

CLUSTER-MODEL EVALUATION OF NEUTRON
CROSS SECTIONS FOR LIGHT-WEIGHT NUCLEI

by 4089

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DEDICATION

To Janet, my wife, who helped more than she will ever know.

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NOMENCLATURE

Symbol	Explanation
$a_{\bar{k}\bar{l}}$	Coefficient defined in Eq. (F-6)
a'	Constant defined in Table I
a''	Arbitrary constant
A, A', A''	Arbitrary constants used in Appendix G
\bar{A}	Matrix of elements $A_{\bar{k}}^{ij}$
$A_{\bar{k}}^{ij}$	Constant of Eq. (2.0-48)
b	Constant representing the magnitude of the Bartlett interaction
$b_{\bar{k}\bar{l}}$	Coefficient defined in Eq. (F-6)
b'	Constant defined in Table I
b''	Arbitrary constant
B	Bartlett exchange operator
B', B'', B'''	Arbitrary constants used in Appendix G
\bar{B}	Matrix of elements $B_{\bar{k}}^{ij}$
$B_{\bar{k}}^{ij}$	Constant of Eq. (2.0-48)
$c_{\bar{k}\bar{l}}$	Coefficient defined in Eq. (F-5)
c'	Constant defined in Table I
d'	Constant defined in Table I
e'	Constant defined in Table I
E	Total energy of the system
$E(n)$	Center-of-mass kinetic energy for neutron-helium-3 configuration
$E(p)$	Center-of-mass kinetic energy for proton-triton configuration
$E_{^3\text{He}}$	Binding energy of the helium-3 nucleus
E_T	Binding energy of the triton nucleus

NOMENCLATURE (cont.)

Symbol	Explanation
f_l	Neutron l^{th} partial wave scattering function defined in (2.0-31)
f_n	Value of the scattering function f_l at the pivotal point r_n
f'	Constant defined in Table I
$f_{\alpha\alpha}^S$	Scattering amplitude as defined in Eq. (2.0-51)
$F(i)$	Scattering function for neutron i
F_l^i	Regular function of the i^{th} channel
$F_l(\eta', x)$	Regular Coulomb function of arguments η' and x
g_l	Proton l^{th} -wave scattering function defined in (2.0-31)
g_n	Value of the scattering function g_l at the pivotal point r_n
$G(i)$	Scattering function of proton i
G_l^i	Irregular function of channel i
$G_l(\eta', x)$	Irregular Coulomb function of arguments η' and x
h	Constant representing the magnitude of the Heisenberg interaction
h'	Interval between two consecutive pivotal points in the numerical integration scheme
\hbar	$h/2\pi$, where h is Planck's constant
H	Heisenberg exchange operator
\hat{i}	Unit vector in x-direction
$I_{l+\frac{1}{2}}(x)$	Modified fractional order Bessel function of the first kind
\hat{j}	Unit vector in y-direction
J	Jacobian of coordinate transformation defined in Eq. (2.0-22)
$J_{l+\frac{1}{2}}(x)$	Fractional order Bessel function of the first kind

NOMENCLATURE (cont.)

Symbol	Explanation
k	Parameter used in Eq. (G-3)
k'	Parameter used in Eq. (G-7)
\bar{k}	Parameter used in Eq. (F-5)
\hat{k}	Unit vector in the z-direction
k_a	Wave number of the incident channel
$K^{DD}(\bar{r}, \bar{r}')$	Kernel defined in Eq. (2.0-28)
$K^{DS}(\bar{r}, \bar{r}')$	Kernel defined in Eq. (2.0-29)
$K^{SD}(\bar{r}, \bar{r}')$	Kernel defined in Eq. (2.0-39)
$K^{SS}(\bar{r}, \bar{r}')$	Kernel defined in Eq. (2.0-40)
$K_l^{IJ}(\bar{r}, \bar{r}')$	Partial kernel for the l^{th} wave
ℓ	Orbital angular momentum quantum number
L^2	Square of the orbital angular momentum operator
m	Constant representing the magnitude of the Majorana interaction
M	Nucleonic mass
M'	Majorana exchange operator
O	Operator defined in Eq. (F-2)
O'	Operator defined in Eq. (F-3)
P_{ij}	Particle exchange operator, which exchanges particles i and j
$P_l(x)$	l^{th} order Legendre polynomial of the argument x
q	Electronic charge
r	Magnitude of vector \bar{r}
\bar{r}	Vector defined in Eq. (2.0-21)
r'	Magnitude of vector \bar{r}'

NOMENCLATURE (cont.)

Symbol	Explanation
\bar{r}'	Vector defined in Eq. (2.0-21)
\bar{r}_i	Position vector of particle i
r_{ij}	Relative distance between particles i and j
\bar{r}_{ij}	Vector distance between particles i and j
$=$	
R	Reactance matrix
R_M	Upper limit to the r' integration
\bar{R}_2	Vector defined in (2.0-21)
\bar{R}_3	Vector defined in (2.0-21)
S	Eigenvalues of spin
\bar{S}	Scattering matrix
$S_{\alpha\alpha'}^l$	Eigenvalues of the scattering matrix
T	Kinetic energy operator
T_m	Weight factors for Gregory's integration
\bar{u}	Vector defined in (2.0-21)
$u(r)$	Function defined in Eq. (3.0-2)
u	Undetermined variable of integration appearing in Eq. (2.0-46)
\bar{v}	Vector defined in (2.0-21)
$v(r)$	Function defined in Eq. (3.0-3)
v_0	Depth of potential well in MeV
v_{ij}	Nuclear potential between the i and j nucleons
v_{ij}^c	Coulomb potential between the i and j nucleons
$v_{DD}(r)$	Direct-potential term defined in Eq. (2.0-26)
$v_{DS}(r)$	Direct-potential term defined in Eq. (2.0-27)

NOMENCLATURE (cont.)

Symbol	Explanation
$v_{SD}(r)$	Direct-potential term defined in Eq. (2.0-38)
$v_{SS}(r)$	Direct-potential term defined in Eq. (2.0-36)
$v_{SS}^{Coul}(r)$	Coulomb-potential term defined in Eq. (2.0-37)
w	Constant determining the magnitude of the Wigner interaction
\bar{y}	Vector defined in (2.0-21)
$y(r)$	Function defined in Eq. (3.0)
$y(x)$	Polynomials defined in Eq. (3.0-10)
$Y_l^m(\theta, \phi)$	Spherical harmonics
x	Constant in Serber exchange force defined in Eq. (41)
x'	Dummy argument
\bar{x}	Vector defined in (2.0-21)
$x(r)$	Function defined in Eq. (3.0-9)
a	Constant defined in Table I
$\alpha(i)$	Spin wavefunction for particle i
β	Constant defined in Table I
$\beta(i)$	Spin wavefunction for particle i
γ	Constant defined in Table I
δ	Constant defined in Table I
δ_{ij}	Kronecker delta symbol
δ^n	n^{th} central difference operator
$\bar{\nabla}$	Gradient operator
∇^2	Laplacian operator
ϵ	Constant defined in Table I

NOMENCLATURE (cont.)

Symbol	Explanation
η	Constant defined in Table I
η'	Parameter defined in Eq. (G-5)
$\eta(ijk)$	Spatial wavefunction for the triton cluster formed by nucleons i, j, and k
$\eta^*(ijk)$	Complex conjugate of $\eta(ijk)$
θ	Polar scattering angle in the center-of-mass system
θ	Angle between position vectors \vec{r} and \vec{r}'
λ	Variationally determined parameter in the triton wavefunction
μ	Parameter describing the range of the Gaussian potential
v	Variationally determined parameter in the helium-3 wavefunction
ρ	Arbitrary variable
$\bar{\rho}_2$	Vector defined in (2.0-21)
$\bar{\rho}_3$	Vector defined in (2.0-21)
$\bar{\rho}_4$	Vector defined in (2.0-21)
σ_S	Spin wavefunction corresponding to the spin S of the system
$\sigma(\theta)$	Differential cross section
ϕ	Azimuthal scattering angle in the center-of-mass system
$\phi(ijk)$	Spatial wavefunction for the helium-3 cluster formed by nucleons i, j, and k
$\phi^*(ijk)$	Complex conjugate of $\phi(ijk)$
ψ	Nuclear wavefunction for the system
V_{ij}	Internucleonic interaction between nucleons i and j
$I_{\ell+\frac{1}{2}}(x)$	Function defined in (2.0-45)

NOMENCLATURE (cont.)

Symbol	Explanation
$\int_{\text{all spin}} d\tau$	Integral over the entire spin space
$\iint_{\text{surface}} ds$	Surface integral
$\int d\tilde{r}_i d\tilde{r}_j d\tilde{r}_k$	9-dimensional integral over the entire coordinate space of the cluster formed by the i, j, and k particles

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1.0 INTRODUCTION

Cross section data for the interaction of neutrons with light-weight nuclei have been obtained by extensive experimental studies, and the results have been compiled for various neutron energies [17,24]. There are, however, significant gaps in the available information, and thus there is a need for theoretical models which can support and supplement the experimental information available. This need is particularly felt for neutron interactions with light-weight nuclei, since the existing models fail, on the whole, to predict accurately the cross section for such nuclei. For instance, collective or statistical models cannot be used with confidence because the number of nucleons present is insufficient to obtain statistically meaningful averages. Attempts to use direct-interaction models are generally hampered by the considerable mathematical difficulty encountered for interactions between nucleons and nuclei of $A > 2$, or interactions where the projectile is not a single nucleon. The optical model, although used with great success in the calculation of neutron cross sections for heavy and medium-weight nuclei [43], can only be replaced by a suitable average potential field. Each nucleon would then move in this average field and exert its influence upon the remaining nucleons only by means of the Pauli principle, which excludes identical particles from occupying the same quantum states [48].

This is clearly not the case for light-weight nuclei, where the detailed structure of the individual nucleus is decisive for the character and yield of the reaction [48].

Some success, however, has been obtained in recent years, by using optical models with a nonlocal potential [33,34]. It will be shown, how-

ever, that the equations ensuing from the model proposed in this work are identical to the equations one must solve for the optical model with non-local potentials, and that furthermore, all optical-model parameters are derived entirely within the framework of the model.

Experimental work on light-weight nuclei has shown strong evidence for "clustering" of nucleons into subgroups within the nucleus [1,35]. In light-weight nuclei, then, it can be safely assumed that some, or all, of the component nucleons are at some instant more closely correlated to each other, to the exclusion of the remaining nucleons (if any).

The configuration, where within the limitations of Pauli's principle some nucleons are more closely correlated, is called a "resonating structure" or a "cluster". Implied in this definition, however, there is no restriction to the number of particles, and in fact, it is entirely appropriate to consider an individual nucleon as a cluster. Also, the cluster configuration of a system is not fixed, but may vary from energy level to energy level and from reaction to reaction.

In the attempt to describe more accurately the behavior of light-weight nuclei, then, one could formulate a model which accounts for the clustering of nucleons in nuclei. In such a model, the wavefunction of the system is written as a superposition of particular wavefunctions describing each of the clusters. The representation need not be unique, and in fact, it will vary from cluster to cluster representation, and also for different excitations of the clusters.

The simpler the cluster representation, the simpler is the mathematical formulation of the model. In the limit, if one were to consider each nucleon of the system as a cluster, the model would revert to the single-particle (shell) model.

The cluster model (or resonating group structure method) [45,48] has been used extensively to analyze scattering problems where both the incident and target nuclei are nucleons or composed of only a few nucleons; and to describe the low-lying energy levels of some light-weight nuclei. To the present, problems treated with this model have been the evaluation of the low-energy levels of ^8Be [47], ^7Li and ^7Be [47], ^9Be [41], and ^{12}C [35], and the elastic scattering of $n+D$ [9,10,11,19], $n+T$ and $p+T$ [3,4], $n+^3\text{He}$ and $p+^3\text{He}$ [3,4], $n+\alpha$ [5,22,23,40], $^3\text{He}+\alpha$ [37], $d+D$ [27], $^3\text{He}+^3\text{He}$ [6], and $\alpha+\alpha$ [8,38,44]. Cross sections for the two-channel five-nucleon system have also been obtained [28].

In the present work, the following two-channel four-nucleon system is formulated using the cluster model:



The cross section for the elastic scattering of neutrons from helium-3 in the presence of the charge-exchange reaction $n+^3\text{He} \rightarrow p+T$ is evaluated by numerical solution of the system of two coupled integro-differential equations arising from the application of the model to the problem.

A Gaussian form of the potential with a Serber-type exchange force is used to represent the potential of the interaction. The parameters contained in the chosen form are adjusted so that the potential will yield the correct values of the binding energies for the helium-3 and triton nuclei. Other authors [4,22] have found this potential to give best agreement with experimental cross sections.

The total and differential cross sections for the $^3\text{He}(n,n)^3\text{He}$ and $^3\text{He}(n,p)\text{T}$ reactions are evaluated at incident neutron energies of 1, 3.6, and 6 MeV.

2.0 THEORY

The wavefunction for the four-nucleon system under consideration, $\Psi(1234)$, is a solution to the Schrödinger equation in the center-of-mass system [2]:

$$[T + \sum_{\text{all pairs}} V_{ij} - E]\Psi(1234) = 0 \quad (2.0-1)$$

where 1 and 3 denote the two neutrons, and 2 and 4 the two protons. From conservation of energy, E , the total energy of the system is:

$$E = E_{^3\text{He}} + E(n) = E_T + E(p) \quad (2.0-2)$$

where $E_{^3\text{He}}$ and E_T are the binding energies of the helium-3 and triton clusters respectively, and $E(p)$ and $E(n)$ are the kinetic energies in the center-of-mass system of the proton-triton and neutron-helium-3 configurations, and are equal to $3/4$ of the kinetic energy of the incident proton or neutron in the laboratory system of coordinates. The kinetic-energy operator T can be written in different forms, each most suitable for a particular particle grouping. For instance, in the case of neutron 1 incident on the helium-3 cluster (234), we can write:

$$T = -\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{2-34}^2 - \frac{2}{3} \frac{\hbar^2}{M} \nabla_{1-342}^2 \quad (2.0-3)$$

whereas, for proton 2 impinging on the Triton cluster (134), we have:

$$T = -\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{34-1}^2 - \frac{2}{3} \frac{\hbar^2}{M} \nabla_{2-341}^2 \quad (2.0-4)$$

V_{ij} is the internucleonic interaction and is assumed to be purely central and of the form:

$$V_{ij} = (w + bB + hH + mM')v_{ij} + v_{ij}^c \quad (2.0-5)$$

where B , H , and M' are the usual Bartlett, Heisenberg, and Majorana operators, and v_{ij}^c is the Coulomb potential given by [3]:

$$v_{ij}^c = \begin{cases} q^2/r_{ij} & \text{if } i,j \text{ are protons,} \\ 0 & \text{otherwise.} \end{cases} \quad (2.0-6)$$

In ordinary spin space, the Bartlett operator, $B = 1/2(1+\bar{\sigma}_i \cdot \bar{\sigma}_j)$, has the effect of interchanging the spins of particles i and j ; the Majorana operator, $M' = -1/4(1+\bar{\sigma}_i \cdot \bar{\sigma}_j)(1+\bar{\tau}_i \cdot \bar{\tau}_j)$, interchanges the spatial coordinates of particles i and j ; and the Heisenberg operator, $H = -1/2(1+\bar{\tau}_i \cdot \bar{\tau}_j)$, interchanges both the spatial and spin coordinates of particles i and j . The actual form of the potential v_{ij} will be discussed later. For the moment, however, it is sufficient to assume that it will be dependent only on $|r_{ij}|$, where \bar{r}_{ij} is the vector distance between particles i and j .

The wavefunction of Eq. (2.0-1) for the composite nucleus can be written as a properly antisymmetrized combination of partial wavefunctions, corresponding to the various ways of distributing the protons and the neutrons into the various groups. Since we denote by 1 and 3 the neutrons, and by 2 and 4 the protons, the properly antisymmetrized wavefunction is given by:

$$\Psi(1234) = (1-P_{13})\phi(234)\sigma_S(1,234)F(1,234) + (1-P_{24})\eta(134)\sigma_S(2,134)G(2,134) \quad (2.0-7)$$

where P_{13} and P_{24} are operators which exchange particles 1 and 3, and particles 2 and 4, respectively. The spin function σ_S corresponds to the total spin of the system ($S = 0,1$). $\phi(234)$ and $\eta(134)$ are the spatial

wavefunctions for the helium-3 and triton clusters, and $F(1,234)$ and $G(2,134)$ are functions describing the motion of the neutron 1 relative to the remaining helium-3 cluster, and of the proton 2 relative to the triton cluster. They are therefore the scattering functions of the corresponding arguments.

Substitution of the properly antisymmetrized wavefunction into the Schrödinger equation yields:

Neutron-helium-3 system

$$[(-\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{2-34}^2 - \frac{2}{3} \frac{\hbar^2}{M} \nabla_{1-234}^2) + \sum_{\text{all pairs}} v_{ij} - E] \{(1-P_{13})\phi(234) \\ \cdot \sigma_S(1234)F(1,234) + (1-P_{24})n(134)\sigma_S(1234)G(2,134)\} \quad (2.0-8)$$

Proton-triton system

$$[(-\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{1-34}^2 - \frac{2}{3} \frac{\hbar^2}{M} \nabla_{2-134}^2) + \sum_{\text{all pairs}} v_{ij} - E] \{(1-P_{13})\phi(234) \\ \cdot \sigma_S(1234)F(1,234) + (1-P_{24})n(134)\sigma_S(1234)G(2,134)\} \quad (2.0-9)$$

The spin for the neutron-helium-3 system can either be 0 or 1. For the singlet case, $S=0$, we have:

$$\sigma_S = \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] [\alpha(2)\beta(4) - \alpha(4)\beta(2)] \equiv \frac{1}{2}\sigma_0 \quad (2.0-10)$$

while for the triplet case, $S=1$:

$$\sigma_S = \begin{cases} \frac{1}{\sqrt{2}} [\alpha(2)\beta(4) - \alpha(4)\beta(2)]\alpha(1)\alpha(3) \equiv {}^3\sigma_1 \\ \frac{1}{2} [\alpha(2)\beta(4) - \alpha(4)\beta(2)] [\alpha(1)\beta(3) + \alpha(3)\beta(1)] \equiv {}^3\sigma_0 \\ \frac{1}{\sqrt{2}} [\alpha(2)\beta(4) - \alpha(4)\beta(2)]\beta(1)\beta(3) \equiv {}^3\sigma_{-1} \end{cases} \quad (2.0-11)$$

The four spin wavefunctions, defined above, are mutually orthogonal, and the spin vectors α and β are defined so that the following relations hold:

$$\int_{\text{all spin space}} \alpha(i)\alpha(i)d\tau = 1 \quad \int_{\text{all spin space}} \beta(i)\beta(i)d\tau = 1$$

$$\int_{\text{all spin space}} \alpha(i)\beta(i)d\tau = 0 \quad (2.0-12)$$

The spin functions for the proton-triton system are similarly written as:

Singlet case:

$$\sigma_S = \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] [\alpha(2)\beta(4) - \alpha(4)\beta(2)] \equiv {}^1\sigma_0 \quad (2.0-13)$$

Triplet case:

$$\sigma_S = \begin{cases} \frac{1}{\sqrt{2}} [\alpha(1)\beta(3) - \alpha(3)\beta(1)]\alpha(2)\alpha(4) \equiv {}^3\sigma_1 \\ \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] [\alpha(2)\beta(4) + \alpha(4)\beta(2)] \equiv {}^3\sigma_0 \\ \frac{1}{\sqrt{2}} [\alpha(1)\beta(3) - \alpha(3)\beta(1)]\beta(2)\beta(4) \equiv {}^3\sigma_{-1} \end{cases} \quad (2.0-14)$$

To develop the equation describing the scattering of a neutron by helium-3, we premultiply Eq. (2.0-8) by the complex conjugate of the helium-3 spatial wavefunction, the spin function, and integrate over

all spin space and all coordinate space of the cluster. By recalling that the wavefunction of the helium-3 cluster itself satisfies its own Schrödinger equation,

$$\left[\left(-\frac{\pi^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\pi^2}{M} \nabla_{2-34}^2 \right) + v_{24}^c + (w+mM'+hH+bB)(v_{24}+v_{23}+v_{34}) - E + E(n) \right] \phi(234) = 0 \quad (2.0-15)$$

one can readily derive an integro-differential equation for the scattering function $F(1,234)$ for both the singlet and triplet spin configuration. Appendix A shows the mathematical operations in detail.

The singlet equation for the neutron-helium-3 system is:

$$\begin{aligned} & \left[\frac{2}{3} \frac{\pi^2}{M} \nabla_{1-234}^2 + E(n) \right] F(1,234) \\ &= \left[(3w-h+m) \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 v_{13} |\phi(234)|^2 \right] F(1,234) + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \\ & \cdot \left[\left(-\frac{h^2}{M} \nabla_{14}^2 - \frac{3}{4} \frac{h^2}{M} \nabla_{2-14}^2 - \frac{2}{3} \frac{h^2}{M} \nabla_{3-124}^2 \right) - E + v_c(24) \right. \\ & + (2w+b+h+2m)(v_{14}+v_{23}) + (w-b-h+m)v_{24} + (3m+w-b)v_{13} \\ & \cdot \phi(142)F(3,124) + (2m+h) \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{14} n(234) G(1,234) \\ & + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \left[2 \left(-\frac{h^2}{M} \nabla_{23}^2 - \frac{3}{4} \frac{h^2}{M} \nabla_{1-23}^2 - \frac{2}{3} \frac{h^2}{M} \nabla_{4-123}^2 \right) \right. \\ & - 2E + 2v_c(24) + (2w+2m+b+h)v_{23} + (4w+4m-b-h)(v_{12}+v_{34}) \\ & \left. \left. + (2w+b)v_{14} \right] n(123) G(4,123) \right] \quad (2.0-16) \end{aligned}$$

The triplet equation for the same system is:

$$\begin{aligned}
 & [\frac{2}{3} \frac{\hbar^2}{M} v_{1-234}^2 + E(n)] F(1,234) \\
 &= [(3w+2b-h-m) \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 v_{13} |\phi(234)|^2] F(1,234) - \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \\
 &\quad \cdot [(-\frac{\hbar^2}{M} v_{14}^2 - \frac{3}{4} \frac{\hbar^2}{M} v_{2-14}^2 - \frac{2}{3} \frac{\hbar^2}{M} v_{3-124}^2) - E + v_c(24) \\
 &\quad + (w+b-3m-2h)v_{13} - (2w+b+h+2m)(v_{14} + v_{34}) - (w-b-h+m)v_{24}] \\
 &\quad \cdot \phi(142)F(3,124) + h \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{12} n(234) G(1,234) \\
 &\quad + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) [b v_{14} - (b+h)(v_{12} + v_{34} - v_{23})] n(123) G(4,123) \quad (2.0-17)
 \end{aligned}$$

The integro-differential equations for the second interaction channel, the proton-triton system, are obtained in an identical procedure as that employed for Eqs. (2.0-16) and (2.0-17), but starting from Eq. (2.0-9), using the spin functions described in (2.0-13) and (2.0-14), and recalling that the triton-cluster wavefunction satisfies

$$\begin{aligned}
 & [(-\frac{\hbar^2}{M} v_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} v_{1-34}^2) + (w+mM+hH+bB)(v_{13} + v_{14} + v_{34}) \\
 &\quad - E + E(p)] n(134) = 0 \quad (2.0-18)
 \end{aligned}$$

The spatial integration is performed over the coordinates of the triton cluster $n(134)$. Again there are two equations corresponding to the singlet and triplet spin configurations of the system. The singlet-state equation is:

$$\begin{aligned}
& \left[\frac{2}{3} \frac{\hbar^2}{M} v_{2-134}^2 + E(p) \right] G(2,134) \\
&= \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 [(3w-h+m)v_{24} + v_c^*(24)] |\eta(134)|^2 G(2,134) \\
&+ \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 \eta^*(134) [(-\frac{h^2}{M} v_{23}^2 - \frac{3}{4} \frac{h^2}{M} v_{1-23}^2 - \frac{2}{3} \frac{h^2}{M} v_{4-123}^2) \\
&- E + v_c(24) + (2w+b+h+2m)(v_{12}+v_{34}) + (w+3m-b)v_{24} + (w+m-h-b)v_{13}] \\
&\cdot \eta(123) G(4,123) + \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 \eta^*(134) (2m+h)v_{12} \phi(134) F(2,134) \\
&+ \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 \eta^*(134) [2(-\frac{h^2}{M} v_{14}^2 - \frac{3}{4} \frac{h^2}{M} v_{2-14}^2 - \frac{2}{3} \frac{h^2}{M} v_{3-124}^2) \\
&- 2E + 2v_c(24) + (2w+b)v_{23} + (2w+2m+b+h)v_{14} + (4w+4m-b-h) \\
&\cdot (v_{12}+v_{34})] \phi(134) F(3,124) \tag{2.0-19}
\end{aligned}$$

and the triplet-state equation is:

$$\begin{aligned}
& \left[\frac{2}{3} \frac{\hbar^2}{M} v_{2-134}^2 + E(p) \right] G(2,134) \\
&= \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 [(3w+2b-h-m)v_{24} + v_c(24)] |\eta(134)|^2 G(2,134) \\
&- \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 \eta^*(134) [(-\frac{h^2}{M} v_{23}^2 - \frac{3}{4} \frac{h^2}{M} v_{1-23}^2 - \frac{2}{3} \frac{h^2}{M} v_{4-123}^2) \\
&- E + v_c(24) + (w+m-b-h)v_{13} + (3m+2h-w-b)v_{24} + (2w+2m+b+h)v_{24}] \\
&\cdot \eta(124) G(4,123) + h \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 \eta^*(134) v_{12} \phi(134) F(2,134) \\
&+ \int d\tilde{r}_1 d\tilde{r}_3 d\tilde{r}_4 \eta^*(134) [b v_{23} - (b+h)(v_{12}+v_{34}-v_{14})] \phi(142) F(3,124) \tag{2.0-20}
\end{aligned}$$

The form of Eqs. (2.0-16) and (2.0-17) can be changed by introduction of a new system of coordinates:

$$\begin{aligned}
 \bar{r} &= \bar{r}_1 - \frac{1}{3}(\bar{r}_2 + \bar{r}_3 + \bar{r}_4) & \bar{r}'' &= \bar{r}_4 - \frac{1}{3}(\bar{r}_1 + \bar{r}_2 + \bar{r}_3) \\
 \bar{r}' &= \bar{r}_3 - \frac{1}{3}(\bar{r}_1 + \bar{r}_2 + \bar{r}_4) & \bar{y} &= \bar{r}_4 - \frac{1}{2}(\bar{r}_2 + \bar{r}_3) = \frac{3}{8}\bar{r} + \frac{9}{8}\bar{r}'' \\
 \bar{v} &= \bar{r}_3 - \frac{1}{2}(\bar{r}_2 + \bar{r}_4) = \frac{3}{8}\bar{r} + \frac{9}{8}\bar{r}' = \bar{\rho}_3 & \bar{R}_2 &= \bar{r}_2 - \bar{r}_3 & (2.0-21) \\
 \bar{\rho}_2 &= \bar{r}_2 - \bar{r}_4 & \bar{R}_3 &= \bar{r}_3 \\
 \bar{\rho}_4 &= \bar{r}_4 & \bar{x} &= \frac{9}{8}\bar{r} + \frac{3}{8}\bar{r}'' \\
 \bar{u} &= \frac{9}{8}\bar{r} + \frac{3}{8}\bar{r}'
 \end{aligned}$$

The Jacobian of the transformation from the coordinate system $(\bar{r}_2, \bar{r}_3, \bar{r}_4)$ to the system $(\bar{\rho}_2, \bar{\rho}_4, \bar{r}')$ is introduced so that:

$$d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 = J d\bar{\rho}_2 d\bar{\rho}_4 d\bar{r}'$$

where

$$J \equiv \begin{vmatrix} \bar{v}_{\bar{\rho}_2, \bar{r}_2} & \bar{v}_{\bar{\rho}_4, \bar{r}_2} & \bar{v}_{\bar{r}, \bar{r}_2} \\ \bar{v}_{\bar{\rho}_2, \bar{r}_3} & \bar{v}_{\bar{\rho}_4, \bar{r}_3} & \bar{v}_{\bar{r}, \bar{r}_3} \\ \bar{v}_{\bar{\rho}_2, \bar{r}_4} & \bar{v}_{\bar{\rho}_4, \bar{r}_4} & \bar{v}_{\bar{r}, \bar{r}_4} \end{vmatrix} = \begin{vmatrix} \{1\} \{0\} \{-\frac{1}{2}\} \\ \{0\} \{0\} \{\frac{9}{8}\} \\ \{-1\} \{1\} \{-\frac{1}{2}\} \end{vmatrix} = \begin{vmatrix} \{\frac{9}{8}\} \{0\} \{0\} \\ \{-\frac{1}{2}\} \{1\} \{0\} \\ \{-\frac{1}{2}\} \{1\} \{1\} \end{vmatrix} = \left(\frac{9}{8}\right)^3$$

where $\{ \}$ denote 3×3 scalar matrices.

Similarly one can show that: $d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 = \left(\frac{9}{8}\right)^3 d\tilde{R}_2 d\tilde{R}_3 d\tilde{r}''$

and

$$d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 = -27 d\tilde{r}'' d\tilde{R}_2 d\tilde{\rho}_2$$

The integrals involving kinetic-energy terms in Eqs. (2.0-16) and (2.0-17) can be reduced to a more workable form by means of Green's Identity.

For instance:

$$\begin{aligned}
 & \int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 \phi(234) \nabla_{3-142}^2 \phi(142) F(3,124) \\
 &= \int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 \phi^*(234) \phi(142) \nabla_{3-142}^2 F(3,124) \\
 &= \int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 F(3,124) \nabla_{3-124}^2 \phi^*(234) \phi(124) \\
 &+ \iint_{\text{surface}} \bar{N} \cdot [\phi^*(234) \phi(124) \bar{\nabla}_{3-124} F(3,124) \\
 &\quad - F(3,124) \bar{\nabla}_{3-124} \phi^*(234) \phi(124)] ds \tag{2.0-23}
 \end{aligned}$$

The surface integral, however, vanishes if one requires the surface of integration to be at infinity, since the wavefunctions vanish there.

Hence:

$$\begin{aligned}
 & \int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 \phi^*(234) \nabla_{3-124}^2 \phi(142) F(3,124) \\
 &= [\int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 \nabla_{3-124}^2 \phi^*(234) \phi(142)] F(3,124)
 \end{aligned}$$

and

$$\begin{aligned}
 & \int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 \phi^*(234) \nabla_{4-123}^2 \eta(123) G(4,123) \\
 &= [\int d\bar{r}_2 d\bar{r}_3 d\bar{r}_4 \nabla_{4-123}^2 \phi^*(234) \eta(123)] G(4,132) \tag{2.0-24}
 \end{aligned}$$

We now use the fact that:

$$\begin{aligned} \nabla_{4-123}^2 \phi^*(234)\phi(124) &= \nabla_{\bar{r}}^2 \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \\ &= \bar{v}_{\bar{r}} \cdot \{\phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \bar{v}_{\bar{r}} \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) + \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \bar{v}_{\bar{r}} \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \end{aligned}$$

and

$$\begin{aligned} \bar{v}_{\bar{r}} \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) &= \frac{\partial}{\partial v_x} \frac{dv_x}{dr'_x} \hat{i} + \frac{\partial}{\partial v_y} \frac{dv_y}{dr'_y} \hat{j} + \frac{\partial}{\partial v_z} \frac{dv_z}{dr'_z} \hat{k} \\ &\quad \cdot \phi^*(v_x \hat{i} + v_y \hat{j} + v_z \hat{k}, \bar{\rho}_2, \bar{\rho}_4) \\ &= \frac{9}{8} (\frac{\partial}{\partial v_x} \hat{i} + \frac{\partial}{\partial v_y} \hat{j} + \frac{\partial}{\partial v_z} \hat{k}) \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \\ &= \frac{9}{8} \bar{v}_{\bar{v}} \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \end{aligned}$$

Therefore

$$\begin{aligned} \nabla_{4-123}^2 \phi^*(234)\phi(124) &= (\frac{9}{8})^2 \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \nabla_{\bar{v}}^2 \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \\ &\quad + (\frac{3}{8})^2 \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \nabla_{\bar{u}}^2 \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \\ &\quad + \frac{27}{32} \bar{v}_{\bar{u}} \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \cdot \bar{v}_{\bar{v}} \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \end{aligned}$$

Furthermore

$$\begin{aligned} (\nabla_{14}^2 + \frac{3}{4} \nabla_{2-14}^2) \phi(142) &= (\nabla_{24}^2 + \frac{3}{4} \nabla_{1-24}^2) \phi(142) \\ &= (\nabla_{\bar{\rho}_2}^2 + \nabla_{\bar{u}}^2) \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \end{aligned}$$

By utilizing the above expressions, and similar ones for the remaining kinetic-energy operators, we can finally write the singlet and triplet equations for the neutron-helium-3 system as

$$\begin{aligned} \left[\nabla^2_{\bar{r}} + \frac{3}{2} \frac{M}{\hbar^2} E(n) \right] F(\bar{r}) &= V_{DD}(r) F(\bar{r}) + V_{DS}(r) G(\bar{r}) \\ &+ \int d\bar{r}' K^{DD}(\bar{r}, \bar{r}') F(\bar{r}') + \int d\bar{r}'' K^{DS}(\bar{r}, \bar{r}'') G(\bar{r}'') \end{aligned} \quad (2.0-25)$$

where, by definition

$$V_{DD}(r) = \frac{M}{\hbar^2} \left(\frac{9}{8} \right)^3 a \int d\bar{r}' d\bar{p}_2 d\bar{p}_4 v(|\bar{u}-\bar{v}|) |\phi(\bar{v}, \bar{p}_2, \bar{p}_4)|^2 \quad (2.0-26)$$

$$V_{DS}(r) = \frac{M}{\hbar^2} \left(\frac{9}{8} \right)^3 a \int d\bar{r}'' d\bar{R}_2 d\bar{R}_3 \phi^*(\bar{y}, \bar{R}_2, \bar{R}_3) v(|\bar{x}-\bar{y}|) n(\bar{y}, \bar{R}_2, \bar{R}_3) \quad (2.0-27)$$

$$\begin{aligned} K^{DD}(\bar{r}, \bar{r}') &= \left(\frac{9}{8} \right)^3 \frac{M}{\hbar^2} \int d\bar{p}_2 d\bar{p}_4 \phi^*(\bar{v}, \bar{p}_2, \bar{p}_4) [\gamma \{ v(|\bar{u} + \frac{1}{2}\bar{p}_2|) \right. \\ &\quad \left. + v(|\bar{u} - \frac{1}{2}\bar{p}_2|) \} + \delta v(|\bar{p}_2|) + \epsilon v(|\bar{u} - \bar{v}|) + n\{ v_c(|\bar{p}_2|) - E \} \right. \\ &\quad \cdot \phi(\bar{u}, \bar{p}_2, \bar{p}_4) + \beta \left(\frac{9}{8} \right)^3 \int d\bar{p}_2 d\bar{p}_4 \left\{ \left(\frac{9}{8} \right)^2 \phi(\bar{u}, \bar{p}_2, \bar{p}_4) \nabla_{\bar{v}}^2 \phi^*(\bar{v}, \bar{p}_2, \bar{p}_4) \right. \\ &\quad \left. + \left(\frac{9}{8} \right)^2 \phi^*(\bar{v}, \bar{p}_2, \bar{p}_4) \nabla_{\bar{u}}^2 \phi(\bar{u}, \bar{p}_2, \bar{p}_4) + \frac{27}{32} \bar{v}_{\bar{u}} \phi(\bar{u}, \bar{p}_2, \bar{p}_4) \right. \\ &\quad \left. \cdot \bar{v}_{\bar{v}} \phi^*(\bar{v}, \bar{p}_2, \bar{p}_4) + \frac{3}{2} \phi^*(\bar{v}, \bar{p}_2, \bar{p}_4) \nabla_{\bar{p}_2}^2 \phi(\bar{u}, \bar{p}_2, \bar{p}_4) \} \right\} \end{aligned} \quad (2.0-28)$$

and

$$\begin{aligned} K^{DS}(\bar{r}, \bar{r}'') &= \left(\frac{9}{8} \right)^3 \frac{M}{\hbar^2} \int d\bar{R}_2 d\bar{R}_3 \phi^*(\bar{y}, \bar{R}_2, \bar{R}_3) [c' v(|\bar{R}_2|) + d' \\ &\quad \cdot \{ v(|\frac{1}{2}\bar{R}_2 - \bar{x}|) + v(|\frac{1}{2}\bar{R}_2 + \bar{y}|) \} + f' v(|\bar{x} - \bar{y}|) - e' E] n(\bar{x}, \bar{R}_2, \bar{R}_3) \end{aligned}$$

$$\begin{aligned}
& + \left(\frac{9}{8}\right)^3 b' \int d\bar{R}_2 d\bar{R}_3 \left\{ \left(\frac{9}{8}\right)^2 \phi^*(\bar{y}, \bar{R}_2, \bar{R}_3) \nabla_{\bar{x}}^2 \eta(\bar{x}, \bar{R}_2, \bar{R}_3) \right. \\
& + \left(\frac{9}{8}\right)^2 \eta(\bar{x}, \bar{R}_2, \bar{R}_3) \nabla_{\bar{y}}^2 \phi^*(\bar{y}, \bar{R}_2, \bar{R}_3) + \frac{27}{32} \bar{v}_{\bar{x}} \eta(\bar{x}, \bar{R}_2, \bar{R}_3) \\
& \cdot \bar{v}_{\bar{y}} \phi^*(\bar{y}, \bar{R}_2, \bar{R}_3) + \frac{3}{2} \phi^*(\bar{y}, \bar{R}_2, \bar{R}_3) \nabla_{\bar{R}_2}^2 \eta(\bar{x}, \bar{R}_2, \bar{R}_3) \\
& \left. - 2(27) \int d\bar{R}_2 d\bar{p}_2 \phi^*(\bar{y}, \bar{R}_2, \bar{p}_2) v_c(|\bar{p}_2|) \eta(\bar{x}, \bar{R}_2, \bar{p}_2) \right\} \quad (2.0-29)
\end{aligned}$$

The constants appearing in (2.0-26) through (2.0-29) are defined for the singlet and triplet cases in Table I.

Since r'' is simply a variable of integration, it can be replaced by r' everywhere, without affecting the equation. Thus:

$$\begin{aligned}
& [\nabla_r^2 + \frac{3}{2} \frac{M}{\hbar^2} E(n)] F(\bar{r}) = V_{DD}(r) F(\bar{r}) + V_{DS}(r) G(\bar{r}) \\
& + \int d\bar{r}' K^{DD}(\bar{r}, \bar{r}') F(\bar{r}') + \int d\bar{r}' K^{DS}(\bar{r}, \bar{r}') G(\bar{r}') \quad (2.0-30)
\end{aligned}$$

Now we let:

$$F(\bar{r}) = \sum_{\ell} \frac{1}{r} f_{\ell}(r) P_{\ell}(\cos\theta), \quad G(\bar{r}) = \sum_{\ell} \frac{1}{r} g_{\ell}(r) P_{\ell}(\cos\theta)$$

$$\text{and } K^{IJ}(\bar{r}, \bar{r}') = \sum_{\ell} \frac{2\ell+1}{4\pi rr'} K_{\ell}^{IJ}(r, r') P_{\ell}(\cos\theta) \quad (2.0-31)$$

where θ = scattering angle in the center of mass system and $\cos\theta = \frac{\bar{r} \cdot \bar{r}'}{rr'}$.

Recalling that

$$\nabla_{\bar{r}}^2 = \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{L^2}{r^2}$$

Table I

Constants for Neutron-Helium-3, and Proton-Triton Scattering.

	<u>Singlet</u>	<u>Triplet</u>
α	$\frac{3}{2}(3w-h+m)$	$\frac{3}{2}(3w+2b-h-m)$
β	-1	+1
γ	$\frac{3}{2}(2w+b+h+2m)$	$-\frac{3}{2}(2w+b+h+2m)$
δ	$\frac{3}{2}(w-b-h+m)$	$-\frac{3}{2}(w-b-h+m)$
η	$\frac{3}{2}$	$-\frac{3}{2}$
ϵ	$\frac{3}{2}(3m+w-b)$	$-\frac{3}{2}(w+b-3m-2h)$
a'	$\frac{3}{2}(2m+h)$	$\frac{3}{2} h$
b'	-2	0
c'	$\frac{3}{2}(2w+2m+b+h)$	$\frac{3}{2}(b+h)$
d'	$\frac{3}{2}(4w+4m-b-h)$	$-\frac{3}{2}(b+h)$
e'	3	-3
f'	$\frac{3}{2}(2w+b)$	$\frac{3}{2} b$

where L^2 is the square of the orbital angular momentum operator, the eigenvalues of which are $-l(l+1)$, then

$$\begin{aligned}
 & \sum_l \left| \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{L^2}{r^2} + \frac{3M}{2\hbar^2} E(n) \right| \frac{1}{r} f_l(r) P_l(\cos\theta) \\
 &= \sum_l V_{DD}(r) \frac{1}{r} f_l(r) P_l(\cos\theta) + \sum_l V_{DS}(r) \frac{1}{r} g_l(r) P_l(\cos\theta) \\
 &+ \sum_{l'} \sum_l \sum_{m=-l}^l \int d\phi' \int d(\cos\theta') \int dr' \frac{2l+1}{4\pi r} K_l^{DD}(r, r') f_{l'}(r') \\
 &\times \sqrt{\frac{4\pi}{2l'+1}} Y_l^0(\theta', \phi') \times \frac{4\pi}{2l+1} Y_l^{*m}(\theta', \phi') Y_l^m(\theta, \phi) \\
 &+ \sum_{l'} \sum_l \sum_{m=-l}^l \int d\phi' \int d(\cos\theta') \int dr' \frac{2l+1}{4\pi r} K_l^{DS}(r, r') f_{l'}(r') \\
 &\times \sqrt{\frac{4\pi}{2l'+1}} Y_l^0(\theta', \phi') \frac{4\pi}{2l+1} Y_l^{*m}(\theta', \phi') Y_l^m(\theta, \phi) \tag{2.0-32}
 \end{aligned}$$

wherein we have used the relations (2.0-25)

$$\begin{aligned}
 P_l(\cos\theta) &= \sqrt{\frac{4\pi}{2l+1}} Y_l^0(\theta) \\
 \text{and } Y_l^0(\theta) &= \sum_{m=-l}^l \sqrt{\frac{4\pi}{2l+1}} Y_l^{*m}(\theta', \phi') Y_l^m(\theta, \phi)
 \end{aligned}$$

Integration over all angular variables and division of the ensuing equation by $P_l(\cos\theta)/r$ will finally yield:

$$\begin{aligned}
 & \left[\frac{d^2}{dr^2} + \frac{3M}{2\hbar^2} E(n) - \frac{l(l+1)}{r^2} \right] f_l(r) = V_{DD}(r) f_l(r) + V_{DS}(r) g_l(r) \\
 &+ \int dr' K_l^{DD}(r, r') f_l(r') + \int dr' K_l^{DS}(r, r') g_l(r') \tag{2.0-33}
 \end{aligned}$$

where use has been made of the orthonormality condition for spherical harmonics.

$$\int_0^{2\pi} d\phi \int_{-1}^1 d(\cos\theta) Y_l^m(\theta, \phi) Y_l^{m'}(\theta', \phi') = \delta_{ll'} \delta_{mm'},$$

The equation for the proton-triton scattering, corresponding to (2.0-33), can be derived in an identical manner from Eqs. (2.0-19) and (2.0-20), with the following change of coordinates:

$$\begin{aligned}
 \bar{r} &= \bar{r}_2 - \frac{1}{3}(\bar{r}_1 + \bar{r}_3 + \bar{r}_4) & \bar{r}'' &= \bar{r}_3 - \frac{1}{3}(\bar{r}_1 + \bar{r}_2 + \bar{r}_4) \\
 \bar{r}' &= \bar{r}_4 - \frac{1}{3}(\bar{r}_1 + \bar{r}_2 + \bar{r}_3) & \bar{R}_2 &= \bar{r}_2 - \bar{r}_4 \\
 \bar{\rho}_2 &= \bar{r}_1 - \bar{r}_3 & \bar{R}_3 &= \bar{r}_4 \\
 \bar{\rho}_4 &= \bar{r}_3 & \bar{x} &= \frac{9}{8} \bar{r} + \frac{3}{8} \bar{r}'' \\
 \bar{u} &= \frac{9}{8} \bar{r} + \frac{3}{8} \bar{r}' & \bar{y} &= \frac{3}{8} \bar{r} + \frac{9}{8} \bar{r}'' \\
 \bar{v} &= \bar{r}_4 - \frac{1}{2}(\bar{r}_1 + \bar{r}_3) = \frac{3}{8} \bar{r} + \frac{9}{8} \bar{r}'
 \end{aligned} \tag{2.0-34}$$

Again, with the definitions (2.0-31) and (2.0-32) we have

$$\begin{aligned}
 \left[\frac{d^2}{dr^2} + \frac{3M}{2\hbar^2} E(p) - \frac{l(l+1)}{r^2} \right] g_l(r) &= v_{SS}(r) g_l(r) + v_{SS}^{Coul}(r) g_l(r) \\
 &+ v_{SD}(r) f_l(r) + \int dr' K_l^{SS}(r, r') g_l(r') + \int dr' K_l^{SD}(r, r') f_l(r')
 \end{aligned} \tag{2.0-35}$$

where:

$$v_{SS}(r) = \left(\frac{9}{8} \right)^3 \frac{M}{\hbar^2} \alpha \int d\tilde{r}' d\tilde{\rho}_2 d\tilde{\rho}_4 v(|\bar{u} - \bar{v}|) \left| n(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \right|^2 \tag{2.0-36}$$

$$v_{SS}^{Coul}(r) = \left(\frac{9}{8}\right)^3 \frac{M}{\hbar^2} \frac{3}{2} \int d\tilde{r}' d\tilde{\rho}_2 d\tilde{\rho}_4 v_c(|\tilde{u}-\tilde{v}|) \left| n(\tilde{v}, \tilde{\rho}_2, \tilde{\rho}_4) \right|^2 \quad (2.0-37)$$

$$v_{SD}(r) = \left(\frac{9}{8}\right)^3 \frac{M}{\hbar^2} a' \int d\tilde{r}' d\tilde{R}_2 d\tilde{R}_3 n^*(\tilde{y}, \tilde{R}_2, \tilde{R}_3) v(|\tilde{x}-\tilde{y}|) \phi(\tilde{y}, \tilde{R}_2, \tilde{R}_3) \quad (2.0-38)$$

$$\begin{aligned} K^{SD}(\tilde{r}, \tilde{r}') &= \left(\frac{9}{8}\right)^3 \frac{M}{\hbar^2} \int d\tilde{R}_2 d\tilde{R}_3 n^*(\tilde{y}, \tilde{R}_2, \tilde{R}_3) [c' v(|\tilde{R}_2|) \\ &\quad + d' \{ v(|\tilde{x}-\frac{1}{2}\tilde{R}_2|) + v(|\tilde{y}+\frac{1}{2}\tilde{R}_2|) \} - e'E + f'v(|\tilde{x}-\tilde{y}|)] \phi(\tilde{x}, \tilde{R}_2, \tilde{R}_3) \\ &\quad + \left(\frac{9}{8}\right)^3 b' \int d\tilde{R}_2 d\tilde{R}_3 \left[\left(\frac{9}{8}\right)^2 n^*(\tilde{y}, \tilde{R}_2, \tilde{R}_3) \nabla_{\tilde{x}}^2 \phi(\tilde{x}, \tilde{R}_2, \tilde{R}_3) \right. \\ &\quad \left. + \left(\frac{9}{8}\right)^2 \phi(\tilde{x}, \tilde{R}_2, \tilde{R}_3) \nabla_{\tilde{y}}^2 n^*(\tilde{y}, \tilde{R}_2, \tilde{R}_3) + \frac{27}{32} \bar{\nabla}_{\tilde{y}} n^*(\tilde{y}, \tilde{R}_2, \tilde{R}_3) \bar{\nabla}_{\tilde{x}} \phi(\tilde{x}, \tilde{R}_2, \tilde{R}_3) \right. \\ &\quad \left. + \frac{3}{2} n^*(\tilde{y}, \tilde{R}_2, \tilde{R}_3) \nabla_{\tilde{R}_2}^2 \phi(\tilde{x}, \tilde{R}_1, \tilde{R}_3) \right] \\ &\quad - 2(27) \int d\tilde{R}_2 d\tilde{\rho}_2 n^*(\tilde{y}, \tilde{R}_2, \tilde{\rho}_2) v_c(|\tilde{x}+\frac{1}{2}\tilde{R}_2|) \phi(\tilde{x}, \tilde{R}_2, \tilde{\rho}_2) \end{aligned} \quad (2.0-39)$$

and

$$\begin{aligned} K^{SS}(\tilde{r}, \tilde{r}') &= \left(\frac{9}{8}\right)^3 \frac{M}{\hbar^2} \int d\tilde{\rho}_2 d\tilde{\rho}_4 n^*(\tilde{v}, \tilde{\rho}_2, \tilde{\rho}_4) [\gamma \{ v(|\tilde{u}-\frac{1}{2}\tilde{\rho}_2|) \right. \\ &\quad \left. + v(|\tilde{v}+\frac{1}{2}\tilde{\rho}_2|) + \delta v(|\tilde{\rho}_2|) + \epsilon v(|\tilde{u}-\tilde{v}|) + n \{ v_c(|\tilde{u}-\tilde{v}|) - E \} \}] \\ &\quad \cdot n(\tilde{u}, \tilde{\rho}_2, \tilde{\rho}_4) + \left(\frac{9}{8}\right)^3 \beta \int d\tilde{\rho}_2 d\tilde{\rho}_4 \left[\left(\frac{9}{8}\right)^2 n^*(\tilde{v}, \tilde{\rho}_2, \tilde{\rho}_4) \nabla_{\tilde{u}}^2 n(\tilde{u}, \tilde{\rho}_2, \tilde{\rho}_4) \right. \\ &\quad \left. + \left(\frac{9}{8}\right)^2 n(\tilde{u}, \tilde{\rho}_2, \tilde{\rho}_4) \nabla_{\tilde{v}}^2 n(\tilde{v}, \tilde{\rho}_2, \tilde{\rho}_4) + \frac{27}{32} \bar{\nabla}_{\tilde{u}} n(\tilde{u}, \tilde{\rho}_2, \tilde{\rho}_4) \bar{\nabla}_{\tilde{v}} n^*(\tilde{v}, \tilde{\rho}_2, \tilde{\rho}_4) \right. \\ &\quad \left. + \frac{3}{2} n^*(\tilde{v}, \tilde{\rho}_2, \tilde{\rho}_4) \nabla_{\tilde{\rho}_2}^2 n(\tilde{u}, \tilde{\rho}_2, \tilde{\rho}_4) \right] \end{aligned} \quad (2.0-40)$$

Again, the constants appearing in the various kernels and direct potentials are defined in Table I for S=1 and S=0.

To evaluate explicitly the direct potentials and kernels in Eqs. (2.0-33) and (2.0-35), one needs to know the form of the nuclear potential, and the wavefunctions representing the helium-3 and triton bound states.

The type of interaction chosen for this study involves a Serber-type exchange force, wherein

$$m = w = \frac{1}{4} (1+x) ; \quad h = b = \frac{1}{4} (1-x) \quad (2.0-41)$$

Such interaction has been found to yield fairly good agreement with experimental results [3,4]. The potential well $V(r)$ is chosen to be of the Gaussian form in order that the kernels may be determined analytically.

$$V(r) = V_0 \exp(-\mu r^2) \quad (2.0-42)$$

For the same reason, we are forced to employ Gaussian wavefunctions for the helium-3 and triton clusters.

$$\phi_{3He} = \frac{1}{N_{3He}} \exp\left(-\frac{\nu}{2} \sum_{ij} r_{ij}^2\right) \quad (2.0-43)$$

$$\eta_T = \frac{1}{N_T} \exp\left(-\frac{\lambda}{2} \sum_{ij} r_{ij}^2\right) \quad (2.0-44)$$

The parameters $V_0 = -45$ MeV, $\mu = 0.2669 \times 10^{26}$ cm⁻², and $x = 0.6$ are those used in previous calculations of four and five-nucleon problems [3,4,22]. These parameters represent a potential which is longer ranged than that suggested by two-body scattering data. On the other hand, the form assumed for the potential is that of a purely central force. Thus,

some equivalent central representation of the tensor force has been postulated, and there is no reason to presume that this equivalent central force is the same for a four-body problem as for the two-body problem. In fact, studies of the binding energy of the alpha particle, in which tensor forces are included, have shown the tensor force to be relatively less effective in producing binding than in the two-body case [22]. Furthermore, the potential used has been shown to be consistent with four-body bound states [3,4], and to predict the correct binding energy of the deuteron [3].

The wavefunction constants

$$\nu = 0.1436 \times 10^{26} \text{ cm}^{-2}$$

$$\lambda = 0.1404 \times 10^{26} \text{ cm}^{-2}$$

used here are those found by Bransden et al. [3] by minimizing the energies $E_{^3\text{He}}$ and E_T in Eqs. (2.0-15) and (2.0-18), which are then automatically satisfied. The minimum values of E_T and $E_{^3\text{He}}$ which they found by a variational method, were:

$$E_{^3\text{He}} = -4.74 \text{ MeV} \quad \text{and} \quad E_T = -5.49 \text{ MeV.}$$

These values are lower than the experimental values, but scattering cross sections are generally insensitive to binding-energy values, as long as one is consistent, and uses the theoretically determined values in the evaluation of the kernels.

With the assumed forms of the potential and nuclear wavefunctions, the kernels and direct-potential terms can be evaluated analytically. Their expressions are given in Table II. Detailed calculations for some typical kernel and direct potential terms are given in Appendices B through D.

Table II
 Direct Potentials and Kernels Appearing in
 Equations (2.0-33) and (2.0-35).

$$v_{DD}(r) = 27 \frac{M}{\hbar^2} \alpha v_0 \left(\frac{v}{2\mu+9v} \right)^{3/2} \exp \left[- \frac{9\mu v}{2\mu+9v} r^2 \right]$$

$$v_{DS}(r) = 216 \frac{M}{\hbar^2} \alpha' v_0 \frac{(\lambda v)^{3/2}}{[9(v+\lambda) + 4\mu]^{3/2} (v+\lambda)^{3/2}} \exp \left[- \frac{9(v+\lambda)}{[9(v+\lambda) + 4\mu]} r^2 \right]$$

$$v_{SS}(r) = 27 \frac{M}{\hbar^2} \alpha v_0 \left(\frac{\lambda}{2\mu+9\lambda} \right)^{3/2} \exp \left[- \frac{9\mu\lambda}{2\mu+9\lambda} r^2 \right]$$

$$v_{SS}^{Coul}(r) = \frac{3}{2} \frac{M}{\hbar^2} \frac{q^2}{r}$$

$$v_{SD}(r) = 216 \frac{M}{\hbar^2} \alpha' v_0 \frac{(\lambda v)^{3/2}}{[9(v+\lambda) + 4\mu]^{3/2} (v+\lambda)^{3/2}} \exp \left[- \frac{9(v+\lambda)}{9(v+\lambda) + 4\mu} r^2 \right]$$

The Kernel $K_l^{(DD)}(r, r')$

$$K_l^{(DD)}(r, r') = \gamma [q_l^{DD}(r, r') + s_l^{DD}(r, r')] + \delta f_l^{DD}(r, r') + \epsilon g_l^{DD}(r, r') \\ + \eta [h_l^{DD}(r, r') - n_l^{DD}(r, r')] + \beta p_l^{DD}(r, r')$$

where

$$q_l^{DD}(r, r') = \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} \frac{81}{2} \frac{v^2}{\sqrt{6v+\mu} (3v+2\mu)} \exp \left[- \frac{9}{16} \frac{v(15v+16\mu)}{6v+\mu} r^2 \right] \\ \times \exp \left[- \frac{9}{16} \frac{v(15v+4\mu)}{6v+\mu} r'^2 \right] I_{l+\frac{1}{2}} \left[\frac{27}{8} v \left(\frac{3v+2\mu}{6v+\mu} rr' \right) \right]$$

Table II (cont.)

$$S_{\ell}^{DD}(r, r') = \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} \frac{81}{2} \frac{v^2}{\sqrt{6v+\mu} (3v+2\mu)} \exp\left[-\frac{9}{16} \frac{v(15v+16\mu)}{6v+\mu} r^2\right]$$

$$\times \exp\left[-\frac{9}{16} \frac{v(15v+16\mu)}{6v+\mu} r'^2\right] I_{\ell+\frac{1}{2}}\left[\frac{27}{8} v\left(\frac{3v+2\mu}{6v+\mu}\right) rr'\right]$$

$$g_{\ell}^{DD}(r, r') = \frac{81}{\sqrt{2\pi}} \frac{MV_0}{\hbar^2} \frac{v^{3/2}}{(6v-4\mu)} \exp\left[-\frac{9}{32}(5v+2\mu)(r^2+r'^2)\right] I_{\ell+\frac{1}{2}}\left[\frac{9}{32}(6v-4\mu) rr'\right]$$

$$n_{\ell}^{DD}(r, r') = \frac{ME}{\hbar^2} \frac{v^{\frac{1}{2}}}{\sqrt{2\pi}} \left(\frac{27}{2}\right) \exp\left[-\frac{45}{32} v(r^2+r'^2)\right] I_{\ell+\frac{1}{2}}\left[\frac{27}{16} vrr'\right]$$

$$f_{\ell}^{DD}(r, r') = 81\sqrt{\frac{3}{\pi}} \left(\frac{MV_0}{\hbar^2}\right)^{\frac{1}{2}} \frac{v^2}{(6v+4\mu)^{3/2}} \exp\left[-\frac{45}{32} v(r^2+r'^2)\right] I_{\ell+\frac{1}{2}}\left[\frac{27}{16} vrr'\right]$$

$$h_{\ell}^{DD}(r, r') = \frac{q^2 M}{\hbar^2} \left(\frac{v}{\pi}\right) \frac{27\sqrt{3}}{2} \exp\left[-\frac{45}{32} v(r^2+r'^2)\right] I_{\ell+\frac{1}{2}}\left[\frac{27}{16} vrr'\right]$$

$$p_{\ell}^{DD}(r, r') = \sqrt{\frac{8v^5}{\pi}} \left(\frac{9}{8}\right)^4 \exp\left[-\frac{45}{32} v(r^2+r'^2)\right]$$

$$\times \left\{ [18(r^2+r'^2) - \frac{608}{27v}] I_{\ell+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) - 28 rr' I_{\ell+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) \right\}$$

The Kernel $K_{\ell}^{DS}(r, r')$

$$K_{\ell}^{DS}(r, r') \equiv d'[q_{\ell}^{DS}(rr') + s_{\ell}^{DS}(r, r')] + c'f_{\ell}^{DS}(rr') + e'[h_{\ell}^{DS}(rr') - n_{\ell}^{DS}(r, r')]$$

$$+ f'g_{\ell}^{DS}(rr') + b'p_{\ell}^{DS}(rr')$$

Table II (cont.)

where:

$$p_{\lambda}^{DS}(r, r') = \left(\frac{9}{8}\right)^4 \sqrt{\frac{(\lambda v)^3}{\pi}} \exp[-\lambda(\frac{81}{64} r^2 + \frac{9}{64} r'^2)] \exp[-v(\frac{9}{64} r^2 + \frac{81}{64} r'^2)]$$

$$\times \left\{ \frac{128}{27(\lambda+v)^{7/2}} [36(\lambda^2+v^2) + 40v\lambda - 54(v+\lambda)^2 + 48\lambda^2 - 48\lambda(v+\lambda)] \right.$$

$$\cdot I_{\lambda+\frac{1}{2}} \left[\frac{27}{32} (v+\lambda) rr' \right] + \left[\frac{(216\lambda^2+24v^2+48\lambda v)r^2 + (216v^2+24\lambda^2+48\lambda v)r'^2}{(\lambda+v)^{5/2}} \right]$$

$$\cdot I_{\lambda+\frac{1}{2}} \left[\frac{27}{32} (v+\lambda) rr' \right] - \left[\frac{144(\lambda^2+v^2) + 160\lambda v}{(\lambda+v)^{5/2}} \right] rr' I_{\lambda+\frac{1}{2}} \left[\frac{27}{32} (v+\lambda) rr' \right]$$

$$q_{\lambda}^{DS}(r, r') = \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} 162 \frac{(\lambda v)^{3/2}}{\sqrt{3(v+\lambda)+\mu} (v+\lambda) (3v+3\lambda+4\mu)}$$

$$\times \exp \left[- \frac{9}{64} \left(\frac{3v^2+30v\lambda+27\lambda^2+28\mu v+36\mu\lambda}{3v+3\lambda+\mu} \right) r^2 \right]$$

$$\times \exp \left[- \frac{9}{64} \left(\frac{27v^2+30v\lambda+3\lambda^2+12v\mu+4\mu\lambda}{3v+3\lambda+\mu} \right) r'^2 \right] I_{\lambda+\frac{1}{2}} \left[\frac{27}{32} \frac{(v+\lambda)(3v+3\lambda+4\mu)}{3(v+\lambda)+\mu} rr' \right]$$

$$s_{\lambda}^{DS}(r, r') = \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} 162 \frac{(\lambda v)^{3/2}}{\sqrt{3(v+\lambda)+\mu} (v+\lambda) (3v+3\lambda+4\mu)}$$

$$\times \exp \left[- \frac{9}{64} \left(\frac{27v^2+30v\lambda+3\lambda^2+12v\mu+4\mu\lambda}{3(v+\lambda)+\mu} \right) r^2 \right]$$

$$\times \exp \left[- \frac{9}{64} \left(\frac{3v^2+30v\lambda+27\lambda^2+28\mu v+36\mu\lambda}{3(v+\lambda)+\mu} \right) r'^2 \right] I_{\lambda+\frac{1}{2}} \left[\frac{27}{32} \frac{(v+\lambda)(3v+3\lambda+4\mu)}{3(v+\lambda)+\mu} rr' \right]$$

Table II (cont.)

$$f_l^{DS}(r, r') = 162 \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} \frac{(\lambda\nu)^{3/2}}{(\nu+\lambda)[3(\nu+\lambda)+4\mu]^{3/2}} \exp\left[-\frac{9}{64}(r^2+9r'^2)\right]$$

$$-\frac{9}{64}\lambda(9r^2+r'^2)I_{l+\frac{1}{2}}[\frac{27}{32}(\nu+\lambda)rr']$$

$$\eta_l^{DS}(r, r') = 162 \sqrt{\frac{3}{\pi}} \frac{M}{\hbar^2} \frac{(\lambda\nu)^{3/2}}{(\nu+\lambda)[3(\nu+\lambda)]^{3/2}} \exp\left[-\frac{9}{64}\nu(r^2+9r'^2)\right]$$

$$-\frac{9}{64}\lambda(9r^2+r'^2)I_{l+\frac{1}{2}}[\frac{27}{32}(\nu+\lambda)rr']$$

$$h_l^{DS}(r, r') = 0$$

$$g_l^{DS}(r, r') = \frac{162}{\sqrt{\pi}} \left(\frac{\lambda\nu}{\nu+\lambda}\right)^{3/2} \frac{MV_0}{\hbar^2} \exp\left\{-\frac{9}{64}[\nu(r^2+9r'^2) + \lambda(9r^2+r'^2) + 4\mu(r^2+r'^2)]\right\}$$

$$\times \frac{1}{3(\nu+\lambda)-4\mu} I_{l+\frac{1}{2}}[\frac{27}{32}(\nu+\lambda) - \frac{9}{8}\mu]rr'$$

The Kernel $K_l^{SD}(r, r')$

$$K_l^{SD}(r, r') \equiv d'[q_l^{SD}(r, r') + s_l^{SD}(r, r')] + c'f_l^{SD}(r, r') + f'g_l^{SD}(r, r')$$

$$+ e'[h_l^{SD}(r, r') - \eta_l^{SD}(r, r')] + b'p_l^{SD}(r, r')$$

where:

$$p_l^{SD}(r, r') = \left(\frac{9}{8}\right)^4 \sqrt{\frac{(\lambda\nu)^3}{\pi}} \exp\left[-\nu\left(\frac{81}{64}r^2 + \frac{9}{64}r'^2\right)\right] \exp\left[-\lambda\left(\frac{9}{64}r^2 + \frac{81}{64}r'^2\right)\right]$$

$$\times \left\{ \frac{128}{27(\lambda+\nu)^{7/2}} [36(\lambda^2+\nu^2) + 40\lambda\nu - 54(\lambda+\nu)^2 + 48\nu^2 - 48\nu(\lambda+\nu)] \right.$$

Table II (cont.)

$$\begin{aligned}
& \times I_{l+\frac{1}{2}} \left[\frac{27}{32} (\nu + \lambda) rr' \right] + \left[\frac{(216\nu^2 + 24\lambda^2 + 48\lambda\nu)r^2 + (216\lambda^2 + 24\nu^2 + 48\lambda\nu)r'^2}{(\lambda + \nu)^{5/2}} \right] \\
& \times I_{l+\frac{1}{2}} \left[\frac{27}{32} (\nu + \lambda) rr' \right] - \left[\frac{144(\lambda^2 + \nu^2) + 160\lambda\nu}{(\lambda + \nu)^{5/2}} \right] rr' I_{l+\frac{1}{2}} \left[\frac{27}{32} (\nu + \lambda) rr' \right] \\
q_l^{\text{SD}}(r, r') &= \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} 162 \frac{(\lambda\nu)^{3/2}}{\sqrt{3(\nu + \lambda) + \mu} (\nu + \lambda) (3\lambda + 3\nu + 4\mu)} \\
&\times \exp \left[- \frac{9}{64} \left(\frac{3\lambda^2 + 30\nu\lambda + 27\nu^2 + 28\mu\lambda + 36\mu\nu}{3(\nu + \lambda) + \mu} \right) r^2 \right] \\
&\times \exp \left[- \frac{9}{64} \left(\frac{3\nu^2 + 27\lambda^2 + 30\lambda\nu + 12\lambda\nu + 4\mu\nu}{3(\nu + \lambda) + \mu} \right) r'^2 \right] I_{l+\frac{1}{2}} \left[\frac{27}{32} \frac{(\nu + \lambda)(3\lambda + 3\nu + 4\mu)}{3(\nu + \lambda) + \mu} rr' \right] \\
s_l^{\text{SD}}(r, r') &= \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} 162 \frac{(\lambda\nu)^{3/2}}{\sqrt{3(\nu + \lambda) + \mu} (\nu + \lambda) (3\lambda + 3\nu + 4\mu)} \\
&\times \exp \left[- \frac{9}{64} \left(\frac{27\lambda^2 + 30\lambda\nu + 3\nu^2 + 12\lambda\nu + 4\mu\nu}{3(\nu + \lambda) + \mu} \right) r^2 \right] \\
&\times \exp \left[- \frac{9}{64} \left(\frac{3\lambda^2 + 30\nu\lambda + 27\nu^2 + 28\mu\lambda + 36\mu\nu}{3(\nu + \lambda) + \mu} \right) r'^2 \right] I_{l+\frac{1}{2}} \left[\frac{27}{32} \frac{(\nu + \lambda)(3\lambda + 3\nu + 4\mu)}{3(\nu + \lambda) + \mu} rr' \right] \\
f^{\text{SD}}(r, r') &= 162 \frac{MV_0}{\hbar^2} \sqrt{\frac{3}{\pi}} \frac{(\lambda\nu)^{3/2}}{(\nu + \lambda) [3(\nu + \lambda) + 4\mu]^{3/2}} \exp \left[- \frac{9}{64} \lambda(r^2 + 9r'^2) \right. \\
&\quad \left. - \frac{9}{64} \nu(9r^2 + r'^2) \right] I_{l+\frac{1}{2}} \left[\frac{27}{32} (\nu + \lambda) rr' \right] \\
\eta_l^{\text{SD}}(r, r') &= 162 \sqrt{\frac{3}{\pi}} \frac{ME}{\hbar^2} \frac{(\lambda\nu)^{3/2}}{(\nu + \lambda) [3(\nu + \lambda)]^{3/2}} \exp \left[- \frac{9}{64} \lambda(r^2 + 9r'^2) \right. \\
&\quad \left. - \frac{9}{64} \nu(9r^2 + r'^2) \right] I_{l+\frac{1}{2}} \left[\frac{27}{32} (\nu + \lambda) rr' \right]
\end{aligned}$$

Table II (cont.)

$$h_{\lambda}^{SD}(r, r') = 0$$

$$g_{\lambda}^{SD}(r, r') = \frac{162}{\sqrt{\pi}} \left(\frac{\lambda v}{\lambda + v}\right)^{3/2} \frac{Mv_o}{n^2} \exp\left\{-\frac{9}{64}[\lambda(r^2 + r'^2) + v(9r^2 + r'^2) + 4\mu(r^2 + r'^2)]\right\} \times \frac{1}{3(v+\lambda)-4\mu} I_{\lambda+\frac{1}{2}}\left[\left\{\frac{27}{32}(v+\lambda) - \frac{9}{8}\mu\right\}rr'\right]$$

The Kernel $K_{\lambda}^{SS}(r, r')$

$$K_{\lambda}^{SS}(r, r') \equiv \gamma[q_{\lambda}^{SS}(r, r') + s_{\lambda}^{SS}(r, r')] + \delta f_{\lambda}^{SS}(r, r') + \epsilon g_{\lambda}^{SS}(r, r')$$

$$+ \eta[h_{\lambda}^{SS}(r, r') + \eta_{\lambda}^{SS}(r, r')] + \beta p_{\lambda}^{SS}(r, r')$$

where:

$$q_{\lambda}^{SS}(r, r') = \frac{Mv_o}{n^2} \sqrt{\frac{3}{\pi}} \frac{81}{2} \frac{\lambda^2}{\sqrt{6\lambda+\mu}} \frac{(3\lambda+2\mu)}{\exp\left[-\frac{9}{16} \frac{\lambda(15\lambda+16\mu)}{6\lambda+\mu} r^2\right]} I_{\lambda+\frac{1}{2}}\left[\frac{27}{8} \lambda \left(\frac{3\lambda+2\mu}{6\lambda+\mu}\right) rr'\right]$$

$$\times \exp\left[-\frac{9}{16} \frac{\lambda(15\lambda+4\mu)}{6\lambda+\mu} r'^2\right] I_{\lambda+\frac{1}{2}}\left[\frac{27}{8} \lambda \left(\frac{3\lambda+2\mu}{6\lambda+\mu}\right) rr'\right]$$

$$s_{\lambda}^{SS}(r, r') = \frac{Mv_o}{n^2} \sqrt{\frac{3}{\pi}} \frac{81}{2} \frac{\lambda^2}{\sqrt{6\lambda+\mu}} \frac{(3\lambda+2\mu)}{\exp\left[-\frac{9}{16} \frac{\lambda(15\lambda+4\mu)}{6\lambda+\mu} r^2\right]} I_{\lambda+\frac{1}{2}}\left[\frac{27}{8} \lambda \left(\frac{3\lambda+2\mu}{6\lambda+\mu}\right) rr'\right]$$

$$\times \exp\left[-\frac{9}{16} \frac{\lambda(16\mu+15\lambda)}{6\lambda+\mu} r'^2\right] I_{\lambda+\frac{1}{2}}\left[\frac{27}{8} \lambda \left(\frac{3\lambda+2\mu}{6\lambda+\mu}\right) rr'\right]$$

$$g_{\lambda}^{SS}(r, r') = \frac{81}{\sqrt{2\pi}} \frac{Mv_o}{n^2} \frac{\lambda^{3/2}}{(6\lambda-4\mu)} \exp\left[-\frac{9}{32}(5\lambda+2\mu)(r^2 + r'^2)\right] I_{\lambda+\frac{1}{2}}\left[\frac{9}{32}(6\lambda-4\mu)rr'\right]$$

Table II (cont.)

$$\eta_{\ell}^{SS}(r, r') = \frac{ME}{\hbar^2} \frac{\lambda^{1/2}}{\sqrt{2\pi}} \left(\frac{27}{2}\right) \exp\left[-\frac{45}{32} \lambda(r^2 + r'^2)\right] I_{\ell+1/2} \left[\frac{27}{16} \lambda rr'\right]$$

$$f_{\ell}^{SS}(r, r') = 81 \sqrt{\frac{3}{\pi}} \left(\frac{MV_0}{h^2}\right) \frac{\lambda^2}{[6\lambda+4\mu]^{3/2}} \exp\left[-\frac{45}{32} \lambda(r^2 + r'^2)\right] I_{\ell+1/2} \left(\frac{27}{16} \lambda rr'\right)$$

$$p_{\ell}^{SS}(r, r') = \sqrt{\frac{8\lambda^5}{\pi}} \left(\frac{9}{8}\right)^4 \exp\left[-\frac{45}{32}(r^2 + r'^2)\right]$$

$$\times \left\{ [18(r^2 + r'^2) - \frac{608}{27\lambda}] I_{\ell+1/2} \left(\frac{27}{16} \lambda rr'\right) - 28rr' I_{\ell+1/2}' \left(\frac{27}{16} \lambda rr'\right) \right\}$$

$$h_{\ell}^{SS}(r, r') = \frac{Mq}{\hbar^2} \left(\frac{9}{8}\right)^3 \frac{\lambda^{3/2}}{\sqrt{\pi}} \frac{64}{3} \exp\left[-\lambda \frac{90}{64} r^2 + \frac{90}{64} r'^2\right]$$

$$\times \int_{-1}^1 dz P_{\ell}(z) e^{-108/64 rr' z} rr' [r^2 + r'^2 - 2rr' z]^{1/2}$$

Inspection of the analytical form of the kernels reveals that the Coulomb terms are absent from the cross-channel kernels. One can show that the Coulomb force contribution to these kernels is zero (Appendix E). Physically this is a consequence of the Coulomb interaction being long ranged; thus it is accounted for in the direct potentials. The exact form for the $h_{\ell}^{SS}(r, r')$ partial kernel can only be determined analytically for each value of ℓ , in that the integral associated with it assumes different expressions for different values of ℓ . Table III lists the values of $h_{\ell}^{SS}(r, r')$ for $\ell=0, 1, 2$; the values of interest in this study.

Table III

Values of $h_{\ell}^{SS}(r, r')$ for Different Values of ℓ .

$$h_0^{SS}(r, r') = \frac{Mq^2}{\pi^2} \frac{81}{4\sqrt{3}\pi} \lambda e^{-\frac{90}{64}\lambda(r^2+r'^2)} \left\{ e^{\frac{108}{64}\lambda rr'} F_0\left[\sqrt{\frac{54\lambda}{64}}(r+r')\right] \right.$$

$$\left. - e^{-\frac{108}{64}\lambda rr'} F_0\left[\sqrt{\frac{54\lambda}{64}}(r-r')\right] \right\}$$

$$h_1^{SS}(r, r') = \frac{Mq^2}{\pi^2} \frac{243\sqrt{2}}{32\sqrt{\pi}} \lambda^{3/2} \exp[-\lambda(\frac{90}{64}r^2 + \frac{90}{64}r'^2)]$$

$$\times \left\{ \left[\left(\frac{r^2+r'^2}{2rr'} \right) \left(\frac{64}{54\lambda} \right)^{1/2} + \frac{1}{4rr'} \left(\frac{64}{54\lambda} \right)^{3/2} \right] \right.$$

$$\left. \times \left[e^{\frac{108}{64}\lambda rr'} F_0\left(\sqrt{\frac{54\lambda}{64}}(r+r')\right) - e^{-\frac{108}{64}\lambda rr'} F_0\left(\sqrt{\frac{54\lambda}{64}}|r-r'|\right) \right] \right\}$$

$$- \frac{1}{4rr'} \left(\frac{64}{54\lambda} \right) \left[e^{\frac{108}{64}\lambda rr'} (r+r') - e^{-\frac{108}{64}\lambda rr'} |r-r'| \right]$$

$$h_2^{SS}(r, r') = \frac{Mq^2}{\pi^2} \frac{243}{32} \frac{2}{\pi} \lambda^{3/2} e^{-\frac{90}{64}\lambda(r^2+r'^2)} \left\{ \left[\frac{3(r^2+r'^2)}{8r^2r'^2} \left(\frac{64}{54\lambda} \right)^{1/2} \right. \right.$$

$$\left. \left. + \frac{3(r^2+r'^2)}{8r^2r'^2} \left(\frac{64}{54\lambda} \right)^{3/2} + \frac{9}{32r^2r'^2} \left(\frac{64}{54\lambda} \right)^{5/2} - \frac{1}{2} \left(\frac{64}{54\lambda} \right)^{1/2} \right] \right\}$$

$$\cdot \left[e^{\frac{108}{64}\lambda rr'} F_0\left(\sqrt{\frac{54\lambda}{64}}(r+r')\right) - e^{-\frac{108}{64}\lambda rr'} F_0\left(\sqrt{\frac{54\lambda}{64}}|r-r'|\right) \right]$$

$$- \left[\frac{3(r^2+r'^2)}{8r^2r'^2} \left(\frac{64}{54\lambda} \right)^2 + \frac{9}{32r^2r'^2} \left(\frac{64}{54\lambda} \right)^2 \right]$$

$$\cdot \left[e^{\frac{108}{64}\lambda rr'} (r+r') - e^{-\frac{108}{64}\lambda rr'} |r-r'| \right]$$

$$+ \frac{3}{16r^2r'^2} \left(\frac{64}{54\lambda} \right) \left[e^{\frac{108}{64}\lambda rr'} (r+r')^3 - e^{-\frac{108}{64}\lambda rr'} |r-r'|^3 \right] \}$$

The functions $I_{\ell+\frac{1}{2}}(\bar{x})$ appearing in the kernels are closely related to the Bessel functions of the first kind and imaginary argument. In fact

$$I_{\ell+\frac{1}{2}}(x') = (-)^{\ell} (\frac{1}{2}\pi x')^{1/\ell} I_{\ell+\frac{1}{2}}(x') \quad (2.0-45)$$

The function $F_0(x)$ in the expressions for $h_{\ell}^{SS}(r, r')$, is the Dawson's integral defined as

$$F_0(x') = e^{-x'^2} \int_0^{x'} e^{u^2} du \quad (2.0-46)$$

which has been tabulated by Miller and Gordon [31] for values of x ranging from 0 to 12.

The equations (2.0-33) and (2.0-35) must now be solved to yield the scattering functions subject to the usual boundary conditions that

$$f_{\ell}(0) = 0 ; \quad g_{\ell}(0) = 0 \quad (2.0-47)$$

and the asymptotic conditions that:

$f_{\ell}(r)$ be represented by a superposition of incoming and outgoing spherical waves in channel I ($n+^3He \rightarrow n+^3He$), and in channel II ($p+T \rightarrow n+^3He$), by a purely outgoing spherical wave.

$g_{\ell}(r)$ be represented in channel II ($p+T \rightarrow p+T$) by a superposition of incoming and outgoing spherical waves, and in channel I ($n+^3He \rightarrow p+T$) by simply an outgoing spherical wave.

Alternatively the functions f_{ℓ} and g_{ℓ} must be found that satisfy (2.0-47) and have two independent solutions such that

$$f_{\ell}^{ij}(r) \sim A_{\ell}^{ij} F_{\ell}^i(r) + B_{\ell}^{ij} G_{\ell}^i(r) \quad i=1,2 \text{ (2 channels)} \quad (2.0-48)$$

$$g_{\ell}^{ik} \sim A_{\ell}^{ik} F_{\ell}^i(r) + B_{\ell}^{ik} G_{\ell}^i(r)$$

where $F_\ell^i(r)$ and $G_\ell^i(r)$ are the regular and irregular wavefunctions for the corresponding channel, and are described in Appendix G.

The reactance matrix is then [28,32]

$$\bar{\bar{R}} = \bar{\bar{B}} \bar{\bar{A}}^{-1} \quad (2.0-49)$$

and the scattering matrix:

$$\bar{\bar{S}} = (1+i\bar{\bar{R}})/(1-i\bar{\bar{R}}) \quad (2.0-50)$$

The scattering amplitude $f_{\alpha\alpha'}^S(\theta)$ corresponding to the total spin S can be written as

$$f_{\alpha\alpha'}^S(\theta) = -\frac{1}{2ik_\alpha} \sum (d_{\alpha\alpha'} - s_{\alpha\alpha'}^\ell) (2\ell + 1) P_\ell(\cos\theta) \quad (2.0-51)$$

where α and α' represent the entrance and exit channels, respectively.

The corresponding differential cross-section is

$$\sigma_{\alpha\alpha'}^S(\theta) \equiv |f_{\alpha\alpha'}^S(\theta)|^2 \quad (2.0-52)$$

The differential cross section for the $n+{}^3He$ interaction is then given by:

$$\sigma(\theta) = \frac{3}{4} \sigma_i(\theta) + \frac{1}{4} \sigma_o(\theta) \quad (2.0-53)$$

For the four-particle system under study, k_α is the wave number of the incident channel, and is equal to $3M/2\hbar^2$ times the energy of the incident particle in the center-of-mass system of coordinates.

3.0 NUMERICAL ANALYSIS

To solve the integro-differential Eqs. (2.0-33) and (2.0-35), the region of integration is divided into two parts, separated by a distance R_M at which the kernels $K_\ell^{IJ}(r, r')$ become vanishingly small. For $r > R_M$, the kernels are set as zero. The integro-differential equations are converted to a set of simultaneous algebraic equations by a method first proposed by Robertson [36]. In the region where the kernels are zero this method becomes entirely equivalent to the method of Fox and Goodwin [16], also known as Cowell's method [30]. The solutions of the equations are then matched to the appropriate regular and irregular functions, at a distance large enough so that the kernels and the direct potentials are zero.

In practice, since the direct potentials also become vanishingly small at the distance R_M where the kernels vanish, it is sufficient to solve the system of simultaneous equations in the region $r \leq R_M$, and match the ensuing solutions to the regular and irregular functions for the respective channels.

For $r \leq R_M$, Eq. (2.0-33) can be written as

$$\frac{d^2 f_\ell(r)}{dr^2} + u(r) f_\ell(r) = v(r) g_\ell(r) + \int_0^{R_M} K_\ell^{DD}(r, r') f_\ell(r') dr' + \int_0^{R_M} K_\ell^{DS}(r, r') g_\ell(r') dr' \quad (3.0-1)$$

$$\text{where } u(r) \equiv \frac{3M}{2\hbar^2} E(n) - \frac{\ell(\ell+1)}{r^2} - v_{DD}(r) \quad (3.0-2)$$

$$\text{and } v(r) \equiv v_{DS}(r) \quad (3.0-3)$$

The range of integration of the kernels on the right hand side of the equation can now be split into a number of pivotal points at equal intervals h' , and the integrals can be evaluated in terms of Gregory's formula, [26], which expresses the integral in terms of the function values at the pivotal points, and the forward and backward differences at the beginning and at the end of the range.

The integrals of the kernels for each value of ℓ can be written as

$$\int_0^{R_M} K^{DD}(r, r') f(r') dr' + \int_0^{R_M} K^{DS}(r, r') g(r') dr' \\ = \sum_{m=0}^N T_m [K_{n,m}^{DD} f_m + K_{n,m}^{DS} g_m] \quad (3.0-4)$$

where $N = R_M/h'$, and T_m are the integration factors derived from Gregory's formula. For this work, the formula was truncated at the fourth difference so that the integral could be expressed solely in terms of the pivotal values of the argument. These integration coefficients are shown in Table IV.

In order to solve the integro-differential equation, the same pivotal points employed for the r' integration are used for the range of r .

The second derivative is expressed in terms of its central difference formula. At the pivotal point r_n we have

$$h'^2 f_n'' = (f_{n-1} - 2f_n + f_{n+1}) - \frac{1}{12} \delta^4 f_n + \frac{1}{90} \delta^6 f_n \quad (3.0-5)$$

Substitution of (3.0-4) and (3.0-5) into (3.0-1) yields for each ℓ .

$$(f_{n-1} - 2f_n + f_{n+1}) + h'^2 u_n f_n = h'^2 v_n g_n$$

$$+ h'^2 \sum_{m=0}^N T_m K_{n,m}^{DD} f_m + h^2 \sum_{m=0}^N T_m K_{n,m}^{DS} g_m + \frac{1}{12} \delta^4 f_n - \frac{1}{90} \delta^6 f_n$$

Thus

$$f_{n-1} - (2 - h'^2 u_n) f_n + f_{n+1} = h'^2 v_n g_n + h'^2 \sum_{m=0}^N T_m K_{n,m}^{DD} f_m$$

$$+ h'^2 \sum_{m=0}^N T_m K_{n,m}^{DS} g_m + \frac{1}{12} \delta^4 f_n - \frac{1}{90} \delta^6 f_n \quad (3.0-6)$$

The central difference operator $(1 + \frac{1}{12} \delta^2)$ is applied throughout Eq. (3.0-6) to yield

$$(1 + \frac{h'^2}{12} u_{n-1}) f_{n-1} - (2 - \frac{10h'^2}{12} u_n) f_n + (1 + \frac{h'^2}{12} u_{n+1}) f_{n+1}$$

$$= \frac{h'^2}{12} v_{n+1} g_{n+1} + \frac{10h'^2}{12} v_n g_n + \frac{h'^2}{12} v_{n-1} g_{n-1}$$

$$+ \frac{h'^2}{12} \sum_{m=0}^N T_m [K_{n-1,m}^{DD} + 10 K_{n,m}^{DD} + K_{n+1,m}^{DD}] f_m$$

$$+ \frac{h'^2}{12} \sum_{m=0}^N T_m [K_{n-1,m}^{DS} + 10 K_{n,m}^{DS} + K_{n+1,m}^{DS}] g_m - \frac{1}{240} \delta^6 f_n \quad (3.0-7)$$

since $\frac{1}{12}[f_{n-2} - 4f_{n-1} + 6f_n - 4f_{n+1} + f_{n+2}] \equiv \frac{1}{12} \delta^4 f_n$

When the above procedure is applied to Eq. (2.0-35), an equation similar to (3.0-7) is obtained.

$$\begin{aligned}
 & (1 + \frac{h'}{12} x_{n-1}) g_{n-1} - (2 - \frac{10h'}{12} x_n) g_n + (1 + \frac{h'}{12} x_{n+1}) g_{n+1} = \frac{h'}{12} y_{n-1} f_{n-1} \\
 & + \frac{10h'}{12} y_n f_n + \frac{h'}{12} y_{n+1} f_{n+1} + \frac{h'}{12} \sum_{m=0}^N T_m [K_{n-1,m}^{SD} + 10 K_{n,m}^{SD} \\
 & + K_{n+1,m}^{SD}] f_m + \frac{h'}{12} \sum_{m=0}^N T_m [K_{n-1,m}^{SS} + 10 K_{n,m}^{SS} + K_{n+1,m}^{SS}] g_m - \frac{1}{240} \delta^6 g_n \quad (3.0-8)
 \end{aligned}$$

where $x(r) \equiv \frac{3M}{2h^2} E(p) - \frac{\ell(\ell+1)}{r^2} - v_{SS}(r) - v_{SS}^{Coul}(r)$ (3.0-9)

and $y(r) \equiv v_{SD}(r)$ (3.0-10)

Robertson [36] showed that the terms $\frac{1}{240} \delta^6 f_n$ and $\frac{1}{240} \delta^6 g_n$ can be set equal to zero, without introducing any appreciable error in the evaluation of the scattering functions.

Equations (3.0-7) and (3.0-8) can now be combined in a matrix homogeneous equation of the form

$$AX = 0 \quad (3.0-11)$$

where X is the column vector formed by the unknown scattering functions,

i.e.:

$$X = \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_N \\ g_0 \\ g_1 \\ \vdots \\ g_N \end{bmatrix}$$

and A is a $(2N-4, 2N)$ matrix.

The elements of each row of the matrix A require the knowledge of the kernels at three n points and all m points. For instance, the equation resulting from multiplication of the first row by X is given by:

$$\begin{aligned}
 & [1 + \frac{h'}{12} u_0 - \frac{h'}{12}(K_{00}^{DD} + 10 K_{10}^{DD} + K_{20}^{DD}) T_0] f_0 - [2 - \frac{10h'}{12} u_1 - \frac{h'}{12}(K_{01}^{DD} + 10 K_{11}^{DD} \\
 & + K_{21}^{DD}) T_1] f_1 + \dots - \frac{h'}{12}(K_{0N}^{DD} + 10 K_{1N}^{DD} + K_{2N}^{DD}) T_N f_N - [\frac{h'}{12} v_0 - \frac{h'}{12}(K_{00}^{DS} \\
 & + 10 K_{10}^{DS} + K_{20}^{DS}) T_0] g_0 - [\frac{10h'}{12} v_1 - \frac{h'}{12}(K_{01}^{DS} + 10 K_{11}^{DS} + K_{21}^{DS}) T_1] g_1 \\
 & - \dots - \frac{h'}{12}(K_{0N}^{DS} + 10 K_{1N}^{DS} + K_{2N}^{DS}) T_N g_N = 0
 \end{aligned} \tag{3.0-12}$$

Table IV

Coefficients of Integration from Gregory's Formula.

$T_0 = 0.340278 h'$	$T_4 = 0.981250 h'$	$T_{N-3} = 1.866667 h'$
$T_1 = 1.195833 h'$	$T_5 = h'$	$T_{N-2} = 0.766667 h'$
$T_2 = 0.766667 h'$	$T_{N-5} = h'$	$T_{N-1} = 1.195833 h'$
$T_3 = 1.866667 h'$	$T_{N-4} = 0.981250 h'$	$T_N = 0.340278 h'$

The remaining $2N-5$ equations are of course similar to the one above, but are for different values of n.

The matrix Eq. (3.0-11) can then be changed into an inhomogeneous equation

$$A'X' = B \tag{3.0-13}$$

by applying the boundary conditions $f_0=0$, $g_0=0$, $f_1=a''$, $g_1=b''$, where a'' and b'' are arbitrary constants, B is then a $(2N-4)$ column vector describing the imposed boundary conditions, and A' is a square $(2N-4, 2N-4)$ matrix.

Equation (3.0-13) is then solved to obtain the scattering functions.

A difficulty arises when terms $u_0 f_0$ and $x_0 g_0$ appear in the boundary condition vector, since u_0 and x_0 may be infinite at the origin. Appendix F shows that those terms are zero for all ℓ 's except $\ell=1$, when they take on the value of 2.

In the numerical evaluation of the kernels, there is need to know the functions $I_{\ell+\frac{1}{2}}(x)$ described in Eq. (2.0-45), and their derivatives.

Two different representations are chosen for the $I_{\ell+\frac{1}{2}}(x)$ depending on whether the argument of the Bessel functions are less or greater (or equal) than one. For arguments less than 1, a power series expansion [46] is employed

$$I_{\ell+\frac{1}{2}}(x) = \sum_{m=0}^{\infty} \frac{(2x)^{\ell+\frac{1}{2}+2m}}{m! \Gamma(\ell+\frac{1}{2}+m+1)} \quad (3.0-14)$$

otherwise, a representation in terms of exponential functions is used.

$$I_{\ell+\frac{1}{2}}(x) = \frac{1}{\sqrt{2\pi x}} [e^x y_\ell(-\frac{1}{x}) + (-)^{\ell+1} e^{-x} y_\ell(\frac{1}{x})] \quad (3.0-15)$$

where

$$y_\ell(x) = \sum_{m=0}^{\ell} \frac{(\ell+m)!}{m!(\ell-m)!2^m} x^m \quad (3.0-16)$$

The derivatives of the $I_{\lambda+\frac{1}{2}}(x)$ functions can easily be calculated by means of the following recursion relation.

$$I'_{\lambda+\frac{1}{2}}(x) = \frac{\lambda+1}{x} I_{\lambda+\frac{1}{2}}(x) - I_{\lambda+3/2}(x) \quad (3.0-17)$$

The function subprograms written to evaluate the values of the function $I_{\lambda+\frac{1}{2}}(x)$ and its derivative for all λ 's and x 's, are reported in Appendix I. Values of the Dawson's integral required in the evaluation of the partial kernels $h_{\lambda}^{SS}(r, r')$ were obtained by interpolation among those tabulated by Miller and Gordon. The interpolation subroutine employed for this purpose is described in detail in Appendix I.

The main programs for calculating the four kernels are designed to compute their values for $r, r' = 0$ (h') $29h'$. That is to say, 900 values of the kernels are calculated. For a fixed value of r , the values for all r' are calculated and punched on cards. The program automatically steps on to the next value of r and repeats the process till the end of the range. In all, 150 cards are punched out for each kernel, each card containing six values of the kernel. A particular feature of the programs, as written, is that the values of the kernels are calculated for the singlet and the triplet cases simultaneously; thus the first card punched contains the first six values of the singlet kernel, the second the first six values of the triplet kernel, and so on, until 300 cards are punched out for each kernel. These cards are then separated into the two 150 card packs for the singlet and triplet kernel respectively.

The kernel programs are listed in Appendix I. Only three programs are necessary, since the kernels K_{λ}^{SD} and K_{λ}^{DS} can be obtained from the same code by simple interchange of the values of λ and v .

From the four 150 card packs containing values of the four kernels for a particular energy, value of ℓ , and total spin, the 56×56 matrix A' is formed.

A problem arises in the inversion of the matrix A' . Because of the size of the matrix involved, numerical noise peculiar to the computer used (IBM-360/50) can introduce large errors if direct inversion is attempted. The matrix A' is therefore partitioned as follows:

$$A' = \left(\begin{array}{c|c} A & B \\ C & D \end{array} \right)$$

The inverse can be calculated from

$$A'^{-1} = \left(\begin{array}{c|c} K & L \\ M & N \end{array} \right)$$

where $N = (D - CA^{-1}B)^{-1}$

$$L = -A^{-1}BN$$

$$M = -NCA^{-1}$$

$$K = A^{-1} - A^{-1}BM$$

The inversion problem is then reduced to that of inverting two 28×28 matrices, namely A and $(D - CA^{-1}B)$, instead of the larger matrix A' . The subroutine RINVRS designed to partition the A' matrix and solve for its inverse is listed in Appendix I.

The subroutine COMPIV employing the standard Gauss-Jordan reduction technique, is used to directly invert the smaller submatrices. A listing of COMPIV is given in Appendix I.

The accuracy of the inverse is tested by multiplying the matrix A' by its inverse, and also by multiplying the inverse by A' . The non-diagonal elements of the resulting matrices are tested and printed if they exceed 1.0×10^{-11} . No such elements were ever printed during the calculations performed.

The main program designed to solve Eq. (3.0-13) for the scattering functions is described in detail in Appendix I.

To obtain the reactance matrix, two independent solutions are required for each reaction channel. The two independent solutions can be readily obtained by choosing different values for the initial slopes of the scattering functions f_λ and g_λ . One such way is to set the arbitrary constants a'' and b'' both equal to 1 for the first independent solution, and to set $a'' = 1$ and $b'' = -1$ for the second one.

Once the scattering functions are known, the reactance matrix can be easily found. Values of the scattering functions at two points near the end of the range are substituted in the system of Eq. (2.0-48), and the set is solved for the unknown coefficients, from which the reactance, and hence the scattering matrix, can be obtained.

The program designed to evaluate the elements of the reactance and scattering matrix is listed in Appendix I.

One can alternatively determine the scattering matrix elements directly by rewriting the system of Eq. (2.0-48) in the form

$$f_\lambda^{ij} = \frac{1}{\sqrt{k_1}} [A^{ij}(G_\lambda^i - iF_\lambda^i) - B^{ij}(G_\lambda^i + iF_\lambda^i)] \quad \begin{matrix} i=1, 2 \text{ channels} \\ j=1, 2 \text{ independent solutions} \end{matrix} \quad (3.0-18)$$

The scattering matrix is then given by

$$\bar{\bar{S}} = \bar{\bar{B}} \bar{\bar{A}}^{-1} \quad (3.0-19)$$

A program developed to determine the scattering matrix elements directly is listed also in Appendix I.

For the purposes of calculating the cross sections, the scattering matrix elements obtained through the reactance matrix are used. The choice is prompted by the fact that if an approximate value of \bar{R} is obtained, then the corresponding scattering matrix is indeed unitary, and hence consistent with the conservation of particles [32]. This is not true, in general, for the approximate S-matrix obtained directly.

It should be stated, however, that the scattering matrix elements obtained by both methods agree generally very well. For the three energies of interest, for instance, the elements of the scattering matrix calculated by one method did not differ from those calculated by the other by more than 15 percent.

The approximate reaction matrix is generally nearly, but not quite, symmetrical. This matrix is thus symmetrized by taking the off-diagonal element to be the arithmetic average of the two calculated off-diagonal elements.

The cross section angular distribution is then calculated according to Eq. (2.0-51) for both the $n+^3He$ elastic scattering and the $^3He(n,p)T$ reaction. The program performing this calculation is listed in Appendix I.

Finally, the total cross sections for the two channels are computed by integration of the corresponding angular distributions over all angles.

4.0 RESULTS AND DISCUSSION

The four kernels K_{ℓ}^{DD} , K_{ℓ}^{DS} , K_{ℓ}^{SD} , and K_{ℓ}^{SS} have been calculated for values of r and r' ranging* from 0 to 7.25 F in steps of 0.25 F for $\ell = 0, 1$, and 2, and the energies of interest. Strictly speaking the kernels are not vanishingly small at 7.25 F. Nevertheless they have decayed to values which are, generally, at least a factor of 100 less than their maximum values. For this reason the value of 7.25 F is considered sufficient as the end point of the integration scheme. After 7.25 F the kernels and direct potentials are set equal to zero.

Values of the four kernels have also been determined for r and r' ranging from 0 to 14.5 F in steps of 0.5 F, for $\ell = 0$.

The decay rate typical of most kernels with r and r' is illustrated in Fig. 1 for the $\ell = 0$, singlet case of the kernel K_{ℓ}^{DD} , and incident neutron energy of 1 MeV. The kernels exhibit a weak dependence on energy, but are markedly affected, particularly in the nuclear region (0 to 4 F) by the chosen values of ℓ and the total spin.

The uniform variation of the kernel with r and r' shown in Fig. 1, is not typical of all the kernels. Several exhibit rapid changes in sign in the nuclear region. This non-uniformity, however, is of no concern for the double integration scheme used to solve for the scattering functions.

Scattering functions have been obtained for incident neutron energies of 1, 3.6, and 6 MeV, $\ell = 0, 1$, and 2, and both $S = 0$, and 1, with the integration spacing being 0.25 F. Figs. 2 and 3 show both the f_{ℓ} and g_{ℓ} scattering functions for $\ell = 0$ and 1 respectively and the two possible values of the spin of the system. The two independent solutions reported, are, of course, required to allow the determination of the scattering and

* Distances are measured in units $1 \text{ F} = 10^{-13} \text{ cm}$.

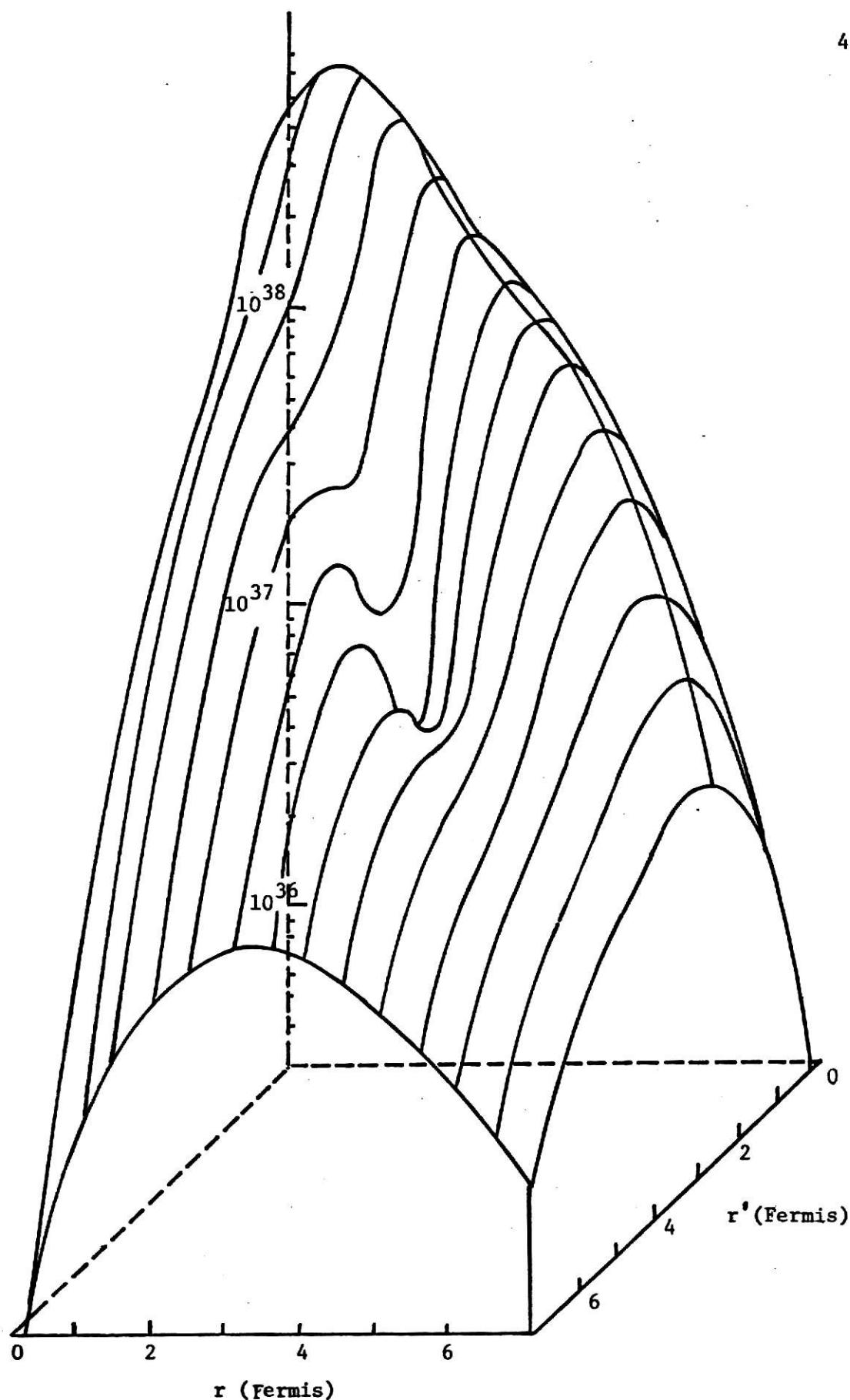


Fig. 1. The kernel $K_{DD}^{(r,r')}$ for $E(n) = 1 \text{ MeV}$, $S = 0$. Ordinate in units of cm^{-3} .

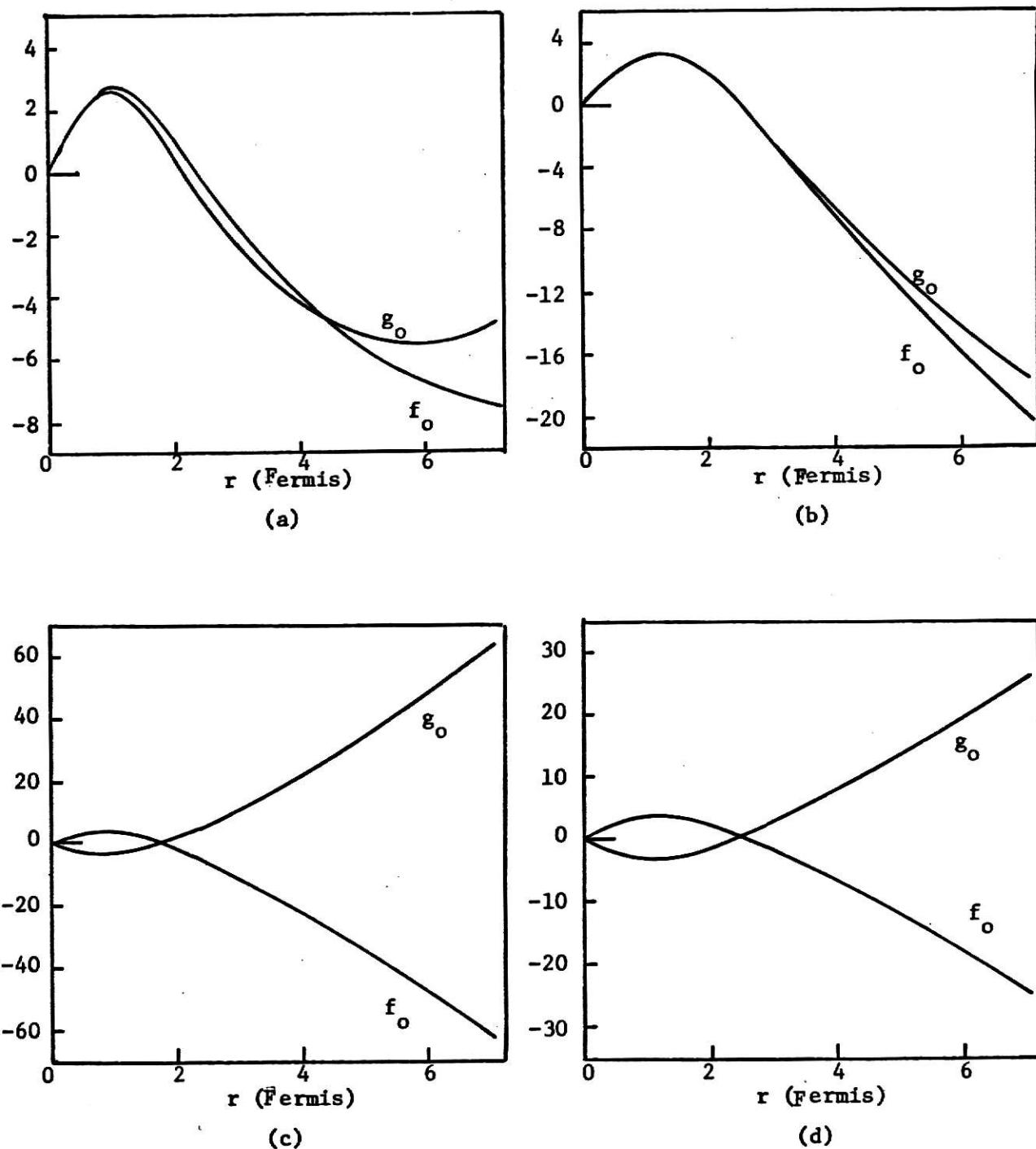


Fig. 2. Scattering functions f_0 and g_0 for incident neutron energy = 1 MeV. The ordinate is in arbitrary units. Integration spacing, $h = 0.25$ Fermis. (a) $S = 0$, 1st independent solution, (b) $S = 1$, 1st independent solution, (c) $S = 0$, 2nd independent solution, (d) $S = 1$, 2nd independent solution.

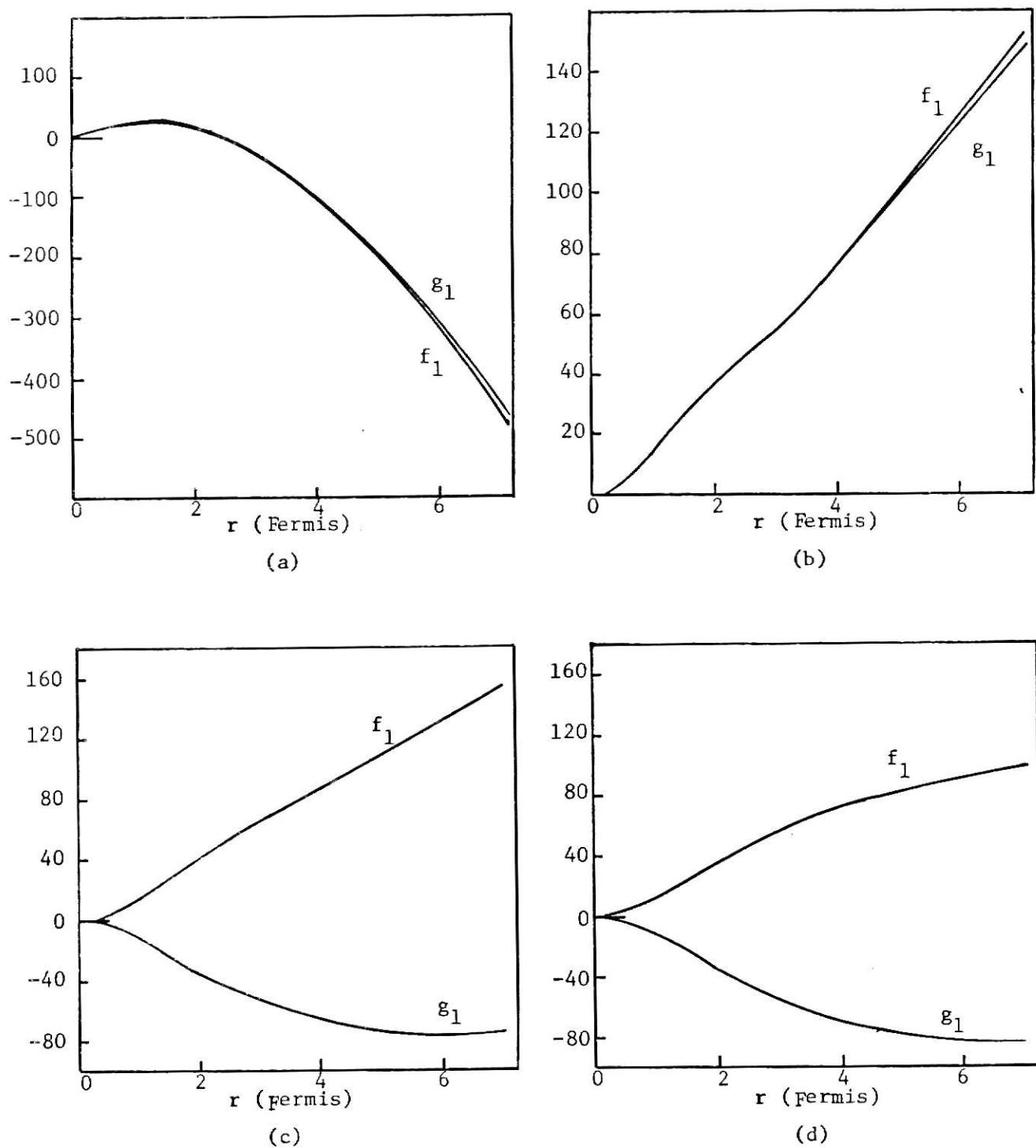


Fig. 3. Scattering functions f_1 and g_1 for incident neutron energy = 1 MeV. The ordinate is in arbitrary units. Integration spacing, $h' = 0.25$ Fermis. (a) $S = 0$, 1st independent solution, (b) $S = 1$, 1st independent solution, (c) $S = 0$, 2nd independent solution, (d) $S = 1$, 2nd independent solution.

reaction cross sections. The scattering functions shown were obtained for an incident neutron energy of 1 MeV.

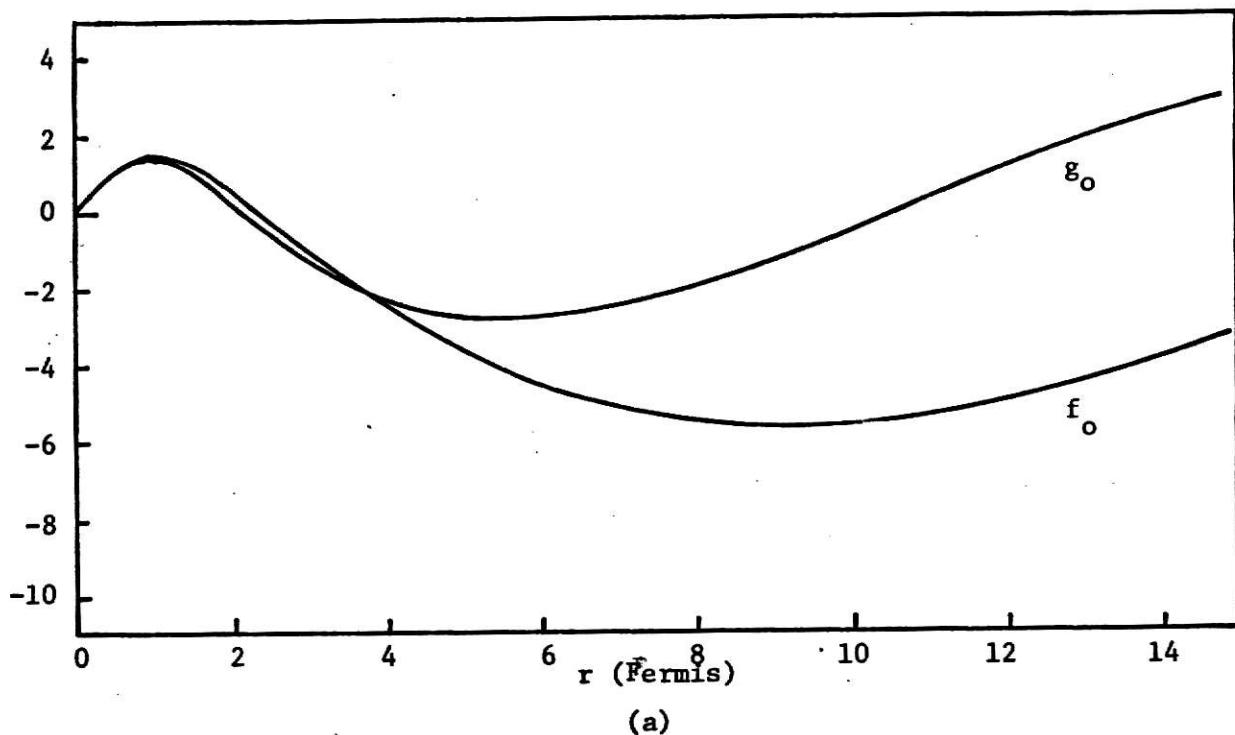
To check the possible validity of the two channel equations, solutions were also obtained for different single channel cases, by approximate modification of the two channel program. Namely, all cross-channel kernels and direct potentials were set equal to zero.

The cross-sections obtained for the sample single channel cases were found to be identical to those reported in the literature [3,4].

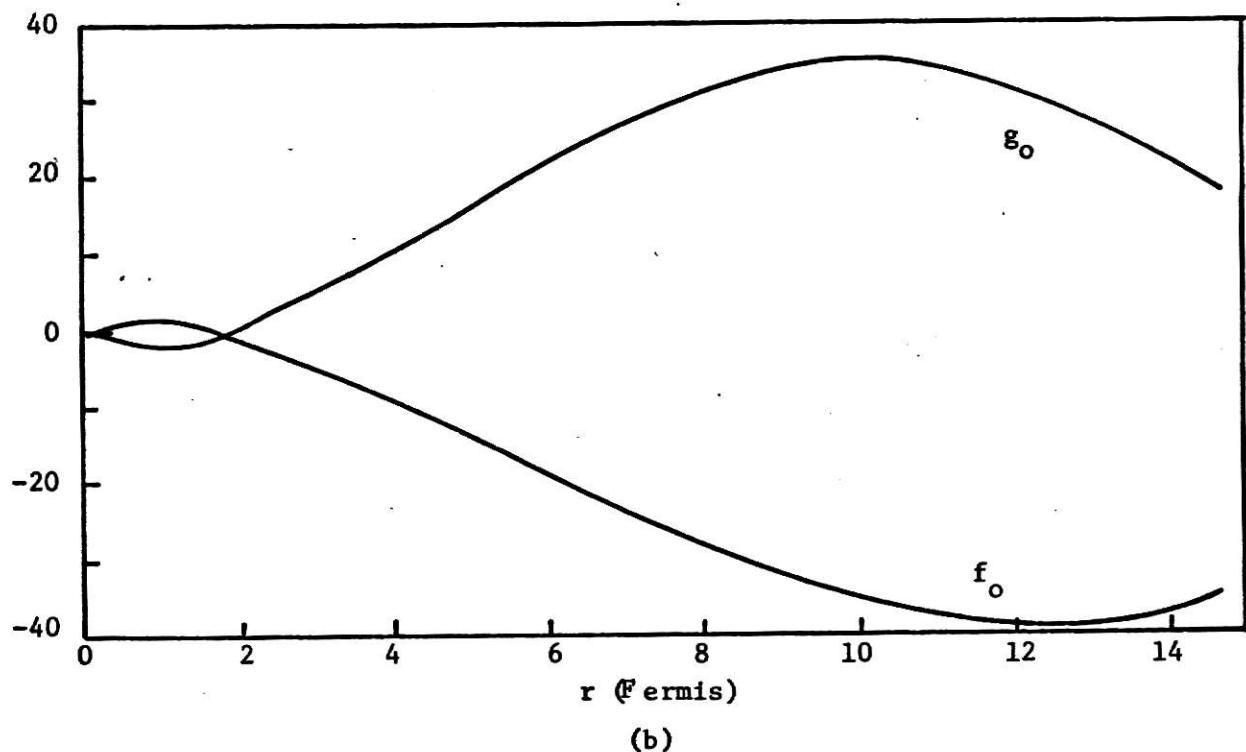
Both independent solutions of the singlet scattering functions f_0 and g_0 , for a 1 MeV incident neutron energy, have also been obtained for an interval between integration points of 0.5 F. The results are shown in Fig. 4. Obviously the features of the scattering functions obtained with $h' = 0.25$ F are retained. Furthermore it is now very evident that both scattering functions do indeed acquire their respective asymptotic behavior.

The elements of the scattering matrices are found by choosing two points at the end of the integration range, 6 F and 7 F respectively, and utilizing values of both independent solutions of the scattering functions at those points. The values of the required regular and irregular Coulomb functions at those points have been obtained by interpolation among values tabulated by references 21, 29, and 42. Interpolation procedures used guarantee a minimum accuracy of two digits.

As a check on the accuracy of the scattering matrix, and thus of the method of solution employed, two different sets of independent solutions were actually used for $\ell = 0$, $E(n) = 1$ MeV, singlet scattering functions. The two different sets were obtained by choosing different values for the initial slope of the g_0 scattering function, i.e., the scattering functions



(a)



(b)

Fig. 4. $S = 0$ scattering functions f and g for incident neutron energy = 1 MeV. The ordinate is in arbitrary units. Integration spacing, $h = 0.5$ Fermis. (a) 1st independent solution, (b) 2nd independent solution.

reported in Figs. 2(a) and 2(c), and Figs. 4(a) and 4(b) were utilized. The values of the scattering matrix elements obtained from the two sets were virtually identical.

Since the interval between integration points, h' , used to compute the scattering functions of Figs. 2 and 4 are different, the results achieved indicate that the value of the scattering matrix is not sensitive to h' , as long as h' is sufficiently small, and the points at which the values of the scattering functions are chosen lie outside the region of the nuclear forces, i.e., in the asymptotic region.

The angular distribution of the cross sections for the elastic scattering and reaction of neutrons with helium-3 have been evaluated for incident neutron energies of 1, 3.6, and 6 MeV. The results are shown in Figs. 5 through 10.

The total cross sections for the two channels at the given energies are found by integration of the differential cross sections over all angles. To determine the accuracy of the angular integration, ascending orders of Gaussian quadrature were used, starting from fifth order. The eighth order integration produced no significant change in the values of the total cross sections obtained with a quadrature of seventh order. The latter figures are then reported in Table V, together with the corresponding experimental values.

The ${}^3\text{He}(n,n){}^3\text{He}$ cross sections, both total and differential, are in fairly good agreement with the experimentally observed cross sections, except at 1 MeV, where the calculated cross sections are too low at all angles. The shape of the angular distribution curve, however, matches quite well the experimental one; in particular the minima of the distribution are predicted correctly. At the higher energies, the larger values of the calculated cross section at large angles could be attributed to the

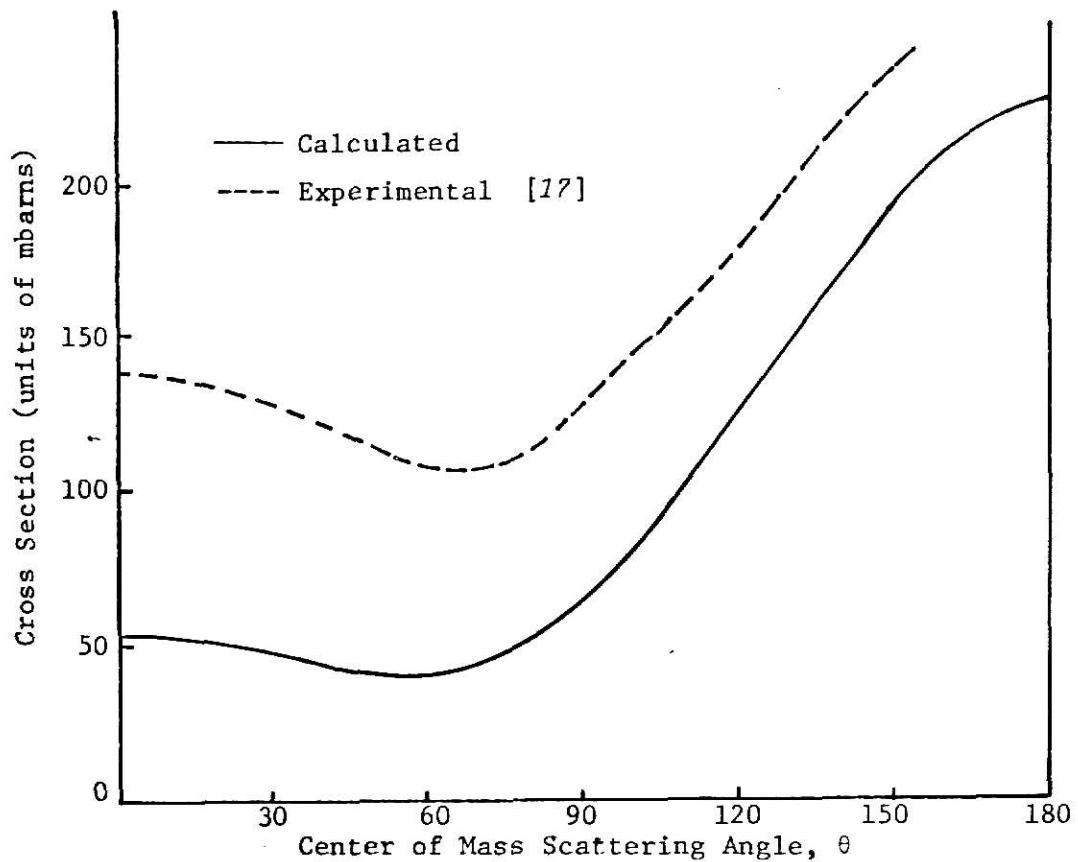


Fig. 5. Angular distribution of 1 MeV neutrons scattered from ${}^3\text{He}$.

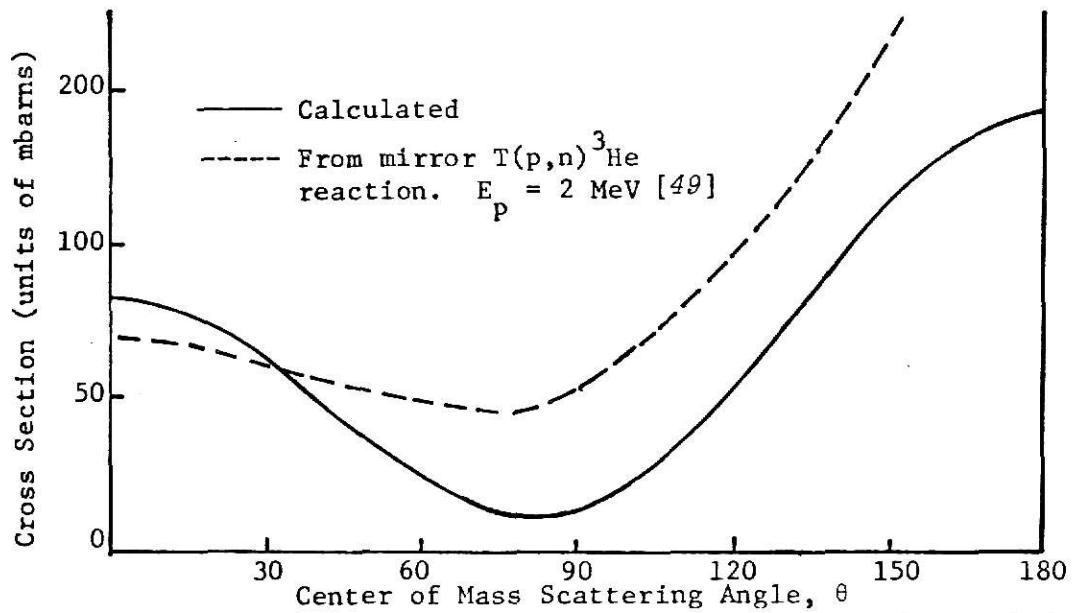


Fig. 6. Angular distribution for the ${}^3\text{He}(n,p)\text{T}$ reaction.
Incident neutron energy = 1 MeV.

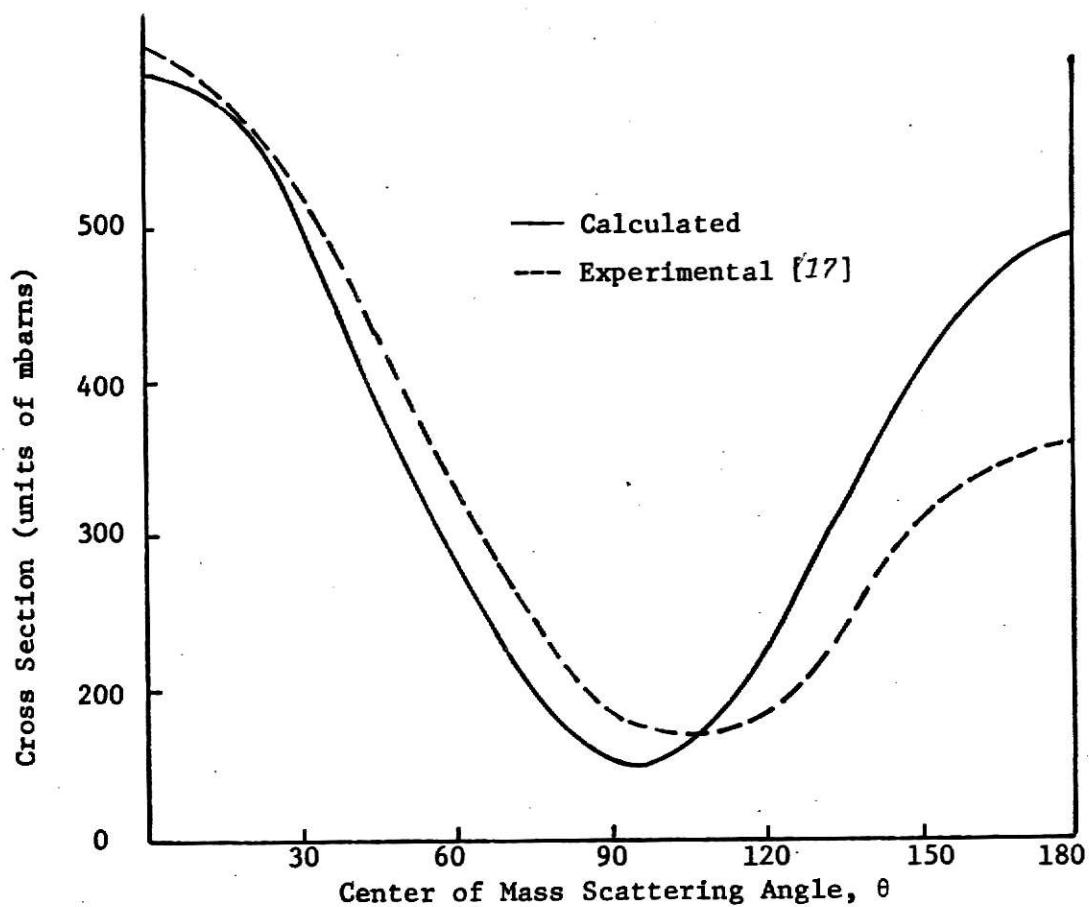


Fig. 7. Angular distribution of 3.6 MeV neutrons scattered from ${}^3\text{He}$.

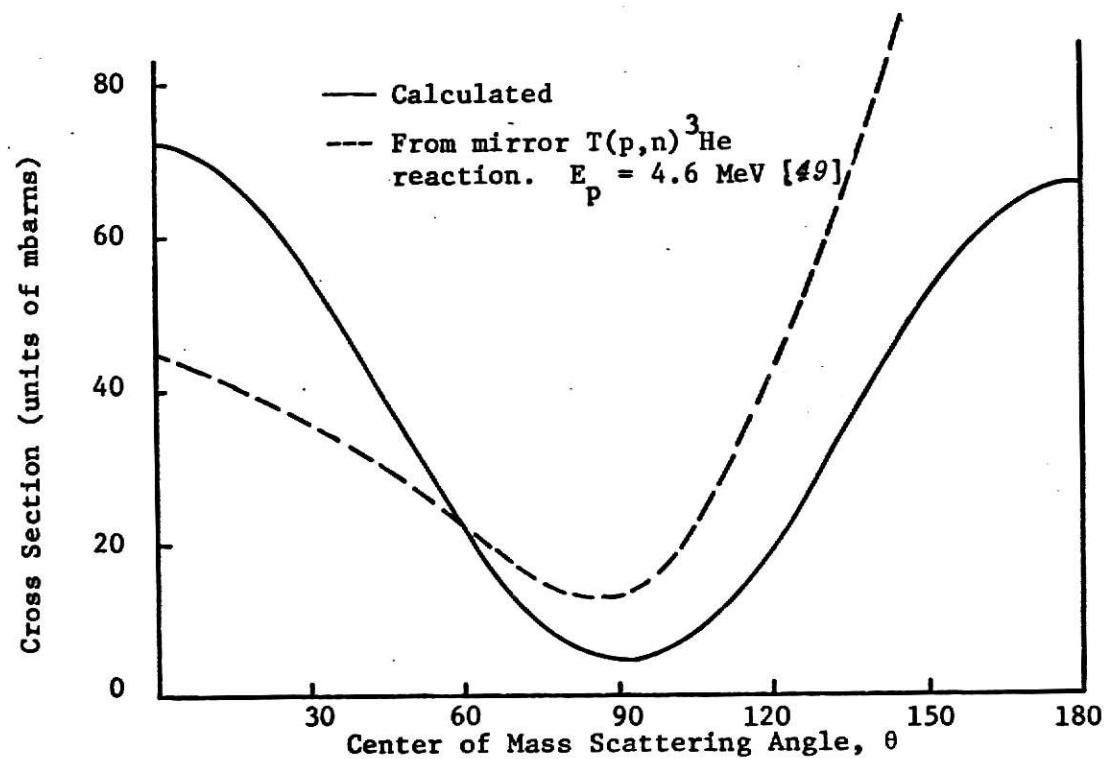


Fig. 8. Angular distribution for the ${}^3\text{He}(n,p)\text{T}$ reaction.
Incident neutron energy = 3.6 MeV.

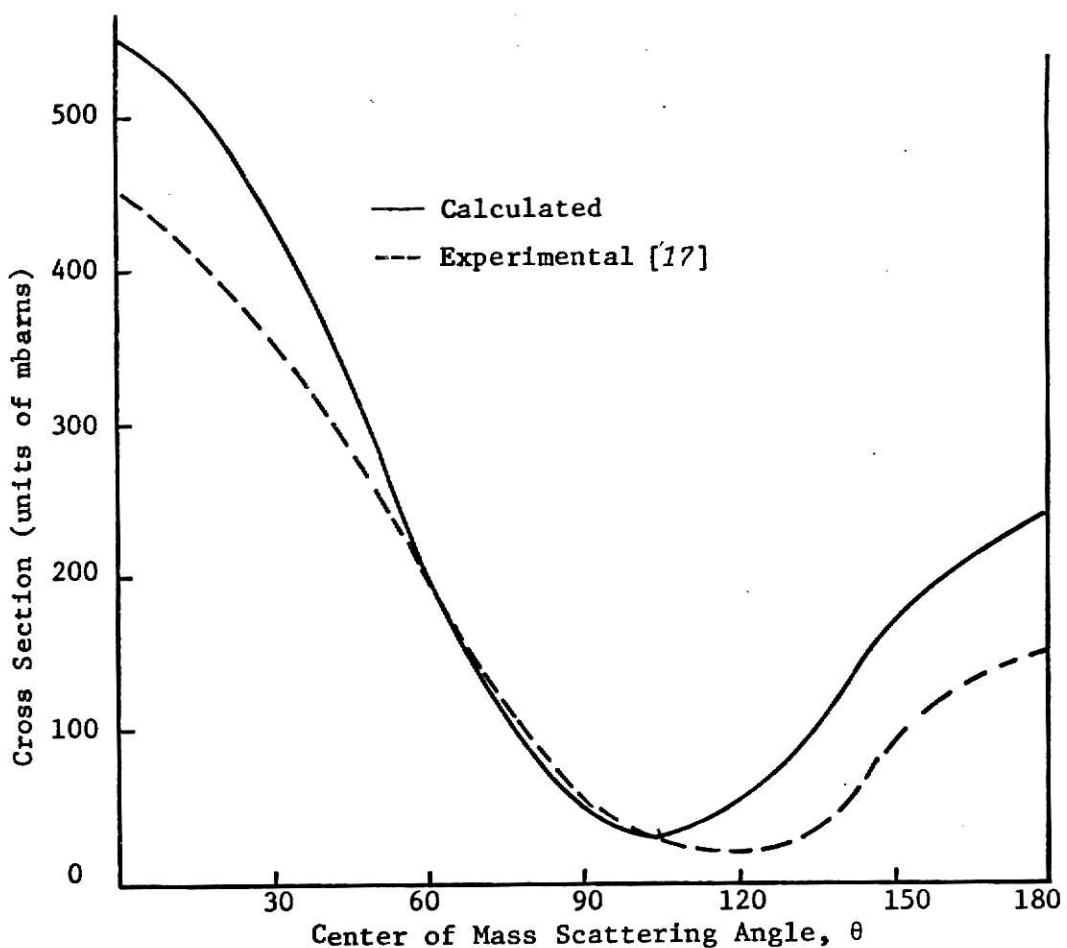


Fig. 9. Angular distribution of 6 MeV neutrons scattered from ${}^3\text{He}$.

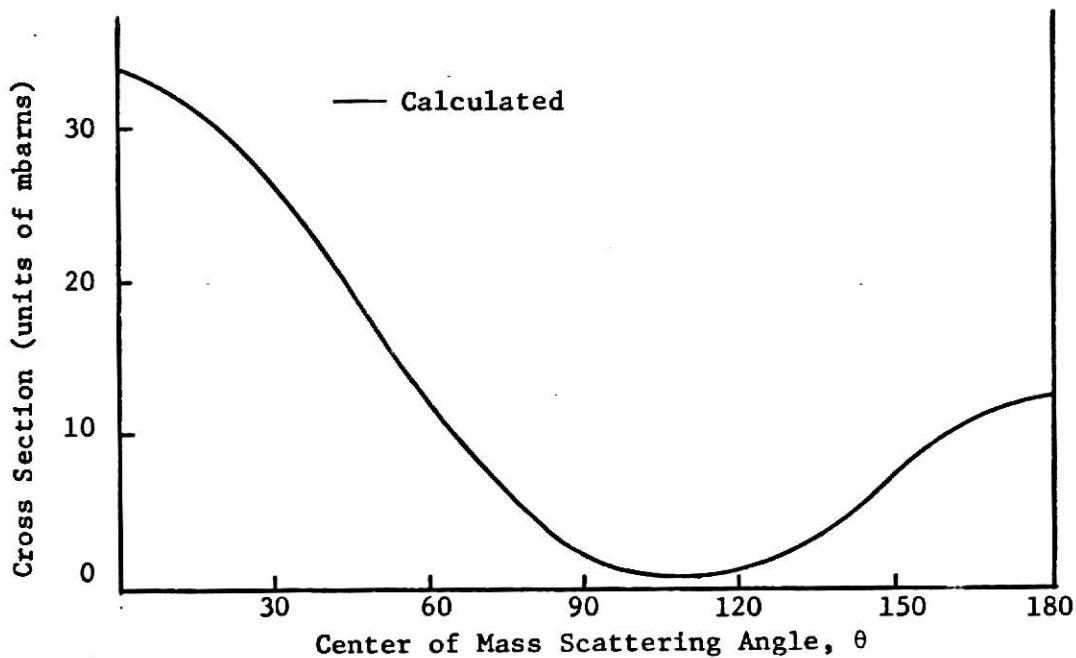


Fig. 10. Angular distribution for the ${}^3\text{He}(n,p)\text{T}$ reaction.
Incident neutron energy = 6 MeV.

Table V
Total Cross Sections

Reaction	Energy (MeV)	Calculated (b)*	Experimental (b) [17]
$^3\text{He}(n,n)^3\text{He}$	1	1.12	1.96
	3.6	2.23	2.34
	6	2.00	1.69
$^3\text{He}(n,p)\text{T}$	1	0.58	0.86
	3.6	0.33	0.54
	6	0.11	0.30

presence of another open channel, $^3\text{He}(n,d)\text{D}$, which is, of course, not accounted for in the theoretical development. When compared with results obtained by other authors with only the elastic scattering channel open, [7,12] the two channel cross sections have almost identical values. This indicates that the one-channel approximation may be sufficient to estimate the elastic scattering cross sections even in the presence of several competing open channels.

The calculated total cross sections for the $^3\text{He}(n,p)\text{T}$ channel are consistently too low. The angular distribution curves exhibit the qualitative features found in the experimental ones, that is, the minima shift toward larger angles as the energy increases, and their position is well predicted. The small values predicted by the Serber interaction at the larger angles are somewhat expected, since this interaction has been found

* Expressed in conventional units of $1 \text{ b} = 10^{-24} \text{ cm}^2$.

to yield too large a value, at those angles, for the elastic scattering cross section.

Because of the discrepancies between experiment and theory introduced partly by use of the Serber exchange in the potential, it is felt that future studies should investigate what mixture of Serber and other types of exchange forces might yield better agreement with experimental results. This study indicates that the percentage of the Serber force in the mixture will probably be high. The results obtained in this study point out that the cluster model could indeed be very successful in predicting cross sections for the interactions of nucleons and elementary particles with light-weight nuclei.

The differences between experiment and theory appear to stem not from the model employed, but mainly from the approximations necessary to reduce the mathematical formulation to a workable level, and the lack of knowledge about the exact nature of the nuclear forces. The latter problem has been briefly investigated, at least for the one-channel problem, by including spin-orbit coupling and tensor forces in the potential [23,40]. The improvement in the agreement between theory and experiment has been encouraging.

Little, however, has been done with regard to the first problem. Future studies, rendered easier by the more sophisticated computers available today, should delve with the possibility of employing wavefunctions and potentials not of the Gaussian type.

With these wavefunctions and potentials, it will no longer be possible to obtain analytical forms for the kernels. The approximations introduced by the numerical solutions thus necessary may, however, be more than offset by the better representation of the wavefunctions of the target nuclei, and the nature of the interaction.

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6.0 VITAE

The author was born on November 25, 1941, in Karlsruhe, Germany. He attended elementary and high schools in Panama City, Panama and Modena, Italy, graduating from the Liceo Scientifico A. Tassoni in Modena.

He came to the United States as a student in the Fall of 1960, enrolling in general engineering curriculum at El Camino Jr. College, Gardena, California.

In September of 1961 the author entered Kansas State University as a student in Nuclear Engineering and received his B.S. in August of 1964, and his M.S. in June 1967.

During this period he was awarded a Title IV NDEA Fellowship. His M.S. Thesis was entitled "Design of Structures for Protection from Window-Collimated, Ceiling-Scattered Fallout Radiation."

During the summer of 1965 the author served as a coordinator of the "Summer Institute on Fundamental Radiation Shielding Problems as Applied to Nuclear Defense Planning," to which he was also a participant. As a result of the successful completion of the Institute, he was classified as a Qualified Fallout Shelter Analysis Instructor.

In May 1967 he became a naturalized citizen of the United States. In September 1968, while pursuing a Ph.D. degree in Nuclear Engineering, he was appointed to the rank of instructor in the Department of Nuclear Engineering.

His responsibilities, which he holds to today, have been to teach undergraduate and graduate level courses, and to serve as the assistant to the director of the Professional Advisory Service Center.

The author is married and has no children.

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8.0 APPENDICES

8.1 APPENDIX A

Derivation of the Singlet Equation for the Neutron-Helium-3 System

Equation (2.0-8), when the spin of the system $S = 0$, is written as:

$$\begin{aligned}
 & \left\{ \left(-\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{2-34}^2 - \frac{2}{3} \frac{\hbar^2}{M} \nabla_{1-234}^2 \right) - E + (w+mM'+hH+bB)(v_{14} + v_{13} + v_{12}) \right. \\
 & + v_{24}^c + (w+mM'+hH+bB)(v_{24} + v_{23} + v_{24}) \} \times \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] \\
 & \cdot [\alpha(2)\beta(4) - \alpha(4)\beta(2)] \{ \phi(234)F(1,234) + \phi(124)F(3,124) + \eta(134)G(2,134) \\
 & \left. + \eta(123)G(4,123) \} \quad (A-1)
 \end{aligned}$$

Since the wavefunction $\phi(234)$ of the Helium-3 cluster satisfies its own Schrödinger equation, and therefore:

$$\begin{aligned}
 & \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \sigma_S \left\{ \left[-\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{2-34}^2 \right] + v_{24}^c + (w+mM'+hH+bB) \right. \\
 & \cdot (v_{24} + v_{23} + v_{34}) - E + E(n) \} \sigma_S \phi(234) = 0
 \end{aligned}$$

then by multiplying Eq. (A-1) by the conjugate of the cluster wavefunction, $\phi^*(234)$, the singlet spin wavefunction $\sigma_S(1,234)$, and integrating over the cluster spatial dependency and the entire spin space, we obtain:

$$\begin{aligned}
 & \int d\tau \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)][\alpha(2)\beta(4) - \alpha(4)\beta(2)] \\
 & \text{all spins} \\
 & \cdot \left\{ \left(-\frac{\hbar^2}{M} \nabla_{34}^2 - \frac{3}{4} \frac{\hbar^2}{M} \nabla_{2-34}^2 - \frac{2}{3} \frac{\hbar^2}{M} \nabla_{1-234}^2 \right) - E + (w+mM'+hH+bB)(v_{14} + v_{13} + v_{12}) \right. \\
 & \left. + v_{24}^c + (w+mM'+hH+bB)(v_{24} + v_{23} + v_{24}) \right\} \times \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] \\
 & \cdot [\alpha(2)\beta(4) - \alpha(4)\beta(2)] \{ \phi(234)F(1,234) + \phi(124)F(3,124) + \eta(134)G(2,134) \\
 & + \eta(123)G(4,123) \} \quad (A-2)
 \end{aligned}$$

$$\begin{aligned}
& + v_{24}^c + (w+mM'+hH+bB)(v_{24}+v_{23}+v_{34}) \frac{1}{2} [\alpha(1)\beta(3)-\alpha(3)\beta(1)] \\
& \cdot [\alpha(2)\beta(4)-\alpha(4)\beta(2)] \{ \phi(234)F(1,234) + \phi(124)F(3,124) + \eta(134)G(2,134) \\
& + \eta(123)G(4,123) \} \tag{A-3}
\end{aligned}$$

and consequently

$$\begin{aligned}
& \int d\tau \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \frac{1}{2} [\alpha(1)\beta(3)-\alpha(3)\beta(1)] [\alpha(2)\beta(4)-\alpha(4)\beta(2)] \\
& \text{all spins} \\
& \cdot \left\{ -\frac{2}{3} \frac{\hbar^2}{M} v_{1-234}^2 - E(n) + (w+mM'+hH+bB)(v_{14}+v_{13}+v_{12}) \right\} \\
& \cdot \phi(234) \frac{1}{2} [\alpha(1)\beta(3)-\alpha(3)\beta(1)] [\alpha(2)\beta(4)-\alpha(4)\beta(2)] F(1,234) \\
& + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \frac{1}{2} [\alpha(1)\beta(3)-\alpha(3)\beta(1)] [\alpha(2)\beta(4)-\alpha(4)\beta(2)] \\
& \cdot \left\{ (T - E - (w+mM'+hH+bB)(v_{12}+v_{13}+v_{14}+v_{23}+v_{24}+v_{34})) + v_{24}^c \right\} \\
& \cdot [\phi(124)F(3,124) + \eta(134)G(2,134) + \eta(123)G(4,123)] \frac{1}{2} [\alpha(1)\beta(3) \\
& - \alpha(3)\beta(1)] [\alpha(2)\beta(4)-\alpha(4)\beta(2)] = 0 \tag{A-4}
\end{aligned}$$

The kinetic energy operator T can again be rewritten in any one of the equivalent forms most suitable for each different grouping. For the neutron 3 and cluster (241) grouping one uses:

$$T = -\frac{\hbar^2}{M} v_{14}^2 - \frac{3}{4} \frac{\hbar^2}{M} v_{2-14}^2 - \frac{2}{3} \frac{\hbar^2}{M} v_{3-142}^2 \tag{A-5}$$

and for the proton 4 and cluster (123) grouping one has:

$$T = -\frac{\hbar^2}{M} v_{23}^2 - \frac{3}{4} \frac{\hbar^2}{M} v_{1-23}^2 - \frac{2}{3} \frac{\hbar^2}{M} v_{4-123}^2 \quad (A-6)$$

Eq. (A-4) is then integrated over all possible spin space. The mathematical manipulations involved in this operation are straightforward but long and tedious. As an example, the integration over spin is carried through for the term:

$$\begin{aligned} & \int d\tau \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] [\alpha(2)\beta(4) - \alpha(4)\beta(2)] \\ & \text{all spins} \\ & \cdot (w + mM' + hH + bB)(v_{14} + v_{13} + v_{12}) \phi(234) \frac{1}{2} [\alpha(1)\beta(3) - \alpha(3)\beta(1)] \\ & \cdot [\alpha(2)\beta(4) - \alpha(4)\beta(2)] F(1, 234) \end{aligned}$$

The Majorana contribution is given by:

$$\begin{aligned} & -m \left[\int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{12} \phi(134) F(2, 134) + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{13} \right. \\ & \cdot \phi(142) F(3, 124) + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{14} \phi(123) F(4, 123)] \\ & \times \int d\tau \frac{1}{4} [\alpha(1)\beta(3) - \alpha(3)\beta(1)]^2 [\alpha(2)\beta(4) - \alpha(4)\beta(2)]^2 \\ & \text{all spins} \end{aligned}$$

The Bartlett operator will yield:

$$\begin{aligned} & b \left[\int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 |\phi(234)|^2 \left\{ v_{12} \frac{1}{4} \int [\alpha(1)\beta(3) - \alpha(3)\beta(1)][\alpha(2)\beta(4) - \alpha(4)\beta(2)] \right. \right. \\ & \text{all spins} \\ & \cdot [\alpha(2)\beta(3) - \alpha(3)\beta(2)][\alpha(1)\beta(4) - \alpha(4)\beta(1)] d\tau - v_{13} \frac{1}{4} \int [\alpha(1)\beta(3) \\ & \text{all spins}] \end{aligned}$$

$$- [\alpha(3)\beta(1)]^2 [\alpha(2)\beta(4)-\alpha(4)\beta(2)]^2 d\tau + v_{14} \frac{1}{4} \int_{\text{all spins}} [\alpha(1)\beta(3)-\alpha(3)\beta(1)]$$

$$\cdot [\alpha(2)\beta(4)-\alpha(4)\beta(2)][\alpha(4)\beta(3)-\alpha(3)\beta(4)][\alpha(2)\beta(1)-\alpha(1)\beta(2)] \{F(1,234)\} d\tau$$

but since $\int d\tau \frac{1}{4} [\alpha(1)\beta(3)-\alpha(3)\beta(1)]^2 [\alpha(2)\beta(4)-\alpha(4)\beta(2)]^2 = 1$,

$$\int d\tau \frac{1}{4} [\alpha(1)\beta(3)-\alpha(3)\beta(1)][\alpha(2)\beta(4)-\alpha(4)\beta(2)][\alpha(2)\beta(3)-\alpha(3)\beta(2)]$$

$$\cdot [\alpha(1)\beta(4)-\alpha(4)\beta(1)] = \frac{1}{2}$$

and the potential v_{ij} is chosen so that

$$\int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 v_{12} |\phi(234)|^2 = \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 v_{13} |\phi(234)|^2 = \text{etc.} \quad (\text{A-7})$$

the Bartlett contribution is 0.

The Heisenberg operator will contribute:

$$-h \left[\int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^{*(234)} v_{12} \phi(134) F(2,134) \frac{1}{4} \int d\tau [\alpha(1)\beta(3)-\alpha(3)\beta(1)] \right]_{\text{all spins}}$$

$$\cdot [\alpha(2)\beta(4)-\alpha(4)\beta(2)][\alpha(2)\beta(3)-\alpha(3)\beta(2)][\alpha(1)\beta(4)-\alpha(4)\beta(1)]$$

$$- \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^{*(234)} v_{13} \phi(124) F(3,124) \frac{1}{4} \int d\tau [\alpha(1)\beta(3)-\alpha(3)\beta(1)]^2$$

$$\cdot [\alpha(2)\beta(4)-\alpha(4)\beta(2)]^2 + \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^{*(234)} v_{14} \phi(123) F(4,123)$$

$$\cdot \frac{1}{4} \int d\tau [\alpha(1)\beta(3)-\alpha(3)\beta(1)][\alpha(2)\beta(4)-\alpha(4)\beta(2)][\alpha(4)\beta(3)-\alpha(3)\beta(4)]$$

all spins

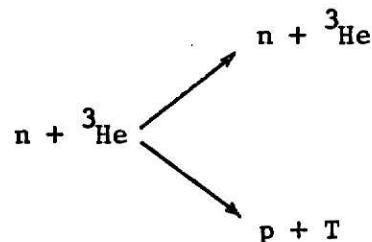
$$\cdot [\alpha(1)\beta(2)-\alpha(2)\beta(1)]]$$

$$\begin{aligned}
 &= -\frac{\hbar}{2} \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{12} \phi(134) F(2,134) \\
 &+ \hbar \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{13} \phi(142) F(3,124) \\
 &- \frac{\hbar}{2} \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 \phi^*(234) v_{14} \phi(123) F(4,123)
 \end{aligned}$$

Finally, the remaining terms can be written as:

$$\begin{aligned}
 &w \int d\tilde{r}_2 d\tilde{r}_3 d\tilde{r}_4 |\phi(234)|^2 (v_{12} + v_{13} + v_{14}) F(1,234) \int_{\text{all spins}} d\tau \frac{1}{4} [\alpha(1)\beta(3)-\alpha(3)\beta(1)]^2 \\
 &\cdot [\alpha(2)\beta(4)-\alpha(4)\beta(2)]^2 \\
 &= 3w \int dr_2 dr_3 dr_4 v_{13} |\phi(234)|^2 F(1,234)
 \end{aligned}$$

When these terms are combined with all the other terms, resulting, in identical fashion, from the integration over all spins of Eq. (A-4), the singlet equation for the first channel:



is obtained. This equation is Eq. (2.0-16).

The triplet equation, Eq. (2.0-17), is obtained in the same way, by using the triplet form of the spin function.

8.2 APPENDIX B

Derivation of the Analytical Form for $v_{DD}(r)$

According to Eq. (2.0-26) the direct potential term $v_{DD}(r)$ is given by

$$v_{DD}(r) = \frac{M}{\hbar^2} \left(\frac{9}{8}\right)^3 \alpha \int d\bar{r}' \int d\bar{\rho}_2 \int d\bar{\rho}_4 v(|\bar{u}-\bar{v}|) |\phi(\bar{v}, \bar{\rho}_2, \bar{\rho}_4)|^2 \quad (2.0-26)$$

It can easily be shown from (2.0-21) and (2.0-43) that

$$\begin{aligned} \phi(\bar{r}_2, \bar{r}_3, \bar{r}_4) &\equiv \frac{1}{N_{^3He}} \exp[-\frac{v}{2}((\bar{r}_2 - \bar{r}_3)^2 + (\bar{r}_2 - \bar{r}_4)^2 + (\bar{r}_3 - \bar{r}_4)^2)] \\ &\equiv \frac{1}{N_{^3He}} \exp[-\frac{v}{2}(2v^2 + \frac{3}{2} \rho_2^2)] \equiv \phi(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \end{aligned} \quad (B-1)$$

Since, then, ϕ has no explicit dependence on $\bar{\rho}_4$ we can write

$$\phi(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) = \phi(\bar{v}, \bar{\rho}_2) = \phi(\bar{\rho}_3, \bar{\rho}_2) \quad (B-2)$$

One can verify that indeed $\bar{v} = \bar{\rho}_3$ from (2.0-21).

The normalization constant $N_{^3He}$ is defined as

$$N_{^3He}^2 \equiv \int d\bar{\rho}_2 \int d\bar{\rho}_3 \int d\bar{\rho}_4 |\phi(\bar{v}, \bar{\rho}_2)|^2$$

Substituting the form (2.0-42) for the potential, one readily obtains

$$v_{DD}(r) = \frac{\left(\frac{9}{8}\right)^3 \frac{M}{\hbar^2} \alpha V_0 \int d\bar{r}' e^{-\mu[\frac{3}{4}(\bar{r}-\bar{r}')]^2} e^{-2v[\frac{3}{8}\bar{r} + \frac{9}{8}\bar{r}']} \int d\bar{\rho}_2 e^{-\frac{3}{2}v\rho_2^2} \int d\bar{\rho}_4}{\int d\bar{\rho}_2 e^{-\frac{3}{2}v\rho_2^2} \int d\bar{\rho}_3 e^{-2v\rho_3^2} \int d\bar{\rho}_4} \quad (B-4)$$

or simply

$$v_{DD}(r) = \frac{M}{\hbar^2} \left(\frac{9}{8}\right)^3 \frac{v^3 \rho_3^{3/2}}{\pi^3} \int d\tilde{r}' e^{-\mu \left[\frac{3}{4}(\tilde{r}-\tilde{r}')\right]^2} e^{-2v \left[\frac{3}{8}\tilde{r} + \frac{9}{8}\tilde{r}'\right]^2} \int d\tilde{\rho}_2 e^{-\frac{3}{2}v\rho_2^2} \quad (B-5)$$

where use has been made of the fact that

$$\int d\tilde{\rho}_3 e^{-2v\rho_3^2} = \frac{\pi^{3/2}}{(2v)^{3/2}}$$

and

$$\int d\tilde{\rho}_2 e^{-\frac{3}{2}v\rho_2^2} = \frac{\pi^{3/2}}{\left(\frac{3}{2}v\right)^{3/2}} \quad (B-6)$$

The argument of the exponential in the \tilde{r}' integral of Eq. (B-5) is transformed to a more suitable form for integration by addition and subtraction of the term $\frac{9\mu vr^2}{2\mu+9v}$; thus:

$$\begin{aligned} & e^{-\frac{9}{16}\mu(\tilde{r}-\tilde{r}')^2} e^{-2v\left(\frac{3}{8}\tilde{r} + \frac{9}{8}\tilde{r}'\right)^2} \\ &= e^{-\left\{\frac{9\mu vr^2}{2\mu+9v} + \frac{9}{32(2\mu+9v)}[(2\mu-3v)r - (2\mu+9v)r']^2\right\}} \end{aligned}$$

Equation (B-5) can then be rewritten as

$$\begin{aligned} v_{DD}(r) &= \left(\frac{9}{8}\right)^3 \frac{v^3 \rho_3^{3/2}}{\pi^3} \frac{M}{\hbar^2} \alpha V_0 e^{-\frac{9}{16}\frac{\mu v}{2\mu+9v}r^2} \int d\tilde{\rho}_2 e^{-\frac{3}{2}v\rho_2^2} \\ &\cdot \int d\tilde{r}' e^{-\frac{9}{32(2\mu+9v)}[(2\mu-3v)\tilde{r} - (2\mu+9v)\tilde{r}']^2} \quad (B-7) \end{aligned}$$

If one defines $x^2 = [(2\mu - 3\nu)\bar{r} - (2\mu + 9\nu)\bar{r}']^2$ then

$$\begin{aligned} v_{DD}(r) &= \left(\frac{9}{8}\right)^3 \frac{\nu^3 3^{3/2}}{\pi^3} \frac{M}{\hbar^2} \alpha V_0 e^{-\frac{9}{16} \frac{\mu\nu}{2\mu+9\nu} r^2} \\ &\cdot \frac{1}{(2\mu+9\nu)^3} \int d\tilde{p}_2 e^{-\frac{3}{2} \frac{\nu p_2^2}{2\mu+9\nu}} \int d\tilde{x} e^{-\frac{9x^2}{32(2\mu+9\nu)}} \end{aligned} \quad (B-8)$$

But

$$\int d\tilde{x} e^{-\frac{9x^2}{32(2\mu+9\nu)}} = \frac{(\pi)^{3/2}}{\left[\frac{9}{32(2\mu+9\nu)}\right]^{3/2}} \quad (B-9)$$

hence

$$v_{DD}(r) = 27 \frac{M}{\hbar^2} \alpha V_0 \left(\frac{\nu}{2\mu+9\nu}\right)^{3/2} \exp\left(-\frac{9\mu\nu}{2\mu+9\nu} r^2\right) \quad (B-10)$$

8.3 APPENDIX C

Derivation of the Analytical Expression for
the Partial Kernel $q_{\lambda}^{DD}(r, r')$

By definition

$$q_{\lambda}^{DD}(r, r') = \left(\frac{9}{8}\right)^3 \frac{M}{\hbar^2} 2\pi rr' \int_0^{\pi} P_{\lambda}(\cos\theta) \sin\theta \left[\int d\tilde{p}_2 d\tilde{p}_4 \phi^*(\bar{u}, \bar{p}_2, \bar{p}_4) \right. \\ \left. \cdot v(|\bar{u} + \frac{1}{2}\bar{p}_2|) \phi(\bar{u}, \bar{p}_2, \bar{p}_4) \right] d\theta \quad (C-1)$$

We make use of Eq. (B-1) and the corresponding expression for $\phi(\bar{u}, \bar{p}_2, \bar{p}_4)$.

$$\phi(\bar{u}, \bar{p}_2, \bar{p}_4) = \phi(\bar{u}, \bar{p}_2) = \frac{1}{N_{3He}} \exp\left[-\frac{v}{2}(2u^2 + \frac{3}{2}p_2^2)\right] \quad (C-2)$$

The potential $v(|\bar{u} + \frac{1}{2}\bar{p}_2|)$ is written in the explicit form of Eq. (2.0-42), wherein \bar{u} is replaced by its proper dependence on \bar{r} and \bar{r}' , as indicated in (2.0-21).

$$v(|\bar{u} + \frac{1}{2}\bar{p}_2|) = v_o \exp\left[-\mu\left(\frac{9}{8}\bar{r} + \frac{3}{8}\bar{r}' + \frac{1}{2}\bar{p}_2\right)^2\right] \quad (C-3)$$

The integration over the \bar{p}_4 coordinates can again be removed by virtue of the fact that identical integrals occur in the kernel and the normalization of the wavefunctions; the normalization constant being identical to (B-3). One can easily verify that

$$q_{\lambda}^{DD}(r, r') = \left(\frac{9}{8}\right)^3 \frac{MV_o}{\hbar^2} \frac{v^3 3^{3/2}}{\pi^2} 2rr' \int_0^{\pi} P_{\lambda}(\cos\theta) \sin\theta \left\{ \int d\bar{p}_2 \exp\left[-v\left(\frac{9}{64}r^2 + \frac{81}{64}r'^2 + \frac{54}{64}\bar{r}\cdot\bar{r}' + \frac{3}{4}p_2^2\right)\right] \right. \\ \left. + \frac{54}{64}\bar{r}\cdot\bar{r}' + \frac{3}{4}p_2^2 \right\} \exp\left[-\mu\left(\frac{81}{64}r^2 + \frac{9}{64}r'^2 + \frac{1}{4}p_2^2 + \frac{54}{64}\bar{r}\cdot\bar{r}' + \frac{9}{8}\bar{r}\cdot\bar{p}_2\right)\right]$$

$$+ \frac{3}{8} \bar{r}' \cdot \bar{\rho}_2) \} \exp[-v(\frac{81}{64} r^2 + \frac{9}{64} r'^2 + \frac{54}{64} \bar{r} \cdot \bar{r}' + \frac{3}{4} \rho_2^2)] \} d\theta \quad (C-4)$$

Collecting terms, and recalling that $\bar{r} \cdot \bar{r}' = rr' \cos\theta$, the following expression is obtained:

$$\begin{aligned} q_\lambda^{DD}(r, r') &= \left(\frac{9}{8}\right)^3 \frac{MV_0}{\pi^2} \frac{2v^3 3^{3/2}}{\pi^2} rr' \int_0^\pi P_\lambda(\cos\theta) \sin\theta \exp[-\frac{9}{16}(\frac{10}{4} v + \frac{9}{4} \mu) r^2] \\ &\cdot \exp[-\frac{9}{16}(\frac{10}{4} v + \frac{1}{4} \mu) r'^2] \exp[-\frac{54}{64}(2v+\mu) rr' \cos\theta] \\ &\cdot \left\{ \int d\bar{\rho}_2 \exp[-\frac{\rho_2^2}{4} (6v+\mu) - \mu(\frac{3}{8} \bar{r}' + \frac{9}{8} \bar{r}) \cdot \bar{\rho}_2] \right\} d\theta \end{aligned} \quad (C-5)$$

Equation (C-5) is then multiplied and divided by the expression

$$\exp[-\frac{9}{16} v \frac{15v+16\mu}{6v+\mu} r^2 + \frac{9}{16} v \frac{15v+4\mu}{6v+\mu} r'^2]$$

The existing exponential terms can then be written as

$$\exp[-\frac{9}{16}(\frac{10}{4} v + \frac{9}{4} \mu - \frac{v(15v+16\mu)}{6v+\mu}) r^2] = \exp[-\frac{81\mu^2 r^2}{64(6v+\mu)}]$$

and

$$\exp[-\frac{9}{16}(\frac{10}{4} v + \frac{1}{4} \mu - \frac{v(15v+4\mu)}{6v+\mu}) r'^2] = \exp[-\frac{9\mu^2 r'^2}{64(6v+\mu)}]$$

so that

$$\begin{aligned}
 q_{\ell}^{DD}(r, r') = & \left(\frac{9}{8}\right)^3 \frac{MV_0}{\pi^2} \frac{2v^3 3^{3/2}}{\pi^2} rr' \int_0^\pi P_\ell(\cos\theta) \sin\theta \exp\left[-\frac{9}{16} - \frac{(15v+16\mu)}{6v+\mu} r^2\right] \\
 & \cdot \exp\left[-\frac{9}{16} v \left(\frac{15v+4\mu}{6v+\mu} r'\right)^2\right] \left\{ \int d\tilde{\rho}_2 \exp\left[-\frac{\tilde{\rho}_2^2}{4} (6v+\mu) - \mu \left(\frac{3}{8} \bar{r}' + \frac{9}{8} \bar{r}\right) \cdot \tilde{\rho}_2 \right. \right. \\
 & \left. \left. - \frac{\frac{81}{64} \mu^2 r^2}{(6v+\mu)} - \frac{\frac{9}{64} \mu^2 r'^2}{(6v+\mu)} \right] \right\} \exp\left[-\frac{54}{64} (2v+\mu) rr' \cos\theta\right] d\theta \quad (C-6)
 \end{aligned}$$

Consider the integral over the $\tilde{\rho}_2$ coordinates. When multiplied and divided by $\exp\left[-\frac{54\mu^2 rr' \cos\theta}{64(6v+\mu)}\right]$ the integral becomes:

$$\begin{aligned}
 & \left[\int d\tilde{\rho}_2 \exp\left\{-\frac{1}{6v+\mu} \left[\frac{\tilde{\rho}_2^2}{4} (6v+\mu) + (6v+\mu)\mu \left(\frac{3}{8} \bar{r}' + \frac{9}{8} \bar{r}\right) \cdot \tilde{\rho}_2 + \left(\frac{3}{8} \mu \bar{r}' + \frac{9}{8} \mu \bar{r}\right)^2\right]\right\} \right. \\
 & \left. \cdot \exp\left[-\frac{27}{8} v \left(\frac{3v+2\mu}{6v+\mu}\right) rr' \cos\theta\right] \right]
 \end{aligned}$$

or simply

$$\exp\left[-\frac{27}{8} v \frac{3v+2\mu}{6v+\mu} rr' \cos\theta\right] \int d\tilde{\rho}_2 \exp\left[-\frac{1}{6v+\mu} \left\{ \left(\frac{3}{8} \bar{r}' + \frac{9}{8} \bar{r}\right) \mu + \frac{6v+\mu}{2} \tilde{\rho}_2 \right\}^2\right]$$

The indicated integration can be performed immediately with the simple substitution

$$x^2 = \left[\left(\frac{3}{8} \bar{r}' + \frac{9}{8} \bar{r}\right) \mu + \frac{6v+\mu}{2} \tilde{\rho}_2 \right]^2$$

and yields $8 \left[\frac{\pi}{6v+\mu}\right]^{3/2}$

Equation (C-6) is now reduced to the form

$$\begin{aligned} q_{\ell}^{DD}(r, r') = & \frac{9^3}{8^2} \frac{2}{\hbar^2} \frac{3^3 3^{3/2} MV}{\pi^{1/2}} \circ \frac{1}{(6v+\mu)^{3/2}} \exp \left[-\frac{9}{16} v \frac{15v+16\mu}{6v+\mu} r^2 - \frac{9}{16} v \frac{15v+4\mu}{6v+\mu} r'^2 \right] \\ & \cdot rr' \int_0^\pi P_\ell(\cos\theta) \sin\theta \exp \left[-\frac{27}{8} v \frac{(3v+2\mu)}{6v+\mu} rr' \cos\theta \right] d\theta \end{aligned} \quad (C-7)$$

We let $z = \cos\theta$, and $k = \frac{27}{8} v \frac{(3v+2\mu)}{6v+\mu} rr'$, then

$$rr' \int_0^\pi P_\ell(\cos\theta) \sin\theta \exp \left[-\frac{27}{8} v \frac{(3v+2\mu)}{6v+\mu} rr' \cos\theta \right] d\theta = \frac{8(6v+\mu)}{27v(3v+2\mu)} \int_{-1}^1 k e^{-kz} P_\ell(z) dz \quad (C-8)$$

In turn the transformation $k = ik$ yields an integral whose value is known [15].

$$\int_{-1}^1 k \ell^{-kz} P_\ell(z) dz = \int_{-1}^1 P_\ell(z)^{-ikz} (ik) dz = ik(-)^{\ell} i^{\ell} \sqrt{2\pi} (\kappa)^{-1/2} J_{\ell+\frac{1}{2}}(\kappa) \quad (C-9)$$

Hence

$$\int_{-1}^1 k \ell^{-kz} P_\ell(z) dz = (-)^{\ell} i^{(\ell+\frac{1}{2})} \sqrt{2\pi k} J_{\ell+\frac{1}{2}}(-ik) \quad (C-10)$$

$$\text{since } J_{\ell+\frac{1}{2}}(-ik) = (-)^{-(\ell+\frac{1}{2})} J_{\ell+\frac{1}{2}}(ik) \quad (C-11)$$

$$\int_{-1}^1 k \ell^{-kz} P_\ell(z) dz = (i)^{\ell-\frac{1}{2}} \sqrt{2\pi k} J_{\ell+\frac{1}{2}}(ik) = 2 I_{\ell+\frac{1}{2}}(k) \quad (C-12)$$

where

$$I_{\ell+\frac{1}{2}}(k) = i^{(\ell-\frac{1}{2})} \sqrt{\pi k/2} J_{\ell+\frac{1}{2}}(ik) = (-)^{\ell} \sqrt{\pi k/2} I_{\ell+\frac{1}{2}}(k) \quad (C-13)$$

Substitution back in Eqs. (C-7) and (C-8) finally yields

$$\begin{aligned}
 q_{\ell}^{DD}(r, r') = & \frac{MV_0}{\hbar^2} \frac{3}{\pi} \left(\frac{81}{2}\right) \frac{v^2}{\sqrt{6v+\mu}} (3v+2\mu) \exp\left[-\frac{9}{16} v \frac{15v+16\mu}{6v+\mu} r^2\right] \\
 & - \frac{9}{16} v \frac{15v+4\mu}{6v+\mu} r'^2 J_{\ell+1/2}\left[\frac{27}{8} v \left(\frac{3v+2\mu}{6v+\mu}\right) rr'\right]
 \end{aligned} \quad (C-14)$$

$J_{\ell+1/2}(x)$ and $I_{\ell+1/2}(x)$ are Bessel functions as defined in reference [21].

8.4 APPENDIX D

Derivation of the Analytical Expression for
the Partial Kernel $p_{\ell}^{DD}(r, r')$

The partial kernel $p_{\ell}^{DD}(r, r')$ is defined as:

$$\begin{aligned}
 p_{\ell}^{DD}(r, r') = & 2\pi rr' \int_0^{\pi} \sin\theta \, P_{\ell}(\cos\theta) \int d\tilde{\rho}_2 \left(\frac{9}{8} \right)^2 \\
 & \cdot \int d\tilde{\rho}_4 \left\{ \left(\frac{9}{8} \right)^2 \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \nabla_{\bar{v}}^2 \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) + \left(\frac{9}{8} \right)^2 \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \nabla_{\bar{u}}^2 \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \right. \\
 & + \left. \frac{27}{32} \bar{v}_{\bar{u}} \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \cdot \bar{v}_{\bar{v}} \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) + \frac{3}{2} \phi^*(\bar{v}, \bar{\rho}_2, \bar{\rho}_4) \nabla_{\bar{\rho}_2}^2 \phi(\bar{u}, \bar{\rho}_2, \bar{\rho}_4) \right\} d\theta
 \end{aligned} \tag{D-1}$$

If the explicit forms of the wavefunctions are then substituted, one will again note that, as in Appendix B, the integrals over the $\bar{\rho}_4$ coordinates can be deleted as they appear identically in the expression for p_{ℓ}^{DD} and the normalization of the wavefunctions. We can then write

$$\begin{aligned}
 p_{\ell}^{DD}(r, r') = & 2\pi \frac{v^3 3^{3/2}}{\pi^3} \int_0^{\pi} rr' \sin\theta \, P_{\ell}(\cos\theta) \\
 & \cdot \left\{ \int d\tilde{\rho}_2 \left(\frac{9}{8} \right)^5 \exp[-v(\frac{81}{64} r^2 + \frac{9}{64} r'^2 + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \right. \\
 & \quad \cdot \left. \nabla_{\bar{v}}^2 \exp[-v(v^2 + \frac{3}{4} \rho_2^2)] \right. \\
 & + \int d\tilde{\rho}_2 \left(\frac{9}{8} \right)^5 \exp[-v(\frac{9}{64} r^2 + \frac{81}{64} r'^2 + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \nabla_{\bar{u}}^2 \exp[-v(u^2 + \frac{3}{4} \rho_2^2)] \\
 & + \left. \frac{27}{32} \int d\tilde{\rho}_2 \left(\frac{9}{8} \right)^3 \bar{v}_{\bar{u}} \exp[-v(u^2 + \frac{3}{4} \rho_2^2)] \cdot \bar{v}_{\bar{v}} \exp[-v(v^2 + \frac{3}{4} \rho_2^2)] \right\}
 \end{aligned}$$

$$\begin{aligned}
& + \int d\tilde{\rho}_2 \left(\frac{9}{8}\right)^3 \frac{3}{2} \exp[-v(\frac{9}{64} r^2 + \frac{81}{64} r'^2 \\
& + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \nabla_{\frac{v}{\rho_2}}^2 \exp[-v(u^2 + \frac{3}{4} \rho_2^2)] \} d\theta
\end{aligned}$$

Now $\nabla_{\frac{v}{v}}^2 \exp[-v(v^2 + \frac{3}{4} \rho_2^2)] = 2v(2vv^2 - 3) e^{-vv^2} e^{-\frac{3}{4} v\rho_2^2}$

$$\nabla_{\frac{v}{u}}^2 \exp[-v(u^2 + \frac{3}{4} \rho_2^2)] = 2v(2vu^2 - 3) e^{-vu^2} e^{-\frac{3}{4} v\rho_2^2}$$

$$\bar{v}_{\frac{u}{u}} \exp[-v(u^2 + \frac{3}{4} \rho_2^2)] \cdot \bar{v}_{\frac{v}{v}} \exp[-v(v^2 + \frac{3}{4} \rho_2^2)]$$

$$= 4v^2 (\bar{v} \cdot \bar{u}) \exp[-v(u^2 + v^2 + \frac{3}{2} \rho_2^2)]$$

$$\nabla_{\frac{v}{\rho_2}}^2 \exp[-v(u^2 + \frac{3}{4} \rho_2^2)] = e^{-vu^2} \frac{3}{2} v(\frac{3}{2} v\rho_2^2 - 3) e^{-\frac{3}{4} \rho_2^2}$$

Therefore $p_l^{DD}(r, r')$ can be written as:

$$p_l^{DD}(r, r') = I_1 + I_2 + I_3 + I_4$$

where:

$$\begin{aligned}
I_1 &= \frac{2v^3 3^{3/2}}{\pi^2} \frac{3}{2} \left(\frac{9}{8}\right)^3 \int_0^\pi rr' p_l(\cos\theta) \sin\theta \left\{ \int d\tilde{\rho}_2 \exp[-v(\frac{9}{64} r^2 + \frac{81}{64} r'^2 \right. \\
&\quad \left. + \frac{54}{64} rr' \cos\theta)] \cdot \frac{3}{2} v(\frac{3}{2} v\rho_2^2 - 3) \exp[-v(\frac{81}{64} r^2 + \frac{9}{64} r'^2 + \frac{54}{64} rr' \cos\theta)] \right. \\
&\quad \left. \cdot \exp(-\frac{3}{2} v\rho_2^2) \right\} d\theta
\end{aligned}$$

$$\begin{aligned}
I_2 &= \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^5 \int_0^\pi rr' p_l(\cos\theta) \sin\theta \left\{ \int d\tilde{\rho}_2 \exp[-v(\frac{81}{64} r^2 + \frac{9}{64} r'^2 \right. \\
&\quad \left. + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \cdot 2v(2v(\frac{9}{64} r^2 + \frac{81}{64} r'^2 + \frac{54}{64} rr' \cos\theta) - 3) \right. \\
&\quad \left. \cdot \exp(-\frac{3}{2} v\rho_2^2) \right\} d\theta
\end{aligned}$$

$$\cdot \exp[-v(\frac{9}{64} r^2 + \frac{81}{64} r'^2 + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \} d\theta$$

$$I_3 = \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^5 \int_0^\pi rr' P_\ell(\cos\theta) \sin\theta \left\{ \int d\rho_2 \exp[-v(\frac{9}{64} r^2 + \frac{81}{64} r'^2 + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \cdot 2v(2v(\frac{81}{64} r^2 + \frac{9}{64} r'^2 + \frac{54}{64} rr' \cos\theta) - 3) \right.$$

$$\left. \cdot \exp[-v(\frac{81}{64} r^2 + \frac{9}{64} r'^2 + \frac{54}{64} rr' \cos\theta + \frac{3}{4} \rho_2^2)] \} d\theta \right.$$

$$I_4 = \frac{2v^3 3^{3/2}}{\pi^2} \frac{27}{32} \left(\frac{9}{8}\right)^5 \int^\pi rr' P_\ell(\cos\theta) \sin\theta \left\{ \int d\rho_2 \exp(-\frac{3}{2} v \rho_2^2) \right.$$

$$\left. \cdot 4v^2 [\frac{27}{64}(r^2 + r'^2) + \frac{45}{32} rr' \cos\theta] \exp[-\frac{45}{32} v(r^2 + r'^2) - \frac{27}{16} v rr' \cos\theta] \} d\theta \right.$$

The integrals are then solved separately for convenience.

If we let $z = \cos\theta$, then I_1 becomes

$$I_1 = \frac{3^{5/2} v^3}{\pi^2} \left(\frac{9}{8}\right)^3 \exp[-\frac{45}{32} v(r^2 + r'^2)] \int_{-1}^1 rr' P_\ell(z) e^{-\frac{27}{16} v rr' z} dz$$

$$\cdot \left[\int d\rho_2 \frac{9}{4} v^2 \rho_2^2 e^{-\frac{3}{2} v \rho_2^2} - \int d\rho_2 \frac{9}{2} v e^{-\frac{3}{2} v \rho_2^2} \right]$$

The integrals over ρ_2 are tabulated in reference [18], and the integral over z has been shown in Appendix C to be equal to $\frac{27}{32v} I_{\ell+1/2}(\frac{27}{16} v rr')$ so that

$$I_1 = -8\sqrt{8} \left(\frac{9}{8}\right)^3 \frac{v^{3/2}}{\pi^2} \exp[-\frac{45}{32} v(r^2 + r'^2)] I_{\ell+1/2}(\frac{27}{16} v rr')$$

The integration of I_2 and I_3 is carried forth simultaneously because of the close resemblance of the two integrals. Performing the indicated products, one can write

$$\begin{aligned}
I_2 + I_3 &= \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^5 4v^2 \frac{45}{32} (r^2 + r'^2) \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \\
&\cdot \int_{-1}^1 dz \ rr' P_\ell(z) \exp\left(-\frac{27}{16} vrr'z\right) \int d\tilde{p}_2 \exp\left(-\frac{3}{2} v p_2^2\right) \\
&+ \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^5 4v^2 \frac{27}{16} \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \\
&\cdot \int_{-1}^1 dz (rr')^2 z P_\ell(z) \exp\left(-\frac{27}{16} vrr'z\right) \int d\tilde{p}_2 \exp\left(-\frac{3}{2} v p_2^2\right) \\
&- \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^5 12v \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \\
&\cdot \int_{-1}^1 dz \ rr' P_\ell(z) \exp\left(-\frac{27}{16} vrr'z\right) \int d\tilde{p}_2 \exp\left(-\frac{3}{2} v p_2^2\right)
\end{aligned}$$

Each of the above terms is integrated separately. The first and third terms can be integrated to yield

$$\left(\frac{9}{8}\right)^4 \frac{v^{5/2}}{\pi^{1/2}} 2\sqrt{2} 15(r^2 + r'^2) \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] I_{\ell+1/2} \left(\frac{27}{16} vrr'\right)$$

and

$$-\left(\frac{9}{8}\right)^4 \frac{v^{3/2}}{\pi^{1/2}} \frac{864}{27} \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] I_{\ell+1/2} \left(\frac{27}{16} vrr'\right)$$

respectively.

The integration over z in the second term, however, presents some difficulty. The solution of such integral is shown separately in Appendix H. Using the result from that appendix, the second term is quickly found to be equal to

$$\left(\frac{9}{8}\right)^4 \frac{v^{3/2}}{\pi^{1/2}} 2\sqrt{2} \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \left\{ \frac{288}{27} I_{\ell+1/2} \left(\frac{27}{16} vrr'\right) - 18vrr' I'_{\ell+1/2} \left(\frac{27}{16} vrr'\right) \right\}$$

Finally

$$\begin{aligned}
 I_4 &= \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^3 \frac{27}{8} v^2 \frac{27}{64} (r^2 + r'^2) \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \\
 &\cdot \int_{-1}^1 dz \, rr' P_l(z) \exp\left(-\frac{27}{16} vrr'z\right) \int d\tilde{p}_2 \exp\left(-\frac{3}{2} v\tilde{p}_2^2\right) \\
 &+ \frac{2v^3 3^{3/2}}{\pi^2} \left(\frac{9}{8}\right)^3 \frac{27}{8} v^2 \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \\
 &\cdot \int_{-1}^1 dz \frac{45}{32} (rr')^2 z P_l(z) \exp\left(-\frac{27}{16} vrr'z\right) \int d\tilde{p}_2 \exp\left(-\frac{3}{2} v\tilde{p}_2^2\right)
 \end{aligned}$$

The first term can be integrated immediately to yield

$$\left(\frac{9}{8}\right)^4 \frac{v^{3/2}}{\pi^{1/2}} 2\sqrt{2} 3(r^2 + r'^2) \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] I_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right)$$

The second term can be solved using the result of Appendix H for the integral over z . Its value is

$$\left(\frac{9}{8}\right)^4 \frac{v^{3/2}}{\pi^{1/2}} 2\sqrt{2} \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \left[\frac{160}{27} I_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) - 10vrr'I'_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) \right]$$

The integral I_4 is then equal to

$$\begin{aligned}
 \left(\frac{9}{8}\right)^4 \frac{v^{3/2}}{\pi^{1/2}} 2\sqrt{2} \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] &\{ 3v(r^2 + r'^2) I_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) \\
 &+ \frac{160}{27} I_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) - 10vrr'I'_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) \}
 \end{aligned}$$

Summing the integrals I_1 , I_2 , I_3 , and I_4 we finally obtain an expression for the partial kernel $p_{\ell}^{DD}(r, r')$.

$$\begin{aligned}
 p_{\ell}^{DD}(r, r') &= \left(\frac{9}{8}\right)^4 \sqrt{\frac{8v^5}{\pi}} \exp\left[-\frac{45}{32} v(r^2 + r'^2)\right] \\
 &\cdot \{ [18(r^2 + r'^2) - \frac{608}{27v}] I_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) - 28vrr'I'_{l+\frac{1}{2}}\left(\frac{27}{16} vrr'\right) \} \quad (D-2)
 \end{aligned}$$

8.5 APPENDIX E

Coulomb Contribution to the Cross-Channel Kernels

The partial kernel H^{DS} is defined as:

$$H^{DS}(r, r') = -27 \frac{M}{\hbar^2} \int d\tilde{R}_2 \int d\tilde{\rho}_2 \phi(\tilde{y}, \tilde{R}_2, \tilde{\rho}_2) v_C(|\tilde{\rho}_2|) n(\tilde{x}, \tilde{R}_2, \tilde{\rho}_2) \quad (E-1)$$

One can easily show that $\phi^*(\tilde{x}, \tilde{R}_2, \tilde{\rho}_2) = \phi(2y^2 + \frac{3}{2} R_2^2)$, and similarly, $n(\tilde{x}, \tilde{R}_2, \tilde{\rho}_2) = (2x^2 + \frac{3}{2} R_2^2)$, so that by the substitution of the explicit forms for the wavefunctions and the Coulomb interaction one obtains:

$$H^{DS}(r, r') = \frac{27 \frac{Mq^2}{\hbar^2} \int d\tilde{R}_2 \int d\tilde{\rho}_2 e^{-\frac{v}{2}(2y^2 + \frac{3}{2} R_2^2)} (1/\rho_2) e^{-\frac{\lambda}{2}(2x^2 + \frac{3}{2} R_2^2)}}{\int d\tilde{r}' d\tilde{R}_2 d\tilde{\rho}_2 e^{-\frac{v}{2}(2y_2^2 + \frac{3}{2} R_2^2)} \int d\tilde{r}' d\tilde{R}_2 d\tilde{\rho}_2 e^{-\frac{\lambda}{2}(2x^2 + \frac{3}{2} R_2^2)}} \quad (E-2)$$

The integrals over the \tilde{r}' and the \tilde{R}_2 variables can be carried through as indicated in previous appendices; the integrals over the $\tilde{\rho}_2$ variables can be written as follows

$$\lim_{A \rightarrow \infty} \frac{\frac{4\pi}{0} \int_0^A \rho_2^2 d\rho_2}{\frac{4\pi}{0} \int_0^A \rho_2^2 d\rho_2} \lim_{A \rightarrow \infty} \frac{3}{2A} = 0$$

Thus the contribution of the Coulomb partial kernel H^{DS} is zero.
An identical result can be obtained for the kernel H^{SD} .

8.6 APPENDIX F

Evaluation of $u(r)f(r)$ and $x(r)g(r)$ at $r=0$

by the Method of Frobenius

Equations (2.0-33) and (2.0-35) can be written in the form

$$\frac{d^2}{dr^2} f_\ell(r) + 0(r)f_\ell(r) + 0'(r)g_\ell(r) = 0 \quad (F-1)$$

For instance, in the case of Eq. (2.0-33) we have

$$0(r) = -\frac{\ell(\ell+1)}{r^2} + \frac{3M}{2\hbar^2} E(n) - V_{DD}(r) - \int dr' K_\ell^{DD}(r, r') \quad (F-2)$$

$$\text{and } 0'(r) = -V_{DS}(r) - \int dr' K_\ell^{DS}(r, r') \quad (F-3)$$

Inspection of 0 and $0'$ reveals that the point $r=0$ is a regular singularity of the equation. Thus one can obtain a solution to the equation in the neighborhood of $r=0$ by using the method of Frobenius [14]. Accordingly Eq. (2.0-33) is multiplied by r^2 .

$$\begin{aligned} & r^2 \frac{d^2}{dr^2} f_\ell(r) - \ell(\ell+1)f_\ell(r) + r^2 \frac{3M}{2\hbar^2} E(n)f_\ell(r) \\ &= r^2 V_{DD}(r)f_\ell(r) + r^2 V_{DS}(r)g_\ell(r) + \int dr' r^2 K_\ell^{DD}(r, r')f_\ell(r') \\ & \quad + \int dr' r^2 K_\ell^{DS}(r, r')g_\ell(r') \end{aligned} \quad (F-4)$$

Now for $f_\ell(r)$ we assume a solution of the form

$$f_\ell(r) = \sum_{k=0}^{\infty} c_{k\ell} r^{\bar{k}+\bar{\alpha}} \quad (F-5)$$

Therefore

$$r^2 f_\ell(r) = \sum_{k=0}^{\infty} (\bar{k} + \bar{\alpha})(\bar{k} + \bar{\alpha} - 1) c_{\bar{k}\ell} r^{\bar{k} + \bar{\alpha}}$$

The point $r=0$ is an ordinary point of the expression $r^2 O(r)$ and $r^2 O'(r)$, hence we can write

$$r^2 O(r) = \sum_{k=0}^{\infty} a_{\bar{k}\ell} r^{\bar{k}}, \text{ and } r^2 O'(r) = \sum_{k=0}^{\infty} b_{\bar{k}\ell} r^{\bar{k}} \quad (F-6)$$

Substituting in the given equation, and equating coefficients of like powers of r , one obtains for $k=0$ the indicial equation

$$\bar{\alpha}(\bar{\alpha}-1)c_{0\ell} + c_{0\ell}a_{0\ell} + c_{0\ell}b_{0\ell} = 0 \quad (F-7)$$

Since $c_{0\ell}$ is completely arbitrary, it follows that

$$\bar{\alpha}(\bar{\alpha}-1) + a_{0\ell} + b_{0\ell} = 0 \quad (F-8)$$

Now, as $r \rightarrow 0$, $r^2 O(r) \rightarrow -\ell(\ell+1)$ and $r^2 O'(r) \rightarrow 0$, so that $a_0 = -\ell(\ell+1)$.

It follows that $\bar{\alpha}(\bar{\alpha}-1) = \ell(\ell+1)$, or $\bar{\alpha} = \ell+1$.

Consequently, as $r \rightarrow 0$, one has:

$$f_\ell(r) \sim a_{0\ell} r^{\ell+1}$$

$$\text{Then } \lim_{r \rightarrow 0} (1/12)h'^2 u(r) f_\ell(r)$$

$$= \lim_{r \rightarrow 0} (1/12)h'^2 \left[\frac{3M}{2\hbar^2} E(n) - V_{DD}(r) - \ell(\ell+1)/r^2 \right] [a_0 r^{\ell+1} + \dots] = 0$$

in all cases except when $\ell=1$.

$$\text{As } \ell=1, \lim_{r \rightarrow 0} (1/12)h'^2 u(r) f_1(r) = (2/12)h'^2 a_{01}.$$

Robertson has shown that the value of $a_{0\ell}$ should be taken as h'^2 [36].

An identical result is obtained when applying Frobenius method to Eq. (2.0-35).

8.7 APPENDIX G

Regular and Irregular Functions of the Reaction Channels

Past a distance R_M , where the direct potentials and the kernels become vanishingly small, the integro-differential equation for f_ℓ , Eq. (2.0-33), takes the form

$$[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{3M}{2\hbar^2} E(n)]f_\ell(r) = 0 \quad (G-1)$$

The above is known as the Riccati-Bessel equation, whose solutions are the Riccati-Bessel functions, i.e., letting $kr=\rho$, where $k^2 = \frac{3M}{2\hbar^2} E(n)$:

$$f_\ell(r) = A\sqrt{\frac{\pi kr}{2}} J_{\ell+\frac{1}{2}}(kr) + (-1)^{\ell+1} B\sqrt{\frac{\pi kr}{2}} J_{-(\ell+\frac{1}{2})}(kr) \quad (G-2)$$

In terms of Coulomb functions the above can be rewritten as [21]

$$f_\ell(r) = AF_\ell(0, kr) - BG_\ell(0, kr) \quad (G-3)$$

Herein $F_\ell(0, kr)$ and $G_\ell(0, kr)$ are the regular and irregular solutions of Eq. (G-1) respectively.

Similarly, where the nuclear potential and the kernels become vanishingly small, but not necessarily the Coulomb potential, the integro-differential equation for g_ℓ can be written as

$$[\frac{d^2}{dr^2} + \frac{3M}{2\hbar^2} E(p) - \frac{\ell(\ell+1)}{r^2} - \frac{3Mq^2}{2\hbar^2 r}]g_\ell(r) = 0 \quad (G-4)$$

We then let $k'^2 = \frac{3M}{2\hbar^2} E(p)$ and $\rho=k'r$. Furthermore we set

$$\eta' = \frac{3Mq^2}{4\hbar^2 k}, \quad (G-5)$$

Then

$$\left[\frac{d^2}{dp^2} + 1 - \frac{\ell(\ell+1)}{p^2} - \frac{2\eta'}{p} \right] g_\ell(p) = 0 \quad (G-6)$$

The above is known as the Coulomb equation, whose solutions are the Coulomb functions. Thus

$$g_\ell(r) = A F_\ell(\eta', k'r) + B G_\ell(\eta', k'r) \quad (G-7)$$

The functions $F_\ell(\eta', p)$ and $G_\ell(\eta', p)$ have been extensively tabulated by Tubis [42] for $\ell=0$. The values for different ℓ 's can be obtained from reference [29], or by appropriate recursion formulas indicated in references [21, 29, 42].

For large enough arguments, the Coulomb functions can be represented by their asymptotic behavior [21], so that the scattering functions f_ℓ and g_ℓ can be described by:

$$f_\ell(r) \xrightarrow[r \rightarrow \infty]{} A \cos \theta_\ell + B \sin \theta_\ell$$

where $\theta_\ell = kr - \frac{\pi}{2} + \sigma_\ell$, with $\sigma_\ell = \arg \Gamma(\ell+1)$; and

$$g_\ell(r) \xrightarrow[r \rightarrow \infty]{} A e^{-i(kr - \frac{\ell\pi}{2} - \eta' \ln 2kr + \sigma_\ell)} + B e^{+i(kr - \frac{\ell\pi}{2} - \eta' \ln 2kr + \sigma_\ell)}$$

where $\sigma_\ell = \arg \Gamma(\ell+1+i\eta')$.

8.8 APPENDIX H

Solution of the Integral $\int_{-1}^1 (rr')^2 z P_\ell(z) e^{-\frac{27}{16} vrr'z} dz$

The integral $\int_{-1}^1 (rr')^2 z P_\ell(z) e^{-\frac{27}{16} vrr'z} dz = I$, can be rewritten as:

$$I = \left(\frac{16}{27v}\right)^2 \int_{-1}^1 z P_\ell(z) e^{-kz} dz \quad (H-1)$$

by letting $k = \frac{27}{16} vrr'$.

The following recursion relation for the Legendre polynomials can then be used.

$$(2\ell+1)zP_\ell(z) = (\ell+1)P_{\ell+1}(z) + \ell P_{\ell-1}(z) \quad (H-2)$$

Substitution into Eq. (H-1) yields two integrals which can be readily evaluated by letting $k = ik$.

$$I = \left(\frac{16}{27v}\right)^2 k^2 \int_{-1}^1 \frac{\ell+1}{2\ell+1} P_{\ell+1}(z) e^{-kz} dz + \int_{-1}^1 \frac{\ell}{2\ell+1} P_{\ell-1}(z) e^{-kz} dz \quad (H-3)$$

With the indicated change, the two integrals above have been solved, and the results shown, in reference [15]. Thus:

$$I = \left(\frac{16}{27v}\right)^2 k^2 (-1)^{\ell-1} (i)^{\ell-\frac{1}{2}} \sqrt{\frac{2\pi}{k}} \left[\frac{\ell}{2\ell+1} J_{\ell-\frac{1}{2}}(k) - \frac{\ell+1}{2\ell+1} J_{\ell+3/2}(k) \right]$$

Since, however,

$$J_{\ell-\frac{1}{2}}(k) = \frac{\ell+\frac{1}{2}}{k} J_{\ell+\frac{1}{2}}(k) + \frac{d J_{\ell+\frac{1}{2}}(k)}{dk} \quad (H-4)$$

and

$$J_{\ell+3/2}(\kappa) = \frac{\ell+\frac{1}{2}}{\kappa} J_{\ell+\frac{1}{2}}(\kappa) - \frac{d J_{\ell+\frac{1}{2}}(\kappa)}{d\kappa} \quad (H-5)$$

one can rewrite:

$$I = \left(\frac{16}{27v}\right)^2 k^2 (-1)^{\ell-1} (i)^{(\ell-\frac{1}{2})} \sqrt{\frac{2\pi}{k}} \left[-\frac{1}{2\kappa} J_{\ell+\frac{1}{2}}(\kappa) + \frac{d J_{\ell+\frac{1}{2}}(\kappa)}{d\kappa} \right] \quad (H-6)$$

After some simple operations, the preceding equation can be changed to the following form:

$$I = \left(\frac{16}{27v}\right)^2 k^2 (-1)^{\ell-1} (i)^{(\ell-\frac{1}{2})} \sqrt{\frac{2\pi}{k}} \left[-\frac{(-1)^{-\ell}}{2k} J_{\ell+\frac{1}{2}}(ik) - (-1)^{-(\ell+\frac{1}{2})} \cdot \frac{d J_{\ell+\frac{1}{2}}(\kappa)}{d(ik)} \right] \quad (H-7)$$

One now defines

$$I_{\ell+\frac{1}{2}}(k) = (i)^{\ell-\frac{1}{2}} \sqrt{\frac{\pi k}{2}} J_{\ell+\frac{1}{2}}(ik) \quad (H-8)$$

so that

$$\frac{d I_{\ell+\frac{1}{2}}(k)}{dk} = (i)^{(\ell-\frac{1}{2})} i \sqrt{\frac{\pi k}{2}} \frac{d J_{\ell+\frac{1}{2}}(k)}{d(ik)} + i^{(\ell-\frac{1}{2})} \frac{\pi}{4} \sqrt{\frac{2}{\pi k}} J_{\ell+\frac{1}{2}}(ik) \quad (H-9)$$

From the preceding equation it follows that

$$\frac{d J_{\ell+\frac{1}{2}}(ik)}{d(ik)} = \sqrt{\frac{2}{\pi k}} i^{-(\ell+\frac{1}{2})} \frac{d I_{\ell+\frac{1}{2}}(k)}{dk} - \frac{1}{2ik} J_{\ell+\frac{1}{2}}(ik) \quad (H-10)$$

The integral studied can then be written as:

$$I = \left(\frac{16}{27v}\right)^2 k^2 (-1)^{\ell-1} (i)^{\ell-\frac{1}{2}} \sqrt{\frac{2\pi}{k}} \left[-\frac{(-1)^{-\ell}}{k} J_{\ell+\frac{1}{2}}(ik) - \sqrt{\frac{2}{\pi k}} (i)^{\ell+\frac{1}{2}} (-1)^{-(\ell+\frac{1}{2})} \cdot \frac{d I_{\ell+\frac{1}{2}}(k)}{dk} \right] \quad (H-11)$$

Again simplification of the above expression by use of Eq. (H-8) reduces it to the desired form.

$$I = \left(\frac{16}{27v}\right)^2 2I_{l+\frac{1}{2}}(k) - \left(\frac{16}{27v}\right)^2 2k \frac{d I_{l+\frac{1}{2}}(k)}{dk} \quad (H-12)$$

8.9 APPENDIX I

Computer Programs

Table VI

Input Data, Variables, and Subprograms Required
for the Scattering Functions Main Program

<u>Symbol</u>	<u>Explanation</u>
ASIN, ALPHSN	Values of the constants a' and α in Table I for either $S=0$ or $S=1$
ANUL	Value of v in the helium-3 wavefunction
VNOT	Potential well depth in MeV
BLMD	Value of λ in the triton wavefunction
BMULL	Value of μ in the form of the potential
DELTAH	Spacing between integration points
PLSOM	Value of $\hbar^2/M \times 10^{-24}$
CHELSQ	Square of the electronic charge
ENNEUT, ENPROT	Energy, in MeV, of the incident neutron, and the equivalent proton energy, respectively
L	Value of the angular momentum for which the scattering functions are sought
W	Arbitrary initial slope for the g_ℓ scattering functions
AKLDD, AKLDS, AKLSD, AKLSS	Tabulated values of the kernels K_ℓ^{DD} , K_ℓ^{DS} , K_ℓ^{SD} , and K_ℓ^{SS} at the grid points of the integration scheme
SCFN	Scattering functions f_ℓ and g_ℓ printed together in succession
RINVRS	Matrix inversion subroutine explained in Table X

```

C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C *
C * THIS IS THE MAIN PROGRAM WHICH YIELDS THE SCATTERING FUNCTIONS *
C * FOR THE TWO CHANNELS. THE PROGRAM REQUIRES THAT THE VALUES OF *
C * THE INPUT KERNELS BE PUNCHED SIX TO A CARD. SUBROUTINE RINVRS *
C * PARTITIONS THE PROGRAM INTO SUBMATRICES WHICH ARE INVERTED BY *
C * THE SUBCUTINE COMPIV. THE PROGRAM THEN CALCULATES SCATTERING *
C * FUNCTIONS AND CHECKS FOR ACCURACY OF THE MATRIX INVERSION *
C *
C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C
C IMPLICIT REAL*8(A-H,O-Z,$)
C DIMENSION A(60,60),B(60,1),AKLDD(30,30),AKLDS(30,30),AKLSD(30,30),
C 1AKLSS(30,30),U(30),V(30),T(30),SCFN(60),XIN(60,60),X(30)
1 FORMAT(6D13.7)
2 FORMAT(4D10.4)
3 FORMAT(3D10.4)
4 FORMAT(2I3)
9 FORMAT(33H           SCATTERING FUNCTIONS,//)
10 FORMAT(L30.7)
109 FORMAT(2I4,D15.7)
READ(1,3)ASIN,ALPFSN,VNCT
READ(1,2)ANUL,BLND,BMULL,DELTAB
112 READ(1,2)PLSUM,ENNEUT,ENPRUT,CHELSQ
READ(1,4)L,w
C
C THESE LOOPS INTRODUCE THE KERNEL DATA WHICH IS PUNCHED SIX TO A
C CARD.      I=ROW NUMBER      J=COLUMN NUMBER
C
J=1
DO 12 I=1,30
11 READ(1,1)AKLDD(I,J),AKLDC(I,J+1),AKLDD(I,J+2),AKLDD(I,J+3),AKLDD(I,
1,J+4),AKLDD(I,J+5)
J=J+6
IF(J.GE.30) GO TO 12
GO TO 11
12 J=1
DO 14 I=1,30
13 READ(1,1)AKLDS(I,J),AKLDS(I,J+1),AKLDS(I,J+2),AKLDS(I,J+3),AKLDS(I,
1,J+4),AKLDS(I,J+5)
J=J+6
IF(J.GT.30) GO TO 14
GO TO 13
14 J=1
DO 15 I=1,30
15 READ(1,1)AKLSD(I,J),AKLSD(I,J+1),AKLSD(I,J+2),AKLSD(I,J+3),AKLSD(I,
1,J+4),AKLSD(I,J+5)
J=J+6
IF(J.GT.30) GO TO 16
GO TO 15
16 J=1
DO 18 I=1,30
17 READ(1,1)AKLSS(I,J),AKLSS(I,J+1),AKLSS(I,J+2),AKLSS(I,J+3),AKLSS(I,
1,J+4),AKLSS(I,J+5)
J=J+6
IF(J.GT.30) GO TO 18
GO TO 17
18 J=1
C
WRITE(3,9)

```

C C C THESE LOOPS EVALUATE THE DIRECT POTENTIAL TERMS

```

CONST=1.5/PLSUM*0.1D+25*ENNEUT
ABCD=1.5/PLSUM*0.1D+25*ENPRT
ARG=9.*BMULL*ANUL/(2.*BMULL+9.*ANUL)*0.1D+27
BAR=9.*BMULL*BLMD/(2.*BMULL+9.*BLMD)*0.1D+27
FIR=(27./PLSUM)*ALPHSN*VNCT*0.1D+25*(ANUL/(2.*BMULL+9.*ANUL))*#1.5
CART=27./PLSUM*ALPHSN*VNCT*0.1D+25*(BLMD/(2.*BMULL+9.*BLMD))*#1.5
CYN=216./PLSUM*ASIN*VNCT*0.1D+25*((BLMD*ANUL)/((9.*BLMD+ANUL)
1+4.*BMULL)*(BLMD+ANUL)))*#1.5
HEL=9.*BMULL*(ANUL+BLMD)/(9.*(ANUL+BLMD)+4.*BMULL)*0.1D+27
IF(L.EQ.1) GO TO 19
U(1)=0.
X(1)=0.
GO TO 20
19 U(1)=2.
X(1)=2.
20 DO 21 I=2,30
R=(I-1)*DELTAB
CENTRF=L*(L+1)/(R**2)
VDD=FIR*1./DEXP(ARG*R**2)
21 U(I)=CENTRF-CONST+VDD
DO 22 I=1,30
R=(I-1)*DELTAB
22 V(I)=CYN*1./DEXP(HEL*R**2).
DO 23 I=2,30
R=(I-1)*DELTAB
COL=CHELSG/PLSUM*C.1D+25/R
VSS=CART*1./DEXP(EAR*R**2)+COL*1.5
CENT=L*(L+1)/(R**2)
23 X(I)=VSS+CENT-ABCC

```

C C C THESE LOOPS CALCULATE THE WEIGHT FACTORS FOR THE GREGORY NUMERICAL INTEGRATION TO SIX DIFFERENCES

```

T0=(0.5-1./12.-1./24.-19./720.-3./360.)*DELTAB
T1=(1.+1./24.+57./720.+12./160.)*DELTAB
T(1)=(1.-1./24.-57./720.-18./160.)*DELTAB
T(2)=(1.+19./24.+12./160.)*DELTAB
T(3)=(1.-3./160.)*DELTAB
GO 33 I=4,23
33 T(I)=DELTAB
T(24)=T(3)
T(25)=T(2)
T(26)=T(1)
T(27)=T1
T(28)=TC

```

C C C THESE LOOPS ASSEMBLE THE BOUNDARY CONDITION CONSTANT VECTOR B

```

AL=DELTAB**2/12.
B(1,1)=(2.+AL*10.*U(2))+AL*(AKLDD(1,2)+10.*AKLDD(2,2)+AKLDD(3,2))*
1*T1+AL*(AKLDS(1,2)+10.*AKLDS(2,2)+AKLDS(3,2))*T1+10.*AL*W*V(2)+AL
2*U(1)
B(2,1)=-(1.-AL*U(2))+AL*(AKLDD(2,2)+10.*AKLDD(3,2)+AKLDD(4,2))*T1+
1*AL*W*V(2)+AL*W*(AKLDS(2,2)+10.*AKLDS(3,2)+AKLDS(4,2))*T1
DO 38 I=3,28
38 B(I,1)=AL*(AKLDD(I,2)+10.*AKLDD(I+1,2)+AKLDD(I+2,2))*T1+AL*W*(AKL
DS(I,2)+10.*AKLDS(I+1,2)+AKLDS(I+2,2))*T1

```

```

B(2',1)=10.*AL*V(2)+AL*(AKLSD(1,2)+10.*AKLSD(2,2)+AKLSD(3,2))*T1+w
1*AL*(AKLSS(1,2)+10.*AKLSS(2,2)+AKLSS(3,2))*T1+w*(2.+10.*AL*X(2))+A
2L*X(1)
B(30,1)=AL*V(2)+AL*(AKLSD(2,2)+10.*AKLSD(3,2)+AKLSD(4,2))*T1+w*(1.
1-AL*X(2))+w*AL*(AKLSS(2,2)+10.*AKLSS(3,2)+AKLSS(4,2))*T1
DO 39 I=31,56
39 U(I,1)=AL*(AKLSD(I-28,2)+10.*AKLSD(I-27,2)+AKLSD(I-26,2))*T1+w*AL*
1(AKLSS(I-28,2)+10.*AKLSS(I-27,2)+AKLSS(I-26,2))*T1

```

```

C THESE LOOPS ARRANGE THE VARIOUS KERNELS AND DIRECT POTENTIALS IN
C THE MATRIX A WHICH IS TO BE INVERTED
C
CC 46 I=1,28
DO 46 J=1,28
IF(I.NE.J) GO TO 44
A(I,J)=1.-AL*U(I+2)-AL*(AKLDD(I,J+2)+10.*AKLDD(I+1,J+2)+AKLDD(I+2,
1J+2))*T(J)
GO TO 46
44 IF(I.GT.J) GO TO 47
A(I,J)=-AL*(AKLDD(I,J+2)+10.*AKLDD(I+1,J+2)+AKLDD(I+2,J+2))*T(J)
GO TO 46
47 IF((I-1).NE.J) GO TO 55
A(I,J)=-(2.+10.*AL*U(J+2))-AL*(AKLDD(I,J+2)+10.*AKLDD(I+1,J+2)
1+AKLDD(I+2,J+2))*T(J)
GO TO 46
55 IF((I-2).NE.J) GO TO 56
A(I,J)=(1.-AL*U(J+2))-AL*(AKLDD(I,J+2)+10.*AKLDD(I+1,J+2)
1+AKLDD(I+2,J+2))*T(J)
GO TO 46
56 A(I,J)=-AL*(AKLDD(I,J+2)+10.*AKLDD(I+1,J+2)+AKLDD(I+2,J+2))*T(J)
46 CONTINUE
DO 70 I=1,28
DO 70 J=29,56
K=J-28
IF(I.NE.K) GO TO 61
A(I,J)=-AL*V(K+2)+AL*(AKLDS(I,K+2)+10.*AKLDS(I+1,K+2)+AKLDS(I+2,K+
12))*T(K)
GO TO 70
61 IF(I.GT.K) GO TO 62
A(I,J)=-AL*(AKLDS(I,K+2)+10.*AKLDS(I+1,K+2)+AKLDS(I+2,K+2))*T(K)
GO TO 70
62 IF((I-1).NE.K) GO TO 63
A(I,J)=-10.*AL*V(K+2)-AL*(AKLDS(I,K+2)+10.*AKLDS(I+1,K+2)+AKLDS(I+
12,K+2))*T(K)
GO TO 70
63 IF((I-2).NE.K) GO TO 64
A(I,J)=-AL*V(K+2)-AL*(AKLDS(I,K+2)+10.*AKLDS(I+1,K+2)+AKLDS(I+2,K+
12))*T(K)
GO TO 70
64 A(I,J)=-AL*(AKLDS(I,K+2)+10.*AKLDS(I+1,K+2)+AKLDS(I+2,K+2))*T(K)
70 CONTINUE
DO 80 I=29,56
DO 80 J=1,28
K=I-28
IF(K.NE.J) GO TO 71
A(I,J)=-AL*V(J+2)-AL*(AKLSD(K,J+2)+10.*AKLSD(K+1,J+2)+AKLSD(K+2,J+
12))*T(J)
GO TO 80
71 IF(K.GT.J) GO TO 72
A(I,J)=-AL*(AKLSD(K,J+2)+10.*AKLSD(K+1,J+2)+AKLSD(K+2,J+2))*T(J)

```

```

GO TO 60
72 IF((K-1).NE.J) GO TO 73
  A(I,J)=-10.*AL*V(J+2)-AL*(AKLSD(K,J+2)+10.*AKLSD(K+1,J+2)+AKLSD(K+2,J+2))*T(J)
  GO TO 80
73 IF((K-2).NE.J) GO TO 74
  A(I,J)=-AL*V(J+2)-AL*(AKLSD(K,J+2)+10.*AKLSD(K+1,J+2)+AKLSD(K+2,J+2))*T(J)
  GO TO 80
74 A(I,J)=-AL*(AKLSD(K,J+2)+10.*AKLSD(K+1,J+2)+AKLSD(K+2,J+2))*T(J)
80 CONTINUE
DO 90 I=29,56
DO 90 J=29,56
K=I-28
M=J-28
IF(K.NE.M) GO TO 81
  A(I,J)=1.-AL*X(M+2)-AL*(AKLSS(K,M+2)+10.*AKLSS(K+1,M+2)+AKLSS(K+2,M+2))*T(M)
  GO TO 90
81 IF(K.GT.M) GO TO 82
  A(I,J)=-AL*(AKLSS(K,M+2)+10.*AKLSS(K+1,M+2)+AKLSS(K+2,M+2))*T(M)
  GO TO 90
82 IF((K-1).NE.M) GO TO 83
  A(I,J)=-(2.+10.*AL*X(M+2))-AL*(AKLSS(K,M+2)+10.*AKLSS(K+1,M+2)+AKLSS(K+2,M+2))*T(M)
  GO TO 90
83 IF((K-2).NE.M) GO TO 84
  A(I,J)=(1.-AL*X(M+2))-AL*(AKLSS(K,M+2)+10.*AKLSS(K+1,M+2)+AKLSS(K+2,M+2))*T(M)
  GO TO 90
84 A(I,J)=-AL*(AKLSS(K,M+2)+10.*AKLSS(K+1,M+2)+AKLSS(K+2,M+2))*T(M)
90 CONTINUE

```

C THIS PART OF THE PROGRAM CALLS THE SUBROUTINE RINVRS DESIGNED TO
C SOLVE THE SYSTEM AX=B, BY PARTITIONING THE MATRIX A AND USING THE
C SUBROUTINE CCPPIV TO INVERT THE SMALLER SUBMATRICES.

```

CALL RINVRS(A,56,XIN)
DO 92 K=1,56
SCFN(K)=0.
DO 91 J=1,56
91 SCFN(K)=SCFN(K)+XIN(K,J)*B(J,1)
92 WRITE(3,10)SCFN(K)

```

C THIS PART OF THE PROGRAM EXECUTES THE CHECK ON THE INVERSE

```

DO 101 I=1,56
DO 101 K=1,56
SUM=0.
DO 102 J=1,56
102 SUM=SUM+A(I,J)*XIN(J,K)
ER1=CAABS(SUM)
IF(ER1.GT.0.1D-10) GO TO 103
GO TO 101
103 WRITE(3,109)I,K,SLM
101 CONTINUE
DO 104 I=1,56
DO 104 K=1,56
SUM=0.
DO 105 J=1,56

```

```
105 SUM=SUM+X IN(1,J)*A(J,K)
      ER2=DABS(SUM)
      IF(ER2.GT.0.1D-10) GO TO 106
      GO TO 104
106 WRITE(3,109) I,K,SUM
104 CONTINUE
      STOP
      END
```

Table VII

Input Data, Variables, and Subprograms Required for the Programs Calculating the Kernels KLDD, KLDS, KLSD, and KLSS

Symbol	Explanation
GAMMA, DELTA, EPSILN, ETA, BETA	Values of the constants γ , δ , ϵ , η , and β , defined in Table I for S=0 (singlet)
GT, DTR, EPTR, ETATRI, BETP	Values of the constants γ , δ , ϵ , η , and β , defined in Table I for S=1 (triplet)
PLSOM	Numerical value of $\hbar^2/M \times 10^{-24}$
VNOT	Potential well depth in MeV
CHELSQ	Square of the electronic charge
ENERGY	Energy of the system in MeV
L	Angular momentum quantum number
DELTAH	Increment of r and r'
RMAX	Variable end-point of the range of the kernels. It is a function of DELTAH
ANU	Value of v in the helium-3 wavefunction for the KLDD and KLDS programs, and of λ in the triton wavefunction for the KLSD and KLSS programs
BMU	Value of μ in the form of the potential
CONU	Value of $ANU \times 10^{-26}$
XLIST(I)	Points at which the values of Dawson's integral are tabulated
YLIST(I)	Values of Dawson's integral at the XLIST points
DSIN, CSN, ESG, FSIN, BSG	Values of the constants d' , c' , e' , f' , and b' , tabulated in Table I for S=0
DTP, CTI, ETRI, FTPL, BTPL	Values of the constants d' , c' , e' , f' , and b' , tabulated in Table I for S=1
ALMDA	Value of λ in the triton wavefunction for the KLDS program, or of v in the helium-3 wavefunction for the KLSD program

Table VII (cont.)

<u>Symbol</u>	<u>Explanation</u>
ALBD	Value of ALMDA $\times 10^{-26}$
BMULL	Value of $\mu \times 10^{-26}$
BNUL	Value of $\nu \times 10^{-26}$ in KLDS, or $\lambda \times 10^{-26}$ in KLSD
TKLD1, AKLD2	Values of KLDD for S=0 and S=1 respectively
TKLDS1, AKLDS2	Values of KLDS (or KLSD) for S=0 and S=1 respectively
TKLS1, AKLS2	Values of KLSS for S=0 and S=1 respectively
INTERP	Interpolation subroutine described in Table XII
COULOMB	Function subprogram described in Table XIII
FL12, FPS12, FRIME	Function subprograms described in Table XIII

```

C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C *
C * THIS PROGRAM CALCULATES THE KERNEL KLDD FOR A GIVEN VALUE OF L *
C * AND ENERGY OF THE SYSTEM AT 30 PIVOTAL POINTS OF R AND RPRIME *
C * IN INCREMENTS DELTAH.      ENERGIES ARE IN MEV. *
C *
C * THIS PROGRAM REQUIRES USE OF THE FOLLOWING FUNCTION ROUTINES *
C * YFN - FL12 - FPS12 - FPRIME - FACT *
C *
C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C
C IMPLICIT REAL*8(A-H,O-Z,$)
1 FORMAT(6E10.4)
2 FORMAT(4D10.4)
25 FORMAT(5D10.4)
3 FORMAT(D11.3,I2,D10.4)
33 FORMAT(6D13.7)
35 FORMAT(D10.4)
4 FORMAT(3I1X,3H L=I2,5X,8H ENERGY=D10.4,///)
5 FORMAT(2D15.3,4D21.8)
6 FORMAT(112H           R           RPRME           KLDISIN
1          PLDD           HLLD           CLDD ,//)

READ(1,1) GAMMA, DELTA, EPSILN, ETA, BETA, PLSOM
READ(1,2) VNCT, ANU, BMU, CHELSC
READ(1,25) GT, DTR, EPTR, ETATRI, BETP
READ(1,3) ENERGY, L, DELTAH
READ(1,35) CCNU
R=0.0
RPRIME=0.C
RMAX=28.*DELTAH
A=VNCT/PLSOM
B=DSQRT(3./3.1415927)
B1=6.*ANU+BMU
C=(ANU**2)/(DSQRT(B1)*(3.*ANU+2.*BMU))
D=(9./16.)*ANU*((15.*ANU+16.*BMU)/B1)
E=(9./16.)*ANU*((15.*ANU+4.*BMU)/B1)
F=(27./8.)*ANU*((3.*ANU+2.*BMU)/B1)
H=6.*ANU-4.*BMU
R2P=1./DSQRT(2.*3.1415927)
S=45./32.*ANU
T=27./10.*ANU
SQDFT0=DSQRT(C.2D+C1)
REWIND 10
WRITE(3,4)L,ENERGY
WRITE(3,6)
7 SGR=R**2+RPRIME**2
PORR=R*RPRIME
IF(PORR.EQ.C.) GO TO 62
GO TO 61
62 TKLD1=0.
AKLD2=C.
ETLDD=C.
GO TO 63
61 ABESF=F*PORR
IF(ABESF-1.)E,9,9
8 TBF=FPS12(ABESF,L)
GOTO10
9 TBF=FL12(ABESF,L)
10 CLPD=A+2*40.5*C*(1./DEXP(D*R**2))+(1./DEXP(E*RPRIME**2))*TBF

```

```

SLD0=A*B*40.5*C*(1./DEXP(E*R**2))*(1./DEXP(D*RPRIME**2))*TBF
GARG=9./32.*H*PCRR
IF(GARG)133,134,134
133 GARG=CABS(GARG)
IF(GARG-1.)121,122,122
121 BESEL=FPS12(GARG,L)
GO TO 123
122 BESEL=FL12(GARG,L)
123 IF(L.EC.1.OR.L.EQ.3) GO TO 135
BESEL=-BESSEL
GO TO 135
134 IF(GARG-1.)11,12,12
11 BESEL=FPS12(GARG,L)
GO TO 135
12 BESEL=FL12(GARG,L)
135 BLID=81.*R2P*A*(ANU**1.5)/H
PLOP=1./DEXP((9./32.)*(5.*ANU+2.*BMU)*SQR)
GLDD=BLID*PLOP*BESSEL
HELP=T*PCRR
IF(HELP-1.)14,15,15
14 FFT=FPS12(HELP,L)
GO TO 16
15 FFT=FL12(HELP,L)
16 Z=(ENERGY/PLSDM)*R2P*DSQRT(ANU)*13.5
THEXP=1./DEXP(S*SCR)
FTLDD=Z*FFT*THEXP
AKAP=(6.*ANU+4.*BMU)**1.5
FLDD=81.*B*(ANU**2)/AKAP*FFT*THEXP*A
HLDD=CHLSQ/PLSDM*B*R2P*27.*FFT*THEXP*ANU/SQ0FT0
SAM=DSQRT(8./3.1415927)*(CONU**2.5)*0.1D+42*((9./8.)**4)*THEXP
CARE=18.*SQR-608./(27.*ANU)
DERBES=FPRIME(HELP,L)
PLDD=SAM*(CARE*FFT-28.*PCRR*DERBES)
TKLD1=(GAMMA*(QLDD+SLDD)+DELTA*FLDD+EPSILN*GLDD+ETA*(HLDD-ETLDD)
1+BETA*PLDD)*0.1D+25
63 WRITE(3,5)R,RPRIME,TKLD1,PLDD,HLDD,GLDD
WRITE(10)TKLD1
IF(RPRIME.LT.RMAX)GO TO 17
GO TO 18
17 RPRIME=RPRIME+DELTAB
GO TO 7
18 RPRIME=0.
IF(R.LT.RMAX)GO TO 19
GO TO 20
19 R=R+DELTAB
GO TO 7
20 REWIND 10
DO 30 I=1,900,6
READ(10)A1
READ(10)A2
READ(10)A3
READ(10)A4
READ(10)A5
READ(10)A6
30 PUNCH 33,A1,A2,A3,A4,A5,A6
STOP
END

```

```

C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C *
C * THE PROGRAM CALCULATES THE KERNEL KLDS (OR KLSD) FOR A GIVEN L *
C * AND ENERGY OF THE SYSTEM AT 30 PIVOTAL POINTS OF R AND RPRIME *
C * IN INCREMENTS DELTAH.          ENERGIES ARE IN MEV *
C *
C * SYNRCLS USED ARE: ALMCA=LAMDA, ANU=NU, BMU=MU,
C *                      ALBD=LAMDA*D-26, BNUL=NU*D-26, BMULL=MU*D-26 *
C *
C * INTERCHANGING THE VALUES OF LAMDA AND NU, WILL YIELD KLSD *
C *
C * THIS PROGRAM REQUIRES USE OF THE FOLLOWING FUNCTION ROUTINES *
C *          YFN - FL12 - FPS12 - FPRIME - FACT *
C *
C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C

```

```

IMPLICIT REAL*8(A-H,D-Z,$)
1 FORMAT(6D10.4)
2 FORMAT(5D10.4)
3 FORMAT(011.3,I2,D10.4)
35 FORMAT(3D10.4)
4 FORMAT(31X,3H L=12,5X,8H ENERGY=D10.4,///)
5 FORMAT(2D15.3,3D21.8)
6 FORMAT(95H           R           RPRME           KLDSSIN
1       KLDSTRI           ETLDS           ,//)
32 FORMAT(8C('*'))
7 FORMAT(6D13.7)
READ(1,1)DSIN,CSN,ESG,FSIN,BSG,PLSOM
READ(1,2)DTP,CTI,ETRI,FTPL,BTPL
READ(1,2)VNCT,ANU,BMU,ALMDA,CHELSQ
READ(1,3)ENERGY,L,DELTAB
READ(1,35)BNUL,BMULL,ALBD
RMAX=58.*DELTAB
U=81./64.
H=9./64.
A=VNCT/PLSOM
B=DSQRT(3./3.1415927)
C=(3.*BNUL+ALBD)+BMULL
D=DSQRT(C)
E=(BNUL+ALBD)*(3.*BNUL+3.*ALBD+4.*BMULL)
G=(BNUL+ALBD)**1.5/(D**E)*0.1D+14
AR1=3.*ANU**2+30.*ANU*ALMDA+27.*ALMCA**2+28.*BMU*ANU+36.*BMU*
1ALMDA
BR2=27.*ANU**2+30.*ANU*ALMDA+3.*ALMDA**2+12.*ANU*BMU+4.*BMU*
1ALMDA
DENOM=3.*(ANU+ALMCA)+BMU
BSF=(27./32.)*(ANU+ALMCA)*(3.*ANU+3.*ALMDA+4.*BMU)
COLL=(BNUL+ALBD)*(3.*BNUL+ALBD)+4.*BMULL)**1.5
UP=((BNUL+ALBD)**1.5)/COLL*0.1D+14
FRAC1=(BNUL+ALBD)**1.5/((BNUL+ALBD)*(3.*BNUL+ALBD)**1.5)*0.1D+14
VALCH=162.*A*((ALBD*BNUL/(ALBD+BNUL))**1.5)*(1./(3.*ALBD+BNUL)-
14.*BMULL)*C.1D+14
PAREN=36.*((ALMCA**2+ANU**2)+4C.*ALMCA*ANU-54.*((ANU+ALMDA)**2
1+48.*ALMDA**2-48.*ALMCA*(ALMDA+ANU)
X=(128./27.)*0.1D-12/((DSQRT(ALBD+BNUL))**7)
X1=(128./27.)*C.1D+14/((ALBD+BNUL)**2.5)
X2=C.1D+14/((ALBD+BNUL)**2.5)
Y=(216.*ALMDA**2+24.*ANU**2+48.*ALMCA*ANU)
Z=(216.*ANU**2+24.*ALMDA**2+48.*ALMCA*ANU)
T=144.*((ALMDA**2+ANU**2)+160.*ALMCA*ANU)

```

```

R=0.0
RPRIME=0.0
REWIND 10
WRITE(3,4)L,ENERGY
WRITE(3,6)
50 PORR=R*RPRIME
ALPHA=ALMDA*(U*R**2+H*RPRIME**2)
BETA=ANU*(H*R**2+L*RPRIME**2)
CONST=((9./8.)*4)*DSQRT((ALBD*BNUL)**3/3.1415927)*(1./DEXP(ALPHA
1))*((1./DEXP(BETA))
BESSEL=(27./32.)*(ANU+ALMDA)*PORR
IF(BESSEL-1.)18,9,9
8 FF=FPS12(BESSEL,L)
GO TO 10
9 FF=FL12(BESSEL,L)
10 FIRST=X*X*PAREN*FF
Y1=Y*R**2
Z1=Z*RPRIME**2
SECOND=X2*(Y1+Z1)*FF
FPR=FPRIME(BESSEL,L)
THIRD=X2*T*PORR*FPR
PLDS=CONST*(FIRST+SECOND-THIRD)
ASK=1./DEXP(H*BR2*RPRIME**2/DENOM)
TOT=1./DEXP(H*R**2*AR1/DENOM)
THUS=BSF*PORR/DENOM
IF(THUS-1.)11,12,12
11 FL=FPS12(THUS,L)
GO TO 13
12 FL=FL12(THUS,L)
13 GLDS=A*B*162.*G*TCT*ASK*FL
BCS=1./DEXP(H*AR1*RPRIME**2/DENOM)
VER=1./DEXP(H*BR2*R**2/DENOM)
SLDS=A*B*162.*G*BCS*VER*FL
TEX=1./DEXP(H*ANU*(R**2+9.*RPRIME**2))
THIES=1./DEXP(H*ALMDA*(9.*R**2+RPRIME**2))
BROWN=27./32.*(ANU+ALMDA)*PCRR
IF(BROWN-1.)14,15,15
14 F12=FPS12(BROWN,L)
GO TO 16
15 F12=FL12(BROWN,L)
16 FLDS=A*B*162.*UP*TEX*THIES*F12
ETALUS=162.*B*ENERGY/PLSCM*TEX*THIES*F12*FRAC
SHIRL=H*(ANU*(R**2+9.*RPRIME**2)+ALMDA*(9.*R**2+RPRIME**2)+4.*I
BMU*(R**2+RPRIME**2))
CSCAR=1./DEXP(SHIRL)
HOMER=(27./32.)*(ANU+ALMDA)-9./8.*BMU)*PORR
IF(HOMER)177,178,178
177 HOMER=DABS(HOMER)
IF(HOMER-1.)186,187,187
186 FICA=FPS12(HOMER,L)
GO TO 188
187 FICA=FL12(HOMER,L)
188 IF(L.EQ.1.CR.L.EQ.3) GO TO 19
FICA=-FICA
GO TO 19
178 IF(HOMER-1.)17,18,18
17 FICA=FPS12(HOMER,L)
GO TO 19
18 FICA=FL12(HOMER,L)
19 GLDS=FICA*DSCAR*VALCH*1./DSQRT(3.1415927)

```

```

TKLDS1=(LSIN*(GLDS+SLDS)+CSN*FLDS-ESG*ETALDS+FSIN*GLDS)*0.1D+25
1+BSG*PLDS
AKLDS2=(DTP*(GLDS+SLDS)+CTI*FLDS-ETRI*ETALDS+FTPL*GLDS)*0.1D+25
1+BTPL*PLDS
WRITE(3,5)R,RPRIME,TKLDS1,AKLDS2,ETALDS
WRITE(10)TKLDS1,AKLDS2
IF(RPRIME.LT.RMAX)GO TO 20
GO TO 21
20 RPRIME=RPRIME+DELTAF
GO TO 80
21 RPRIME=0.
IF(R.LT.RMAX)GO TO 22
GO TO 23
22 R=R+DELTAF
GO TO 80
23REWIND 10
WRITE(6,32)
DO 30 I=1,3600,6
READ(10)A1,B1
READ(10)A2,B2
READ(10)A3,B3
READ(10)A4,B4
READ(10)A5,B5
READ(10)A6,B6
PUNCH 7,A1,A2,A3,A4,A5,A6
30 WRITE(6,7)B1,B2,B3,B4,B5,B6
STOP
END

```

```

C ****
C *
C * THIS PROGRAM CALCULATES THE KERNEL KLSS FOR A GIVEN VALUE OF L *
C * AND ENERGY OF THE SYSTEM AT 30 PIVOTAL POINTS OF R AND RPRIME *
C * IN INCREMENTS DELTAF.    ENERGIES ARE IN MEV. *
C *
C * THIS PROGRAM REQUIRES USE OF THE FOLLOWING FUNCTION ROUTINES *
C * YFN - FL12 - FPS12 - FPRIME - FACT - COULMB - SUBROUTINE INTERP*
C *
C ****

```

```

IMPLICIT REAL*8(A-H,O-Z,$)
DIMENSION XLIST(90),YLIST(90)
36 FORMAT(2D15.8)
1 FORMAT(6D10.4)
2 FORMAT(4D10.4)
25 FORMAT(5D10.4)
3 FORMAT(D11.3,I2,D10.4)
33 FORMAT(6D13.7)
35 FORMAT(D10.4)
4 FORMAT(3I2,X,3H L=I2,5X,8H ENERGY=D10.4,///)
5 FORMAT(2D15.3,3D21.8)
6 FORMAT(95H           R           RPRME           KLSSIN
1       KLSSTRI          HLSS          ,//)
READ(1,1)GAMMA,DELTA,EPSILN,ETA,BETA,PLSDM
READ(1,2)VN01,ANU,BMU,CHELSQ
READ(1,25)GT,DTR,EPTR,ETATRI,BETP
READ(1,3)ENERGY,L,DELTAF
READ(1,35)CONU

```

```

CC 65 I=1,30
65 READ(1,36)XLIST(I),YLIST(I)
R=0.0
RPRIME=0.0
RMAX=28.*DELTAH
A=VNOT/PLSFIM
B=DSQRT(3./3.1415927)
B1=6.*ANU+BMU
C=(ANU**2)/(DSQRT(B1)*(3.*ANU+2.*BMU))
D=(9./16.)*ANU*((15.*ANU+16.*BMU)/B1)
E=(9./16.)*ANU*(15.*ANU+4.*BMU)/B1
F=(27./8.)*ANU*(3.*ANU+2.*BMU)/B1
H=6.*ANU-4.*BMU
R2P=1./DSQRT(2.*3.1415927)
S=45./32.*ANU
T=27./16.*ANU
REWIND 1C
WRITE(3,4)L,ENERGY
WRITE(3,6)
7 SCR=R**2+RPRIME**2
PORR=R*RPRIME
IF(PORR.EQ.0) GO TO 77
GO TO 61
77 TKLS1=0.
AKLS2=0.
ETLDD=0.
GO TO 62
61 ABESF=F*PORR
IF(ABESF-1.)8,9,9
8 TBF=FPS12(ABESF,L)
GOTO10
9 TBF=FL12(ABESF,L)
10 QLDD=A*B*40.5*C*(1./DEXP(D*R**2))*(1./DEXP(E*RPRIME**2))*TBF
SLDD=A*B*40.5*C*(1./DEXP(E*R**2))*(1./DEXP(D*RPRIME**2))*TBF
GARG=9./32.*H*PORR
IF(GARG)133,134,134
133 GARG=DABS(GARG)
IF(GARG-1.)121,122,122
121 BESEL=FPS12(GARG,L)
CO TO 123
122 BESEL=FL12(GARG,L)
123 IF(L.EQ.1.OR.L.EQ.3) CO TO 135
BESEL=-BESEL
GO TO 135
134 IF(GARG-1.)11,12,12
11 BESEL=FPS12(GARG,L)
GO TO 135
12 BESEL=FL12(GARG,L)
135 BLID=81.*R2P*A*(ANU**1.5)/H
PLUP=1./DEXP((9./32.)*(5.*ANU+2.*BMU)*SQR)
GLDD=BLID*PLUP*BESEL
HELP=T*PORR
IF(HELP-1.)14,15,15
14 FFT=FPS12(HELP,L)
GO TO 16
15 FFT=FL12(HELP,L)
16 Z=(ENERGY/PLSFIM)*R2P*DSQRT(ANU)*13.5
THEXP=1./DEXP(S*SCR)
ETLDD=Z*FFT*THEXP
AKAP=(6.*ANU+4.*BMU)**1.5

```

```

FLIND=81.*B*(ANU**2)/AKAP*FFT*THEXP*A
AAA=DSCRT((54./64.)*ANU)
SX1=AAA*(R+RPRIME)
DIFF=DABS(R-RPRIME)
SX2=AAA*DIFF
CALL INTERP(30,XLIST,YLIST,3,SX1,F01)
CALL INTERP(30,XLIST,YLIST,3,SX2,F02)
TESP=1./DEXP((90./64.)*ANU*SQR)
HLDD=(CHELSC/PLSUM)*243.*1.414/(32.*DSCRT(3.1415927))*(ANU**1.5)*
1TESP*CCULINB(F01,FC2,R,RPRIME,ANU,L)
SAM=DSCRT(8./3.1415927)*(CONU**2.5)*0.1D+42*((9./8.)**4)*THEXP
CARE=18.*SQR-608./(27.*ANU)
DERBES=FPRIME(HELP,L)
PLDD=SAM*(CARE*FFT-28.*PCRR*DERBES)
TKLS1=(GAMMA*(GLDD+SLDD)+DELTA*FLDD+EPSILN*ULDD+ETA*(HLDD-ETLDD)-
1+BETA*PLDD)*0.1D+25
AKLS2=(GT*(GLDD+SLDD)+CTR*FLDD+EPTR*GLDD+ETATRI*(HLDD-ETLDD)+
1BETP*PLDD)*0.1D+25
62 WRITE(3,5)R,RPRIME,TKLS1,AKLS2,HLDD
      WRITE(10)TKLS1,AKLS2
      IF(RPRIME.LT.RMAX)GO TO 17
      GO TO 18
17 RPRIME=RPRIME+DELTAB
      GO TO 7
18 RPRIME=0.
      IF(R.LT.RMAX)GO TO 19
      GO TO 20
19 R=R+DELTAB
      GO TO 7
20 REWIND 10
      DO 30 I=1,900,6
      READ(10)A1,B1
      READ(10)A2,B2
      READ(10)A3,B3
      READ(10)A4,B4
      READ(10)A5,B5
      READ(10)A6,B6
      PUNCH 33,A1,A2,A3,A4,A5,A6
30 PUNCH 33,B1,B2,B3,B4,B5,B6
      STOP
      END

```

Table VII

Input Data and Variables Required in the
Reaction and Scattering Matrices Programs

<u>Symbol</u>	<u>Explanation</u>
HEAD	Alphabetic data reference card, which is printed as heading to the desired results
FLOR1, FLOR2	Values of the regular Coulomb functions $F_\ell(0, R)$ at two points R1 and R2
GLOR1, GLOR2	Values of the irregular Coulomb functions $G_\ell(0, R)$ at two points R1 and R2
FLNR1, FLNR2, FLEK1, FLEKR2	Values of the regular Coulomb functions $F_\ell(\eta^i, R)$ at two points R1 and R2
GLNR1, GLNR2, GLEK1, GLEKR2	Values of the irregular Coulomb functions $G_\ell(\eta^i, R)$ at two points R1 and R2
F1R1, F2R2	Values of the scattering function f_ℓ from the 1st independent solution at the points R1 and R2
F2R1, F2R2	Values of the scattering function f_ℓ from the 2nd independent solution at the points R1 and R2
G1R1, G1R2	Values of the scattering function g_ℓ from the 1st independent solution at the points R1 and R2
G2R1, G2R2	Values of the scattering function g_ℓ from the 2nd independent solution at the points R1 and R2
AK1, AK2	Wave numbers of the first and second channel, respectively
L	Angular momentum quantum number
S00, S01, S10, S11	Scattering matrix elements (complex)
CNTN, CNTP, ELSCNT, REACTN	Partial wave cross sections for neutron reactions
CPTN, CPTP, REACPT, ELSCTP	Partial wave cross sections for proton reactions

Table VIII (cont.)

Symbol	Explanation
R11, R12, R21, R22	Reactance matrix elements
RES11, RES12, RES21, RES22	Real part of the scattering matrix elements
TIMS11, TIMS12, TIMS21, TIMS22	Imaginary part of the scattering matrix elements

```

C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * ****
C *** * THIS PROGRAM EVALUATES THE SCATTERING MATRIX AND THEN **** *
C *** * CALCULATES THE VARIOUS SCATTERING AND REACTION X-SECTS **** *
C *** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * ****
C **** * IMPLICIT REAL*8(A-H),COMPLEX*16(C-Z,$)
C COMPLEX*16 DCMPLX,DCONJG
C DIMENSION HEAD(20)
1 FORMAT(4D15.7)
2 FORMAT(2D15.7,I3)
3 FORMAT(//,60H      RE-S00          IM-S00          RE-S01          IM-
1S01    ,/)
4 FORMAT(//,60H      RE-S10          IM-S10          RE-S11          IM-
1S11    ,/)
5 FORMAT(G15.7,G15.7,G15.7,G15.7)
6 FORMAT(//,60H      N+HE=N+FE          N+HE=P+T          P+T=N+FE          P+T
1=P+T    ,/)
7 FORMAT(2CA4)
8 FORMAT(///,20A4)
9 READ(1,7)HEAD
  READ(1,1)FLOR1,FLCR2,GLOR1,GLOR2
  READ(1,1)FLNR1,FLNR2,GLNR1,GLNR2
  READ(1,1)F1R1,F2R1,F1R2,F2R2
  READ(1,1)G1R1,G2R1,G1R2,G2R2
  READ(1,2)AK1,AK2,L
  A=DSQRT(AK1)
  B=DSQRT(AK2)
  C1R1=DCMPLX(GLCR1,FLOR1)
  O1R2=DCMPLX(GLCR2,FLOR2)
  P1R1=DCCNJG(O1R1)
  P1R2=DCCNJG(O1R2)
  O2R1=DCMPLX(GLNR1,FLNR1)
  O2R2=DCMPLX(GLNR2,FLNR2)
  P2R1=DCCNJG(O2R1)
  P2R2=DCCNJG(O2R2)
  ZDN=P1R1*C1R2-P1R2*O1R1
  VDN=P2R1*C2R2-P2R2*O2R1
  PA11=A*(F1R1*O1R2-F1R2*O1R1)/ZDN
  QB11=A*(P1R1*F1R2-P1R2*F1R1)/ZDN
  PA12=A*(F2R1*O1R2-F2R2*C1R1)/ZDN
  OB12=A*(P1R1*F2R2-P1R2*F2R1)/ZDN
  SA21=B*(G1P1*O2R2-G1R2*O2R1)/VDN
  TB21=B*(P2R1*G1R2-P2R2*G1R1)/VDN
  SA22=B*(G2R1*O2R2-G2R2*O2R1)/VDN
  TB22=B*(P2R1*G2R2-P2R2*G2R1)/VDN
  Q=PA11*SA22-SA21*PA12
  S00=-(QB11*SA22-QB12*SA21)/Q
  S01=-(QB12*PA11-QB11*PA12)/Q
  S10=-(TB21*SA22-TB22*SA21)/Q
  S11=-(TB22*PA11-TB21*PA12)/Q
  WRITE(3,8)HEAD
  WRITE(3,3)
  WRITE(3,5)S00,S01
  WRITE(3,4)
  WRITE(3,5)S10,S11
  UMS00=(0.1D+01,0.0D+00)-S00
  UMS11=(0.1D+01,0.0D+00)-S11
  AQR=(CDABS(UMSC0))**2

```

```

BQR=(CDABS(UMS11))**2
CR=(CDABS(SC1))**2
CR=(CDABS(S101))**2
APA=3.1415627*(2*L+1)
CNTN=APA*ACR/AK1**2
CNTP=APA*CR/AK1**2
CPTN=APA*DR/AK2**2
CPTP=APA*BGR/AK2**2
WRITE(3,6)
WRITE(3,1)CNTN,CNTP,CPTN,CPTP
GO TO 9
STOP
END

```

```

*****
C **** THIS PROGRAM EVALUATES THE REACTION MATRIX AND THEN ****
C **** CALCULATES THE VARIOUS SCATTERING AND REACTION X-SECTS ****
C ****
***** IMPLICIT REAL*8(A-H,O-Z,$)
DIMENSION HEAD(20)
1 FORMAT(4D15.7)
2 FORMAT(2D15.7,I3)
3 FORMAT(//,9H R-MATRIX,/)
4 FORMAT(/,35H      REAL-S           IMAG-S      ,/)
5 FFORMAT(//,60H      N+HE=N+HE      N+HE=P+T      P+T=N+HE      P+T
1=P+T      ,/)
7 FFORMAT(///,20A4)
8 FORMAT(2CA4)
6 READ(1,8)HEAD
READ(1,1)FLOR1,FLCR2,GLOR1,GLOR2
READ(1,1)FLEKR1,FLEKR2,GLEKR1,GLEKR2
READ(1,1)F1R1,F2R1,F1R2,F2R2
READ(1,1)G1R1,G2R1,G1P2,G2R2
READ(1,2)AK1,AK2,L
C
C EVALUATE THE R-MATRIX
C
A=DSQRT(AK1)
B=DSQRT(AK2)
DENOM=FLOR1*GLOR2-FLOR2*GLCR1
A11=A*(F1R1*GLOR2-F1R2*GLOR1)/DENOM
B11=A*(FLCR1*F1R2-FLOR2*F1R1)/DENOM
A12=A*(F2R1*GLOR2-F2R2*GLOR1)/DENOM
B12=A*(F2R2*FLCR1-FLOR2*F2R1)/DENOM
DNM=FLEKR1*GLEKR2-FLEKR2*GLEKR1
A21=B*(G1R1*GLEKR2-G1R2*GLEKR1)/DNM
B21=B*(FLEKR1*G1R2-FLEKR2*G1R1)/DNM
A22=B*(G2R1*GLEKR2-GLEKR1*G2R2)/LNM
B22=B*(G2R2*FLEKR1-FLEKR2*G2R1)/DNM
BELOW=A11*A22-A21*A12
R11=(B11*A22-B12*A21)/BELOW
R12=(B12*A11-B11*A12)/BELOW
R21=(B21*A22-B22*A21)/BELOW
R22=(B22*A11-B21*A12)/BELOW

```

```

      WRITE(3,7)HEAD
      WRITE(3,3)
      WRITE(3,1)R11,R12,R21,R22
C
C      ASSEMBLE THE S-MATRIX
C
      WRITE(3,4)
      R12=0.5*(R12+R21)
      ADENT=(1.-R22*R11+R12**2)**2+(R11+R22)**2
      RES11=((1.+R11*R22-R12**2)*(1.-R11*R22+R12**2)-(R11+R22)*(R11-R22)
1)/ADENT
      TIMS11=(2./ADENT)*(R11-R22*R12**2+R11*R22**2)
      WRITE(3,2)RES11,TIMS11
      RES12=-2.*R12*(R11+R22)/ADENT
      TIMS12=(2./ADENT)*R12*(1.-R11*R22+R12**2)
      WRITE(3,2)RES12,TIMS12
      RES22=((1.+R11*R22-R12**2)*(1.-R11*R22+R12**2)-(R22-R11)*(R11+R22)
1)/ADENT
      TIMS22=(2./ADENT)*(R22+R22*R11**2-R11*R12**2)
      WRITE(3,2)RES22,TIMS22
      S1=1.-RES11
      S2=1.-RES22
C
C      EVALUATE CROSS SECTIONS
C
      WRITE(3,5)
      ELSCNT=3.1415927*(S1**2+TIMS11**2)/(AK1**2)*(2*L+1)
      REACNT=3.1415927*(RES12**2+TIMS12**2)/(AK1**2)*(2*L+1)
      REACPT=REACNT*(AK1**2/AK2**2)
      ELSOPT=3.1415927*(S2**2+TIMS22**2)/(AK2**2)*(2*L+1)
      WRITE(3,1)ELSCNT,REACNT,REACPT,ELSOPT
      GO TO 6
      STOP
      END

```

Table IX

Input Data, Variables, and Subprograms Required
in the Cross Section Angular Distribution Program

<u>Symbol</u>	<u>Explanation</u>
HEAD	Alphameric data reference card, which is printed as a heading to the results
AK1, AK2	Wave numbers of the first and second channel, respectively
L	Angular momentum quantum number
N	Number of angles at which the value of the cross section is desired
S00(I)	Complex values of the scattering matrices first diagonal element listed in increasing values of L
S01(J)	Complex values of the scattering matrices off-diagonal elements listed in increasing values of L
PL	Function subprogram described in Table XIII
X1	Differential cross section for the elastic scattering channel at an angle THETA
X3	Differential cross section for the reaction channel at an angle THETA
THETA(J)	J values of the angle at which the cross sections are sought

```

C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C **** * THIS PROGRAM DETERMINES THE DIFFERENTIAL SCATTERING **** *
C **** * AND REACTION CROSS SECTIONS FOR THE N-HELlUM-3 AND **** *
C **** * PROTON-TRITON SYSTEMS AT N VALUES OF THE SCATTERING **** *
C **** * ANGLE FOR VALUES OF L RANGING UP TO 2. **** *
C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *
C **** * **** * **** * **** * **** * **** * **** * **** * **** * **** * **** *

```

```

IMPLICIT REAL*8(A-H,O-Z,$)
COMPLEX*16 SCO,SC1,DCONJG,AR,CR,DUM,SUM
DIMENSION SCO(20),SC1(20),AR(20),CR(20),HEAD(20),THETA(20)
1 FORMAT(G15.7,G15.7)
2 FORMAT(2E15.7,2I3)
3 FORMAT(2CA4)
4 FORMAT(//,3E8      N+HE=N+HE          N+HE=P+T          THETA,/ )
5 FORMAT(2D15.7,F8.2)
9 FORMAT(F10.2)
READ(1,3)HEAD
READ(1,2)AK1,AK2,L,N
M=L+1
DO 6 I=1,M
6 READ(1,1)SCO(I)
DO 7 J=1,M
7 READ(1,1)SC1(J)
WRITE(3,3)HEAD
WRITE(3,4)
DO 10 J=1,N
READ(1,9)THETA(J)
X=THETA(J)
T=X*3.1415927/180.
DUM=(0.0D+00,0.0D+00)
SUM=(0.0D+00,0.0D+00)
DO 11 I=1,M
K=I-1
SUM=SUM+(1.-SCO(I))*(2*K+1)*PL(T,K)
AR(I)=DCONJG(SCO(I))
11 DUM=DUM+(1.-AR(I))*(2*K+1)*PL(T,K)
X1=(1./(4.*AK1**2))*SUM*DUM
SUM=(0.0D+00,0.0D+00)
DUM=(0.0D+00,0.0D+00)
DO 13 I=1,M
K=I-1
SUM=SUM-SC1(I)*(2*K+1)*PL(T,K)
CR(I)=DCONJG(SC1(I))
13 DUM=DUM-CR(I)*(2*K+1)*PL(T,K)
X3=(1./(4.*AK1**2))*SUM*DUM
10 WRITE(3,5)X1,X3,X
STOP
END

```

Table X

Input Data and Subprograms Required for the Subroutine
RINVRS Performing the Matrix Inversion by Partitioning

<u>Symbol</u>	<u>Explanation</u>
RINVRS	Symbolic name of the subroutine subprogram
R	Original matrix which is to be inverted
ISIZE	Size of the original matrix
XCT	Inverse matrix
A	Array used in the program to successively store the inverse of the submatrix A resulting from partition of R, and the submatrix K of the final inverse
B	Array used in the program to successively store the submatrix B resulting from partition of R, and the matrix product $A^{-1}B$
C	Array used in the program to successively store the submatrix C resulting from partition of R, the matrix product CA^{-1} , and the submatrix M of the final inverse SCT
D	Submatrix resulting from partition of R
L	Submatrix of the partitioned inverse XCT
F	Array used in the program to successively store the submatrix A resulting from partition of R, and the submatrix N of the partitioned inverse XCT
COMPIV	Matrix inversion subroutine described in Table XI. This routine must be used with KODE=2

```

SUBROUTINE RINVR5(R,ISIZE,XCT)
C THIS SUBROUTINE PARTITIONS THE MATRIX R AND INVERTS IT.
C THE MATRIX R AND ITS INVERSE XCT ARE PARTITIONED AS FOLLOWS:
C
C          R          XCT
C          A B        K L
C          C D        M N
C
C IMPLICIT REAL*8(A-H,O-Z,$)
REAL*8L
DIMENSION R(60,60),A(31,31),B(31,30),C(30,31),DUM(32),L(30,30),
1XCT(60,60),D(31,31),F(31,32)
ISIZE=ISIZE
SIZE=SIZE+.0CCCCCCCC01
KSIZE=SIZE/2.
JSIZE=ISIZE-KSIZE
NNN=JSIZE+1
C***** THESE LCCPS PARTITION THE MATRIX R *****
DO 100 I=1,JSIZE
DO 200 J=1,JSIZE
200 F(I,J)=R(I,J)
DO 100 J=NNN,ISIZE
K=J-JSIZE
100 B(I,K)=R(I,J)
DO 300 I=NNN,ISIZE
K=I-JSIZE
DO 400 J=1,JSIZE
400 C(K,J)=R(I,J)
DO 300 J=NNN,ISIZE
M=J-JSIZE
300 D(K,M)=R(I,J)
C***** THESE LCCPS INVERT THE MATRIX R *****
CALL COMPIV(JSIZE,2,F)
C***** A(-1) STORED IN F *****
DO 19 I=1,JSIZE
DO 19 J=1,JSIZE
19 A(I,J)=F(I,J)
C***** A(-1) STORED IN A *****
DO 4 J=1,KSIZE
DO 3 I=1,JSIZE
DUM(I)=0.
DO 3 K=1,JSIZE
3 DUM(I)=DUM(I)+F(I,K)*B(K,J)
DO 4 I=1,JSIZE
4 B(I,J)=DUM(I)
C***** A(-1)*B STORED IN B *****
DO 7 J=1,KSIZE
DO 7 I=1,KSIZE
TERM=0.
DO 6 K=1,JSIZE
6 TERM=TERM+C(I,K)*E(K,J)
7 E(I,J)=C(I,J)-TERM
CALL CCPPIV(FSIZE,2,F)
C***** N = (D-C*A(-1)*B)-1 IS STORED IN F *****
DO 9 J=1,KSIZE
DO 8 I=1,JSIZE
DUM(I)=C.
DO 8 K=1,KSIZE

```

```

9 L(KK,J)=CUM(KK)                                *****
C*****          L = -A(-1)*B*N IS STORED IN L      *****
DO 11 I=1, KSIZE
DO 10 J=1, JSIZE
CUM(J)=0.
DO 10 K=1, JSIZE
10 CUM(J)=CUM(J)+C(I,K)*A(K,J)
DO 11 J=1, JSIZE
11 C(I,J)=CUM(J)                                *****
C*****          C*A(-1) STORED IN C      *****
DO 13 J=1, JSIZE
DO 12 I=1, KSIZE
CUM(I)=0.
DO 12 K=1, KSIZE
12 CUM(I)=CUM(I)-F(I,K)*C(K,J)
DO 13 I=1, KSIZE
13 C(I,J)=CUM(I)                                *****
C*****          M = -N*C*A(-1) IS STORED IN C      *****
DO 15 J=1, JSIZE
DO 15 I=1, JSIZE
TERM=0.
DO 14 K=1, KSIZE
14 TERM=TERM+B(I,K)*C(K,J)
15 A(I,J)=A(I,J)-TERM
C*****          K = A(-1) - A(-1)*B*M IS STORED IN A      *****
C*****          THESE LOOPS RECONSTITUTE THE INVERSE MATRIX XCT *****
DO 21 I=1, JSIZE
DO 20 J=1, JSIZE
20 XCT(I,J)=A(I,J)
DO 21 K=1, KSIZE
J=K+JSIZE
21 XCT(I,J)=L(I,K)
DO 23 J=1, JSIZE
DO 23 K=1, KSIZE
KK=K+JSIZE
23 XCT(KK,J)=C(K,J)
DO 22 J=1, KSIZE
DO 22 K=1, KSIZE
KK=K+JSIZE
JK=J+JSIZE
22 XCT(KK,JK)=F(K,J)
RETURN
END

```

Table XI

Input Data and Variables Required for the
Direct Matrix Inversion Subroutine COMPIV

Symbol	Explanation
COMPIV	Symbolic name of the subroutine subprogram
LN	Number of rows of the matrix to be inverted
KODE	Dummy variable whose value determines whether the subroutine is to perform direct matrix inversion (KODE=2), or is to solve a system of linear algebraic equations (KODE=1)
B	If KODE=1, B is the augmented matrix from the system of linear algebraic equations. If KODE=2, B is the matrix whose inverse is sought, and the return inverse matrix

```

SUBROUTINE COMPIV(LN,KODE,B)
IMPLICIT REAL*8(A-H,O-Z,1)
DIMENSION NROW(31),NCOL(31),ABA(31),CCNST(31),ABB(31),A(31,32)
1,C(31,32),B(31,32)
C      KODE = 1      SOLUTION OF LINEAR ALGEBRAIC EQUATIONS
C      KODE = 2      MATRIX INVERSION BY GAUSS-JORDAN REDUCTION
LNN=LN+1
492 FORMAT(1H1,28HSINGULAR MATRIX, EQUATIONS =,I4,2X,6HRANK =,I4)
DET=1.0
DO 2001 I=1,LN
NROW(I)=I
NCOL(I)=I
   DO 2001 J=1,LNN
2001 A(I,J)=B(I,J)
   DO 2000 ILEFT=1,LN
      FIND LARGEST ELEMENT
      BIG=0.
      DO 2200 J=ILEFT,LN
      DO 2200 I=ILEFT,LN
      BURPE=DABS(B(I,J))
      IF(BIG-BURPE)2039,2200,2200
2039 BIG=BURPE
      IRW=I
      JCCL=J
2200 CONTINUE
      IF(IROW-ILEFT)2092,2091,2092
2092 DET=-DET
2091 IF(JCCL-ILEFT)2094,2093,2094
2094 DET=-DET
2093 CONTINUE
C      INTERCHANGE TWO ROWS
      DO 2050 J=1,LN
      D=B(IRW,J)
      B(IROW,J)=B(ILEFT,J)
2050 B(ILEFT,J)=D
      KEEP=NROW(ILEFT)
      NROW(ILEFT)=NROW(IROW)
      NROW(IRW)=KEEP
C      INTERCHANGE TWO COLUMNS
      DO 2051 I=1,LN
      D=B(I,JCUL)
      B(I,JCCL)=B(I,ILEFT)
2051 B(I,ILEFT)=D
      KEEP=NCOL(ILEFT)
      NCOL(ILEFT)=NCOL(JCUL)
      NCOL(JCUL)=KEEP
      DIV=B(ILEFT,ILEFT)
      DET=DET*DIV
      IRANK=ILEFT-1
      IF(DIV)2351,2350,2351
2351 DIV=1.0/DIV
      DO 2098 I=1,LN
2098 B(I,LNN)=0.0
      B(ILEFT,LNN)=1.0
C      GAUSS-JORDAN REDUCTION
      DO 2060 K=1,LNN
2060 B(ILEFT,K)=B(ILEFT,K)*DIV
      DO 2080 I=1,LN
      IF(I-ILEFT)2065,2080,2065
2065 ATJ=-B(I,ILEFT)

```

```

    DO 2070 K=1,LNN
2070  B(I,K)=B(I,K)+AIJ*B(ILEFT,K)
2080  CONTINUE
    DO 2029 I=1,LN
2029  B(I,ILEFT)=B(I,LNN)
2090  CONTINUE
    IRANK=LNN
2100  IF(LNN.GT.IRANK)GO TO 2011
C      REARRANGE INVERSE MATRIX
    DO 2031 J=1,LN
      K=IROW(J)
      DO 2031 I=1,LN
2031  C(I,K)=B(I,J)
      DO 2032 I=1,LN
      K=NCOL(I)
      DO 2032 J=1,LN
2032  B(K,J)=C(I,J)
C      B IS THE INVERSE MATRIX
      IF(KODE.EQ.2)RETURN
C      CALCULATE SOLUTION VECTOR
    DO 2019 I=1,LN
      ABA(I)=0.0
2019  CONST(I)=A(I,LNN)
2020  DO 2005 K=1,LN
      ABB(K)=0.
      DO 2006 J=1,LN
2006  ABB(K)=ABB(K)+B(K,J)*CONST(J)
2005  ABA(K)=ABA(K)+ABB(K)
      DO 2007 I=1,LN
        IF(DABS(ABA(I)/ABA(I)).GT.1.0-18)GO TO 2009
2007  CONTINUE
      DO 2020 I=1,LN
2020  B(I,LNN)=ABA(I)
      RETURN
C      DETERMINE RESIDUES
    DO 2003 I=1,LN
      DO 2003 J=1,LN
2003  CONST(I)=CONST(I)-A(I,J)*ABB(J)
C      IMPROVE SOLUTION VECTOR
      GO TO 2010
2011  WRITE(3,492)LN,IRANK
      RETURN
      END

```

Table XII

Input Data and Variables Required for the Interpolation Subroutine

<u>Symbol</u>	<u>Explanation</u>
INTERP	Symbolic name of the subroutine subprogram
IMAXTP	Length of interpolation list
XABCIS	Abcissa of interpolation list; must be entered into computer in either ascending or descending order
FORDIN	Ordinate of interpolation list
NPTSTP	Number of interpolation points
TVX	Interpolation point in abscissa list
TVF	Desired interpolated value in ordinate list
XOTP	Floating point variable used in ordering interpolation points
INTP	Fixed point variable used in ordering interpolation points; INTP=1 is the argument of the XABCIS (and FORDIN) nearest TVX, INTP=2 is next nearest, etc.
ATP	Variable used in ordering interpolation points made equal to absolute value of difference between TVX and each XABCIS
ITP	Position in list of XABCIS nearest TVX
INNTP	Integer oscillating between +1 and -1 to obtain the Gaussian arrangement
XN	Abcissa list ordered so that successive values are at greater distances from TVX
FN	Ordinate list ordered so that successive values are at greater distances from TVF
IQTP	Variable which determines if end of list has been reached
FACT	Factor which modifies the divided differences

```

SUBROUTINE INTERP(IMAXTP,XABCIS,FORDIN,NPTSTP,TVX,TVF)
C   IMAXTP=LENGTH OF INPUT DATA LIST
C   XABCIS=ABSCISSAS OF LIST
C   FORDIN=ORDINATES OF LIST
C   NPTSTP=ORDER OF INTERPOLATION
C   TVX=VALUE OF THE ABSCISSA AT WHICH THE ANSWER IS DESIRED
C   TVF=DESIRED ANSWER
C   IMPLICIT REAL*8(A-H,O-Z,$)
C   DIMENSION XABCIS(90),FORDIN(90),XN(30),FN(30)
300 IF(IMAXTP.GT.1)GO TO 830
    GO TO 801
801 IF(IMAXTP.EQ.1)GO TO 820
810 TVF=C.
    RETURN
820 TVF=FORDIN(1)
    RETURN
C   THESE ORDERS TAKE CARE OF ECCENTRICALLY SHORT LISTS
830 IF(NPTSTP.LT.IMAXTP)GO TO 850
840 NPTSTP=IMAXTP-1
C   ORDER OF INTERPOLATION IS DECREASED IF LIST IS TOO SHORT
850 XOTP=1.0+60
    DO 890 INTP=1,IMAXTP
        ATP=TVX-XABCIS(INTP)
        IF(ATP.GE.0.)GO TO 870
860 ATP=-ATP
870 IF(ATP.GE.XOTP) GO TO 890
880 ITP=INTP
    XOTP=ATP
890 CONTINUE
C   THIS LOOP SELECTS THE VALUE OF XABCIS CLOSEST TO TVX
    IF((IMAXTP-ITP).GT.1) GO TO 889
    GO TO 892
889 IF(ITP.GT.1) GO TO 891
892 INNTP=1
    GO TO 894
891 IF(DABS(TVX-XABCIS(ITP+1)).GT.DABS(TVX-XABCIS(ITP-1))) GO TO 893
    GO TO 892
893 INNTP=-1
894 NPTSTP=NPTSTP+
C   THESE ORDERS DETERMINE ON WHICH SIDE OF TVX IS THE NEXT XABCIS
    DO 970 INTP=1,NPTSTP
        XN(INTP)=XABCIS(ITP)
        FN(INTP)=FORDIN(ITP)
        IF(INNTP.GT.0)GO TO 910
900 IQTP=ITP-INTP
    GO TO 940
930 ITP=ITP-1
    GO TO 970
910 IQTP=ITP+INTP
920 IF(IMAXTP.LT.IQTP) GO TO 930
940 IF(IQTP.GT.0) GO TO 960
950 ITP=ITP+1
    GO TO 970
960 ITP=IQTP
    INNTP=-INNTP
970 CONTINUE
C   THIS LOOP ORDERS THE INTERPOLATION POINTS
C   FOR INCREASING DISTANCES FROM TVX
    NPTSTP=NPTSTP-1
    TVF=0.

```

```
FICT=1.  
DO 990 JNTP=1,NPISTP  
    TVF=TVF+FICT*FN(1)  
    DO 980 INTP=JNTP,APTSTP  
        ICTP=INTP-JNTP+1  
        FN(ICTP)=(FN(ICTP+1)-FN(ICP)))/(XN(INTP+1)-XN(ICP))  
980    FICT = FICT*(TVX-XN(JNTP))  
C     THIS IS THE MAIN LOOP FOR CALCULATING THE DIVIDED DIFFERENCES  
1000 RETURN  
END
```

Table XIII

Function Subprograms Required for the Calculation of the
Kernels and the Cross Section Angular Distributions

Symbol	Explanation
PL(THETA,L)	Yields values of the L-th order Legendre polynomial of argument THETA for values of L=0,1,2
FACT(N)	Calculates N factorial
YFN(ARG,L)	Yields values of the polynomials $y(x)$ necessary to compute $I_{l+1/2}(x)$ from $x=ARG>1$, and all values of L. Requires use of FACT(N)
FL12(ARG,L)	Calculates $I_{l+1/2}(x)$ for $x=ARG>1$, and all values of L. Requires use of YFN(ARG,L)
FPS12(ARG,L)	Calculates $I_{l+1/2}(x)$ by power series expansion when $x=ARG<1$, and for all values of L. Requires use of FACT(N)
FPRIME(ARG,L)	Computes the derivative of $I_{l+1/2}(x)$ for all arguments and values of L. Requires use of FL12(ARG,L) and FPS12(ARG,L)
COULMB(FF1,FF2, X,Y,A,L)	Returns values of the Coulomb contribution to the KLSS kernel for L=0,1,2

```

FUNCTION PL(THETA,L)
IMPLICIT REAL*8(A-H,D-Z,$)
IF(L.GT.0) GO TO 111
PL=1.
GO TO 113
111 IF(L.GT.1) GO TO 112
PL=DCOS(THETA)
GO TO 113
112 PL=1.5*(DCOS(THETA))**2-C*5
113 RETURN
END

```

```

FUNCTION FACT(N)
IMPLICIT REAL*8(A-H,D-Z,$)
1C18 FORMAT( 2CH ARG OF FACT = NEG , I3,/ )
IF( N ) 1C13,1C14,1C15
1C13 WRITE(3,1C18) N
GO TO 1C17
1C15 FACT = 1.
DO 1C19 I=1,N
XI = I
1C19 FACT = FACT*XI
GO TO 1C17
1C14 FACT=1.
1C17 RETURN
END

```

```

FUNCTION YFN(ARG,L)
IMPLICIT REAL*8(A-H,D-Z,$)
M=0
YFN=1.0
IF(L.EQ.0) GO TO 998
999 M=M+1
IL=L+M
IM=L-M
F=FACT(IL)/((FACT(IM))*(FACT(M))*(2**M))
YFN=YFN+F*(ARG**M)
IF(M.LT.L) GO TO 999
998 RETURN
END

```

```

FUNCTION FL12(ARG,L)
IMPLICIT REAL*8(A-H,O-Z,$)
AR1=1.0/ARG
AR2=-AR1
A=DEXP(ARG)
FL12=0.5*((A*YFN(AR2,L)*((-1)**L))+((-1)**(2*L+1))*YFN(AR1,L))/A
RETURN
END

```

```

FUNCTION FPS12(ARG,L)
IMPLICIT REAL*8(A-H,O-Z,$)
M=0
AR=L+0.5
BR=L+1.5
IF(ARG.GT.0.) GO TO 2221
FPS12=0.0
GO TO 2223
2221 TNUM=(0.5*ARG)**AR
RUT=DSQRT(0.5*3.1415927*ARG)
FPS12=(((-1)**L)*RUT*TNUM)/DGAMMA(BR)
2222 M=M+1
AR=L+2*M+0.5
BR=L+M+1.5
TNUM=(0.5*ARG)**AR
SUM=(((-1)**L)*RUT*TNUM)/DGAMMA(BR)
FPS12=FPS12+SUM
IF((SUM/FPS12).GT.0.0000001) GO TO 2222
2223 RETURN
END

```

```

FUNCTION FPRIME(ARG,L)
IMPLICIT REAL*8(A-H,O-Z,$)
K=L+1
IF(ARG.GT.0.) GO TO 776
CONTINUE
IF(L.EQ.0.) GO TO 774
FPRIME=0.
GO TO 778
774 FPRIME=1.0
GO TO 778
776 IF(ARG.LT.1.0) GO TO 777
FPRIME=((L+1)/ARG)*FL12(ARG,L)-FL12(ARG,K)
GO TO 778
777 FPRIME=((L+1)/ARG)*FPS12(ARG,L)-FPS12(ARG,K)
778 RETURN
END

```

```

FUNCTION COULMB(FF1,FF2,X,Y,A,L)
IMPLICIT REAL*8(A-H,D-Z,>)
RR=X**Y
RZP=X**2+Y**2
POS=DEXP((1C8./64.)*A*RR)
ANEGL=1./POS
R=DSQRT(64./(54.*A))
IF(L.GT.0) GO TO 441
COULMB=L*(POS*FF1-ANEGL*FF2)
GO TO 445
441 CONTINUE
IF(L.GT.1) GO TO 442
C=(RZP/(2.*RR))*B
D=(1./(4.*RR))*B**3
E=(1./(4.*RR))*B**2
COULMB=(C+D)*(POS*FF1-ANEGL*FF2)-E*(POS*(X+Y)-ANEGL*DABS(X-Y))
GO TO 445
442 CONTINUE
IF(L.GT.2) GO TO 443
T=3*(3.*RZP**2)/(8.*RR**2)+(3.*RZP/(8.*RR**2))*B**3+(9./(32.*RR**1.5))-0.5*B
U=(3.*RZP/(8.*RR**2))*B**2+(9./(32.*RR**2))*B**4
Z=(3./(16.*RR**2))*B**2
COULMB=T*(POS*FF1-ANEGL*FF2)-U*(POS*(X+Y)-ANEGL*DABS(X-Y))+Z*(POS*(X+Y)**3-ANEGL*(DABS(X-Y))**3)
443 CONTINUE
GO TO 445
C THIS SPACE IS RESERVED FOR FUTURE ADDITIONS TO THIS COULOMB
C FUNCTION WHENEVER HIGHER VALUES OF L ARE CALCULATED
445 RETURN
END

```

CLUSTER-MODEL EVALUATION OF NEUTRON
CROSS SECTIONS FOR LIGHT-WEIGHT NUCLEI

by

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B.S., Kansas State University, 1964
M.S., Kansas State University, 1967

AN ABSTRACT OF A DOCTOR'S DISSERTATION

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1970

ABSTRACT

The four-nucleon reaction is formulated using the resonating group (cluster) model for the neutron-helium-3 and proton-triton groupings. Two coupled integro-differential equations describing the possible reactions are derived for each value of the total spin and angular momentum of the system.

Analytical forms for the nonlocal and direct interactions are obtained by employing an equivalent central potential with a Gaussian shape, and wavefunctions for the ground states of the helium-3 and triton clusters also of Gaussian shape.

The exchange dependence of the potential is chosen to be of the Serber type. Other authors have shown this type to yield satisfactory agreement with experimental values for the range of energies considered.

The coupled integro-differential equations are solved numerically and the total and differential cross sections for the ${}^3\text{He}(\text{n},\text{n}){}^3\text{He}$ and ${}^3\text{He}(\text{n},\text{p})\text{T}$ reactions are reported for incident neutron energies of 1, 3.6, and 6 MeV. The ${}^3\text{He}(\text{n},\text{n}){}^3\text{He}$ cross sections, both total and differential, are in fairly good agreement with the experimental values except at 1 MeV, where the calculated cross section is too low at all angles. The shape of the angular distribution curve, however, matches quite well with the experimental one; in particular the minima of the distribution are predicted correctly. At the higher energies, the larger values of the calculated cross section at large angles could be attributed to the presence of another open channel, ${}^3\text{He}(\text{n},\text{d})\text{D}$, which is of course not accounted for in the present theoretical treatment.

The elastic scattering cross sections do not significantly differ from those calculated by other authors, who considered the elastic-scattering channel as the only open exit channel.

The calculated total cross section for the ${}^3\text{He}(n,p)T$ channel are consistently too low. The angular distribution curves exhibit the qualitative features found in the experimental ones, i.e., the minima shift toward larger angles as the energy increases, and their position is well predicted. The small values predicted for the Serber interaction at the larger angles are expected, since this interaction yields too large a value at those angles for the elastic scattering cross section.