)\Psi_ia(2 \ldots A) \quad (2a)
\]

\[
\Psi_f(1 \ldots A) = A^{-1/2} \sum_b \varphi_b(1)\Psi_fb(2 \ldots A) \quad (2b)
\]

The scattering amplitude then becomes

\[
T_{if} = \sum_{ab} \langle \Psi_{fb} | \Psi_{ia} \rangle T_{ab} \quad (3)
\]

where the single-particle transition amplitude \( T_{ab} \) is given by

\[
T_{ab} = \langle \psi_f(+)0(1)|t(0,1)|\psi_i(-)0(1)\rangle \quad (4)
\]

It is convenient to express both \( T_{if} \) and \( T_{ab} \) as sums of amplitudes for transfer of total angular momentum \((J,M)\)\(^1\)

\[
T_{if} = \sum_{JM} \langle J_i M_i, JM | J_f M_f \rangle T_{if}^{JM} \quad (5a)
\]

\[
T_{ab} = \sum_{JM} \langle j_a m_a, JM | j_b m_b \rangle T_{ab}^{JM} \quad (5b)
\]

\(^1\)Condon and Shortley conventions are used for the Clebsch-Gordon coefficients \( \langle J_1, m_1, j_2 m_2 | JM \rangle \). Reduced matrix elements, W-coefficients and the 9-J coefficients, are defined in ref. 13. The U-coefficient was introduced by H. A. Jahn (ref. 14).
And also to express $\psi_{ia}$ and $\psi_{fb}$ in terms of angular momentum eigenstates:

$$\psi_{ia} = \sum_{J_A M_A} \langle J_A M_A, j_a m_a | J_{i M_{i}} \rangle \psi^{J_A M_A}_{ia}$$  \hspace{1cm} (6a)$$

$$\psi_{fb} = \sum_{J_B M_B} \langle J_B M_B, j_b m_b | J_{f M_{f}} \rangle \psi^{J_B M_B}_{fb}$$  \hspace{1cm} (6b)$$

Then the relation

$$T^J_{if} = \sum_{ab} S_{J}(i|ab)T^{JM}_{ab}$$  \hspace{1cm} (7)$$

holds, where the spectroscopic amplitude $S_J$ is given by

$$S_{J}(i|ab) = \sum_{J_{A}} U(j_{a}J_{A}J_{f}|J_{i}b) \left\langle \psi^{J_{A}}_{fb} | \psi^{J_{A}}_{ia} \right\rangle$$  \hspace{1cm} (8)$$

In the event that the distorted waves do not have spin-orbit coupling, one can decompose $T^{JM}$ still further into amplitudes for transfer of definite $L$ and $S$:

$$T^{JM} = \sum_{LM_{L}, SM_{S}} \langle S_{0}^{\mu_{i}}, SM_{S} | S_{0}^{\mu_{f}} \rangle \langle LM_{L}, SM_{S} | JM \rangle T^{LSJM}_{L}$$  \hspace{1cm} (9)$$

$$T^{LSJM}_{L} = \sum_{ab} S_{J}(i|ab)T^{LSJM}_{ab}$$  \hspace{1cm} (10)$$

Here $S_{0}$ is the spin of the projectile, and $\mu_{i}$ and $\mu_{f}$ are its initial and final projections on the z-axis. The sum over initial and final states of the entire system is incoherent in this case, so that we obtain
\[
\left( \frac{d\sigma}{d\Omega} \right)_{if} = \left( \frac{m}{2\pi \hbar^2} \right)^2 \frac{k_f}{k_i} \frac{2J_f + 1}{2J_i + 1} \sum_{LSJ} \frac{\sigma_{LSJ}}{(2L + 1)(2S + 1)}
\]  

where

\[
\sigma_{LSJ} = \sum_{M_L} \left| T_{i f}^{LSJM_L} \right|^2
\]

Single-Particle Transition Amplitude

With equation (7) the first step of the program, namely, to separate details of the reaction mechanism (given by \( T_{ab} \)) from details of the nuclear structure (given by \( S_J \)), is complete. The single-particle transition amplitude is of secondary concern; it may be evaluated in a number of ways (ref. 6), depending on the specific forms of \( t(0, 1) \) and the distorted waves. For example, when the optical potential has no spin-orbit term, and the spin dependence of the two-body interaction can be expressed in terms of the spin tensors \( \sigma_0 = 1 \) and \( \sigma_1 = 2S \) as

\[
t(0, 1) = \sum_S t_S (\vec{r}_0, \vec{r}_1) \vec{\sigma}_S(0) \cdot \vec{\sigma}_S(1)
\]

the equation

\[
T_{ab}^{LSJM_L} = \langle S_0 | \sigma_S | S_0 \rangle g_{LSJ}^{ab} T_{ab}^{LSM_L}
\]

is obtained, where

\[
g_{LSJ}^{ab} = \sqrt{2(2l_b + 1)(2j_a + 1)(2S + 1)(2J + 1)} \begin{pmatrix} l_a & 1/2 & j_a \\ L & S & J \\ l_b & 1/2 & j_b \end{pmatrix}
\]
If $T_s$ is central, an expansion in Legendre polynomials yields

$$t_s(r_0, r_1) = \sum_{L} \frac{2L+1}{4\pi} P_L(r_0 \cdot r_1) t_{LS}(r_0, r_1)$$

(17)

where the single-particle form factor $f_{LS}^{ab}$ is given by

$$f_{LS}^{ab}(r_0) = \langle \ell_b | Y_L | \ell_a \rangle \int_0^\infty \varphi_b^*(r_1) t_{LS}(r_0, r_1) \varphi_a(r_1) r_1^2 \, dr_1$$

(19)

A convenient way to express this result is to define a nuclear form factor, $f_{LSJ}^{if}(r_0)$, such that

$$T_{if}^{LSJM} = \langle S_0 | \sigma_S | S_0 \rangle \int \psi_f^{(-)}(r_0)^* \int \varphi_b^*(r_1) t_{LSJ}(r_0) Y_L^* Y_L \varphi_a^*(r_0) \psi_a^*(r_0) \, dr_0$$

(20)

and then to write it in terms of the single-particle form factors:

$$f_{LSJ}^{if}(r_0) = \sum_{ab} S_J^{if(ab)} g_{LSJ}^{ab} f_{LS}^{ab}(r_0)$$

(21)

If the two-body interaction $t(0, 1)$ is isospin-dependent, $t_{LS}(r_0, r_1)$ will be a function of the isospin coordinates of the projectile and the bound nucleon. One could introduce a general formalism for handling the isospin at this point. When Hartree-Fock wave functions are used, however, there occurs a natural separation of the spectroscopic amplitude
S_\text{J} into a neutron part S_\text{J}^n and a proton part S_\text{J}^p. Examples of the isospin treatment will therefore be deferred to the section Spectroscopic Factor.

Exchange term for inelastic nucleon scattering. - In the case of inelastic nucleon scattering, Amos, et al. (ref. 3) have shown that the exchange term is nearly in phase with the direct term, and makes a substantial contribution to the cross section. To include this term, when the spin-dependence of t(0, 1) is as in equation (13), t_S(\vec{r}_0, \vec{r}_1) in equation (16) must be replaced by

$$t_S(\vec{r}_0, \vec{r}_1) - \sum_{S'} \epsilon_{SS'} t_S(\vec{r}_0, \vec{r}_1) p_{01}^{MT}$$

where $p_{01}^{MT}$ is an operator which exchanges the space and isospin coordinates of nucleons 0 and 1 and where

$$\epsilon_{SS'} = (-1)^{S+S'-1}(2S' + 1)W(\frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} | SS') = \frac{1}{2} - \frac{2}{3} \delta_{S1} \delta_{S'1}$$

The exchange terms cannot be put in a form like equation (18), of course, so no form factor can be defined.

Form factors for coupled channel calculation. - In some reactions, transition rates to various excited states of the nucleus are comparable in magnitude to the ground state (elastic) transition rate. Consequently, even an approximate wave function should have considerable projection onto these excited states, and the resulting analysis is a coupled-channels calculation. For such a calculation a set of effective projectile-target interactions of the form

$$t_{if}(0) = A \langle \psi_i(1 \ldots A) | t(0, 1) | \psi_f(1 \ldots A) \rangle$$

$$= \sum_{JM} \langle J_i M_i, JM | J_f M_f \rangle t_{if}^{JM}(0)$$

is needed, where the integration extends over the nuclear coordinates and the internal coordinates of the projectile and $i$ and $f$ now label the nuclear states included in the expansion of the total wave function. Proceeding exactly as before, a single-particle effective interaction is introduced.
The two equations are related by

\[ t_{ab}(0) = \langle \varphi_b(1) | t(0, 1) | \varphi_a(1) \rangle \]

\[ = \sum_{JM} \langle j_a m_a, JM | j_b m_b \rangle t_{ab}^{JM}(0) \]  (25)

When \( t(0, 1) \) can be expanded in spin tensors and spherical harmonics as in equations (13) and (17), the equation

\[ t_{ab}^{JM}(0) = \sum_{ab} S_{j}(if|ab)t_{ab}^{JM}(0) \]  (26)

is obtained, where \( f_{LSJ}^{if} \) is defined in equation (21) and the spin-angle tensor \( \mathcal{Y}_{LSJ}^{M} \) is given by

\[ \mathcal{Y}_{LSJ}^{M}(0) = \sum_{M_L M_S} \langle LM_L, SM_S | JM \rangle Y_{LM_L}(r_0) \mathcal{Y}_{SM_S}(0) \]  (28)

**Spectroscopic Factor**

The evaluation of \( S_J \) is performed using Hartree-Fock wave functions. As is well known, the Hartree-Fock method consists of approximating the nuclear wave function by a single Slater determinant,

\[ \Phi = (A!)^{-1/2} \det \{ \varphi_\lambda \} \]  (29)

where \( \{ \varphi_\lambda \} \) is a set of single-particle wave functions, or orbitals. These functions are determined by the requirement that \( \Phi \) minimizes the expectation value of the nuclear Hamiltonian \( H \), which leads to the coupled eigenvalue equations

\[ \hbar \varphi_\lambda = \epsilon_\lambda \varphi_\lambda \]  (30)
where

\[ h(i) = \frac{p_i^2}{2m} + \sum_{\mu} \int d\tau_j \phi^+_{\mu}(j)v(i, j) \left(1 - P^H_{ij}\right) \phi_{\mu}(j) \]  

(31)

with the \(\mu\)-sum restricted to those orbitals used to construct \(\Phi\).

The intrinsic HF wave function does not depend on the orientation of the deformed field relative to the space-fixed system, and, clearly, the single-particle energies of the nucleons in the deformed field do not depend on this orientation. Thus, states of the intrinsic system which are based on the same deformed field are degenerate with respect to orientation; any two such states are simply related by

\[ \varphi_K(\vec{x}') = R(\Omega)\varphi_K(\vec{x}'') \]  

(32)

where \(\Omega\) is the orientation of \(\vec{x}''\) relative to \(\vec{x}'\). Also, it should be noted that the states \(\varphi_K\) are not states of good \(J\). However, it is possible to construct states of good \(J\) and \(M\) in the space-fixed system by taking appropriate linear combinations of the degenerate states \(\varphi_K(\vec{x}')\).

In order to determine the expansion coefficients, a particular \(\varphi_K(\vec{x}')\) is expanded in a complete set of states \(\{\psi^K_J(\vec{x}')\}\) which are normalized eigenstates of \(J^2\) and \(J_z\) in the body-fixed system:

\[ \varphi_K(\vec{x}') = \sum_J a_J \psi^K_J(\vec{x}') \]  

(33)

Here, \(\vec{x}'\) stands for all the coordinates in the body-fixed frame. If \(\psi^K_J(\vec{x}')\) is now expressed in terms of the states \(\psi^M_J(\vec{x})\) in the space-fixed frame

\[ \psi^K_J(\vec{x}') = R(\Omega)\psi^K_J(\vec{x}) = \sum_M D^J_{MK}(\Omega)\psi^M_J(\vec{x}) \]  

(34)

where \(\Omega\) is the orientation of the body-fixed frame relative to the space-fixed frame, then

\[ \varphi_K(\vec{x}') = \sum_{JM} a_J D^J_{MK}(\Omega)\psi^M_J(\vec{x}) \]  

(35)
This expression may be inverted to give

\[ \psi^M_J(\mathbf{x}) = \frac{2J + 1}{8\pi^2 \alpha_J} \int d\Omega D^J_{MK}(\Omega)^* \varphi_K(\mathbf{x}') \]  

(36)

A linear combination of intrinsic states, with

\[ \frac{2J + 1}{8\pi^2 \alpha_J} D^J_{MK}(\Omega)^* \]  

(37)

as the weighting coefficients, gives rise to a state of good \( J \) and \( M \) in the space-fixed frame (eq. (17)). It is not necessary to calculate each \( q_K(zT) \) individually, because

\[ \varphi_K(\mathbf{x}') = R(\Omega) \varphi_K(\mathbf{x}) \]

hence, equation (17) can be written

\[ \psi^M_J(\mathbf{x}) = \frac{2J + 1}{8\pi^2 \alpha_J} \int d\Omega D^J_{MK}(\Omega)^* R(\Omega) \varphi_K(\mathbf{x}) \]  

(38)

Thus, it is sufficient to calculate \( \varphi_K \) in the space-fixed frame and carry out integration (18), which is denoted symbolically by

\[ \psi^M_J(\mathbf{x}) = D^J_{MK} \varphi_K(\mathbf{x}) \]  

(39)

It is clear that, from one intrinsic state \( \varphi_K \), many states \( \psi^M_J \) may be generated; these are usually associated with the rotational bands found in deformed nuclei. The Slater determinant \( \varphi_K(\mathbf{x}) \) may be written as the antisymmetrized product of two determinants, one of which represents the spherical closed-shell core and the other the \( M \) nucleons outside the core. Because the core determinant has \( J = 0 \), it will be unaffected by the rotation operator \( R(\Omega) \). Hence, the net effect of the rotation operator in equation (18) will be to rotate each of the orbits in the extracore determinant only, or equivalently, to rotate only the extracore orbitals in \( \varphi_K \).

Of course, the state \( \psi^M_J(\mathbf{x}) \) yields a higher expectation value of \( H \) than \( \Phi \) does, because of the cross terms, but it is hoped that the discrepancy is not large. Calculations in the s-d shell confirm this hope, at least for low-lying nuclear levels (refs. 10 and 11).
A better procedure would be to determine the set \{\varphi_\lambda\} by minimizing \langle\Psi|H|\Psi\rangle directly, but this is a formidable task and until recently (ref. 9) has not been attempted.

Quite commonly the nucleus is represented as N nucleons outside a closed-shell core, and the core orbitals are not varied in the Hartree-Fock procedure. In that case equation (37) becomes

$$h(i) = h_c(i) + \sum_\mu' \int d\tau_j \varphi_\mu^+(j) v(i, j) \left(1 - P_{ij}^H\right) \varphi_\mu(j)$$

(40)

where \(h_c(i)\) is the Hamiltonian (eq (31)) for the core orbitals and the sum over \(\mu\) is limited to the extracore orbitals in \(\Phi\). Usually \(h_c\) is not dealt with directly; instead, its eigenfunctions are assumed to be shell model orbitals (harmonic oscillator functions, for instance), and its eigenvalues are taken from experiment (ref. 15). As before, eigenstates of \(J^2\) and \(J_z\) are obtained using equation (32), but, because of the closed-shell core, a simplification occurs. The determinant \(\Phi\) may be written as the antisymmetrized product of two determinants, one of which represents the core nucleons. This latter determinant has \(J^2 = 0\) and is thus invariant under rotations. Hence, the net effect of the rotation operator in equation (32) is to rotate only the extracore orbitals in \(\Phi\).

Whatever method is used to determine \(\{\varphi_\lambda\}\), we assume that the nuclear wave functions are single Slater determinants projected onto states of good \(J\) and \(M\) by means of equation (18). We also assume the existence of a closed-shell core, identical in initial and final states, because, in the final results, the core can always be taken to contain no particles. Finally, we assume that the set \(\{\varphi_\lambda\}\) has been made orthonormal, because any nonorthogonal components would make no contribution to the Slater determinants.

The first task is to show that the summation over single-particles in equation (3), and consequently in equation (7), is restricted to states outside the core. This is easiest to show in the notation of second quantization, using fermion creation and annihilation operators, for, then, the overlap integral in equation (3) may be written

$$\langle\Psi_{fb}|\Psi_{ia}\rangle = \langle\Psi_f|\eta_b^+\eta_a|\Psi_i\rangle$$

$$= \delta_{ab} \langle\Psi_f|\Psi_i\rangle - \langle\Psi_f|\eta_a\eta_b^+|\Psi_i\rangle$$

(41)

The first term on the right side of equation (34) vanishes for inelastic transitions, because the initial and final nuclear states are orthogonal. The second term will also vanish, if either a or b refers to a core state, because the core has been unaffected.
by the projection procedures of equation (32) (except for antisymmetrization) and is consequently still filled.

We next turn to evaluation of the spectroscopic amplitude $S_J$. If the nucleus is not spherical, the orbits $\varphi_\lambda$ will, in general, be of the form

$$\varphi_\lambda = \sum_{jm} C_{jm}^\lambda \varphi_{jm}$$  \hfill (42)

where $\{\varphi_{jm}\}$ is the complete set used earlier. Consequently, an expansion of the determinant $\Phi$ leads to

$$\Phi = A^{-1/2} \sum_{\lambda jm} C_{jm}^\lambda \varphi_{jm}(1) \Phi_\lambda(-1)$$  \hfill (43)

where $\Phi_\lambda(-1)$ is the cofactor of $\varphi_\lambda$ in $\Phi$ and is itself a normalized Slater determinant for $A-1$ nucleons.

The projection operator $P_{MK}^J$ must now be applied to $\Phi$. From the definition of $\Phi$, it may be shown that $P_{MK}^J$ picks out states whose $J^2$ and $J_z$ eigenvalues are $J(JH)$ and $K$, respectively, and then changes the $J_z$ eigenvalue from $K$ to $M$. Consequently, $P_{MK}^J$ transforms under rotations like an irreducible tensor $A_{jm}$. The product of another irreducible tensor $A_{jm}$ with $P_{M'K'}^J$ may therefore be written

$$A_{jm} P_{M'K'}^J = \sum_{J_1 M_1} \langle J'M', jm | J_1 M_1 \rangle B_{J_1 M_1} (j; J'K')$$  \hfill (44)

and application of $P_{MK}^J$ then yields

$$P_{MK}^J A_{jm} P_{M'K'}^J = \langle J'M', jm | JK \rangle B_{JM} (j; J'K')$$

$$= \langle J'M', jm | JK \rangle \sum_{m' \mu} \langle J' \mu, jm' | JM \rangle A_{jm, \mu K'} P_{\mu K'}$$  \hfill (45)

(Note that $B_{JK}$ has been singled out and then transformed to $B_{JM'}$.) Setting $K' = M'$ and summing both sides of equation (45) over all $J'$ and $M'$ results in
\[ P_{MK}^{JM} = \sum_{m}^{J'} A_{jm'} \sum_{JM'} \langle J'M', jm | JK \rangle \langle J'M', jm' | JM \rangle P_{JM'}^{JM} \]  

which is the desired theorem.

Using equations (43) and (46) to construct the nuclear wave function \( \Psi_{JM} \) yields

\[ \Psi_{JM} = \sum_{K} P_{MK}^{JM} \Phi \]

\[ = A^{-1/2} \sum_{jm} \varphi_{jm}(1) \sum_{JM} \langle J'M', jm | JM \rangle \sum_{\lambda K M' m'} C_{jm', JM'} \langle J'M', jm' | JK \rangle P_{JM'}^{JM} \Phi_{\lambda}(-1) \]  

From the definitions of \( \psi_{ia}^{JAMA} \) and \( \psi_{fb}^{JBMB} \), given by equations (2) and (6), it follows by comparison with equation (47) that

\[ \psi_{ia}^{JAMA} = \sum_{\lambda_1 M'_{A} m_a K_i} C_{A}^{\lambda_1} \langle J'M'_{A}, j_a m_a | J_1 K_i \rangle P_{M_{A} M_{A}}^{JM} \Phi_{\lambda_1}(-1) \]  

\[ \psi_{fb}^{JBMB} = \sum_{\lambda_2 M'_{B} m_b K_f} C_{B}^{\lambda_2} \langle J'M'_{B}, j_b m_b | J_f K_f \rangle P_{M_{B} M_{B}}^{JM} \Phi_{\lambda_2}(-1) \]  

The overlap integral needed for evaluation of \( S_J \) is therefore given by

\[ \langle \psi_{fb}^{J} || \psi_{ia}^{J} \rangle = \sum_{\lambda_1 \lambda_2} \sum_{m_a m_b} \langle C_{b}^{\lambda_2} \rangle^{*} C_{A}^{\lambda_1} \sum_{M_{A} M_{B}} \langle J_{A} M_{A}, j_a m_a | J_1 K_i \rangle \]

\[ \times \langle J_{A} M_{A}, j_b m_b | J_f K_f \rangle \langle \Phi_{\lambda_2} || P_{M_{B} M_{B}}^{JM} \Phi_{\lambda_1} \rangle \]  

For simplicity, the normalization of the initial and final nuclear states has been ignored in the derivation of equation (49). It is clear, however, that
\[ \sum_{K} P_{MK}^{J} \Phi \]

will not be normalized to unity, even if \( \Phi \) is, and equation (49) should therefore be multiplied by the normalization factor

\[ N = \left( N_{1} N_{f} \right)^{-1/2} \]  

(50)

where

\[ N_{1} = \langle \psi_{1} | \psi_{1} \rangle = \sum_{KK'} \langle \Phi_{1} | J_{i} | P_{KK'} \Phi_{1} \rangle \]  

(51a)

\[ N_{f} = \langle \Phi_{f} | \psi_{f} \rangle = \sum_{KK'} \langle \Phi_{f} | J_{f} | P_{KK'} \Phi_{f} \rangle \]  

(51b)

The integrals appearing in equations (49) and (51) are evaluated by means of the integral representation (32) for \( P_{MK}^{J} \). Consider the normalization integral, which contains terms of the form

\[ \int d\Omega D_{MK}^{J}(\Omega)^{*} \langle \Phi | \widetilde{\Phi} \rangle \]  

(52)

where \( \widetilde{\Phi} = R(\Omega) \Phi \). The effect of \( R(\Omega) \) on \( \Phi \) is to rotate each of the \( N \) extracore orbitals in \( \Phi \). The core orbitals in \( \Phi \) and \( \widetilde{\Phi} \) are identical, and so we find that

\[ \langle \Phi | \widetilde{\Phi} \rangle = \det \{ B \} \]  

(53)

where \( B \) is an \( N \times N \) matrix with elements

\[ B_{\lambda \mu} = \langle \varphi_{\lambda} | \widetilde{\varphi}_{\mu} \rangle = \langle \varphi_{\lambda} | R(\Omega) | \varphi_{\mu} \rangle \]  

(54)

The integral in equation (49) is treated in a similar fashion, except that now terms of the form

\[ \int d\Omega D_{MK}^{J}(\Omega)^{*} \langle \Phi_{1\lambda} | \widetilde{\Phi}_{1\mu} \rangle \]  

(55)
are encountered. Here $\Phi_{\lambda}^\lambda$ and $\Phi_{\mu}^\mu$ are normalized Slater determinants for $A-1$ particles, again with identical core orbitals. It can be shown in this case that $\langle \Phi_{\lambda}^\lambda | \Phi_{\mu}^\mu \rangle$ is equal to the cofactor of $B_{\lambda\mu}$ in the determinant $\det \{ B \}$. An elementary theorem concerning cofactors of determinants then permits us to write

$$\langle \Phi_{\lambda}^\lambda | \Phi_{\mu}^\mu \rangle = b_{\mu\lambda} \det \{ B \} \quad (56)$$

where $b_{\mu\lambda}$ is an element of the matrix $b = B^{-1}$.

Most Hartree-Fock calculations are made without isospin mixing, which means that each orbital is either a pure neutron state or proton state. The summation in equation (49) is therefore restricted by the condition $\tau_1 = \tau_2$, and the result vanishes unless $\tau_a = \tau_b$. One may thus speak of the proton part $S_p^J$ or the neutron part $S_n^J$ of the spectroscopic factor defined in equation (8).

**FORM FACTORS FOR 2s-1d SHELL NUCLEI**

**Structure of s-d Shell Nuclei**

The general procedure that is used to obtain nuclear states of good $J^2$ and $J_Z$ was discussed in the previous section. In the calculation of the "intrinsic" state defined in equation (29), we have assumed that oxygen 16 constitutes the inert closed-shell core. The 2s-1d shell nuclei are considered to be axially symmetric, although there have been some calculations which indicate regions of asymmetry (namely, $^{24}\text{Mg}$, $^{32}\text{S}$). However, because the prediction of asymmetric regions in the s-d shell is based only on the examination of the intrinsic spectra and because the assumption of axial symmetry has already yielded excellent structure results (ref. 8), we believe that the assumption is justified. In this case, equation (32) becomes

$$\Psi_{JM}^J = \Phi_{MK}^J \Phi_K^J \quad (57)$$

and the orbitals $\varphi_{\lambda}$ will be of the form

$$\varphi_{\lambda} = \sum_j c_{j\lambda}^\lambda \varphi_{j\lambda} \quad (58)$$

The subspace of the basis states is limited to the 2s-1d shell (i.e., $1d_{5/2}$, $2s_{1/2}$, $1d_{3/2}$), with harmonic oscillator radial dependence. The spherical single-particle
energies are taken from experiment, and the two-body interaction which appears in equation (33) is chosen to be a Rosenfeld mixture with a Gaussian radial dependence:

\[ v(i, j) = V_0 e^{-\mu r^2} \frac{\tau_i - \tau_j}{3} (0.3 + 0.7 \sigma_i - \sigma_j) \]

with \( V_0 = +55 \text{ MeV} \). The harmonic oscillator constant, \( \nu = m\omega/\hbar \), was chosen such that \( \mu = \nu \). There has been no correction for center-of-mass motion.

The determinate wave function \( \Phi_K \) is constructed in such a way that, along with each single-particle state, one also includes the time reversed state

\[ \varphi_{-\lambda} = \sum_j C_j^\lambda (-1)^{j-m_\lambda} \varphi_{j-m_\lambda} \] (59)

that is, a proton and neutron are put in the state (58) and the state (59). This gives rise to a fourfold degeneracy of each orbit in an even-even nucleus; the resulting determinate wave function is then the time reversed invariant. The construction of such states for odd nuclei is more involved and will not be considered.

**TABLE I. - ENERGIES AND WAVE FUNCTIONS FOR NEON 20 AND MAGNESIUM 24**

<table>
<thead>
<tr>
<th>Nucleus and Hartree-Fock energy</th>
<th>Hartree-Fock single-particle energy, ( e_\lambda ), MeV</th>
<th>Projection of angular momentum onto z-axis, ( m_\lambda )</th>
<th>Projection of Hartree-Fock orbits onto spherical basis, ( C_j^\lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne(^{20}) (( E_{HF} = -38.95 \text{ MeV} ))</td>
<td>-16.42</td>
<td>1/2</td>
<td>\begin{tabular}{lll} 1d_{5/2} &amp; 2s_{1/2} &amp; 1d_{3/2} \ 0.7155 &amp; -0.5731 &amp; -0.3996 \end{tabular}</td>
</tr>
<tr>
<td>Mg(^{24}) (( E_{HF} = -75.68 \text{ MeV} ))</td>
<td>-18.66</td>
<td>1/2</td>
<td>\begin{tabular}{lll} 1d_{5/2} &amp; 2s_{1/2} &amp; 1d_{3/2} \ 0.6997 &amp; -0.6400 &amp; -0.3175 \end{tabular}</td>
</tr>
<tr>
<td></td>
<td>-12.14</td>
<td>3/2</td>
<td>\begin{tabular}{lll} 1d_{5/2} &amp; 2s_{1/2} &amp; 1d_{3/2} \ 0.9616 &amp; 0 &amp; -0.2744 \end{tabular}</td>
</tr>
</tbody>
</table>

The \( C_j^\lambda \)'s for neon 20 and magnesium 24 (Ne\(^{20}\) and Mg\(^{24}\)) have been obtained from a computer code (private communication, W. Bassichis) which solves the variational problem by an iterative procedure. In table I, the results of these calculations are given for

\( ^2 \)A Yukawa radial dependence was also investigated and yielded results almost identical to the Gaussian dependence.
occupied proton (or neutron) orbits with positive m-projection. The orbits for the time-reversed states may be obtained by application of equation (3). The degenerate orbits are specified by the HF single-particle energies, $e_\lambda$ (see eq. (33)).

It is clear from examination of table I that the orbits in both Ne\(^{20}\) and Mg\(^{24}\) are strongly deformed. These results are in agreement with results obtained by other researchers (ref. 16).

**Direct Interaction**

The calculation of microscopic form factors for inelastic scattering requires a knowledge of the projectile-nucleon interaction. At the present stage of development, the theories of the nucleus and reactions are not sufficient to provide such a force. Instead, either a phenomenological interaction or the two-nucleon t-matrix must be used. From this point on, the projectile is assumed to be a nucleon.

We have chosen a phenomenological spin-dependent interaction which was used by Glendenning and Veneroni in a recent study of inelastic scattering (ref. 4). These authors assumed the two-body interaction to be important only in even states, and used an interaction of the form

$$V(\mathbf{r}) = -52e^{-(r/1.95)^2}(P_{TE} + 0.6 P_{SE})$$

where $P_{TE}$ and $P_{SE}$ are projection operators for the triplet-even and single t-even states, respectively. In terms of single-particle operators,

$$V(\mathbf{r}) = -52 \left[ 0.3 \left( 1 - \frac{1}{2} \vec{\tau}_0 \cdot \vec{\tau}_1 \right) - 0.1 \left( \frac{1}{2} + \vec{\tau}_0 \cdot \vec{\tau}_1 \right) \vec{\sigma}_0 \cdot \vec{\sigma}_1 \right] e^{-(r/1.85)^2}$$

where $\vec{\tau}_0$ and $\vec{\tau}_1$ refer to the isospin of the projectile and bound nucleon, respectively.

Comparing equation (61) with equation (13), it is shown that (with $r = |\mathbf{r}_0 - \mathbf{r}_1|$)

$$t_0(\mathbf{r}_0, \mathbf{r}_1) = -15.6 \left( 1 - \frac{1}{2} \vec{\tau}_0 \cdot \vec{\tau}_1 \right) e^{-(r/1.85)^2}$$

and

$$t_1(\mathbf{r}_0, \mathbf{r}_1) = 5.2 \left( \frac{1}{2} + \vec{\tau}_0 \cdot \vec{\tau}_1 \right) e^{-(r/1.85)^2}$$
Because the projectile is in a pure isospin state and because the charge exchange is not considered an inelastic scattering event, the matrix element of $\overrightarrow{r}_1 \cdot \overrightarrow{r}_0$ will be +1 when projectile and target nucleon are like nucleons and -1 when they are unlike nucleons. Hence, the form factor can be written as the sum of the two terms, one for protons and one for neutrons.

**Form Factors for Neon 20 and Magnesium 24**

We have computed the form factors $f_{LSJ}^{if}$ for excitation of the first $2^+$ state of Ne$^{20}$ and Mg$^{24}$, assuming the projectile to be a proton. In figures 1 to 4, the Hartree-Fock form factors are compared with those obtained from the shell model and the macroscopic collective model. The shell-model states are obtained by filling the $1d_{5/2}$ spherical orbits to obtain either Ne$^{20}$ or Mg$^{24}$, and then states of good $J^2$ and $J_z$ are projected from the resulting intrinsic state. The macroscopic form factor is proportional to the derivative of the real part of the optical potential which is used to fit the elastic scattering (ref. 17). In keeping with convention, this form factor is assumed spin dependent, and has a derivative Woods-Saxon radial dependence:

$$f_{JOJ}(r_0) = C_J \left[ 2 + \exp \left( r_0 - \frac{R_S}{a_S} \right) + \exp \left( -r + \frac{R_S}{a_S} \right) \right]^{-1}$$

(62)

where $C_J$ depends on multipolarity of the transition, the optical model parameters, and the deformation $\beta_J$ of the nucleus. The well parameters, $R_S$ and $a_S$, refer to the radius and diffuseness of the real part of the optical potential $V_{op}(r_0)$ and $r_0$ is the separation between the projectile and the nuclear surface. If $U_0$ as the strength of the optical potential,

$$C_J = \frac{\beta_J U_0 R_S}{a_S (2J + 1)^{1/2}}$$

In figures 1 and 2, the HF form factors for Ne$^{20}$ and Mg$^{24}$ are compared with the corresponding shell-model form factors. For both Ne$^{20}$ and Mg$^{24}$, the scalar parts ($S = 0$) of the HF form factors are enhanced over the shell-model results by a factor of about 1.5. At small values of $r(<1f)$ the form factors for Ne$^{20}$ are essentially identical. However, as $r$ increases, the difference becomes quite significant, and, at roughly $r = 4f$ and beyond, the HF form factor is larger by approximately a factor of 2. A similar behavior is observed for the case of Mg$^{24}$, except that the scalar part of the HF form
Figure 1. - Form factors for inelastic proton scattering from neon $^{20}$. (The $s = 1$ curve has been magnified to make it visible.)

Figure 2. - Form factors for inelastic proton scattering from magnesium $^{24}$.

Factor and the shell-model results are the same only at $r \leq 0.4$ fermi (or fm). Another, perhaps less important, feature is that the HF ($S = 0$) and the shell-model form factors peak at different values of $r$ for both Ne$^{20}$ and Mg$^{24}$. In both cases, the HF results have their maxima nearer the accepted values of the nuclear radius ($R = 1.25 \ A^{1/3}$ fm) than do the shell-model results.

The HF vector form factor ($S = 1$), which gives rise to spin-flip transitions, is difficult to analyze because its shell-model counterpart vanishes identically. (This is
due to the fact that $g_{LSJ}^{ab}$ which appears in equation (21) is zero for the shell model states. However, note that the HF vector form factors for Ne$^{20}$ and Mg$^{24}$ are about 300 times smaller than the scalar parts. If the direct interaction which has been chosen (eq. (60)) is realistic, then the meaning of this result is simply that, for excitation of the $2^+$ states in Ne$^{20}$ and Mg$^{24}$, the spin-flip part of the reaction mechanism is unimportant. A more reliable investigation of this question must be relegated to later studies in which angular distributions are compared with experiment.

The macroscopic form factors are compared with the HF results in figures 3 and 4. Only the scalar part of the HF form factor is plotted, because the macroscopic model does not yield a vector form factor in the approximation which leads to equation (56). The normalizations $C_J$ for the macroscopic form factors are based on the parameters which appear in the figure captions. These parameters are obtained from elastic scattering studies (ref. 18) and the measurement of the lifetime of the $2^+$ states (ref. 19).

![Figure 3. Form factors for inelastic proton scattering from neon 20. Radius of Wood-Saxon well, 3.393 femtometers; deformation parameter, 0.87; diffuseness of Wood-Saxon well, 0.6 femtometer; strength of real part of optical potential, 45 MeV.](image-url)
Figures 3 and 4 show that, although the collective form factors for Ne$^{20}$ and Mg$^{24}$ have the same shapes as the HF results, they are enhanced by factors of about 5 (for Ne$^{20}$) and 4 (for Mg$^{24}$). When the differential cross section is calculated, because it is related to the square of the form factor, the enhancement in magnitude of the cross sections will be of the order of 20 times larger for the collective model. In figure 3, the maxima of the form factors occur at about the same radius, whereas, in figure 4, the macroscopic result has its maximum at a slightly larger radius.

SUMMARY OF RESULTS

The inelastic scattering of nucleons and composite particles from nuclei has been formulated in terms of a projectile-nucleon interaction and a many-body variational wave
function which is obtained from structure calculations. The actual nuclear states are generated from the variational wave function by projection - a method which has been quite successful in the study of low-lying levels of s-d shell nuclei.

The form factors for inelastic scattering of protons from Ne$^{20}$ and Mg$^{24}$ have been computed, based on the assumptions given above, and compared with the form factors based on the projected shell model and the macroscopic collective model. The vector part of the HF form factor is very small, as one might expect because the shell model counterpart vanishes identically. The scalar part is larger than the corresponding shell-model form factor. The macroscopic form factor is even larger than the HF result, however, indicating that cross sections which are calculated using the HF method with projection, will be too small by a factor of about 20.

The model which has been used in these calculations is based on the assumption that the core is spherical and inert. Calculations by the present authors of B(E2) rates have yielded results which are also smaller than experiment. This is in agreement with the form factor study presented for both Gaussian and Yukawa interactions. Thus, the HF theory appears to be inadequate to provide the correct magnitude for cross sections, etc., if the inert core assumptions is retained.

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"The aeronautical and space activities of the United States shall be conducted so as to contribute ... to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."

—National Aeronautics and Space Act of 1958

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