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The Effect of Orthogonality and Antisymmetrisation in the Strong - Coupling Model of Nuclear Cluster Reactions

A thesis presented in partial fulfilment
of the requirements for the degree of
Doctor of Philosophy
at the University of Auckland

Ian Joseph Thompson
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Abstract

The possibility and feasibility is investigated of including in the modelling of nuclear cluster reactions a unified treatment of the effects both of the non-orthogonalities between transfer channels, and of the antisymmetrisation required by the Pauli Principle. The deuteron - nucleus interaction, the simplest cluster reaction, is considered in detail within the Coupled Channels framework. The Coupled Channels formalism was chosen because it accurately handles inelastic and transfer couplings of arbitary strengths.

The fact that transfer channels are orthogonal to each other only asymptotically is taken into account by reallocating the wave function in the internal region, from the deuteron channels to the transfer channels, taking components from the deuteron channels in ways exactly analogous to the way the antisymmetrisation requirements remove blocked deuteron-core components. Thus a unified treatment of the two effects is facilitated.

It is found further that when all possible transfer channels are included, along with all Pauli blockings from the core nucleons, then under certain conditions at low energies, the wave function in the deuteron channel is small and oscillatory in the internal region, leaving the deuteron as a cluster to have largely asymptotic significance. In this limit, the exact non-local potential governing the deuteron channel simplifies considerably in one approximation to be replaceable by just several orthogonality conditions, and these are easily modelled in solving the coupled equations for the radial wave functions. This simplified and unified model has the advantage, since the deuteron's internal wave form is significant only asymptotically, of allowing automatically for arbitary deuteron polarisation by the core (though not vice-versa). Furthermore, the asymptotic matching is not at a fixed radius as in R-matrix theory, but is a continuous process that depends on the binding energies of the actual proton & neutron bound states in the residual nucleus.

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Table of Contents

Chapter 1 Introduction

When two clusters of nucleons approach each other, they may interact in several ways. The primary interaction results from the inter-nucleon two-body force, which has an average effect found by folding over the internal states of the two clusters. The clusters move in the folded potential subject to the Pauli Principle, and as they move they may be excited internally, and nucleons may be transferred from one cluster to the other. The purpose of the present work is to investigate how the Pauli Principle, inelastic excitations, transfer reactions, and their multi-step combinations may all be satisfactorily included in a model of a simple cluster reaction : the reaction of the simplest cluster, the deuteron, with another cluster of arbitary size.

Deuteron stripping reactions have traditionally been important in nuclear spectroscopy for determining the quantum numbers and spectroscopic factors of single-particle states that can be filled by transferring a proton or a neutron from an incident deuteron. Spectroscopic factors for these states are found by using the observed cross-sections to normalise a theoretical calculation of the reaction rates. The calculations generally use the plane-wave or the distorted-wave Born approximations (PWBA or DWBA), which are easy to perform and widely used.

These first-order Born approximations can however be extended, to accurately model multi-stage processes involving e.g. inelastic cluster excitations. For in certain resonance reactions, the excited states occur with large amplitude and form an essential 'doorway state' in the reaction path. In these and other cases where strong

couplings are evident, to obtain accurate predictions the DWBA etc. must in general be replaced by the Coupled Channels method, which takes into account all orders of interactions and accurately handles couplings of arbitary strengths.

The Coupled Channels method has been extended to include all transfer channels as well as the inelastic doorway states, and thus can model all the processes outlined in Figure 1.1 . Note that the model naturally includes two- and higher-step reactions, and also the exact reverse couplings physically necessary.

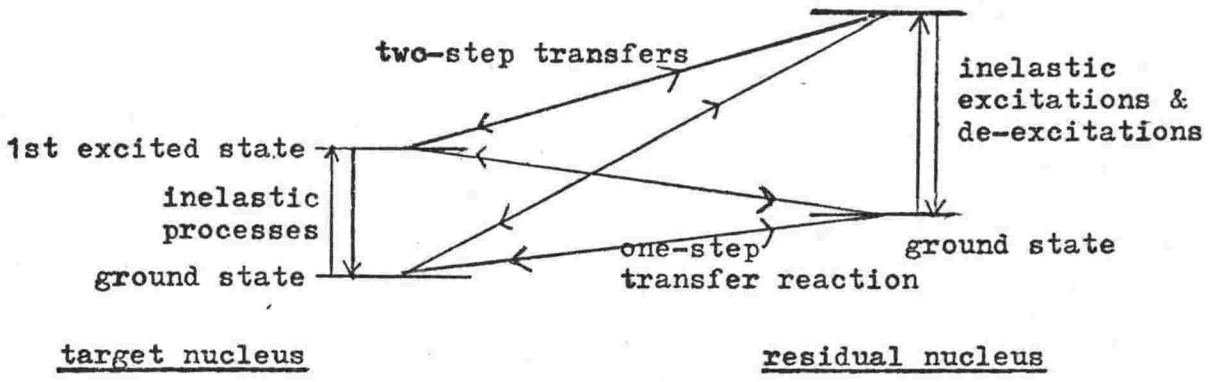


Figure 1.1

When the transfer channels are included however, the complication arises that the reaction channels are no longer orthogonal to each other in the internal region. The present work is concerned primarily with finding satisfactory treatments of the Pauli Principle and the non-orthogonality problems within the Coupled Channels framework.

In the thesis, chapters 2 & 3 are largely summary chapters that deal respectively with the standard Coupled Channels formalism, and with the single-particle scattering theory that includes the Pauli Principle. In both cases a number of minor extensions are presented. Chapter 2 begins with the usual application of the coupled channels procedure to deuteron stripping: in particular to neutron-transfer reactions of deuterons on a target nucleus that can be inelastically excited to a quadrupole excited state. Sections 2.5 & 2.6 then extend the basic formalism to take into account (a) orthogonality conditions on the radial wave functions, and (b) non-local potentials, both of which will arise in later chapters.

Chapter 3 gives a summary of Feshbach's Unified Reaction Theory (see Feshbach, 1968) applied to the scattering of single nucleons by nuclei, when the Pauli Principle (i.e. antisymmetrisation) is taken into account. Later sections extend the theory to allow for configuration mixing in the core, and also its inelastic excitation. Similar techniques have already been used to find energy eigenstates of the nucleon-plus-nucleus system: see for example Friedman(1967)

Chapter 4 extends the Feshbach theory again to model deuteron - nucleus interactions, the simplest cluster - nucleus interaction. In this case the magnitude of the antisymmetrisation effects is particularly important at low scattering energies (e.g. several Mev.), where it is clear from the simple model of section 4.1 that they should be much more significant. Döhnert(1971) does some preliminary analysis with realistic wave functions, while Buck, Friedrich & Wheatley(1977) have recently proposed a 'symmetric $(1-K)^{\frac{1}{2}}$ ansatz' for the effective Hamiltonian for the relative wave function between the

clusters, and give several justifications for it. In chapter 4 an alternative approach is used to derive the $(1-K)^{\frac{1}{2}}$ approximation in a semi-rigorous manner for the specific cluster reaction of deuterons on nuclei, and to investigate in detail the assumptions sufficient for the result. The chapter uses the proton & neutron operators $1-K_p$ & $1-K_n$ (derived e.g. from the standard theory of chapter 3) to derive a $1-K_d$ operator for the deuteron-nucleus relative wave function. It will be seen that the effects of the 1-K operators of both kinds may be split into two parts: the projecting out of fully-blocked components, and secondly the renormalisation by $(1-K)^{-\frac{1}{2}}$ of partially-blocked components of the relative wave function. It is shown that with certain assumptions, the same split may be made in the antisymmetrised Hamiltonian too. This enables all the renormalising effects to merely renormalise the wave function by $(1-K)^{-\frac{1}{2}}$, so that only the projection-operator effects remain in the final channel equations.

The proper inclusion of transfer channels in the coupled channels framework is next considered. Although recent work (see e.g. Cotanch & Vincent, 1976; Udagawa et al,1973; Goldfarb & Takeuchi,1972 & 1974; and Döhnert, 1971) has questioned the assumption, most models of transfer reactions have assumed that the deuteron and transfer channels have internal states that are mutually orthogonal. If this were so, the transfer coupling would involve only the $\mathcal{V}_f$ part of the Hamiltonian, and there would be no coupling terms involving the kinetic energy operators or the optical potentials. In fact, as is shown in chapter 5, the states are <u>not</u> orthogonal, principally because the internal states of the two kinds of channels are defined with different coordinates and are eigenstates of different partitions of the Hamiltonian.

Chapter 5 is devoted to the non-orthogonality problem. An analogy is found between the non-orthogonality of the internal states and the non-orthogonality of two non-perpendicular vectors in the plane, and a number of proposals for redefining internal states are illustrated on this basis. One such proposal is found to be suitable for further development: one in which the internal state of the proton's exit channel is kept unchanged, and used to orthogonalise the internal state of the deuteron channel. The process may be repeated for multiple exit channels, and the orthogonalised deuteron state may or may not be renormalised. This method is used because it gives cumulative effects when one deuteron channel is orthogonalised to many transfer channels. Reaction calculations are typically of that form, but in any case it is here that significant consequences may be expected. This is illustrated numerically for deuteron reaction on ^{12}C leading to many $p + {}^{13}C^*$ transfer channels.

Chapter 6 brings together the treatments of antisymmetrisation and of non-orthogonalities of chapters 4 & 5 respectively. We see here that the full advantage is brought out of the method of orthogonalising chosen in chapter 5. For now we find that this orthogonalising reallocates the wave function in the reaction region from the deuteron channels to the transfer channels, taking components from the deuteron channels in ways exactly additive to the way the antisymmetrisation requirements remove blocked deuteron-core components. Further, when <u>all</u> possible transfer channels are included, along with all Pauli blockings from core nucleons, then at low energies the deuteron channel is fully blocked in the internal region, leaving the deuteron as a bound state to be significant only asymptotically. In this limit, the exact non-local potential governing the deuteron channel

simplifies dramatically in one approximation to be replaceable by just several orthogonality conditions on the relative wave function, and these can be modelled easily when solving the radial coupled channel equations as explained in section 2.5 . This simplification is examined numerically again with respect to the $^{12}C(d,p)^{13}C^*$ set of reactions.

Finally, some general observations are made concerning the importance of the the Pauli Principle and non-orthogonality effects in a wider range of reaction calculations.

Chapter 2 Systems of Coupled Channels

In this chapter we present the usual coupled channel theory for the elastic and inelastic scattering of two clusters, and also include the transfer channels on an equal footing. In this procedure the channels' internal wave functions are assumed to be orthogonal, and a set of coupled differential equations involving local potentials is obtained.

In section 2.1 we give the approximations required to obtain the standard coupled channel (CC) equations when the channel wave functions define the interacting clusters. Section 2.2 presents the Hamiltonian in a form which may be partitioned according to the various channels, and which also permits the usual folding procedure to be used to obtain the distorting potential for the channel clusters. In section 2.3 the radial equations are presented, which are obtained by the usual procedure of substituting the total wave function into Schrödinger's equation $H\Psi = E\Psi$, and using the internal 'angular' channel wave functions as projection operators which are here assumed to be mutually orthogonal. (In chapter 5 we do not assume this orthogonality, and are led to non-local terms in the CC equations.) We present in section 2.4 the results of a numerical calculation for a particular reaction which includes the reverse coupling of the transfer channels to the incoming (deuteron) channels. We compare our results with the earlier CCBA, and will use this CC model in investigating the effects of taking the non-orthogonality and antisymmetrisation terms into account.

In the final sections 2.5 & 2.6 we first present the mathematical methods which will be used latter to enforce orthogonality between radial scattering wave functions and other bound radial functions, and then we find methods to deal with non-local terms.

2.1 Coupled deuteron and transfer channels

In later chapters the reactions of deuterons on ^{12}C nuclei will be used as a test case to determine the validity of certain approximations and the size of several effects concerning the assumptions listed below. Several deuteron reactions will be modelled: elastic scattering; inelastic scattering with the excitation of the $^{12}C_{0^+}$ core to its 2^+ state at 4.43 Mev, and neutron-transfer reactions leading to a proton and a ^{13}C (= ^{12}C + n) residual nucleus. All these possible reactions channels will be considered not as small perturbations of the incoming deuteron channel, but on an equal footing with it. This is done using a standard coupled-channels (CC) formalism, which solves for all channels simultaneously, and effectively includes all orders of perturbations.

For the sake of completeness, this section gives the detailed channel equations of the CC system. As outlined in chapter 1, however, the standard CC approach ignores effects such as

1) Pauli Principle effects between the core and scattering nucleons,
2) the non-orthogonality of the transfer channels to each other, which strictly should generate further coupling terms between them,
3) polarisation of the deuteron as it approaches the charged target nucleus
4) deuteron break-up reactions (d,np) giving 3-body final states.

The aim of the present work is to try to remedy the first two shortcomings within the CC framework, and indirectly the third. Other approaches (Farrell et al. 1976, & Eppel et al. 1978) must be used to model break-up reactions.

The total wavefunction for the chosen model contains two kinds of channels (i) deuterons around the target nucleus A (^{12}C here), and (ii) protons around the residual nucleus B = A + n (^{13}C here). These two kinds have wavefunctions of the forms $u_d(\underline{R})\ \phi_d(\underline{r})\ \phi_A(\underline{r}_1,..,\underline{r}_A)$ and $u_p(\underline{r}_p)\ \phi_B(\underline{r}_n,\underline{r}_1,\ ..\ ,\underline{r}_A)$ respectively, where

$\phi_A(\underline{r}_1,\ ..\ ,\underline{r}_A)$ is the wavefunction of the target nucleus of A nucleons

$\phi_B(\underline{r}_n,\underline{r}_1,\ ,\underline{r}_A)$ is the state of the residual nucleus B = A + neutron

$\phi_d(\underline{r})$ is the internal deuteron state

$u_d(\underline{R})$ is the relative deuteron-target wavefunction

& $u_p(\underline{r}_p)$ is the relative proton-residual nucleus wavefunction,

and where

$\underline{r}_1\ ..\ \underline{r}_A$ are the coordinates of the A nucleons of the target A relative to the centre-of-mass of A

$\underline{r}_n$ is coord. of the neutron relative to the cm. of A

$\underline{r}_p$ is coord. of the proton relative to the cm. of nucleus B

$\underline{R}$ is coord. of the cm. of the deuteron relative to the A cm.

$\underline{r}$ is coord. of the proton relative to the neutron position.

When the states ϕ_A to u_p are expanded in terms of angular momentum eigenfunctions, the full model space has two kinds of sums over angular-momentum quantum numbers. In the entrance channel the chosen model allows for excitation of the target nucleus A, to various states $\phi_I(\underline{r}_1,\ ..,\underline{r}_A)$, by an incoming deuteron in state $(L_a s_a)J_a$ where the deuteron spin is s_a=1. In the exit channel it allows for an outgoing proton in state $(L_b s_b)J_b$ (proton spin $s_b=\frac{1}{2}$) and a residual nucleus B in state 'n' with total angular momentum J_B. Its states $\phi^{M_B}_{J_B}(\underline{r}_n,\underline{r}_1,..,\underline{r}_A)$ are expanded as sums of neutron-plus-target states with coefficients of fractional

parentage $A^{jIJ_B n}_{lsj}$ describing the amplitude of neutron single-particle state $(ls)j$ (neutron spin $s = \frac{1}{2}$) with target state I in the final B-state number n with angular momentum J_B.

The overall Ψ-field for total angular momentum J with z-component M is now written in the model form

$$\Psi^{JM} = \sum_{\substack{I\mu \\ L_a M_a m_a J_a}} \psi^{m_a}_{s_a}(\underline{d})\ \psi^{o}_{d}(\underline{r})\ \phi^{\mu}_{I}(\underline{r}_1 \cdots \underline{r}_A)\ i^{L_a}\ Y^{M_a}_{L_a}(\hat{\underline{R}}) \cdot C^{L_a s_a J_a}_{M_a m_a M_a + m_a} \cdot C^{J_a\ I\ J}_{M_a + m_a\ \mu M} \cdot \frac{1}{R} f^{J}_{(L_a s_a) J_a I}(R)$$

$$+ \sum_{\substack{J_B M_B n \\ L_b M_b m_b J_b}} \psi^{m_b}_{s_b}(\underline{p})\ \phi^{M_B}_{J_B n}(\underline{r}_n, \underline{r}_1, \ldots)\ i^{L_b}\ Y^{M_b}_{L_b}(\hat{\underline{r}}_p) \frac{1}{r_p} g^{J}_{(L_b s_b) J_b J_B n}(r_p) \cdot C^{L_b s_b J_b}_{M_b m_b M_b + m_b} \cdot C^{J_b\ J_B\ J}_{M_b + m_b\ M_B M} \qquad (1)$$

where

$$\phi^{M_B}_{J_B n}(\underline{r}_n, \underline{r}_1, \ldots) = \sum_{\substack{ljI \\ \mu}} A^{jIJ_B n}_{lsj}\ C^{j\ I\ J_B}_{M_B - \mu\ \mu M_B}\ \phi^{\mu}_{I}(\underline{r}_1, \ldots)\ \chi^{M_B - \mu}_{lj}(\underline{r}_n), \qquad (2)$$

$$\chi^{m}_{lj}(\underline{r}_n) = \sum_{m'} C^{l\ s\ j}_{m\ m-m'\ m}\ i^{l}\ Y^{m'}_{l}(\hat{\underline{r}}_n)\ \psi^{m-m'}_{s}(\underline{n})\ R_{lsj}(r_n), \text{ and} \qquad (3)$$

$$\psi^{o}_{d}(\underline{r}) = \frac{1}{(4\pi)^{\frac{1}{2}}} \phi_d(r), \qquad (4)$$

assuming that the internal deuteron wave function is completely that of an s-state.

2.2 Hamiltonian Partitions

Let 'H' be the Hamiltonian for the full system of a proton at $\underline{r}_p$, a neutron at $\underline{r}_n$, and a target nucleus consisting of 'Z' protons and 'N' neutrons at r_{p_j}, $j=1,..,Z$ & r_{n_i}, $i=1,..,N$ respectively, with $N + Z = A$. In terms of the three internucleon potentials V_{pp}, V_{nn}, & $V_{pn}=V_{np}$, and with T_p & T_n the kinetic energy operators for a proton & neutron respectively, H may be written as

$$\begin{aligned} H = {} & T_p(r_p) + T_n(r_n) + V_{pn}(r_p,r_n) \\ & + \left[\sum_j^Z V_{pp}(r_p,r_{p_j}) + \sum_i^N V_{pn}(r_p,r_{n_i}) \right] \\ & + \left[\sum_j^Z V_{pn}(r_{p_j},r_n) + \sum_i^N V_{nn}(r_n,r_{n_i}) \right] \\ & + H_A \end{aligned} \tag{5}$$

where H_A is the Hamiltonian for the nucleus 'A' :

$$\begin{aligned} H_A = {} & \sum_i^N \left[T_n(r_{n_i}) + \tfrac{1}{2} \sum_{k\neq i}^N V_{nn}(r_{n_i},r_{n_k}) \right] \\ & + \sum_j^Z \left[T_p(r_{p_j}) + \tfrac{1}{2} \sum_{l\neq j}^Z V_{pp}(r_{p_j},r_{p_l}) \right] \\ & + \sum_i^N \sum_j^Z V_{pn}(r_{p_j},r_{n_i}) \ . \end{aligned} \tag{6}$$

The nucleus states ϕ_I^μ are eigenstates of H_A for energies e_I :

$$H_A \phi_I^\mu = e_I \phi_I^\mu . \tag{7}$$

The external nucleons at $\underline{r}_p$ & $\underline{r}_n$ experience a collective potential from all the core nucleons. This potential is customarily divided into two parts, called the 'folded potential' and the 'inelastic excitation potential', that respectively are diagonal for, and couple, different internal states of the nucleus ϕ_I for distinct quantum numbers 'I'. The collective potential of the core nucleons in their state $\phi_I(r_1,..,r_A)$ is most conveniently derived in terms of the one-particle density operators $\rho_1^{II'} \equiv K^{II'}(r,r')$ for the protons &

neutrons separately : $K_p^{II'}$ & $K_n^{II'}$ where

$$K_p^{II'}(r_p,r_p') = \langle \phi_{I'}(r_p',r_{p_2},\ldots,r_{n_1},\ldots) | \phi_I(r_p,r_{p_2},\ldots,r_{n_1},\ldots)\rangle$$
$$\text{and} \quad K_n^{II'}(r_n,r_n') = \langle \phi_{I'}(r_{p_1},\ldots,r_n,r_{n_2},\ldots) | \phi_I(r_{p_1},\ldots,r_n',r_{n_2},\ldots)\rangle \quad . \tag{8}$$

Ignoring antisymmetrisation, which is to be treated in Chapters 3 & 4, the two parts of the collective potential may now be written

$$\begin{aligned} & V_p^I(\underline{r}_p)\,\delta_{II'} + V_p^{ex}(\underline{r}_p,I,I') \\ &= \mathrm{Tr}_n(V_{pn}(\underline{r}_p,)\,K_n^{II'}) + \mathrm{Tr}_{p'}(V_{pp}(\underline{r}_p,\underline{r}_p')\,K_p^{II'}(\underline{r}_p',\underline{r}_p')) \\ &= \int V_{pn}(\underline{r}_p,\underline{r}_n)\,K_n^{II'}(\underline{r}_n,\underline{r}_n)\,d\underline{r}_n \\ &\quad + \int V_{pp}(\underline{r}_p,\underline{r}_p')\,K_p^{II'}(\underline{r}_p',\underline{r}_p')\,d\underline{r}_p' \quad , \text{ expanding the Trace operators.} \end{aligned} \tag{9}$$

and

$$\begin{aligned} & V_n^I(\underline{r}_n)\,\delta_{II'} + V_n^{ex}(\underline{r}_n,I,I') \\ &= \mathrm{Tr}_p(V_{pn}(,\underline{r}_n)\,K_p^{II'}) + \mathrm{Tr}_{n'}(V_{nn}(\underline{r}_n,\underline{r}_n')\,K_n^{II'}(\underline{r}_n',\underline{r}_n')\,). \end{aligned} \tag{10}$$

Using these definitions, the potentials and couplings of H between two target states ϕ_I & $\phi_{I'}$, (fixed and presumed known) are the 'matrix elements' of H : $H_2^{II'} = \langle \phi_{I'} | H | \phi_I \rangle$ that are still functions of the 2 variables $\underline{r}_p$ & $\underline{r}_n$:

$$\begin{aligned} H_2^{II'} = & \left[T_p(\underline{r}_p)+V_p^I(\underline{r}_p) + T_n(\underline{r}_n)+V_n^I(\underline{r}_n) + V_{np}(\underline{r}_p-\underline{r}_n) + e_I \right] \delta_{II'} \\ & + V_p^{ex}(\underline{r}_p,I,I') + V_n^{ex}(\underline{r}_n,I,I') \end{aligned} \tag{11}$$

The above expression for H_2 is called the 'post' form, H_f, of the Hamiltonian, as it is most naturally suited to the outgoing proton channels in a (d,p) reaction, when the proton and neutron move largely independently. In the deuteron channels, the proton and neutron by

contrast are most frequently in the specific relative state $\phi_d(\underline{r})$. Now the kinetic energy operators $T_p + T_n$ can be rearranged to equal $T_d + T_{di}$, where $T_{di}(\underline{r})$ is the kinetic energy internal to the proton - neutron pair, and $T_d(\underline{R})$ is the kintic energy of the deuteron cluster relative to the target cluster. The Hamiltonian is then nearer its 'prior' form H_i :

$$H_i = \left(T_d(\underline{R}) + V_p^I(\underline{r}_p) + V_n^I(\underline{r}_n) + T_{di}(\underline{r}) + V_{np}(\underline{r}) + e_I\right)\delta_{II'} + V_d^{ex} \qquad (12)$$

where

$$V_d^{ex} = V_p^{ex} + V_n^{ex}.$$

The deuteron internal state $\phi_d(\underline{r})$ is an eigenfunction of the part Hamiltonian $T_{di} + V_{np}$,

$$\left(T_{di}(\underline{r}) + V_{np}(\underline{r})\right)\phi_d(\underline{r}) = e_d\ \phi_d(\underline{r}) \qquad (13)$$

for eigen-energy $e_d = -2.226$ Mev.

The states $\phi_{J_B n}$ of the residual nucleus 'B' are eigenstates at energies $e_{J_B n}$ of the part Hamiltonian $H_B(\underline{r}_n, \underline{r}_1, \ldots, \underline{r}_A)$ composed of the T_n kinetic energy operator, the folded and excitation potentials for the neutron, along with the core Hamiltonian H_A:

$$H_B = T_n(\underline{r}_n) + \sum_{j=1}^{Z} V_{pn}(\underline{r}_{p_j}, \underline{r}_n) + \sum_{i=1}^{N} V_{nn}(\underline{r}_n, \underline{r}_{n_i}) + H_A .$$

It is now usual to define averaged potentials, first for the deuteron-core interaction by averaging ('folding') over the deuteron's internal state ϕ_d:

$$W_d(\underline{R}) = \int \phi_d(\underline{r})^* \; (V_p(\underline{r}_p(\underline{R},\underline{r})) + V_n(\underline{r}_n(\underline{R},\underline{r})) \; \phi_d(\underline{r}) \quad d\underline{r} \; , \tag{14}$$

and secondly for the proton - residual-nucleus (B), by summing the proton-core potential V_p with an averaged effect from the extra neutron:

$$W_p^{J_B n}(\underline{r}_p) = V_p(\underline{r}_p) + \iint |\phi_{J_B n}(\underline{r}_n,\underline{r}_1,..)|^2 \; V_{np}(\underline{r}_p-\underline{r}_n) \; d\underline{r}_n \; d\underline{r}_1 \; .. \tag{15}$$

We now rearrange the post and prior Hamiltonians to

$$H_i = T_d(\underline{R})+W_d(\underline{R}) + T_{di}(\underline{r})+V_{np}(\underline{r}) + \mathcal{V}_i(\underline{R},\underline{r}) + V_d^{ex} + H_A \tag{16}$$

$$\text{defining } \mathcal{V}_i(\underline{R},\underline{r}) = V_p(\underline{r}_p) + V_n(\underline{r}_n) - W_d(\underline{R}), \tag{17}$$

$$= H_d(\underline{R}) + H_{di}(\underline{r}) + \mathcal{V}_i(\underline{R},\underline{r}) + V_d^{ex} + H_A \; , \text{ defining } H_d \; \& \; H_{di} \tag{18}$$

$$\& \; H_f = T_p(\underline{r}_p)+W_p(\underline{r}_p) + T_n(\underline{r}_n)+V_n(\underline{r}_n)+V_n^{ex}+H_A + \mathcal{V}_f(\underline{r}_p,\underline{r}_n) + V_p^{ex} \tag{19}$$

$$= H_p(\underline{r}_p) + H_B(\underline{r}_n,\underline{r}_1,..) + {}_f(\underline{r}_p,\underline{r}_n) + V_p^{ex}$$

$$\text{where} \quad \mathcal{V}_f(\underline{r}_p,\underline{r}_n) = V_{np}(\underline{r}_p-\underline{r}_n) + V_p(\underline{r}_p) - W_p(\underline{r}_p) \tag{20}$$

The only terms depending on more than one channel variable (ie. on both $\underline{R}$ and $\underline{r}_p$) are $\mathcal{V}_i$ and $\mathcal{V}_f$, and they couple the incoming and transfer channels. Compared with $\mathcal{V}_i$, however, $\mathcal{V}_f$ is much simpler and more convenient to use, in that for (d,p) reactions, most of $\mathcal{V}_f$ can be replaced by V_{np}, 'about which we presume to have some knowledge,' as in, for example, the zero-range approximation

$$V_{np}(\underline{r}) = + D_o \; / \; \phi_d(\underline{0}) \; . \; \delta(\underline{r}) \; , \text{ with } D_o = -122.5 \text{ Mev.fm}^{\frac{3}{2}}$$

from for example McCarthy, 1968, section 13 A(iii).

2.3 Coupled Radial Equations

The channel equations for the deuteron radial wavefunctions $f^J_{(L_a s_a)J_a I}(R)$ are therefore in detail

$$\left[\frac{-1}{.0478\mu_d}\frac{d^2}{dR^2} + V^d_{opt}(R) + \frac{L_a(L_a+1)}{.0478\mu_d R^2} - E_{d_I}\right] f^J_{(L_a s_a)J_a I}(R)$$

$$+ \sum_{L'_a J'_a I'} V^{J\ (d-ex)}_{(L_a s_a)J_a I:(L'_a s_a)J'_a I'} \cdot F_d(R) \cdot f^J_{(L'_a s_a)J'_a I'}(R)$$

$$+ \sum_{L_b J_b J_B n} V^{J\ (dp)}_{(L_a s_a)J_a I : (L_b s_b)J_b J_B n}(R) \cdot \left(\frac{M_B}{M_A}\right)^{-\frac{1}{2}} \cdot g^J_{(L_b s_b)J_b J_B n}\left(\frac{M_A}{M_B} R\right) = 0 \qquad (21)$$

where $\mu_d = \frac{m_d \cdot M_A}{M_A + m_d}$, m_d = mass of deuteron, M_A = mass of target A in amu,

$V^d_{opt} = V^d_{nucl} + V^d_{coul} + V^{d(L_a s_a)Ja}_{spin\text{-}orbit}$ in Mev.

$V^d_{nucl} = -V_{od}/(1+\exp\frac{1}{a}(R-R_o A^{\frac{1}{3}})) \equiv -V_{od}/E_d(R)$, the Saxon-Woods form,

and $F_d(R) = (E_d(R)-1) \cdot E_d(R)^{-2}$ is the inelastic-excitation form factor.

The couplings are

$$V^{J\ (d-ex)}_{(L_a s_a)J_a I : (L'_a s_a)J'_a I'} \cdot F_d(R) \qquad \text{(Quadrupole core excitation Q=2)}$$

$$= F_d(R) \cdot i^{Q+L'_a-L_a} \cdot i^{Q+I'-I} \cdot (4\pi)^{-\frac{1}{2}} \hat{I}\,\hat{I}'$$
$$\cdot (IOI'0|QO) \cdot (L_a O L'_a 0|QO)$$
$$\cdot \hat{J}_a \hat{J}'_a \hat{L}_a \hat{L}'_a \; W(L_a J_a L'_a J'_a; s_a Q) \cdot W(I J_a I' J'_a; JQ)$$
$$\cdot (-1)^{-J+s_a+I+L_a+L'_a}$$
$$\cdot \beta \cdot R_o A^{\frac{1}{3}} \cdot (-V_{od}) \,/\, (a \cdot 5^{\frac{1}{2}}) \qquad (22)$$

where the excitatory effect of the deuteron is now assumed to be that from a single particle of unit charge and mass 2 amu, so

$$V^{ex}_d(\underline{R},I,I') = \sum_{\substack{q \\ Q=2}} T^q_Q(\hat{\underline{R}})^* \, i^2 \frac{\beta R_o A^{\frac{1}{3}}(-V_{od})}{a} F_d(R) \langle \phi_{I'} | D^2_{qo} | \phi_I \rangle \qquad (23)$$

with β = deformation parameter of nucleus 'A'.

The couplings $V^{J\ (dp)}$ are the d-p transfer couplings, here derived from the zero-range approximation $\mathcal{V}_f \doteq V_{np}(\underline{r}) \doteq D_o\,\delta(\underline{r}) \,/\, \phi(\underline{0})$:

$$V^{J\ (dp)}_{(L_a s_a)J_a I\ :\ (L_b s_b)J_b J_B n}(R)$$

$$= \sum_{lj} D_o\ \hat{J}_B\ \hat{J}_a\ W(IjJJ_b;\ J_B J_a)\ .\ \begin{bmatrix} L_b & s_b & J_b \\ l & s & j \\ L_a & s_a & J_a \end{bmatrix}$$

$$\cdot\ A^{jIJ_B n}_{lsj}\ \ i^{l+L_b-L_a}\ \ (4\pi)^{-\frac{1}{2}}\ \hat{l}\ \hat{L}_b\ (-1)^{L_b-l}\ \begin{pmatrix} l & L_a & L_b \\ 0 & 0 & 0 \end{pmatrix}\ R_{lsj}(R) \qquad (24)$$

The proton radial wavefunctions $g^J_{(L_b s_b)J_b J_B n}(r_p)$ satisfy the channel equations

$$\left[\frac{-1}{.0478\mu_p}\frac{d^2}{dr_p^2} + V^p_{opt}(r_p) + \frac{L_b(L_b+1)}{.0478\mu_p r_p^2} - E_{p\,J_B n}\right] g^J_{(L_b s_b)J_b J_B n}(r_p)$$

$$+ \sum_{L_a J_a I} V^{J\ (dp)}_{(L_b s_b)J_b J_B n\ :\ (L_a s_a)J_a I}(r_p)\ \cdot\ \left(\frac{M_A}{M_B}\right)^{-\frac{1}{2}}\cdot\ f^J_{(L_a s_a)J_a I}\left(\frac{M_B}{M_A}\, r_p\right)$$

$$+ \sum_{L'_b J'_b J'_B n'} V^{J\ (p\text{-}ex)}_{(L_b s_b)J_b J_B n\ :\ (L'_b s_b)J'_b J'_B n'}\ \ g^J_{(L'_b s_b)J'_b J'_B n'}(r_p)$$

$$+ \sum_{L'_b J'_b J'_B n'} V^{J\ (Vnp)}_{(L_b s_b)J_b J_B n\ :\ (L'_b s'_b)J'_b J'_B n'}\ \ g^J_{(L'_b s'_b)J'_b J'_B n'}(r_p) \ = \ 0 \qquad (25)$$

where $\mu_p = \dfrac{m_p \cdot M_B}{M_B + m_p}$, m_p = mass of proton, M_B = mass of residual nucleus B

$V^p_{opt}(r_p)$ = proton - B optical potential with the usual nuclear, Coulomb, spin-orbit & imaginary absorbtion terms.

The three couplings V^J: dp, p-ex, & Vnp are respectively

(a) $V^{J\ (dp)}_{\#b\ :\ \#a} = V^{J\ (dp)}_{\#a\ :\ \#b}$ from above : the transfer coupling is symmetric

(b) The p-p' coupling caused by excitation of the core A, with the neutron as a passive bystander:

$$V^{J\ (p\text{-}ex)}_{(L_b s_b)J_b J_B n\ :\ (L'_b s_b)J'_b J'_B n'}(r_p)$$

$$= \sum_{\substack{lj \\ I\ I'\ J_c}} A^{jIJ_B n}_{lsj}\ A^{jI'J'_B n'}_{lsj}\ \hat{J}_B\ \hat{J}_c\ W(jIJJ_b;\ J_B J_c)\ \hat{J}'_B\ \hat{J}_c\ W(jI'JJ'_b;\ J'_B J_c)$$

$$\cdot\ (-1)^{J_B + J'_B - I - I' - 2J_c}$$

$$\cdot\ V^{J_c\ (d\text{-}ex)}_{(L_b s_b)J_b I\ :\ (L'_b s_b)J'_b I'}$$

$$\cdot\ F_p(r_p)$$ except with $R_o A$, V_{od}, & a replaced by the parameters of the <u>proton's</u> optical potential. (26)

(c) The p-p' coupling between proton channels caused by the $V_{np}(r_p - r_n)$ potential between an outgoing proton and a bound neutron. The proton and neutron can scatter off each other; the core is a passive bystander. In the zero-range approximation, $V^{J\ (Vnp)}$ is

$$V^{J\ (Vnp)}_{(L_b s_b)J_b J_B n\ :\ (L'_b s_b)J'_b J'_B n'}(r_p)$$

$$= \frac{D_o}{\phi_d(0)} \sum_{lj\ l'j'} R_{lsj}(r_p)^*\ R_{l'sj'}(r_p)\ \cdot\ i^{L_b + l - L'_b - l'}$$

$$\cdot \sum_{L\ S\ J_a} \frac{\hat{L}_b \hat{L}'_b \hat{l}\ \hat{l}'}{4\pi} \begin{pmatrix} L_b & l & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L'_b & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{bmatrix} L_b & l & L \\ s_b & s & S \\ J_b & j & J_a \end{bmatrix} \begin{bmatrix} L'_b & l' & L \\ s_b & s & S \\ J'_b & j' & J_a \end{bmatrix}$$

$$\cdot \sum_{I} A^{jIJ_B n}_{lsj}\ A^{j'\ I\ J'_B n'}_{l'sj'}\ \hat{J}_B\ \hat{J}_a\ W(IjJJ_b;\ J_B J_a)$$

$$\cdot\ \hat{J}'_B\ \hat{J}_a\ W(Ij'JJ'_b;\ J'_B J_a) \qquad (27)$$

The asymptotic boundary conditions for the radial functions are, as R & r_p become large,

$$f^J_{(L_a s_a)J_a I}(R) \rightarrow \tfrac{1}{2}i\,\delta(L_a J_a I, L^i_a J^i_a I^i) \left[G_{L_a}(k_I R) - iF_{L_a}(k_I R) \right]$$

$$-\tfrac{1}{2}iS^J_{(L_a s_a)J_a I} \left[G_{L_a}(k_I R) + iF_{L_a}(k_I R) \right] \qquad (28)$$

where $L^i_a J^i_a I^i$ specify the incoming channel,

$$k_I^2 = .0478\ \mu_d\ E_{d_I},$$

and 'S' is the S-matrix element for $L_a^i J_a^i I^i \rightarrow L_a J_a I$ scattering. The proton radial wavefunction becomes

$$g^J_{(L_b s_b) J_b J_B n}(r_p) \rightarrow \begin{cases} -\frac{1}{2}i\ S^J_{L_a^i J_a^i I^i : L_b J_b J_B n} \left[G_{L_b}(k_{J_B n} r_p) + i F_{L_b}(k_{J_B n} r_p) \right] \\ \qquad \text{for scattering } E_{p J_B n} > 0 \\ \frac{1}{2}\ S^J_{L_b J_b J_B n}\ W_{L_b}(|k_{J_B n}| r_p) \\ \qquad \text{for bound states } E_{p J_B n} < 0. \end{cases} \tag{29}$$

The transfer cross-sections for a spin-zero target ($I^i=0$) are

$$\frac{d\sigma_n}{d\Omega} = \frac{1}{2s_a+1} \sum_{m_a M_b M_B} |f^{m_b M_B n}_{m_a}(\theta)|^2 \tag{30}$$

with $$f^{m_b M_B n}_{m_a}(\theta) = \frac{4\pi}{k_I^2 i} \sum_{\substack{J_a^i L_a^i \\ M_a = 0}} e^{i\sigma_{L_a^i}(k_I i)} \left(\frac{2L_a^i+1}{4\pi}\right)^{\frac{1}{2}} (L_a^i M_a s_a m_a | J_a^i\ M_a+m_a)$$

$$\sum_{L_b J_b} (L_b M_b s_b m_b | J_b M_a+m_a-M_B)\ (J_b M_a+m_a-M_B\ J_B M_B | J_a^i M_a+m_a$$

$$\cdot e^{i\sigma_{L_b}}\ Y^{M_b}_{L_b}(\theta,0)\ \frac{1}{2i}\ S^J_{L_a^i J_a^i I_a^i : L_b J_b J_B n} \tag{31}$$

These channel equations have been derived assuming that the deuteron-channel internal states $\phi_d \cdot \phi_A$ are orthogonal in the region of interaction to the proton-channel internal states $\phi_{J_B n}$. They are in fact not orthogonal, and the effect of this non-orthogonality will be investigated in detail in chapter 5. In the standard coupled-channels approach, the assumption of orthogonality means that the full set of N coupled equations is of the mathematical form

$$\left[a_i \frac{d^2}{dr^2} + b_i(r) \right] f_i(r) + \sum_{j=1}^{N} V_{ij}(r)\ f_j(r) = 0,\ i=1 \ldots N,$$

with everywhere local terms $b_i(r)$ and $V_{ij}(r)$. This allows the CC system of equations to be solved directly using using the numerical integration procedure described in Buck, Stamp & Hodgson(1963).

2.4 Numerical Calculations

To determine the numerical effects of the Pauli Principle and of transfer channels, the coupled-channel formalism will be applied to the reactions of deuterons on carbon-12, allowing inelastic excitation of the target to the $^{12}C_{2+}$ state at 4.43 Mev., and neutron transfers to the lowest several states of ^{13}C, as listed in Table 2.4.1.

Particular attention is given to the deuteron resonance at an incident energy of E_d = 2.71 Mev. in the lab. frame. This resonance is believed (Stamp, 1974) to be formed as a $^{14}N_{3+}$ intermediate state, when the ^{12}C target is excited to $I = 2^+$ and the deuteron is captured into the bound $2s_1$ eigenstate of the deuteron-core collective potential. Because in this type of intermediate 'doorway state' the deuteron amplitude is very large in the reaction region, it was believed that the non-orthogonality and antisymmetrisation effects would be large. Stamp modelled this reaction by solving the coupled-channel set of elastic and inelastic deuteron channels, followed by a T-matrix calculation of transfer amplitudes from these deuteron channels: what has been called the Coupled Channels Born Approximation CCBA. One aim of the present work has been to look at the above reaction with a similar set of physical parameters to those used in Stamp(1974) - see Tables 2.4.2 to 2.4.4 - but to take into account the reverse neutron-pickup coupling (ie. the effects of the coupling $V^{J\,(dp)}$ in eqn. 2.1.24), to include deuteron - core antisymmetrisation, and to treat properly the non-orthogonality of the deuteron to the proton channels. The treatment of these second and third features is the subject of chapters 4, 5, & 6, so their effects on the differential cross-sections are determined later, and the results presented in sections 5.4 & 6.5.

Table 2.4.1

^{13}C states : their coefficients $A_{lsj}^{jIJ_Bn}$ of fractional parentage from $^{12}C_I$.

n	E_B(Mev)	J_B	^{12}C core I = 0 + neutron state : $A_{l\frac{1}{2}j}^{j0J_Bn}$	^{12}C core I = 2 +neutron state: $A_{l\frac{1}{2}j}^{j2J_Bn}$
1	0.0	$\frac{1}{2}^-$	+ $0p_{\frac{1}{2}}$: -.7090	+ $0p_{3/2}$: -.6981
				+ $0f_{5/2}$: +.1003
2	3.086	$\frac{1}{2}^+$	+ $0s_{\frac{1}{2}}$: -.9454	+ $0d_{3/2}$: .1118
				+ $0d_{5/2}$: .3062
3	3.684	$\frac{3}{2}^-$	+ $0p_{3/2}$: -.8918	+ $0p_{\frac{1}{2}}$: .2921
				+ $0p_{3/2}$: .2619
				+ $0f_{5/2}$: .0546
				+ $0f_{7/2}$: .2187
4	3.854	$\frac{5}{2}^+$	+ $0d_{5/2}$: -.9261	+ $0s_{\frac{1}{2}}$: .1410
				+ $0d_{3/2}$: .0686
				+ $0d_{5/2}$: .3433
5	6.864	$\frac{5}{2}^+$	+ $0d_{5/2}$: .0623	+ $0s_{\frac{1}{2}}$: -.8556
				+ $0d_{3/2}$: +.0324
				+ $0d_{5/2}$: .5129
6	7.68	$\frac{3}{2}^+$	+ $0d_{3/2}$: .0464	+ $0s_{\frac{1}{2}}$: -.8204
				+ $0d_{3/2}$: -.2026
				+ $0d_{5/2}$: +.5327

These coefficients were obtained by diagonalising the interaction between a neutron (moving in the potential of Table 2.4.3) and the deformed ^{12}C core (in either its I=0 ground state, or its I=2 first excited state at 4.43 Mev) with deformation $\beta = -0.4$, along the lines of Robson & Van Megen(1972b), to derive results similar to those of Barker(1961).

Table 2.4.2

Bound neutron states in ^{13}C (in Stamp 1974, from Lovas 1966)

State	Binding energy(Mev.)	Well depth -V (Mev.)	V_{ls} (Mev.)
$0s_{\frac{1}{2}}$	32.15	57.6	7.4
$0p_{3/2}$	16.68	"	"
$0p_{\frac{1}{2}}$	11.70	"	"
$0d_{5/2}$	2.19	"	"
$1s_{\frac{1}{2}}$	1.87	"	"
$0f_{5/2}$ & $3/2$	1.00	117.4	7.4

Saxon-Woods potentials with $R = 1.25\ A^{1/3}$ fm., & a = .65 fm.

Table 2.4.3

Central potentials of ^{12}C : parameters for Saxon-Woods forms

projectile	-V Mev	r_o fm	a fm	V_{ls} Mev	r_o' fm	a' fm
deuteron 'B'	113.5	0.9	0.9	5.0	0.9	0.9
'C'	116.5	0.9	1.0	5.0	0.9	0.9
proton	54.0	1.25	0.65	7.4	1.25	0.65
neutron	57.6	1.25	0.65	7.4	1.25	0.65

(No imaginary absorbtion parts were present)

Table 2.4.4 Channel coupling parameters

d-d' & p-p' coupling by rotational excitation of a deformed ^{12}C core Deformation parameter $\beta = -0.4$
d-p & p-p' coupling by $V_{np}(\underline{r})$, the proton-neutron interaction $D_o = -122.5$ Mev $fm^{3/2}$ in the zero-range approx.

The effect of first including the reverse pickup coupling is shown in Figure 2.4.1. The main effect of increasing the coupling from the proton back to the deuteron channels is to reduce and broaden the resonance peaks. The figure shows how cross-sections, at 160°, of transfer reactions from the $L_a=2$, $J_a=3$ incoming partial wave change as D_o of the reverse dp coupling terms $V^{(dp)}$ is increased from a small value of -4.0 up to the physical value of -122.5. (Potential 'C' of Table 2.4.3 gives the resonance at 3.025 not 2.71 Mev., but the mechanism is believed the same.) The limit of $D_o \rightarrow 0$ reproduces the CCBA results of Stamp's calculations, allowing for slightly different coefficients of fractional parentage. Increasing D_o is now shown to broaden the resonance and reduce its peak amplitudes. In the $^{13}C_{5/2^+}$ exit channels the curves are changed by interference with a non-resonant direct cross-section of approximately 10 mb/sr.

When D_o has its full value of -122.5 Mev $fm^{3/2}$, the resonance is so broad that to reconstruct a resonance of reasonable width, the diffuseness 'a' of the deuteron-core potential well has to be decreased from a = 1.0 fm to around a = 0.9 fm. Potential well 'B' of Table 2.4.3, with a = 0.9 fm., gives a resonance 34 kev wide (with $D_o=-122.5$), not far from the observed width of 47 kev. It is a general observation that as more inelastic channels are coupled, the diffuseness of the surface regions of both the imaginary and real parts of the optical potential have to be reduced to maintain the same overall width of, say, a resonance.

FIGURE 2·4·1

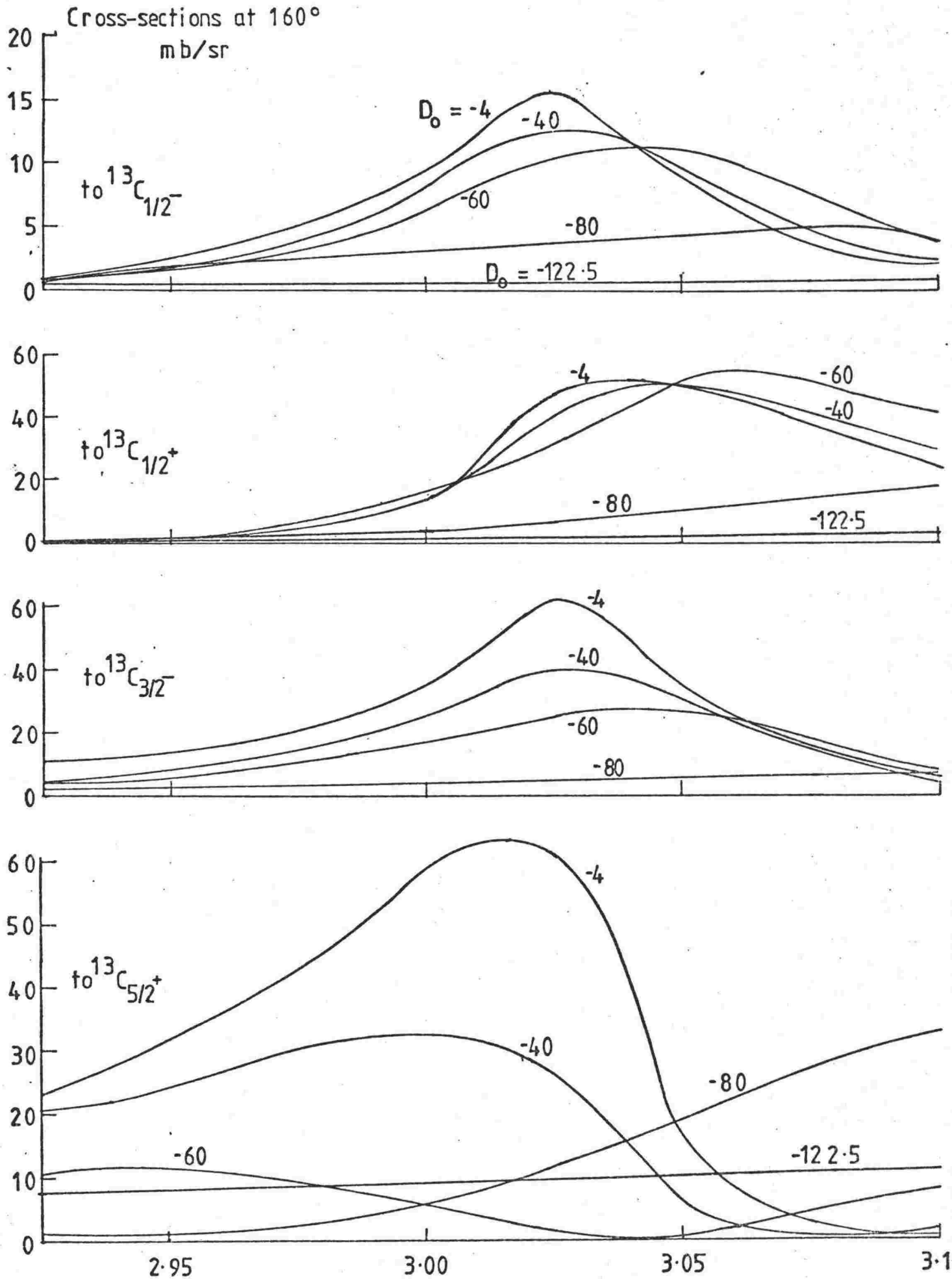

Cross-sections at 160°
mb/sr
20
15
10
5
0
D_o = -4
-40
-60
-80
D_o = -122·5
to $^{13}C_{1/2^-}$
60
40
20
0
-4
-60
-40
-80
-122·5
to $^{13}C_{1/2^+}$
60
40
20
0
-4
-40
-60
-80
to $^{13}C_{3/2^-}$
60
50
40
30
20
10
0
-4
-40
-80
-60
-122·5
to $^{13}C_{5/2^+}$
2·95
3·00
3·05
3·1
INCIDENT DEUTERON ENERGY, Mev

Figure 2.4.2 shows how the cross-sections vary across the resonance in potential 'B', again from solely the $L_a=2$ $J_a=3$ deuteron partial wave. To compare with experiment, the non-resonant contributions from other incoming partial waves have to be included. Figure 2.4.3 shows the angular distribution of the resonant cross-sections from the 9 partial waves up to & including $L_a=3$ $J_a=3$. The absorption from the two $L_a=3$ partial waves is 9.4 & 2.5 mb., so it is surmised that the higher waves not included contribute less than this. Also shown in the figure are the experimental cross-sections observed by Davison et al(1974) and Tryti et al(1975). No effort has been made to fit the experimental cross-sections by adjusting parameters of the model, and antisymmetrisation & channel-nonorthogonality effects have not yet been taken into account. The present results should be compared with those of Stamp using the CCBA. It is noted that when the reverse coupling is included, the magnitudes of all the cross-sections to the (d,p) channels are in approximate agreement with experiment.

FIGURE 2·4·2

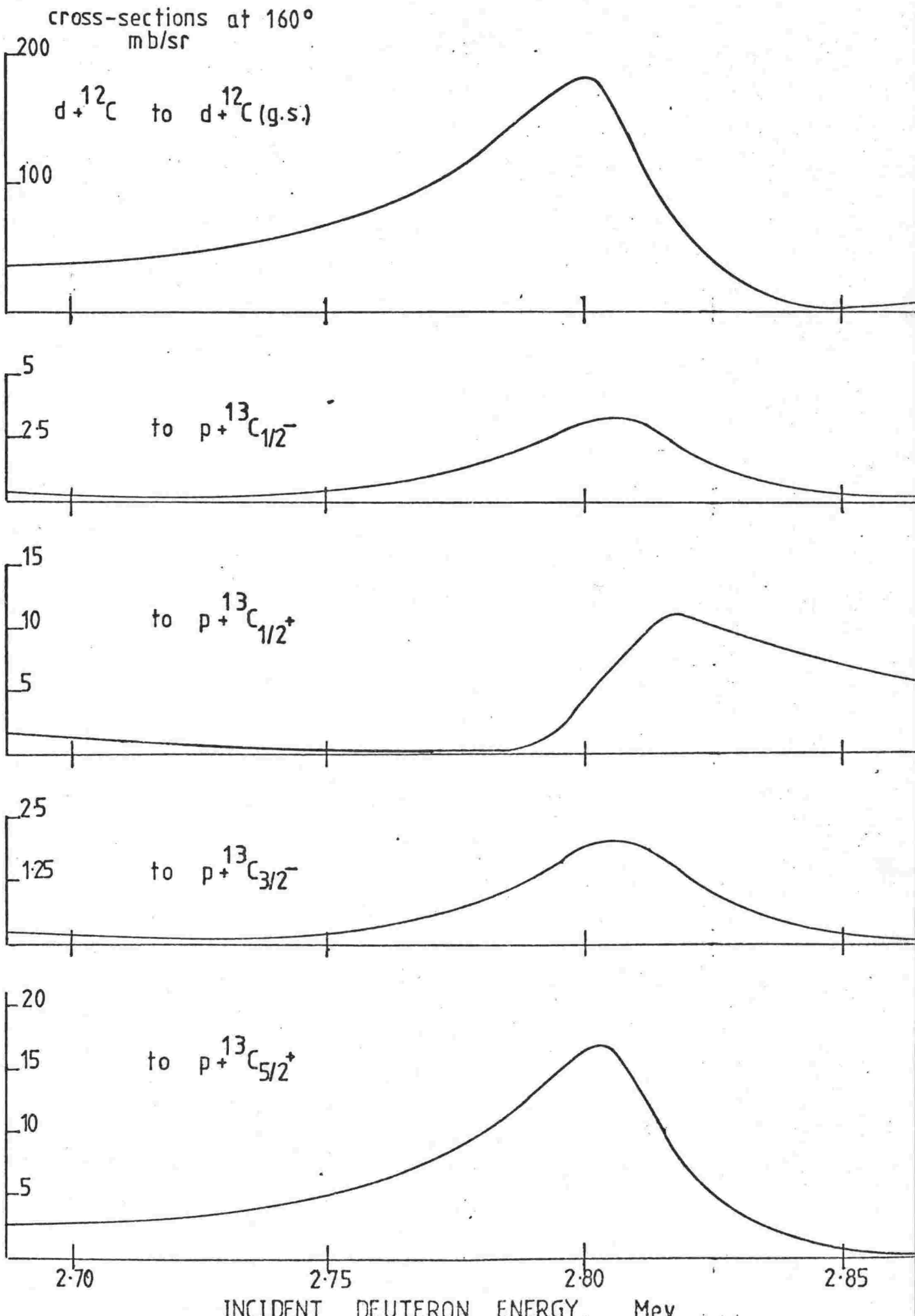

cross-sections at 160°
mb/sr
200
d + 12C to d + 12C (g.s.)
100
5
2·5
to p + 13C1/2−
15
10
to p + 13C1/2+
5
25
1·25
to p + 13C3/2−
20
15
to p + 13C5/2+
10
5
2·70
2·75
2·80
2·85
INCIDENT DEUTERON ENERGY, Mev

FIGURE 2.4.3

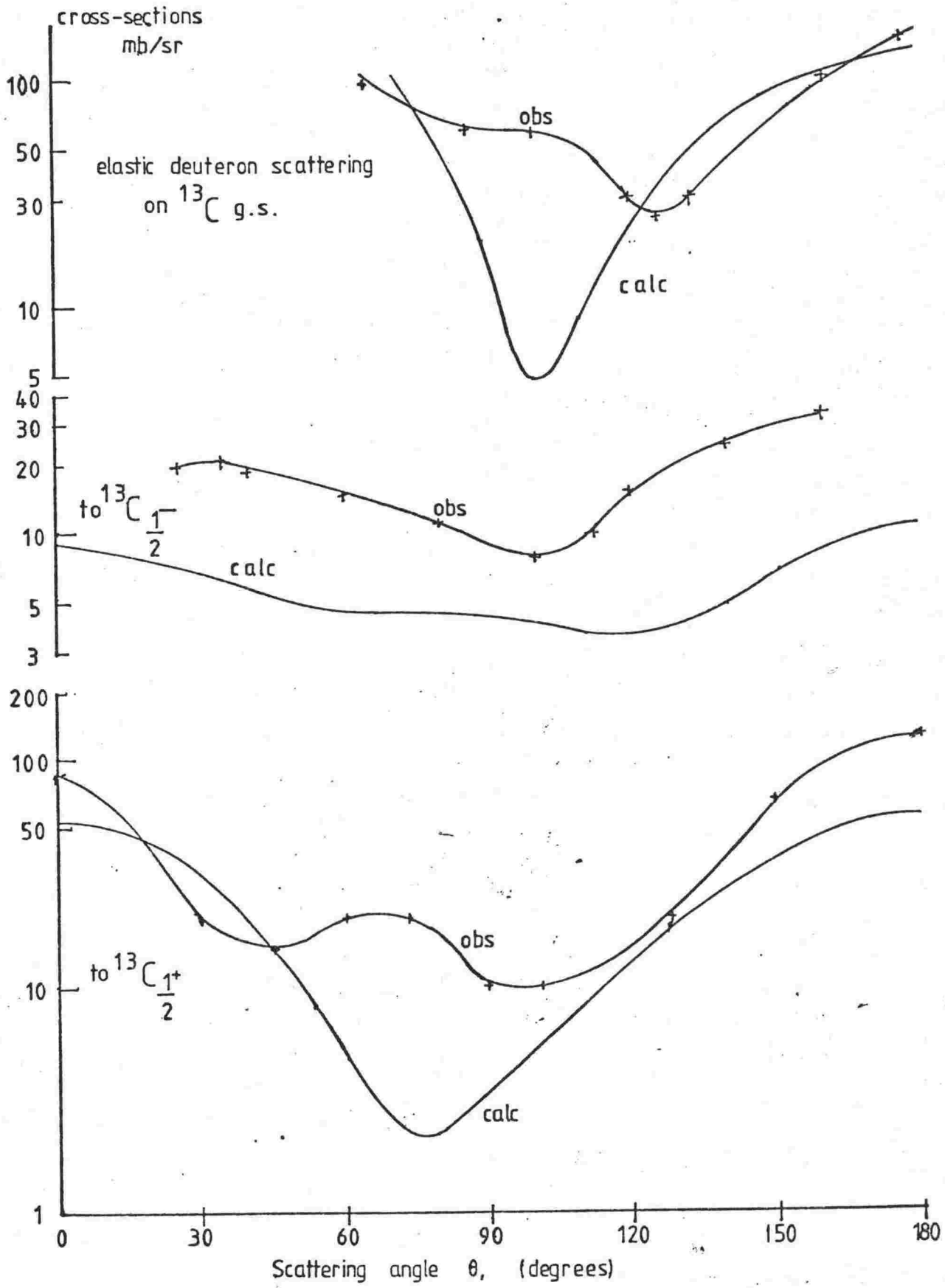
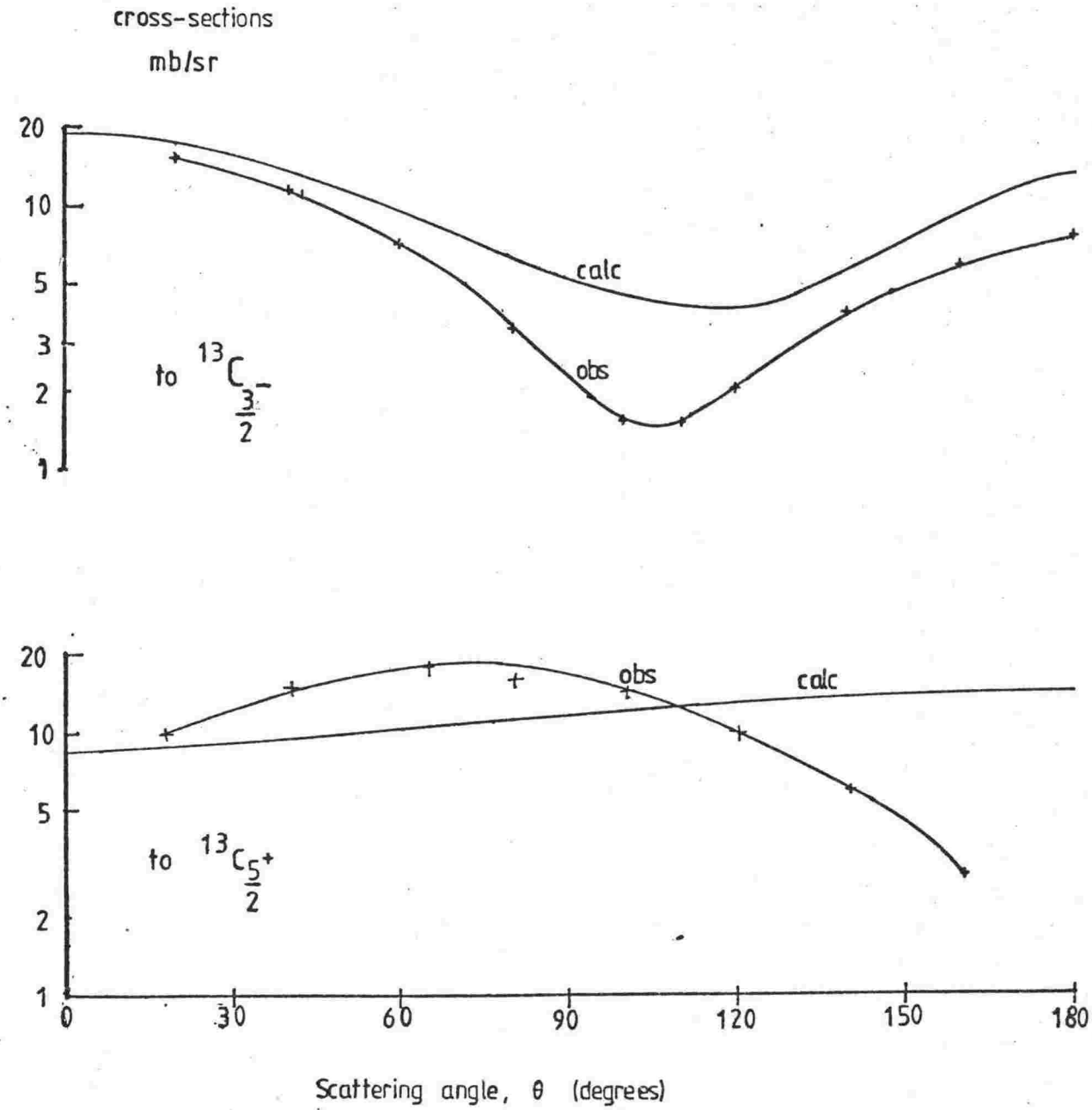

cross-sections
mb/sr
elastic deuteron scattering
on ^{13}C g.s.
obs
calc
to ^{13}C $\frac{1}{2}^-$
obs
calc
to ^{13}C $\frac{1}{2}^+$
obs
calc
Scattering angle θ, (degrees)

Figure 2.4.3 (continued)



2.5 Including Orthogonality Conditions in the Channel Equations

When the CC system of equations is derived without making all the assumptions listed in section 2.1, the channel operators and coupling potentials are often no longer local. The general problem of arbitary nonlocal terms will be examined in section 2.6, while this section considers the simpler case where only orthogonality conditions on the radial wave functions are imposed by the introduction of the nonlocal potentials. (The existence of these orthogonality conditions is not necessarily related to the non-orthogonality of the channels' internal states as mentioned in section 2.1 & dealt with in chapter 5.) Several ways that orthogonality conditions can be fitted into the CC formalism will now be given, in anticipation of their appearance later.

First, consider reformulating the Schrödinger equation $(H - E)\, f = 0$ so as to require all solutions f to be orthogonal to some arbitary vector 'u' : $\langle u|f\rangle = 0$. If projection operators P & Q are constructed by $P = |u\rangle\langle u|$ and $Q = 1 - P$, the orthogonality condition is $Pf = 0$, or $(1-P)f = Qf = f$. Note, however, that because of this condition, the original Schrödinger equation $Hf = Ef$ is not in general satisfied. Thus, the rest of section 2.5 strictly looks not at reformulations of Hf=Ef, but at reformulations within an equivalence-class of Schrödinger equations that differ from Hf=Ef only in the addition of kinematic projection terms, etc., without changing the dynamics of the potentials etc. in the Hamiltonian H.

The simplest change to $(H-E)f=0$ to enforce Qf=f is to apply H-E to Qf instead of to f, and later use Qf=f in the E term.

Thus $(H - E)\, Qf = 0$

so $HQf = EQf$

so $QHQf = EQ^2f = EQf$ as Q is a projection operator,

finally $QHQ\, f = E\, f$ as Qf=f.

The form QHQ is Feshbach's standard form (see Feshbach, 1968) for an Hermitian effective Hamiltonian which restricts solutions to the subspace Qf=f, ie. Pf=0. For if we multiply QHQf = Ef by P, and use PQ=0, we have E.Pf=0. If the total energy is not zero, $E \neq 0$ implies Pf=0, so the orthogonality condition $\langle u | f \rangle = 0$ is satisfied as required. This result may also be seen by the following reasoning: The effective Hamiltonian QHQ has the state 'u' as an eigensolution at zero energy E=0. As QHQ is Hermitian and independent of 'E', the solutions f to QHQf=Ef at all other energies must therefore be orthogonal to 'u'.

Secondly, the orthogonality condition may be imposed by a non-local potential V_u (depending on 'u') in $(H + V_u - E)f = 0$. These potentials are not uniquely defined. One form may be derived from the effective Hamiltonian QHQ of above, following Saito(1969):

$$QHQ\ f = E\ f$$

$$(H - E)f = (H - QHQ)f$$

$$= PH.f + (1-P)HP.f$$

Note that any multiple of $(1-P)APf = (1-P)\,[A,P]f$, for any operator 'A', can be added to the right-hand side of the above equation and, provided $E \neq 0$, we can still prove that Pf=0 by pre-multiplying by P. Choosing A = -H, the equation simplifies to

$$(H - E)f = PHf$$

$$= u \langle u | H | f \rangle \text{ , using the defintion of P,}$$

so that, in its simplest form, the Saito potential V_u is -PH.

Both of the above methods are successful since they shift any solution f=u to zero energy E=0. It is possible however to write down a potential to shift this unwanted eigenstate to any nominated energy E = e. The potential is $V_u^e = eP$, and it can be added to either of the above equations to shift the spurious eigenstate f = u:

$$(QHQ + eP - E)f = 0$$

or $(H - PH + eP - E)f = 0$, respectively.

Premultiplying either of these by P, we have $(e-E)Pf=0$, so that $E \neq e$ implies $Pf = 0$. The shifted level 'e' should be chosen as far from typical working energies E as possible. If desired, e can be made dependent on E, as suggested by Schmid et al(1976). For example, the function $e(E) = (E^2 + e_o^2)^{\frac{1}{2}}$ with $e_o \neq 0$ would impose the required orthogonality conditions without the presence of any spurious bound states at finite energies.

An alternative proposed by Kukulin et al(1978) is to take the limit $e \to \infty$ directly, in which case the Saito potential is not necessary. If $(H + eP - E)f_e = 0$, Kukulin et al prove that $\lim_{e\to\infty} Pf_e = 0$, so that the orthogonality condition is satisfied in the limit. There is no spurious bound state for any energy E.

In actually solving numerically the coupled-channel equations subject to orthogonality conditions, either we use one of the potential forms given above, or we use a more direct numerical condition. Because all the potentials are non-local, the methods of section 2.6 will be needed to handle them. This means that enforcing the conditions by a potential is more complicated than the following method which puts them in as extra numerical conditions when solving the coupled differential equations. The method dates back to Frantz et al(1958):

let f_1 be a homogeneous soln. of $(H-E)f_1 = 0$, and

let f_u be a particular soln. of $(H-E)f_u + u = 0$ that has only outgoing waves asmptotically. Then the linear combination $f = f_1 + cf_u$ satisfies $\langle u|f\rangle = 0$ for some c, in fact for $c = -\langle u|f_1\rangle / \langle u|f_u\rangle$. The method can be easily generalised to any number of orthogonality conditions on any selection of channels in the coupled-channels system.

2.6 Non-local Potentials

In this section, we seek to solve coupled equations that include non-local potentials and couplings. When non-localities are present, the step-by-step radial integration procedure of Buck, Stamp, & Hodgson is no longer applicable unchanged, and to solve sets of equations like

$$\left(a_i \frac{d^2}{dr^2} + b_i(r) - E \right) f_i(r) + \sum_{j=1}^{N} \int_0^\infty K_{ij}(r,r') \, f_j(r') \, dr' = 0$$

(ie. like $\left(H_i - E \right) f_i + \sum_{j=1}^{j=N} K_{ij} \, f_j = 0$,

where H_i are local and K_{ij} are non-local operators)

various approximations have to be used.

Two kinds of approaches are possible. The first is to look for some local equivalent to the full nonlocal potential, and then to use that local potential in the CC calculation in the usual manner. The second approach is to use the full non-local potential itself in the CC calculations, either iteratively, or via eigenvalue expansions into sums of separable nonlocal potentials.

The first approach uses a local equivalent potential. If the exact wavefunction were known, $f_i(r)$, then a local potential exactly equivalent to K_{ij} would be simply

$$U_{ij}^{\text{exact}}(r) = \frac{\int K_{ij}(r,r') \, f_j(r') \, dr'}{f_j(r)} .$$

However this expression, as well as being complex-valued, has poles where f_j has zeros. Thus it is usual to seek approximate expressions that yield well-behaved local equivalents $U_{ij}(r)$, and that do not require knowing the exact $f_i(r)$. The task is made much easier when K_{ij} has only short-ranged nonlocalities, ie. when $K_{ij}(r,r')$ becomes

small when $|r-r'|$ is larger than some 'nonlocal range'. For the range less than the wavelength of $f_i(r)$, Frahn & Lemmer(1957) present an 'effective mass' formula for U_{ij}. Perey et al(1962,1964) give a 'local energy approximation' that still holds when the range $|r-r'|$, though a small fraction of r or r', is larger than the local f_i wavelength - as is the case with short-ranged potentials at high energies. Georgiev et al(1978) and Sinha(1975) use related methods. When the nonlocal potential is directionally-dependent (eg. the potential when the Pauli Principle is included), Austern(1970,1975) uses a similar 'local-momentum approximation' of the WKB method.

Almost all of the above methods use a 'local wavelength' $\lambda(r) = 2\pi/k(r)$, where k(r) is the modulus of the local momentum $k(r) = \frac{2m}{h^2}(E - V(r))^{\frac{1}{2}}$. The V(r) is the total potential, either an empirical optical-model potential, or one derived self-consistently to include the final local equivalent potential itself, as suggested by Georgiev & Mackintosh(1978).

When the nonlocalities of a potential are not short-ranged (eg. with separable potentials such as the Saito orthogonalising potential), these methods for local-equivalences are not expected to be so accurate. This has not been investigated in detail in the present work: methods have instead been found which can handle nonlocal potentials of arbitary range.

The simplest such method is to iterate on the non-local terms. A sequence f_i^o .. f_i^n is calculated using

$$(H_i - E)\, f_i^o = 0$$

and

$$(H_i - E)\, f_i^n = - \sum_{j=1}^{j=N} K_{ij}\, f_j^{n-1} \qquad \text{for } n=1,2,3,..$$

This sequence will converge everywhere if the maximum eigenvalue of $(H_i - E)^{-1}\, K_{ij}$ has absolute value less than unity. It could diverge

either when the $K_{ij}(r,r')$ are large, or when an eigenvector of K_{ij} is near a resonance of H_i-E, that is, near a pole of $(H_i-E)^{-1}$. It is clear that if E is near the energy level of a resonance of H_i, then the method is numerically unsound, as slight changes in the Kf^{n-1} driving terms lead to large changes in the resonant wavefunction f^n.

When the K_{ij} have small effects and resonances are unimportant, Buckingham & Massey(1942) found the Λ iterative method to be most satisfactory for including in their model the residual nonlocalities of the antisymmetrised folded potentials in neutron-deuteron scattering.

When the eigenvalues of the K_{ij} are not small, but resonances are still known to be unimportant, it is feasible (following Perey & Buck, 1962, and Reeves & Owen, 1969) to improve the convergence of the method by subtracting a certain local potential U_{ij} from K_{ij}, and adding it to H_i. The iteration equations are then

$$(H_i - E)\, f_i^o + \sum_{j=1}^{N} U_{ij}(r)\, f_j^o(r) = 0$$

and

$$(H_i-E)\, f_i^n + \sum_{j=1}^{N} U_{ij}\, f_j^n = -\sum_{j=1}^{N} (K_{ij} - U_{ij})\, f_j^{n-1}.$$

This holds for any U_{ij}, but if we choose something near a local equivalent of K_{ij}, then the maximum eigenvalues of the residual $K_{ij}-U_{ij}$ would be much reduced, and the convergence of the iterations improved. The U_{ij} cannot however be the exactly-equivalent local potentials U_{ij}^{exact} defined earlier. For, although the U_{ij}^{exact} have imaginary parts, these do not lead to overall absorbtion or generation of flux because, when the K_{ij} are Hermitian ($K_{ij}(r,r')=K_{ji}(r',r)$), there is a conservation condition asserting that any flux absorbed must also reappear elsewhere: $\int_0^\infty \mathrm{Im}(U^{exact}(r))\,|f(r)|^2\,dr = 0$. Because the U_{ij} will be used with wave functions f^n different from

any used to form any precalculated U_{ij}, this conservation will not be exactly satisfied, and unitarity of the coupled-channels system will not hold. I think it is safest not to allow U_{ij} to have any imaginary parts at all. Thus parts of K_{ij} – the flux-transferring parts – must always be treated iteratively. This limits the cancellation in the $(K_{ij}-U_{ij})$ residual, and restricts the convergence improvement attainable.

A precise method of treating the nonlocal parts of K_{ij} (one that preserves unitarity exactly) is in fact possible, provided they can be written as sums of separable forms. For the CC equations can be solved exactly with a separable nonlocal potential: one of the form $|w\rangle k \langle w|$, or $K_{ij}(r,r') = w(r)\ k\ w(r')$, for some vector 'w', and some magnitude 'k'. The solution is as follows: let f_1 and f_w be the homogeneous and particular solutions of $(H-E)f_1=0$ and $(H-E)f_w + w = 0$, respectively. It can then be easily verified that the linear combination $f = f_1 + c.f_w$ with $c = k\langle w|f_1\rangle/(1-k\langle w|f_w\rangle)$ satisfies $(H + |w\rangle k\langle w| - E)\ f = 0$.

Furthermore, by an eigenvalue expansion, any finite non-local potential K_{ij} can be approximated to any desired accuracy by a finite sum of separable potentials $K_{ij}(r,r') = \sum_{p}^{Q_{ij}} |u_{ijp}(r)\rangle k_{ijp} \langle w_{ijp}(r')|$. The full CC system thus becomes

$$(H_i-E)\ f_i + \sum_{j=1}^{N} \sum_{p=1}^{Q_{ij}} |u_{ijp}\rangle k_{ijp} \langle u_{ijp}|f_j\rangle = 0,$$

which can be solved exactly by a multi-channel generalisation of the above method.

Chapter 3 The Pauli Principle

According to the Pauli Exclusion Principle, no two indistinguishable nucleons may be in the same quantum-mechanical state. This can be maintained by requiring that the system's wavefunction $\Psi(r_1, .. ,r_n)$ be antisymmetric for nucleon exchanges. That is, using the exchange operator P_{ij} that interchanges the coordinates of the i'th & j'th particles, $P_{ij}\Psi(. r_i . r_j .) = \Psi(. r_j . r_i .)$, the Pauli Principle requires

$$P_{ij}\Psi(. r_i . r_j .) = -\Psi(. r_i . r_j .).$$

The negative sign in $P_{ij}\Psi = -\Psi$ marks anti-symmetrisation, which holds for Fermi-Dirac particles such as protons and neutrons. It is also sufficient to imply that two protons (or two neutrons) can not be found in the same state. For example, consider two indistinguishable nucleons in states $w_1(r_1)$ and $w_2(r_2)$. We can then easily construct an anti-symmetrised (but not necessarily normalised) system state $\Psi(r_1,r_2)$ as

$$\Psi(r_1,r_2) = 2^{-\frac{1}{2}} (w_1(r_1)w_2(r_2) - w_1(r_2)w_2(r_1)) .$$

It is readily verified that $\Psi(r_1,r_2) = -\Psi(r_2,r_1)$, and that if $w_1=w_2$ then $\Psi = 0$. This is a mathematical statement of the fact that if the two individual states are identical, then the total wavefunction vanishes, and hence cannot be normalised. Such a situation is therefore physically impossible. Conversely, if the system wavefunction is not to vanish, the individual states must all be distinct.

Consider now the idealised scattering situation of a nucleus of 'A' identical nucleons being approached by another nucleon in a state $u(r_o)$ relative to the nucleus. Assume that the internal state of the nucleus is known to be at all times $\phi_A(r_1, .. ,r_A)$ (normalised and antisymmetrised internally), and that we wish to construct an anti-

symmetric wavefunction Ψ for the total system of A+1 indistinguishable nucleons. That is, we seek an antisymmetrising operator $\mathcal{A}$ so that $\Psi(r_o, r_1, \ldots, r_A) = \mathcal{A}\, u(r_o)\, \phi_A(r_1 \ldots r_A)$ is antisymmetric. Such an operator $\mathcal{A}$ can in fact be given in terms of the permutation operators P_{ij}:

$$\mathcal{A} = (A+1)^{-\frac{1}{2}} \left(1 - \sum_{j=1}^{j=A} P_{oj} \right).$$

Thus the antisymmetrised Ψ contains a sum ie.

$$u(r_o)\phi_A(r_1,\ldots) - u(r_1)\phi_A(r_o,r_2,\ldots) - u(r_2)\phi_A(r_1,r_o,r_3,\ldots) - \ldots$$

Now that an antisymmetric wavefunction for the system has been constructed, it is used in Schrodingers' equation in conjunction with a Hamiltonian for the A+1 nucleons. Since the state ϕ_A of the nucleus is assumed constant and known, the Schrodinger equation in A+1 variables can be reduced to a single nucleon equation in only the scattering coordinate r_o. The possibility of Ψ becoming zero because of two individual states becoming identical must be taken into account, and here the best treatment is the now standard one of Feshbach(1958, 1962, & 1968). This treatment is summarised in section 3.1.

3.1 Feshbach's Theory of Antisymmetrisation

In Feshbach's Unified Reaction Theory, a distinction is made between the physical wavefunction Ψ and the wavefunction used in any model. Since the model wavefunction must always be the more restricted, it is denoted by $P\Psi$, for some projection operator 'P' which projects from the physical space to the model subspace. In the present case, the model subspace for $P\Psi$ is the space of all antisymmetrised products of a scattering wavefunction $u(r_o)$ with a known nucleus ground state $\phi_A(r_1 \,..\, r_A)$: $\quad P\,\Psi(r_o, r_1\,..) = \mathcal{A}\, u(r_o)\, \phi_A(r_1\,..)$.

Since we seek a one-particle Schrodinger equation for the scattering state $u(r_o)$, we further project $P\Psi$ onto the nucleus state ϕ_A, and as usual integrate over all the internal coordinates $r_1 \,..\, r_A$, to define a new 'projected' scattering wavefunction $U(r_o)$:

$$U(r_o) = \langle \phi_A \,|\, P\Psi \rangle = \langle \phi_A \,|\, \mathcal{A}\, u\, \phi_A \rangle \qquad (1)$$

$$= u(r_o) - A \langle \phi_A(r_1,..,r_A) \,|\, \phi_A(r_o, r_2,..,r_A) \rangle\, u(r_1) \qquad \begin{matrix}(2)\\(3)\end{matrix}$$

$$= (1 - K)\, u$$

where 'K' is a new integral operator defined by its kernel function $k(r_o, r_1) = A \langle \phi_A(r_1 \,..\, r_A) \,|\, \phi_A(r_o, r_2 \,..\, r_A) \rangle$, so $U = (1-K)u$ means $U(r_o) = u(r_o) - \int k(r_o, r_1)\, u(r_1)\, dr_1$. If $P\Psi = \mathcal{A} u \phi_A$ is normalised $\langle \mathcal{A} u \phi_A | \mathcal{A} u \phi_A \rangle = 1$ e.g. for a bound state, then $\langle u | 1-K | u \rangle = \langle u | U \rangle = 1$. Note that neither u nor U by themselves are normalised.

The scattering wavefunctions $u(r_o)$ and $U(r_o)$ (which multiply ϕ_A, and are projected by ϕ_A, respectively) are asymptotically equal, and hence give identical scattering cross-sections etc. But they are different in the internal region because of the operator K which describes all the kinematic effects of antisymmetrisation. The effect of 1-K in $U = (1-K)\, u$ is to remove all components of u that overlap

with any internal states of the core nucleons: it is a kind of 'blocking operator' for the Pauli Exclusion Principle. If the core state ϕ_A were a simple Slater determinant made of orthonormal wavefunctions w_i,

$$\phi_A(r_1,r_2,\ldots,r_A) = A^{-\frac{1}{2}} \begin{vmatrix} w_1(r_1) & \cdots & w_A(r_1) \\ w_2(r_1) & \cdots & w_A(r_2) \\ \vdots & & \vdots \\ w_A(r_1) & \cdots & w_A(r_A) \end{vmatrix}, \qquad (4)$$

then 1-K is just a projection operator removing any w_i-parts of u :

$$1 - K = 1 - \sum_{i=1}^{A} |w_i\rangle\langle w_i| , \qquad (5a)$$

$$\text{or} \quad k(r_o,r_1) = \sum_{i=1}^{A} w_i(r_o)\, w_i(r_1)^* . \qquad (5b)$$

Thus if u were equal to one of the core states w_i, then Ku=u, and U = (1-K)u would be zero. The total wavefunction PΨ would also be zero, as $a w_i \phi_A = 0$, and so could be added in arbitary multiples to any other term $a u \phi_A$ without changing the latter. Feshbach calls in the general case the solutions w_i^1 that are totally blocked $(1-K)w_i^1 = 0$ the 'supererogatory solutions', and points out that the elimination of these superfluous terms would of course be useful from the points of view of efficiency and convenience. More importantly, in any numerical method it would be intolerable if the desired solutions were not unique, and could be swamped by the addition of arbitarily large multiples of these supererogatory solutions. It is most advisable to identify in advance and project out these superfluous solutions, to ensure unique solutions to a numerically stable method.

To identify the supererogatory solutions (those fully blocked by 1-K), we need to find the actual form of the blocking operator K, and consider its eigenvalue expansion $K\, w_i^{\lambda_i} = \lambda_i\, w_i^{\lambda_i}$. The operator K is in fact just the single-particle density-matrix operator for the antisymmetrised nucleus state ϕ_A. Sometimes this is known from other nuclear structure calculations, but more often than not the density

operator K has to be constructed from simplified nuclear models.

If the nucleus state ϕ_A is taken to be a product of 'A' single-particle states w_i, i=1 .. A, with no dynamic correlations apart from antisymmetrisation, then ϕ_A has the Slater-determinant form of above. The K operator is the projection operator given earlier, and has eigenvectors $w_i^1 = w_i$ all corresponding to unit eigenvalues $\lambda_i = 1$.

If the nucleus has multi-nucleon correlations, and has to be written as a linear combination of product wavefunctions, and/or has excited states whose angular momentum couples to that of the incoming particle, then K is correspondingly more complicated, and has one of the forms derived in Appendices 1 & 2.

Whatever the density matrix K of the nucleus may be, it always has the following properties :

(1) K is Hermitian, so the eigenvalues λ_i are all real,

(2) K is positive definite : for any u, $\langle u|K|u\rangle \geq 0$,
so all the λ_i are positive definite : $\lambda_i \geq 0$. (6a)

(3) 1-K is also positive definite :
for any u, $\langle u|1-K|u\rangle = \frac{1}{A+1} \langle \mathcal{A} u\, \phi_A | \mathcal{A} u\, \phi_A \rangle \geq 0$.
so all the $\lambda_i \leq 1$. (6b)
With (2), we have $0 \leq \lambda_i \leq 1$. (6c)

(4) Tr K = A : the density matrix describes A nucleons.

(5) K is bounded : $\int dr_1 \int dr_0 \, |k(r_0,r_1)|^2 \leq A$. (7)
Thus $k(r_0,r_1) \to 0$ as either r_0 or r_1 becomes large.
This is the reason for the remark earlier that $u(r_0)$ and $U(r_0) = (1-K)u$ are asymptotically equal, and hence give identical phase shifts, cross-sections, etc.

In general the operator K can always be expanded in terms of its eigenvectors $w_i^{\lambda i}$ as

$$k(r_o,r_1) = \sum_i w_i^{\lambda i}(r_o)\ \lambda_i\ w_i^{\lambda i}(r_1)^* . \qquad (8)$$

The case where an eigenvalue $\lambda_i = 1$ requires special consideration, because when we solve $U = (1-K)u$ for u, the expansion of $(1-K)^{-1}$ in terms of the eigenfunctions of K will show a pole whenever a λ_i eigenvalue is unity. The corresponding eigenvector will be w_i^1, and because $K\, w_i^1 = 1.w_i^1$, we have $(1-K)w_i^1 = 0$, and hence $\langle w_i^1 | U\rangle = 0$. We find further that $\mathcal{A} w_i^1\, \phi_A = 0$, so w_i^1 is one of the supererogatory solutions that are completely blocked by antisymmetrising, and should be avoided in solving the equations. From $\langle w_i^1 | U\rangle = 0$, U must have no component proportional to any w_i^1, so the inversion $u = (1-K)^{-1}\ U$ can be carried out without difficulty by simply leaving out all the eigenvectors of K that correspond to unit eigenvalues. Define K' to be the remaining operator

$$K' = \sum_{i,\ \lambda_i \neq 1} |w_i^{\lambda i}\rangle\ \lambda_i\ \langle w_i^{\lambda i}| , \qquad (9)$$

so the solution for u is $(1-K')^{-1}\ U$, always well defined and containing no supererogatory components when U has none :

$$u(r_o) = \sum_{i,\lambda_i \neq 1} \frac{\langle w_i^{\lambda i} | U\rangle}{1-\lambda_i}\ w_i(r_o) .$$

Note: If we define P_A to be that part of K <u>not</u> in K', then $K = K' + P_A$ and $(1-K) = (1-K')(1-P_A)$; P_A is the projection operator of fully-blocked states : $P_A = \sum_{i,\ \lambda_i=1} |w_i^1\rangle\langle w_i^1|$; and $P_A\ U = 0$.

Now that the model wavefunction $P\Psi = \mathcal{A} u \phi_A$ has been defined, and any ambiguities removed, Feshbach's theory now gives a Schrodinger equation in only one variable r_o for the scattering wave functions $u(\underline{r}_o)$ and/or $U(\underline{r}_o)$.

First, a wave equation for $P\Psi$ is obtained by restricting the full Hamiltonian 'H_{full}' for the complete A+1 - body system to the model subspace defined by the projection operator P. The model Hamiltonian 'H' in the subspace, in which the core nucleons are always in the state ϕ_A, is in terms of H_{full}

$$H = P H_{full} P + P H_{full} Q (E^+ - Q H_{full} Q)^{-1} Q H_{full} P, \text{ where } Q=1-P.$$

More often though, the effect of the remaining 'Q' part is neglected, and H is written down directly for the scattering-particle + nucleus-in-state-ϕ_A system, e.g.

$$H(\underline{r}_o, \underline{r}_1 .. \underline{r}_A) = T(\underline{r}_o) + V_{oA}(\underline{r}_o, \underline{r}_1, ..) + H_A(\underline{r}_1, .. , \underline{r}_A)$$

where

$T(\underline{r}_o)$ is the kinetic energy operator for the scattering nucleon,

V_{oA} is the sum of potentials between the scattering nucleon and the core nucleons : $V_{oA} = \sum_{j=1}^{A} V_2(\underline{r}_o, \underline{r}_j)$ where $V_2(\underline{r}_o, \underline{r}_1)$ is the nucleon-nucleon interaction, and

H_A is the nuclear Hamiltonian : $H_A \phi_A = e_A \phi_A$ for some energy e_A.

Applied to the model subspace $P\Psi = \mathcal{A} u \phi_A$, the model Hamiltonian H gives, for total energy E, the Schrodinger equation in A+1 variables

$$H | \mathcal{A} u \phi_A \rangle = E | \mathcal{A} u \phi_A \rangle , \qquad (10a)$$

which may be rewritten as

$$H | \mathcal{A} . \phi_A \rangle u = E | \mathcal{A} . \phi_A \rangle u , \qquad (10b)$$

where henceforth $| \mathcal{A} . \phi_A \rangle$ denotes the antisymmetrisation operator on one-variable functions $u(\underline{r}_o)$ giving the A+1 - variable wavefunction $\mathcal{A} u \phi_A$. Its Hermitian transpose $\langle \mathcal{A} . \phi_A |$ is the operator $\langle \phi_A | \mathcal{A}$.

To derive an equation in the one variable r_o, we project onto the core state, using one of the operators $\langle\phi_A|$, $(1-P_A)\langle\phi_A|$, $\langle\mathcal{A}.\phi_A| \equiv \langle\phi_A|\mathcal{A}$, or $(1-P_A)\langle\mathcal{A}.\phi_A|$. The first choice $\langle\phi_A|$ is the simplest and is used by Feshbach; the second and fourth make explicit the treatment of the supererogatory components; while the third and fourth are better in giving Hermitian operators, and lead in section 4.2 to a useful series of Hermitian approximations. Applied to the equation $H\,|\mathcal{A}.\phi_A\rangle u = E\,|\mathcal{A}.\phi_A\rangle u$, the four operators are equivalent, as on the right-hand side $\langle\phi_A|\mathcal{A}.\phi_A\rangle$, $(1-P_A)\langle\phi_A|\mathcal{A}.\phi_A\rangle$, $\langle\mathcal{A}.\phi_A|\mathcal{A}.\phi_A\rangle$, and $(1-P_A)\langle\mathcal{A}.\phi_A|\mathcal{A}.\phi_A\rangle$ all equal $(1-K)$. As the left-hand side starts with the $(A+1)$-body Hamiltonian H (symmetric for two-particle interchanges) operating on an antisymmetrising '$\mathcal{A}$', we have

$$\langle\phi_A|H\mathcal{A} = \langle\phi_A|H\mathcal{A}^2 = \langle\phi_A|\mathcal{A}H\mathcal{A} \qquad \text{as H is symmetric}$$
$$= \langle\mathcal{A}.\phi_A|\,H\,\mathcal{A} \qquad \text{by the definition of } \langle\mathcal{A}.\phi_A|,$$

$$\langle\mathcal{A}.\phi_A|\,H\mathcal{A} = (1-P_A)\langle\mathcal{A}.\phi_A|\,H\mathcal{A} \qquad \text{as } \mathcal{A}w_i^1\phi_A \equiv 0$$
$$= (1-P_A)\,\langle\phi_A|\,H\mathcal{A},$$

and hence the equivalence of the four equations

$$\langle\phi_A\,|\,H\,|\,\mathcal{A}.\,\phi_A\rangle u = E\,(1-K)\,u \qquad (11a)$$
$$(1-P_A)\,\langle\phi_A\,|\,H\,|\,\mathcal{A}.\,\phi_A\rangle u = E\,(1-K)\,u\,, \qquad (11b)$$
$$\langle\mathcal{A}.\,\phi_A\,|\,H\,|\,\mathcal{A}.\,\phi_A\rangle u = E\,(1-K)\,u\,, \quad \text{and} \qquad (11c)$$
$$(1-P_A)\,\langle\mathcal{A}.\,\phi_A\,|\,H\,|\,\mathcal{A}.\,\phi_A\rangle u = E\,(1-K)\,u\,. \qquad (11d)$$

As Krause & Mulligan(1975) correctly point out, these four equations all admit in their solutions, for any value of E, the addition of arbitary multiples of the supererogatory components w_i^1. Although the w_i^1 are non-zero only in the inner region and therefore do not affect the scattering phase-shifts, etc., it is advisable as mentioned earlier to remove all components w_i^1 from the solutions by

requiring $\langle w_i^1 | u \rangle = 0$, to ensure unique solutions to a numerically stable method. We must therefore change the equations so that all their solutions have <u>zero</u> multiples of the supererogatory components w_i^1 ; and this should be checked by verifying that the modified channel equation by itself implies that its solutions are all orthogonal to the w_i^1, ie that $P_A u=0$. The solutions of all 4 equations will be otherwise the same, to answer a query of Krause & Mulligan.

Any supererogatory additions to the solutions 'u' of the equations are removed by changing their right-hand sides from $E(1-K)\ u = E(1-K')(1-P_A)\ u$ to $E(1-K')\ u$, so

$$\langle \phi_A \mid H \mid \mathcal{a} \cdot \phi_A \rangle\ u = E\ (1-K')\ u, \qquad (12a)$$

and similarly for the other 3 forms. By operating on any of these 4 modified equations with $\langle w_i^1|$, and using $(1-P_A)w_i^1 = 0$, & $\mathcal{a} w_i^1 \phi_A = 0$, we can prove when $E \neq 0$ that $\langle w_i^1 | u \rangle = 0$, ie. $P_A u=0$, so all solutions 'u' of these equations have no supererogatory components.

Instead of changing the u-equations to remove the w_i^1, equations could have been derived for the 'U' function using the $u = (1-K')^{-1}U$ relation given above. Four equivalent equations for U are hence

$$\langle \phi_A \mid H \mid \mathcal{a} \cdot \phi_A \rangle\ (1-K')^{-1}\ U = E\ U, \qquad (13a)$$

and similarly for the other 3 projections (b,c,d). It can easily be shown that, by again projecting with $\langle w_i^1|$, the solutions U to (13a-d) all satisfy $\langle w_i^1 | U \rangle = 0$, and that when H is symmetric the 4 equations have identical solutions. If an approximate 'H' is used that is not exactly symmetric, then in general only the sets' (b), (c), & (d) equations still give $\langle w_i^1 | U \rangle = 0$. Of these three, the (b) & (d) are better in that with their $(1-P_A)$ factor, they explicitly remove the supererogatory components whatever approximations may be used for $\langle \phi_A | H | \mathcal{a} \cdot \phi_A \rangle$ or $\langle \mathcal{a} \cdot \phi_A | H | \mathcal{a} \cdot \phi_A \rangle$.

None of the above equations for U or for u are of the form $H_{eff}\, f = E\, f$ for some Hermitian effective Hamiltonian H_{eff}. To derive such an equation, Feshbach describes how it is necessary to define a third scattering wavefunction $\Omega(r_o)$ by

$$\Omega = (1-K)^{\frac{1}{2}}\, u = (1-K')^{-\frac{1}{2}}\, U \,. \qquad (14)$$

The square-root operator is always real, as all of the eigenvalues of K' are less than unity, by construction, inequality (6b), and

$$(1-K')^{\frac{1}{2}} = \sum_{\substack{i \\ \lambda_i \neq 1}} |w_i^{\lambda_i}\rangle (1-\lambda_i)^{\frac{1}{2}} \langle w_i^{\lambda_i}| \,. \qquad (15)$$

The $\Omega(r_o)$ is again asymptotically equal to both U and u, so any one of the three is sufficient for cross-sections etc. The Schrodinger equation for Ω is obtained from eqn. (11c), or better from (12c), and is

$$(1-K')^{-\frac{1}{2}} \langle \mathcal{A}.\, \phi_A | H | \mathcal{A}.\, \phi_A \rangle \, (1-K')^{-\frac{1}{2}}\, \Omega(r_o) = E\, \Omega(r_o), \qquad (16)$$

which can be abbreviated $H_{eff}\, \Omega = E\, \Omega$, with Hermitian H_{eff}.

One advantage of Ω against u or U is that Ω can be directly normalised. For example, for a bound state

$$\langle \mathcal{A}\, u\, \phi_A | \mathcal{A}\, u\, \phi_A \rangle = 1$$

ie. $\langle \Omega | (1-K')^{-\frac{1}{2}} \langle \mathcal{A}.\, \phi_A | \mathcal{A}.\, \phi_A \rangle (1-K')^{-\frac{1}{2}} | \Omega \rangle = 1$

ie. $\langle \Omega | (1-K')^{-\frac{1}{2}} (1-K) \, (1-K')^{-\frac{1}{2}} | \Omega \rangle = 1$

ie. $\langle \Omega | (1-P_A) | \Omega \rangle = 1$

ie. $\langle \Omega | \Omega \rangle = 1$ once supererogatory components are removed by requiring

$$P_A\, \Omega = 0.$$

For scattering states in the continuum, the $\Omega_E(r)$ still form an orthonormal set $\langle \Omega_E | \Omega_{E'} \rangle = \delta(E-E')$. These orthonormal properties of Ω reflect the fact that it is the eigensolution of an Hermitian operator.

Summarising, there are three physically equivalent equations for the three kinds of scattering wavefunctions u, U, Ω :

$$(1-K')^{-1}\,(1-P_A)\,\langle\phi_A|\,H\,|\,a.\,\phi_A\rangle\,u \;=\; E\,u\,, \qquad (12a')$$

$$\langle a.\,\phi_A|\,H\,|\,a.\,\phi_A\rangle\,(1-K')^{-1}\,U \;=\; E\,U\,, \qquad (13a)$$

and $$(1-K')^{-\frac{1}{2}}\,\langle a.\,\phi_A|\,H\,|\,a.\,\phi_A\rangle\,(1-K')^{-\frac{1}{2}}\,\Omega \;=\; E\,\Omega\,. \qquad (16)$$

(Where the forms $(1-P_A)\langle\phi_A|$ and $\langle a.\,\phi_A|$ are interchangeable here.)

All three equations are sufficient by themselves to imply $P_A\,u = P_A\,U = P_A\,\Omega = 0$, in each case relying on $\langle w_i^1|\langle a.\,\phi_A| = 0$ or $\langle w_i^1|\,(1-P_A) = 0$ for fully blocked components w_i^1 .

The Hamiltonian expressions $\langle\phi_A|H|\,a.\,\phi_A\rangle$ and $\langle a.\phi_A|H\,|\,a.\phi_A\rangle$ that occur in the above Schrodinger equations are called 'matrix elements' of H : the expectation values of H for model basis directions along $|\,\phi_A\rangle$ or $|\,a.\phi_A\rangle$. It should be noted that any approximations to these matrix elements should still block the w_i^1 exactly: any numerical expression of $|a.\phi_A\rangle$, for example, should satisfy $|a.\phi_A\rangle|w_i^1\rangle=0$. This may be ensured by constructing P_A from the numerical w_i^1 solutions, and then including an extra $(1-P_A)$ factor in the matrix elements. Thus the channel equation for Ω , say, that is numerically the more stable is

$$(1-P_A)\left[(1-K')^{-\frac{1}{2}}\,\langle a.\phi_A|\,H\,|\,a.\phi_A\rangle\,(1-K')^{-\frac{1}{2}}\right]\Omega \;=\; E\,\Omega\,, \qquad (16')$$

where the term in the square brackets may be replaced by some expression that is closely equivalent numerically.

The general forms for the matrix elements will be derived in Chapter 4, in the context of examining the antisymmetrised interactions between a deuteron and a nucleus. The case of one nucleon outside a nucleus of 'A' identical nucleons is simpler, and, anticipating Chapter 4 a little, the two matrix elements have the following slightly different approximations :

$$\langle \phi_A \mid T(r_o) + V_{oA} + H_A \mid \mathcal{A} \cdot \phi_A \rangle$$

$$\simeq \left(T(r_o) + V_a + e_A \right) (1-K) \qquad (17)$$

and $\langle \mathcal{A} \cdot \phi_A \mid T(r_o) + V_{oA} + H_A \mid \mathcal{A} \cdot \phi_A \rangle$

$$\simeq (1-K)^{\frac{1}{2}} \left(T(r_o) + V_a + e_A \right) (1-K)^{\frac{1}{2}} \qquad (18)$$

where V_a is the overall core-nucleon potential. The V_a potential has a local 'direct' part V_D and a non-local 'exchange' part V_E :

$$V_a\, u(r_o) = V_D(r_o)\, u(r_o) - \int V_E(r_o,r_1)\, u(r_1)\, dr_1 \quad \text{for any 'u'}$$

where

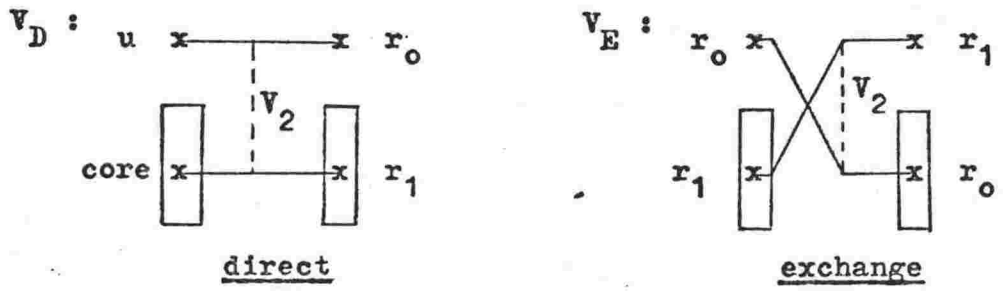
$$V_D(r_o) = \int V_2(r_o,r_1)\; k(r_1,r_1)\, dr_1 = \mathrm{Tr}(V_2 K) \text{ in short,}$$

and $V_E(r_o,r_1) = V_2(r_o,r_1)\; k(r_o,r_1) = (V_2 \cdot K)$ in short;

$V_2(r_o,r_1)$ = nucleon-nucleon two-body potential;

& $k(r,r')$ is the kernel of the density operator K of the nucleus.

For notational convenience, write $V_a = \mathrm{Tr}(V_2K) - (V_2 \cdot K)$. The two parts may be represented diagrammatically by



The direct part V_D, also called the 'folded potential', is the only part present in models which ignore antisymmetrisation.

As will be explained in Chapter 4, the above approximations for the matrix elements are exact when the nucleus has no nucleon-nucleon correlations apart from those implied by antisymmetrisation, that is when ϕ_A is a Slater-determinant wavefunction and K is a projection operator (then, $K=P_A$ & $K'=0$). Both approximations are consistent with respect to shifts of the E=0 origin when K is not a projection operator.

The three channel equations (12a', 13a & 16) can be written using the matrix element $(1-P_A) \langle \phi_A | H | \mathcal{A}.\phi_A \rangle$, and, with this matrix element simplified as above, they become

$$(1-K')^{-1} (1-P_A) \left[T + V_a + e_A \right] (1-P_A) (1-K') u = E\, u(r_o) , \qquad (19a)$$

$$(1-P_A) \left[T + V_a + e_A \right] (1-P_A) U = E\, U(r_o) , \qquad (19b)$$

$$\text{and } (1-K')^{-\frac{1}{2}} (1-P_A) \left[T + V_a + e_A \right] (1-P_A) (1-K')^{\frac{1}{2}} \Omega = E\, \Omega(r_o) . \qquad (19c)$$

These three equations may also be written using the Hermitian matrix element $\langle \mathcal{A}.\phi_A | H | \mathcal{A}.\phi_A \rangle$, and, with its simplified form of above, to a slightly different approximation the three equations become

$$(1-K')^{-\frac{1}{2}} (1-P_A) \left[T + V_a + e_A \right] (1-P_A) (1-K')^{\frac{1}{2}} u = E\, u(r_o) , \qquad (20a)$$

$$(1-K')^{\frac{1}{2}} (1-P_A) \left[T + V_a + e_A \right] (1-P_A) (1-K')^{-\frac{1}{2}} U = E\, U(r_o) , \qquad (20b)$$

$$\text{and } (1-P_A) \left[T + V_a + e_A \right] (1-P_A) \Omega = E\, \Omega(r_o) . \qquad (20c)$$

To summarise the notation

$T + V_a$ = one-body Hamiltonian for scattering particle,

V_a = $V_D + V_E$ = folded potential + some residual non-local ptl.,

$E - e_A$ = scattering energy in the c.m. frame

$(1-P_A)$ on each side of $(T+V_a)$ ensures that $P_A\, u = 0$, etc., i.e. that the scattering wavefunctions are all orthogonal to the components fully blocked by the Pauli Principle,

$(1-K')$ renormalises those components that are not fully blocked.

Only the equations (19b) & (20c) above have channel Hamiltonians which are symmetric and Hermitian, so these two will be preferred to the other four equations.

3.2 The Kinematic Assumption

The Schrodinger equations derived in the previous section are different in two ways from those derived by ignoring the Pauli Principle and the antisymmetrisation it requires. First, there is the presence of the $1-P_A$ and $1-K'$ operators, and second, the overall core-nucleon potential V_a has a non-local exchange term in addition to the usual local term. The first difference, as it affects primarily the wave function definitions and projections, is largely kinematic. The second difference, as it affects primarily the detailed dynamics of the nucleon-nucleus potentials, is largely dynamic.

The kinematic assumption is to assume that all the significant antisymmetrisation effects are adequately accounted for kinematically. That is, once the kinematic terms are included, it is a good approximation to replace the non-local potential V_a by some local effective potential V_L such as an optical-model potential. Given this 'kinematic assumption' and the use of such a local effective potential (not necessarily just the direct part of V_a), the non-local effects appear only with the terms $(1-K')$ which renormalise components not fully blocked, and with terms $(1-P_A)$, which block the supererogatory components. With Buck et al(1977), "we take the view that the specific effects of the Pauli Principle should not be sensitive to the detailed dynamics of the nuclear scattering as expressed in assumptions about the inter-nucleon forces. We should like therefore to have a theory in which antisymmetrisation constraints and dynamical conditions appear in a factorised form instead of being 'inextricably mixed up' as in the usual resonating group method (RGM)." The RGM uses the full antisymmetrised Hamiltonian H, constructed directly from nucleon-nucleon forces, in

matrix elements like $\langle a.\phi_A \mid H \mid a.\phi_A \rangle$, and makes no distinction between 'kinematic' and 'dynamic' effects of antisymmetrisation. Not surprisingly, the detailed integro-differential equations of the RGM are complicated to write down and hard to solve numerically.

Let it be clear what effects are precluded when we leave out the dynamic exchange terms. Consider the case, say of modelling ^{13}C structure as a neutron around a ^{12}C core. The 0p shell in the ^{12}C core is only 2/3 full, so the neutron can go there, as well as into the s-d shell at a higher energy. There will be few antisymmetrisation effects of any kind when the neutron is in an s-d state, but we would expect both the kinematic and dynamic terms to be large for a p-state neutron. The 'kinematic' terms will first block the neutron from any fully-occupied p-shell state, and then renormalise the neutron's amplitude where it overlaps with any state only partially occupied by a ^{12}C neutron. The 'dynamic' terms would block the occupied states too, if this were not already done by the kinematic terms. But more importantly, only the dynamic terms will shift the energy levels of the neutron + core eigenstates. That this does happen is obvious experimentally : the $p_{\frac{1}{2}}$ and $p_{3/2}$ states of ^{13}C are within an Mev of the $s_{\frac{1}{2}}$ and $d_{5/2}$ states, indicating that somehow the energies of the p-shell neutron eigenstates are much higher than would be expected for the neutron occupying an eigenstate of a local potential. This rise in the p-state eigenenergy can be attributed to the large <u>dynamic</u> effects of antisymmetrisation, when a neutron interacts with 4 other neutrons in a shell that is altogether 5/6 occupied.

Thus when the dynamic exchange terms are neglected, though scattering resonances and bound eigenstates may be renormalised to the correct amplitudes (zero, if fully blocked!), they may well occur

at the wrong energies, especially if kinematically they are partially or largely blocked by core nucleons. So when we use a local potential V_L instead of the more accurate non-local V_a, we should be aware of this shortcoming, and if necessary slightly adjust the parameters of the local potential so that its resonances and eigenstates appear at their observed energies (as to some extent is common practice already).

The shortcomings of using only a local approximation to V_a are hence not nearly so serious in scattering calculations as they would be in structure calculations. In structure calculations that include antisymmetrisation properly (eg. those of Friedman, 1967), the primary results are energy-level diagrams, whereas in scattering analyses, the primary results are the wave function amplitudes, especially their phase shifts. The energy levels of eigenstates have only a second-order effect on the scattering amplitudes, through the placing and widths of resonances. We must therefore expect, when using a scattering model derived with the kinematic assumption, to have to feed in the positions of any resonances. Given that, they should then appear with good amplitudes and widths.

Using the kinematic assuption, the Schrodinger equations of section 3.1 are simplified : the channel operator $T+V_a+e_A$ is replaced by $H_L = T + V_L + e_A$, which is entirely a local differential operator. This begins to make the numerical problem more straightfoward.

We now deal specifically with the kinematic terms $(1-P_A)$, $(1-K')$, and $(1-K) = (1-P_A)(1-K')$ still in the channel equations. The first investigators (eg. Saito, 1969) neglected the partially-blocked components, and assumed that all scattering wave components were either fully blocked, or not significantly blocked at all. That is, they assumed that all the eigenvalues of K were either unity or zero, so $1-K = 1-P_A$,

and $K' = 0$. In this case, all the channel equations of section 3.1 reduce to $(1-P_A)\, H_L\, (1-P_A)\, u(r_o) = E\, u(r_o)$, and identically for $U(r_o)$ and $\Omega(r_o)$. As shown in section 2.5, this equation is equivalent to the ordinary local Schrodinger equation $H_L\, u = E\, u$ with the associated orthogonality conditions $P_A u = 0$, or $\langle w_i^1 \mid u \rangle = 0$, and is easy to solve numerically.

This final result is the Orthogonality Condition Model (OCM) of Saito(1969), and has since been used extensively for a wide range of scattering problems: see Shakin & Weiss(1975) or Saito(1977).

Buck et al(1977) now point out the important fact that the OCM not only works well when the eigenvalues of K are zero or unity (or close to these limits, as Saito et al.,1973, show), but also gives excellent results in other cases when the spectrum of eigenvalues of K goes rather smoothly from 0 to 1. We can of course still orthogonalise to the fully-blocked states with unit eigenvalues, but it is hard to take account of eigenstates which have eigenvalues not very near to either limit. Hence it is difficult to justify replacing $1-K$ by $1-P_A$, and the neglect of K', even if we include in P_A some 'almost forbidden states' which are only fully blocked in some limit, as advocated by Saito et al.(1973).

In fact, we already have a wave equation which clarifies the situation. Taking the symmetric matrix element $\langle a.\phi_A | H | a.\phi_A \rangle$, the wave equation for $\Omega(r_o)$ of section 3.1 becomes (with the kinematic assumption) $(1-P_A)\, H_L\, (1-P_A)\, \Omega = E\, \Omega(r_o)$ for <u>any</u> operator K ! That is, we still have an OCM-like equation which can be easily solved, without neglecting the possibility of partially-blocked states. Instead, the wave equation uses a renormalised wave function Ω, and

this renormalisation completely absorbs the effects of states being only partially blocked : $\Omega = (1-K')^{\frac{1}{2}} u = (1-K')^{-\frac{1}{2}} U$.

Thus, to quote from Buck et al., "the applicability of the OCM is not necessarily restricted to systems where there are only exactly forbidden and almost totally allowed states. If there are many partially redundant states ($\lambda \neq 0$ or 1), the OCM may still be valid, but it must be interpreted as an equation for $(1-K')^{\frac{1}{2}}$ times the RGM wave function u. Since u and $\Omega = (1-K')^{\frac{1}{2}}u$ differ only for small separations, they have the same asymptotic forms and give the same phase shifts in scattering calculations. This may be the reason that the point has not been generally noticed previously."

To end this section, I note that occasionally it is possible to even further simplify the OCM equations, which are

$$(1-P_A)\, H_L\, (1-P_A)\, \Omega = E\, \Omega$$

or $$H_L\, \Omega = E\, \Omega \quad \text{with } P_A \Omega = 0,$$

where

$$H_L = T + V_L + e_A$$

and $$P_A = \sum_i |w_i^1\rangle\langle w_i^1| \ .$$

For suppose that the potential V_L supported some bound states similar to the forbidden states $w_i^1(r_o)$. Then it is obvious that the higher-energy bound states and the scattering wave functions of the Hermitian operator H_L would be orthogonal to the lower 'redundant' solutions, as H_L does not explicitly depend on the energy E. The orthogonality conditions would then be fulfilled just by disregarding such solutions. If the w_i^1 were eigenstates of $T+V_L$ at energies e_i, say,

$$\text{i.e.} \quad (T + V_L)\, w_i^1 = e_i\, w_i^1 \ ,$$

then $$(T + V_L + e_A)\, \Omega = E\, \Omega$$

$$\text{implies} \quad \langle w_i^1 | T + V_L | \Omega\rangle = \langle w_i^1 | E - e_A | \Omega\rangle \ ,$$

ie. $e_i \langle w_i^1 | \Omega \rangle = (E - e_A) \langle w_i^1 | \Omega \rangle$

so $E \neq e_A + e_i$ implies $\langle w_i^1 | \Omega \rangle = 0$, the orthogonality conditions.

This phenomenom, which I call 'natural orthogonality', occurs when the scattering nucleon is subject to approximately the same collective forces as are the nucleons internal to the nucleus. This is true to some approximation : whether it occurs accurately in fact must be examined in particular cases. One way is to find the commutator $[P_A, H_L] = P_A H_L - H_L P_A$. If this is zero or small, then as P_A & H_L commute they have a common set of eigenvectors. That is, the eigenvectors w_i^1 of P_A are then eigenstates of the Hamiltonian H_L for some eigenenergy, e_i say.

If P_A & H_L do commute, and the scattering states are 'naturally orthogonal' to the fully blocked states, then even the OCM orthogonality conditions become redundant. The sufficient wave equation for Ω is finally just $H_L \Omega = E \Omega$, in which all terms are strictly local. This is what is presumed when fitting local optical potentials to nucleon scattering data.

One warning about 'natural orthogonality' : it is only useful when the scattering energy $E-e_A$ is well separated from any energy levels e_i of the fully blocked states. Presumably all the e_i would be negative, being approximately the eigen-energies of the core nucleons. The scattering energy $E-e_A$ is usually at least positive, so all is well; but should inelastic doorway excitations occur, then $E-e_A$ will become negative. The actual energy levels could be checked, but it would probably be safer to include the OCM conditions explicitly in any such marginal cases.

Chapter 4 Elastic Deuteron Scattering with Antisymmetrisation

After having discussed in Chapter 3 the case of a single nucleon outside a core of many indistinguishable nucleons, we now consider the case of two distinguishable nucleons outside a nucleus. It will be found that two-particle antisymmetrisation effects are naturally larger than those for one-particle scattering, basically because of the variable partitioning of the total energy between the two nucleons. This will be demonstrated in section 4.1 for the ideal case of all states being harmonic-oscillator states. The actual physical situation is of course more complicated, so in section 4.2 the full Hamiltonian for the whole nucleus-plus-2-nucleon system is written down. This Hamiltonian is then averaged, in a fully Hermitian and symmetric manner, over the state of the nucleus, presumed known, to leave an effective three-body Hamiltonian for the general motion of two nucleons outside a core. Section 4.3 goes on to find a wave equation for these two particles' joint wave function in configuration space $\Omega_2(\underline{r}_p,\underline{r}_n)$ for a neutron at $\underline{r}_n$ and a proton at $\underline{r}_p$.

This joint wave function still includes all deuteron reactions : it includes bound deuterons with the form $\phi_d(\underline{r})\ u_d(\underline{R})$, neutron-transfer channels $\phi_n(\underline{r}_n)\ u_p(\underline{r}_p)$ with bound neutrons, proton-transfer channels $\phi_p(\underline{r}_p)\ u_n(\underline{r}_n)$, and breakup states $u_n(\underline{r}_n)\ u_p(\underline{r}_p)$. (The ϕ's denote normalised bound states, and the u's scattering states.) The simplest deuteron reaction is elastic scattering, for which it seems Ω_2 need only include $\phi_d(\underline{r})\ u_d(\underline{R})$. Section 4.4 investigates the work of Pong & Austern(1975) in finding the effect of core-deuteron antisymmetrisation on elastic scattering with $\Omega_2 = \phi_d\ u_d$ only. This is done in some detail to see specifically the nature of the assumptions made.

4.1 Estimates using Harmonic-Oscillator States

The Pauli Principle implies that two indistinguishable nucleons may not occupy the same quantum-mechanical state. In the scattering of deuterons on nuclei, this means that the neutron in the deuteron must not overlap any of the states of the neutrons in the nucleus, and the proton similarly. To compare the wave functions of the scattering nucleons with those of the nucleons in the target, however, the states of the incoming nucleons have to found in terms of $\underline{r}_n$ & $\underline{r}_p$ (coordinates with respect to the nucleus centre of mass), instead of in terms of $\underline{r}$, the internal p-n coordinate of the deuteron, and $\underline{R}$, the distance between the clusters collectively. If the nucleus is much heavier than the deuteron, we have immediately $\underline{r} = \underline{r}_p - \underline{r}_n$ and $\underline{R} = \frac{1}{2}(\underline{r}_p + \underline{r}_n)$, but it is more difficult to find the 'core state' of a scattering nucleon, given only that it is in a deuteron with internal state $\phi_d(\underline{r})$ that is moving as a whole with wave function $u_d(\underline{R})$. In Chapter 5 we will investigate overlap expressions like $\langle\phi_n|\,\phi_d\rangle\, u_d$ for specific neuteron states $\phi_n(\underline{r}_n)$, and find that they are in general complicated integral-operator expressions. However, if both the states ϕ_d & u_d were eigenstates $|nl\rangle$ & $|NL\rangle$ respectively of simple harmonic oscillators with length constants 'b' in the ratio 2:1, then an exact transformation of states is possible.

Given the approximation that the relative p-n state of the deuteron ϕ_d is the s.h.o. state $|nl\rangle$ for some quantum numbers nl (most likely n=l=0), and that the collective deuteron - core state u_d is $|NL\rangle$ for some N & L, we can use a Moshinsky transformation (Brody & Moshinsky, 1960) to find the amplitudes of the s.h.o. neutron states

$|n_1 l_1\rangle$ and of the proton states $|n_2 l_2\rangle$ (defined to the nucleus' c.m.). Each pair has a certain numerical amplitude $\langle n_1 l_1\ n_2 l_2\ J\rho|\ nl\ NL\ J\rho\rangle$:

$$|nl\ NL\ J\rho\rangle = \sum_{\substack{n_1 l_1 \\ n_2 l_2}} \langle n_1 l_1\ n_2 l_2\ J\rho|\ nl\ NL\ J\rho\rangle\ |n_1 l_1\ n_2 l_2\ J\rho\rangle$$

where

$$\rho = 2n_1+l_1 + 2n_2+l_2 = 2n+l + 2N+L$$

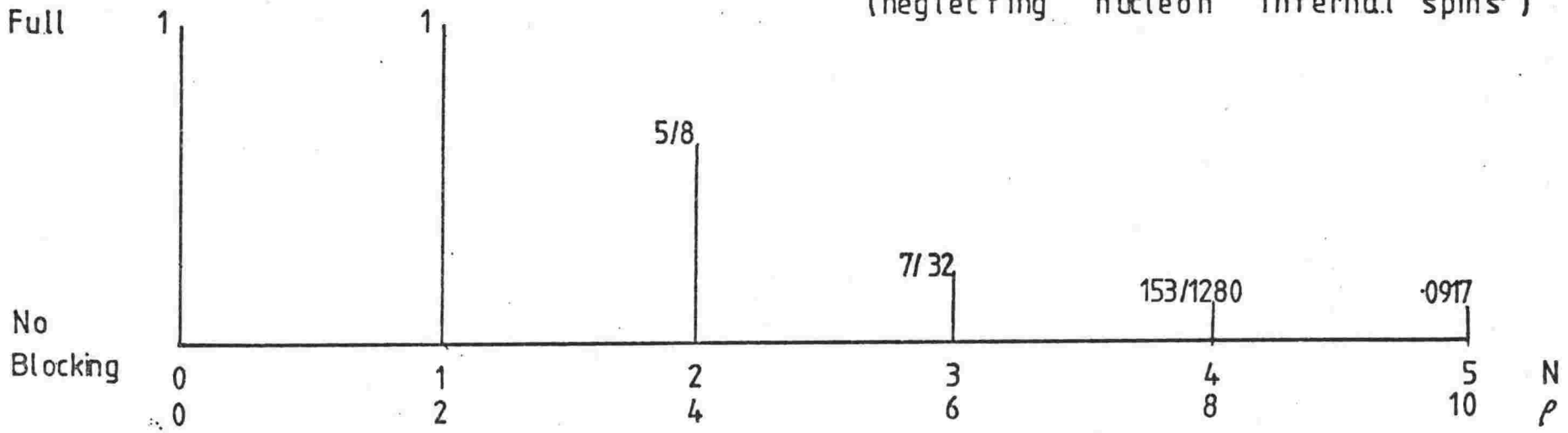
is the total excitation quantum number

and J is the total angular momentum (neglecting spins).

It is now a simple matter to modify this combined state to take the Pauli Principle into account: we just omit from the above sum for $|nl\ NL\rangle$ all those terms $n_1 l_1\ n_2 l_2$ in which either the neutron state $n_1 l_1$ or the proton state $n_2 l_2$ is already occupied by a core nucleon of the same kind. If for example the target nucleus were ^{16}O with its 0s & 0p shells full for both protons & neutrons, then the above sum would be for all $n_1 l_1\ n_2 l_2$ except for either $n_1 l_1$ or $n_2 l_2$ being 00 or 01. If the deuteron internal state ϕ_d is assumed to be exactly $|00\rangle$, then we can calculate the numerical effect of the Pauli Principle for a variety of collective states $|NL\rangle$. Figure 4.1.1 shows the sums of the squares of the removed components, versus $N = 0,1, \ldots ,5$, for $L=0$ and $L=2$. The deuteron's energy increases as $\rho = 2N+L$ above the lowest 0s bound eigenstate, with the scattering continuum $E > 0$ beginning around $\rho=4$.

These results show that even when the core is a simple set of closed shells with no configuration mixing, there is a significant Pauli blocking effect of deuteron states well into the continuum. This is in distinct contrast to the effect of the Pauli Principle on single-particle scattering states. Indeed, the blocking of such single-particle states, using the harmonic oscillator approximation, is exactly zero, because in the harmonic oscillator all states at

FIGURE 4·1·1 Blocking of deuterons by full 0s & 0p shells (i.e. by ^{16}O)
(neglecting nucleon internal spins)

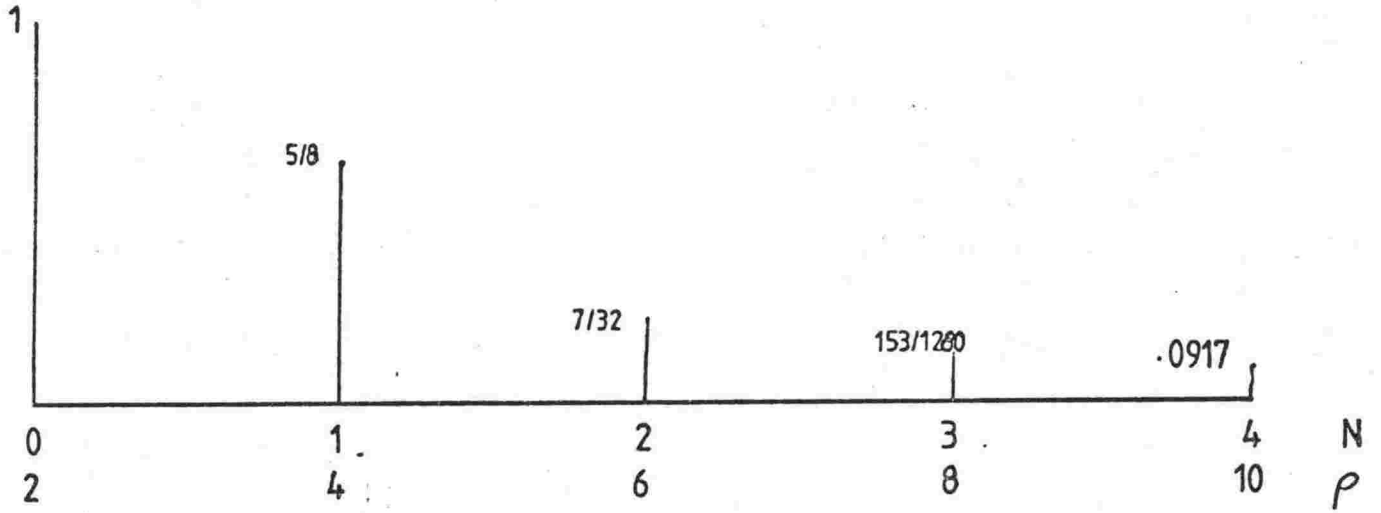


L = 0 s - states J = 2

Deuteron internal state is n=0, l=0

so

$\rho = 2N + L$



L = 2 d - states J = 2

different energies are exactly orthogonal. The energy of a deuteron scattering state, by contrast, is only the average of the neutron and proton energies : one nucleon can go up in energy if the other goes down by the same amount. And as soon as either nucleon would try to drop in energy as far as an occupied shell, that whole pair component is blocked by the Pauli Principle.

This fact - that two-particle antisymmetrisation effects are naturally larger than those for one particle scattering - persists when more realistic scattering states are used. It also allows us very conveniently to make more severe simplifying assumptions and still have non-trivial effects that specifically result from anti-symmetrisation. It becomes practicable, for example, to assume that the internal nucleons of the core move in eigenstates of the potential that governs the scattering of a further nucleon around the core. The widely-used Hartree-Fock approximation assumes all the internal nucleons are in eigenstates of the same potential, but here the additional assumption is that this collective potential is the same for the 'A' core nucleons and the 'A+1' nucleon system, including the scattering nucleon. With single-particle scattering, this assumption would mean no specific antisymmetrisation effects, since all nucleon states would be eigenstates of the same potential, but at different energies and hence all naturally orthogonal to each other. Not so, however, with the scattering of multi-nucleon clusters, for as explained above, there is Pauli blocking even if only one nucleon drops in energy to the occupied levels of the core. This is quite likely, as the energy of a cluster is only the average of its single-nucleon energies.

4.2 Antisymmetrised Matrix Elements for Deuteron - Core Interactions

In this section, formulae are derived for the matrix elements of realistic Hamiltonians, when fully antisymmetrised wave functions are used to describe the state of a proton and a neutron outside an inert core of both protons and neutrons. In sections 4.2 & 4.3 the external pair of nucleons will be described only by their joint wave function $u_2(\underline{r}_p,\underline{r}_n)$, so to begin with we will derive a three-body Hamiltonian H_2 for those 2 nucleons interacting with the core.

The total model state P for the system is defined by the form

$$P\Psi(\underline{r}_p,\underline{r}_n,\underline{r}_1 \cdot\cdot \underline{r}_A) = |\mathcal{A}_{2-A}\ u_2(\underline{r}_p,\underline{r}_n)\ \phi_A(\underline{r}_1 \cdot\cdot \underline{r}_A)>$$
$$\equiv |\mathcal{A}_{2-A} \cdot \phi_A> \ u_2 \text{ , an abbreviated notation,}$$

where

$\phi_A(\underline{r}_1 \cdot\cdot \underline{r}_A)$ is the core state of the 'A' nucleons. The ϕ_A wave function is assumed to be already antisymmetrised.

The $\mathcal{A}_{2-A}$ is the antisymmetrising operator between the external neutron and proton and their indistinguishable corresponding nucleons in the core.

If the core consists of 'N' neutrons and 'Z' protons, A = N + Z, then

$$P\ (\underline{r}_p,\underline{r}_n,\underline{r}_{n_1} \cdot\cdot \underline{r}_{n_N},\underline{r}_{p_1} \cdot\cdot \underline{r}_{p_Z})$$
$$= |\mathcal{A}_{2-NZ}\ u_2(\underline{r}_p,\underline{r}_n)\ \phi_{NZ}(\underline{r}_{n_1} \cdot\cdot \underline{r}_{n_N},\underline{r}_{p_1} \cdot\cdot \underline{r}_{p_Z})>$$

where

$$\mathcal{A}_{2-NZ} = (N+1)^{-\frac{1}{2}}\left(1 - \sum_{i=1}^{N} P_{ni}\right)(Z+1)^{-\frac{1}{2}}\left(1 - \sum_{j=1}^{Z} P_{pj}\right),$$

P_{ni} exchanges the $\underline{r}_n$ coordinate with $\underline{r}_{n_i}$, that of the i'th neutron in the core,

and P_{pj} exchanges proton coordinates $\underline{r}_p$ & $\underline{r}_{p_j}$ similarly.

The Hamiltonian H for the full system of N+1 neutrons and Z+1 protons has been given in section 2.2 . We now wish to calculate antisymmetrised matrix elements of H, such as $\langle \phi_{NZ} | H | \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle$ or $\langle \mathcal{A}_{2-NZ} \cdot \phi_{NZ} | H | \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle$, for both the one-particle operators (ie. the kinetic energy operators T(r)) and the two-particle operators (ie. the internucleon potentials V(r,r')) that occur in H.

The simplest matrix element is the 'zero-particle' overlap integral $1-K_2 \equiv \langle \phi_{NZ} | \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle$, as appears, for example, in

$$\begin{aligned} U_2(\underline{r}_p,\underline{r}_n) &= \langle \phi_{NZ} | \mathcal{A}_{2-NZ}\ u_2(\underline{r}_p,\underline{r}_n)\ \phi_{NZ} \rangle \\ &= \langle \phi_{NZ} | \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle\ u_2 \\ &= (1 - K_2)\ u_2 . \end{aligned}$$

This defines the two-particle operator K_2 for the Feshbach theory, a generalisation of the one-particle K operator of section 3.1.

Using the definition of $\mathcal{A}_{2-NZ}$ given above, explicit calculation of $U_2(\underline{r}_p,\underline{r}_n)$ yields

$$\begin{aligned} U_2(\underline{r}_p,\underline{r}_n) = u_2(\underline{r}_p,\underline{r}_n) &- \int K_n(\underline{r}_n,\underline{r}'_n)\ u_2(\underline{r}_p,\underline{r}'_n)\ d\underline{r}'_n \\ &- \int K_p(\underline{r}_p,\underline{r}'_p)\ u_2(\underline{r}'_p,\underline{r}_n)\ d\underline{r}'_p \\ &+ \iint K_{np}(\underline{r}_n,\underline{r}_p;\ \underline{r}'_n,\underline{r}'_p)\ u_2(\underline{r}'_p,\underline{r}'_n)\ d\underline{r}'_n\ d\underline{r}'_p , \end{aligned}$$

where

K_n & K_p are the one-particle density operators for neutrons & protons (resp.) in the core state ϕ_{NZ} : see section 2.1,

and K_{np} is the two particle density operator for neutrons & protons jointly.

If the neutron and proton motions in the core are uncorrelated, then K_{np} factorises simply, giving

$$K_{np}(\underline{r}_n,\underline{r}_p;\ \underline{r}'_n,\underline{r}'_p) = K_n(\underline{r}_n,\underline{r}'_n)\ K_p(\underline{r}_p,\underline{r}'_p),$$

so $U_2 = (1 - K_n)\ (1 - K_p)\ u_2$.

That is, $1 - K_2 = (1 - K_n)(1 - K_p)$, where both sides operate on arbitary 2-particle states of the form $u_2(\underline{r}_p, \underline{r}_n)$.

The next simplest matrix element is the explicitly Hermitian form $\langle \mathcal{A} \cdot \phi_A \mid \mathcal{A} \cdot \phi_A \rangle$, as appears for example in the expression

$$\begin{aligned} \|P\Psi\|^2 &= \langle P\Psi \mid P\Psi \rangle \\ &= \langle \mathcal{A} u_2 \phi_A \mid \mathcal{A} u_2 \phi_A \rangle \\ &= \langle u_2 \mid \langle \mathcal{A} \cdot \phi_A \mid \mathcal{A} \cdot \phi_A \rangle \mid u_2 \rangle \ . \end{aligned}$$

Detailed calculations show that this form is equal to the first one:

$$\langle \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \mid \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle = 1-K_2 = (1-K_n)(1-K_p) \ .$$

When we consider a one-particle operator, the two kinds of matrix elements of $T_p(\underline{r}_p)$, say, are first

$$\langle \phi_{NZ} \mid T_p(\underline{r}_p) \mid \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle = T_p(\underline{r}_p)\ (1-K_2) \ .$$

Unfortunately this result is not Hermitian, as in general $(1-K_2)T_p \neq T_p(1-K_2)$ because T_p & K_p do not necessarily commute. It would be better if the matrix element were clearly Hermitian, as then probabilities and fluxes are explicitly conserved. To this end, I prefer using the second form of matrix element $\langle \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \mid T_p \mid \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle$ which, although more complicated algebraically, is always Hermitian whether or not K_p & T_p commute.

This Hermitian matrix element of $T_p(\underline{r}_p)$ becomes after detailed calculation (and after assuming $K_{np} = K_n K_p$ again)

$$\begin{aligned} &\langle \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \mid T_p(\underline{r}_p) \mid \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle \\ &= \frac{1}{Z+1} \left[T_p - K_p T_p - T_p K_p + \mathrm{Tr}(T_p K_p) - \mathrm{Tr}_2(T_p K_{pp}) \right] (1-K_n) \end{aligned}$$

where $Tr(T_p K_p) = \int T_p(\underline{r}_p)\, K_p(\underline{r}_p, \underline{r}_p)\, d\underline{r}_p$,

the kinetic energy of protons in the core,

$$Tr_2(T_p K_{pp}) = \int T_p(\underline{r}_p)\, K_{pp}(\underline{r}, \underline{r}_p; \underline{r}', \underline{r}_p)\, d\underline{r}_p ,$$

and K_{pp} is the two-proton density matrix :

$$K_{pp}(\underline{r}_1, \underline{r}_2; \underline{r}_1', \underline{r}_2') = Z(Z-1) \langle \phi_{NZ}(.., \underline{r}_{n_N}, \underline{r}_1', \underline{r}_2' ..) | \phi_{NZ}(.. \underline{r}_{n_N}, \underline{r}_1, \underline{r}_2 ..) \rangle,$$

integrating over $\underline{r}_{p_3}, .. \underline{r}_{p_Z}$ and all the $\underline{r}_{n_i}$, i=1 .. N.

The matrix element may be simplified again if the proton motions in the core have no correlations beyond those required by the Pauli Principle, as then K_{pp} factorises in an antisymmetric fashion:

$$K_{pp}(\underline{r}_1, \underline{r}_2; \underline{r}_1', \underline{r}_2') = K_p(\underline{r}_1, \underline{r}_1')\, K_p(\underline{r}_2, \underline{r}_2') - K_p(\underline{r}_1, \underline{r}_2')\, K_p(\underline{r}_2, \underline{r}_1').$$

The matrix element of $T_p(\underline{r}_p)$ becomes

$$\frac{1}{Z+1} \left(T_p - T_p K_p - K_p T_p + Tr(T_p K_p) - K_p Tr(T_p K_p) + K_p T_p K_p \right) (1-K_n)$$

$$= \frac{1}{Z+1} \left((1-K_p) T_p (1-K_p) + Tr(T_p K_p)\, (1-K_p) \right) (1-K_n) .$$

The above assumption of independent motion in the core is equivalent to assuming that ϕ_{NZ} is a product of proton & neutron Slater-determinant states, i.e. that K_n & K_p and hence K_2 are projection operators. If K_p is a projection operator $(1-K_p) = (1-K_p)^{\frac{1}{2}}$, so under the same assumption the matrix element becomes

$$\frac{1}{Z+1} \left((1-K_p)^{\frac{1}{2}}\, T_p\, (1-K_p)^{\frac{1}{2}} + Tr(T_p K_p)\, (1-K_p) \right) (1-K_n)$$

$$= \frac{1}{Z+1} (1-K_2)^{\frac{1}{2}} \left(T_p + Tr(T_p K_p) \right) (1-K_2)^{\frac{1}{2}} .$$

The advantage of this $(1-K)^{\frac{1}{2}}$ reformulation is that although it is exact for K_p a projection operator, it is also consistent with the original matrix-element expression in the limit T_p a scalar : both this reformulation and $\langle \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \mid T_p \mid \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle$ become equal to just $t(1-K_2)$ in the limit $T_p = t$, for t any scalar. This result holds

for any K_p, and is independent of whether or not K_p & T_p commute.

A consistent approximation for $\langle \mathcal{A}_{2-NZ}\cdot\phi_{NZ} \mid T_n(\underline{r}_n) \mid \mathcal{A}_{2-NZ}\cdot\phi_{NZ}\rangle$ would by analogy be

$$\frac{1}{N+1}\ (1-K_2)^{\frac{1}{2}} \left[T_n(\underline{r}_n) + \mathrm{Tr}(T_nK_n)\right]\ (1-K_2)^{\frac{1}{2}} .$$

Similar $(1-K)^{\frac{1}{2}}$ approximations are available for two-particle operators such as $V_{pp}(\underline{r}_p,\underline{r}'_p)$, $V_{nn}(\underline{r}_n,\underline{r}'_n)$, and $V_{np}(\underline{r}_n,\underline{r}_p) = V_{pn}(\underline{r}_p,\underline{r}_n)$. The matrix element of V_{pp} is, for example, after considerable algebra

$$\langle \mathcal{A}_{2-NZ}\cdot\phi_{NZ} \mid V_{pp}(\underline{r}_p,\underline{r}'_p) \mid \mathcal{A}_{2-NZ}\cdot\phi_{NZ}\rangle$$

$$= \frac{2}{Z(Z+1)} \left[(1-K_p)\ V_a(p)\ (1-K_p) + \mathrm{Tr}_{12}(V_{pp}K_{pp})\ (1-K_p)\right]\ (1-K_n)$$

where $V_a(p) = \mathrm{Tr}(V_{pp}(\underline{r}_p,)K_p) - (V_{pp}\cdot K_p)$

the antisymmetrised proton-to-core potential,

$\mathrm{Tr}(V_{pp}(\underline{r}_p,)K_p) = \int V_{pp}(\underline{r}_p,\underline{r}'_p)\ K_p(\underline{r}'_p,\underline{r}'_p)\ d\underline{r}'_p$

the direct part of the proton-core potential (local),

$(V_{pp}\cdot K_p)u = \int V_{pp}(\underline{r}_p,\underline{r}'_p)\ K_p(\underline{r}_p,\underline{r}'_p)\ u(\underline{r}'_p)\ d\underline{r}'_p$

the non-local exchange part of the potential,

and $\mathrm{Tr}_{12}(V_{pp}K_{pp}) = \iint V_{pp}(\underline{r}_p,\underline{r}'_p)\ K_{pp}(\underline{r}_p,\underline{r}'_p;\ \underline{r}_p,\underline{r}'_p)\ d\underline{r}_p\ d\underline{r}'_p$

the attraction between two protons both in the core.

By assuming $(1-K_p) = (1-K_p)^{\frac{1}{2}}$ as explained earlier, this becomes

$$\frac{2}{Z(Z+1)}\ (1-K_2)^{\frac{1}{2}} \left[V_a(p) + \mathrm{Tr}_{12}(V_{pp}K_{pp})\right]\ (1-K_2)^{\frac{1}{2}} .$$

A derivation along these lines of the matrix element of V_{pn} gives

$$\frac{1}{(N+1)(Z+1)}\ (1-K_2)^{\frac{1}{2}} \left[V_{pn} + \mathrm{Tr}_n(V_{pn}K_n) + \mathrm{Tr}_p(V_{pn}K_p) + \mathrm{Tr}_{np}(K_pV_{pn}K_n)\right]\ (1-K_2)^{\frac{1}{2}} .$$

Using these $(1-K_2)^{\frac{1}{2}}$ matrix elements for T(r) and V(r,r'), the total Hamiltonian H of section 2.2 has the fully antisymmetrised and explicitly Hermitian matrix element

$$\langle \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \,|\, H \,|\, \mathcal{A}_{2-NZ} \cdot \phi_{NZ} \rangle$$

$$= (1-K_2)^{\frac{1}{2}} \Big[T_p(\underline{r}_p) + V_a(p) + T_n(\underline{r}_n) + V_a(n) + V_{pn}(\underline{r}_p, \underline{r}_n) + e_A \Big] (1-K_2)^{\frac{1}{2}},$$

where $V_a(p)$ & $V_a(n)$ are the antisymmetrised single-particle potentials from the core to the proton & neutron respectivley,

and e_A is the constant energy internal to the core, $H_A \phi_{NZ} = e_A \phi_{NZ}$,

$$e_A = Tr_p(T_p K_p) + Tr_n(T_n K_n) + Tr_{12}(V_{nn} K_{nn}) + Tr_{12}(V_{pp} K_{pp}) + Tr_{12}(K_p V_{pn} K_n) .$$

This form should be familar, as when antisymmetrisation is not taken into account the only changes are the $(1-K_2)^{\frac{1}{2}}$ factors being unity and $V_a(p)$ & $V_a(n)$ being entirely local potentials.

The effects of antisymmetrisation, according to the more complete analysis presented here, are therefore of two kinds. First, they result in the individual nucleon-to-core potentials having non-local components. The existence of the non-local exchange terms has long been known, but it is found that local equivalent potentials (see section 2.6) often exist which accurately reproduce the same cross-sections. The 'kinematic assumption' of section 3.2 assumes local approximations V_p & V_n to $V_a(p)$ & $V_a(n)$ respectively, so the only efffect of antisymmetrisation is of the second 'kinematic' kind: the existence of the $(1-K_2)^{\frac{1}{2}}$ factors.

4.3 Wave Equations for two particles outside the core

In the previous section, it was shown that the total Hamiltonian for the neutron-plus-proton-plus-core system has a fully-antisymmetrised and explicitly Hermitian matrix element of the form

$$(1-K_2)^{\frac{1}{2}} \; H_2 \; (1-K_2)^{\frac{1}{2}}$$

where $H_2 = T_p+V_n + T_n+V_n + V_{np} + e_A$,

V_p & V_n are the full $V_a(p)$ & $V_a(n)$ or some other equivalent,

$1-K_2 = (1-K_p)(1-K_n)$,

and the whole expression operates on 2-particle joint wave functions of the form $u_2(\underline{r}_p,\underline{r}_n)$.

The operator $1-K_2$ may now be divided into two parts

$$1-K_2 = (1-P_2)\,(1-K_2')$$

where P_2 is the projection operator onto those vectors that $1-K_2$ blocks fully,

and K_2' is the remaining part of K_2 : $K_2' = K_2 - P_2$.

That is, exact in analogy with the single-particle case of section 3.1, if in an eigenvalue expansion

$$K_2 = \sum_i |w_i\rangle \lambda_i \langle w_i| \text{ , with } \{w_i\} \text{ an orthonormal set,}$$

then $$P_2 = \sum_{\lambda_i=1} |w_i\rangle\langle w_i| \quad \text{and} \quad K_2' = \sum_{\lambda_i\neq 1} |w_i\rangle \lambda_i \langle w_i| \;,$$

so $K_2 = P_2 + K_2'$ and $P_2K_2' = 0$. The P_2 is a projection operator, so $P_2 \cdot P_2 = P_2$ and $P_2^{\frac{1}{2}} = P_2$. The square-root operator $(1-K_2)^{\frac{1}{2}}$ is defined by $(1-K_2)^{\frac{1}{2}} = \sum_i |w_i\rangle(1-\lambda_i)^{\frac{1}{2}}\langle w_i|$. If the neutron and proton motions in the core are independent, then $1-P_2$ factorises to $(1-P_n)(1-P_p)$ where both P_n and P_p are projection operators with $P_2 = P_n + P_p - P_nP_p$.

Schrodinger's equation for the deuteron-plus-core system at energy 'E' is

$$\left[H - E \right] \, | \mathcal{A}_{2\text{-}NZ} \; u_2(\underline{r}_p, \underline{r}_n) \; \phi_{NZ} > = 0 \; .$$

Thus

$$< \mathcal{A}_{2\text{-}NZ} \cdot \phi_{NZ} \; | \; H - E \; | \; \mathcal{A}_{2\text{-}NZ} \cdot \phi_{NZ} > \; u_2(\underline{r}_p, \underline{r}_n) \; = \; 0,$$

so

$$(1-K_2)^{\frac{1}{2}} \left[H_2 - E \right] (1-K_2)^{\frac{1}{2}} \; u_2(\underline{r}_p, \underline{r}_n) \; = \; 0 \; ,$$

or

$$(1-K_2')^{\frac{1}{2}}(1-P_2) \quad H_2 - E \quad (1-P_2)(1-K_2')^{\frac{1}{2}} \; u_2 \; = \; 0 \; .$$

Proceeding as in the single-particle case of section 3.1, we absorb K_2' (the partially-blocking part of K_2) into a wave function redefinition, and leave the totally-blocking part P_2 to put orthogonality conditions into the channel equations :

$$(1-P_2) \left[H_2 - E \right] (1-P_2) \; \Omega_2(\underline{r}_p, \underline{r}_n) \; = \; 0,$$

where

Ω_2 is defined by $\Omega_2 = (1-K_2')^{\frac{1}{2}} \; u_2$,

and the division by $(1-K_2')^{\frac{1}{2}}$ is always possible as K_2' has no unit eigenvalues, by construction.

The P_2 is a projection operator, so the above equation projects Ω_2 onto the not-totally-forbidden subspace $P_2 \Omega_2 = 0$ before applying the channel Hamiltonian. However, an equation of the form $(1-P)\left[H-E\right](1-P)f = 0$ does not (yet) remove the forbidden components from the wave function : the above equation does <u>not</u> imply $Pf=0$, it only nullifies the effect of such components for the Hamiltonian. It is possible nevertheless, to construct another, related, equation for $f' \equiv (1-P)f$ which has all the forbidden components specifically removed : $\left[H - E - PH \right] f' = 0$ implies $Pf'=0$ for $E \neq 0$.

Applying this construction to the equation for Ω_2, we get

$$\left[H_2 \; - \; E \; - \; P_2 . H_2 \right] \Omega_2(\underline{r}_p, \underline{r}_n) \; = \; 0.$$

From this equation, by premultiplying by P_2, and by assuming E is not exactly zero, we can easily prove $P_2\Omega_2=0$. And then, if $P_2 = P_n + P_p - P_nP_p$, $P_n\Omega_2 = P_p\Omega_2 = 0$ can be proved too.

Expanding $H_2 = H_p(\underline{r}_p) + H_n(\underline{r}_n) + V_{np}(\underline{r}_p-\underline{r}_n) + e_A$, we can get

$$\left(H_p + H_n + V_{np} + e_A - E\right)\Omega_2 - P_2\left(H_p + H_n + V_{np}\right)\Omega_2 = 0,$$

which leads to $P_2\Omega_2=0$ provided $E \neq e_A$. The first term is that usually taken to describe deuteron interactions with a core nucleus; the second term is a specific effect of antisymmetrisation. It is an additional effective potential (often called the 'Saito Potential') that forces the orthogonality of any solution Ω_2 to the fully-blocked vectors $|w_i^1\rangle$ ($\lambda_i=1$) that constitute P_2 : $P_2\Omega_2=0$.

In numerically solving the system of coupled differential equations like that above, one would more readily use the direct orthogonalising technique described in section 2.5 than use the full Saito potential in the form above. But knowing that form can be useful, as in the next section, for example, it will be simplified considerably in the case of elastic scattering only, and then the resulting expression will be found to be more useful as a perturbing potential than as one that forces orthogonality conditions.

4.4 Elastic Deuteron Scattering

The previous section derived an equation for the general motion of a neutron and a proton outside a core nucleus, including anti-symmetrisation with the core nucleons. In this section, a channel equation is derived for the relative motion of the deuteron to the core when they interact only elastically. If $\underline{R}$ is the coordinate distance between their centres of mass, then we will be considering components $\phi_d(\underline{r})\ u_d(\underline{R})$ of the general joint wave function $\Omega_2(\underline{r}_p,\underline{r}_n)$, where $u_d(\underline{R})$ is the cluster-to-cluster relative wave function.

To derive a channel equation in $\underline{R}$ that is sufficient to determine $u_d(\underline{R})$, we project the equation of Ω_2 onto the deuteron's internal state:

$$\int d\underline{r}\ \phi_d(\underline{r})^*\ (1-P_2)\ [H_2 - E]\ (1-P_2)\ \Omega_2 = 0,$$

where, as explained in sections 2.2 and 4.3, the orthogonality condition $P_2\Omega_2=0$ may be used to remove any supererogatory components in Ω_2. With elastic scattering only, $\Omega_2 = \phi_d\ u_d$, so

$$\langle \phi_d | (1-P_2)\ [H_2-E]\ (1-P_2) | \phi_d \rangle\ u_d(\underline{R}) \ = \ 0\ .$$

There are at least three ways of treating this sort of channel equation:

(1) One way is to expand it in full, using $1-P_2 = (1-P_n)(1-P_p)$ and the eigenvalue expansions $P_n = \Sigma_i\ |\phi_{ni}\rangle\langle\phi_{ni}|$ & $P_p = \Sigma_j\ |\phi_{pj}\rangle\langle\phi_{pj}|$ for the neutron & proton projection operators respectively. This is done in section 6.2, and will be seen there to lead to a great many terms in a complicated final result.

(2) A second method is to approximate

$$\langle\phi_d|(1-P_2)\,[H_2-E](1-P_2)\,|\phi_d\rangle$$

by $\langle\phi_d|1-P_2|\phi_d\rangle^{\frac{1}{2}}\,[H_d(\underline{R}) + e_d + e_A - E]\langle\phi_d|1-P_2|\phi_d\rangle^{\frac{1}{2}} + H_{res}$

and then by

$$\langle\phi_d|1-P_2|\phi_d\rangle^{\frac{1}{2}}\,[H_d(\underline{R}) + V_{res} + e_d + e_A - E]\,\phi_d\,|1-P_2|\phi_d\rangle^{\frac{1}{2}}\,.$$

This "square-root approximation" will be examined in more detail in sections 5.5 & 6.1 in the context of orthogonalisation to specific neutron states. It has the advantage that many of the orthogonalising effects can be absorbed by redefining the wave function $u_d(\underline{R})$.

(3) A third method is that of Pong & Austern(1975), and is now investigated in more detail. It uses the orthogonality condition $P_2\Omega_2=0$ (ie. $P_2\phi_d u_d=0$) to simplify $\langle\phi_d|(1-P_2)[H_2-E](1-P_2)|\phi_d\rangle\ u_d = 0$. They get therefore

$$\langle\phi_d|(1-P_2)\,[H_p + H_n + V_{np} + e_A - E]\,|\phi_d\rangle\,u_d(\underline{R}) = 0.$$

They next assume that H_p & H_n commute with P_2, ie. that the scattering and core nucléons move in the same collective potential. This is not unreasonable, as explained in section 4.1, so

$$\langle\phi_d|[H_p + H_n + (1-P_2)V_{np} + e_A - E]|\phi_d\rangle\ u_d = 0,$$

ie. $$\langle\phi_d|[H_2 - P_2V_{np} - E]|\phi_d\rangle\,u_d = 0,$$

ie. $$[T_d + W_d - \langle\phi_d|P_2V_{np}|\phi_d\rangle - E_d]\ u_d(\underline{R}) = 0,$$

where $W_d(\underline{R})$ is the deuteron folded potential - see section 2.1,

and $E_d=E-e_A-e_d$ is the deuteron incident energy in the cm. frame.

The effect of antisymmetrisation is the positive correction $-\langle\phi_d\,|\,P_2V_{np}\,|\,\phi_d\rangle$ to the deuteron's folded potential W_d. As it

stands, $-\langle \phi_d | P_2 V_{np} | \phi_d \rangle$ is non-local and not Hermitian, but after some effort Pong & Austern find a local approximation for it (by a method outlined in my section 2.6), so that it may be very conveniently added to the folded potential as a second-order correction to the shape of the potential well.

They find that the local equivalent to the correction term reduces by about 10 Mev the depth of the potential well for d - ^{16}O scattering around 5 to 20 Mev incident energy, and has a radial dependence very similar to that of the nuclear density. This sort of correction to the folded potential is approximately that shown to be necessary by Perey & Satchler(1967), who calculate for each of a wide range of nuclei the folded potentials W_d, and compare these with the optical potentials obtained directly from the observed deuteron - nucleus elastic scattering data. They consistently find for the optical potential two well depths at $78^{\pm 2}$ & $110^{\pm 2}$ Mev that equally well match the experimental data : the two wells differ by an integer in the number N (cf. section 4.1) of oscillations of the deuteron wave function in the inner region. Unfortunately for the folding model, the calculated folded potentials W_d fall almost midway between these two sets of optimum depths, so the folding model theory cannot decide between them. From their data, Perey & Satchler "may be able to deduce the magnitude of the higher-order corrections ($\simeq$ 20 Mev) to the model, but not their sign." With the result of Pong & Austern that the second-order corrections they calculated are repulsive about 10 Mev, they have clearly accounted for part of the discrepancy, and point towards the shallower optical well as being more realistic.

This general agreement with experiment of Pong & Austern's second-order correction is very encouraging, but the trouble is that two of their assumptions are mutually inconsistent! They assumed that the orthogonality condition $P_2\Omega_2=0$ could still be held in the restricted model space $\Omega_2 = \phi_d\, u_d$, but this in fact is not true: $P_2\, \phi_d\, u_d = 0$ implies that u_d is zero everywhere except asymptotically! And their master equation for u_d certainly does not imply that the orthogonality condition is fulfilled, as we checked for the channel equations derived in the previous section. The only term additional to the usual local Hamiltonian is at most 5 to 10 Mev, and in retrospect we see that this additional potential is only an approximation to even the equation derived in section 4.3, even though its derivation looked reasonably rigorous.

To discover exactly how good this approximation is, we need a model space for Ω_2 in which the condition $P_2\Omega_2 = 0$ <u>can</u> hold. We will find we need to include at least transfer channels in the model space, but this brings up the problem of the non-orthogonality between deuteron and transfer channels, and in the next two chapters it will be seen how the twin problems of nonorthogonalities and antisymmetrisation are very much interrelated, and need to be treated simultaneously.

There are very definite physical reasons, which may be given in the meantime, why the magnitudes of these twin effects are of about the same magnitude, and add together. For transfer reactions involve a scattering nucleon going into an unoccupied bound state around the core, whereas the Pauli Primciple is the opposite : it requires that any scattering nucleon <u>not</u> overlap any bound state around the core if that state is already occupied. Chapter 5 shows how to deal with

the nonorthogonality of transfer channels : by orthogonalising the deuteron wave function to all the unoccupied bound states. We deal with antisymmetrisation requirements by orthogonalising the deuteron wave function to all the occupied bound states. Although the physical processes are opposite, because they are exactly opposite, the approximate magnitudes of the twin effects will depend on largely the same principles, and on largely the same features of particular reactions. It is therefore desireable that they be included in models and analyses together.

If we now go back to Pong & Austern's method, we can consider how their model space $\Omega_2 = \phi_d\ u_d$ must be extended if the orthogonality condition $P_2\Omega_2=0$ is to ever hold. Take for convenience the simplest case of a core nucleus of just one neutron, in a state $\phi_n(\underline{r}_n)$. The Pauli operator P_2 is then just $|\phi_n><\phi_n|$, and the condition $P_2\Omega_2 = 0$ becomes $\langle\phi_n|\ \Omega_2 = 0$. In the light of the physical arguments above, we may alternatively view this Pauli Principle requirement as the 'blocking' of a possible neutron transfer to the state ϕ_n. So let us include in the model a mathematical description of such a transfer :

$$\Omega_2(\underline{r}_p,\underline{r}_n) = \phi_d(\underline{r})\ u_d(\underline{R}) + \phi_n(\underline{r}_n)\ u_p(\underline{r}_p)$$

for some variable wave function $u_p(\underline{r}_p)$. The Pauli requirement is now

$$0 = <\phi_n|\Omega_2 = <\phi_n|\phi_d> u_d + u_p,$$

where, as explained in chapter 5 in detail, the nonorthogonality problem is that the overlap $<\phi_n|\phi_d> \neq 0$. The condition $u_p = -<\phi_n|\phi_d>\ u_d$ may quite reasonably hold, with both u_d and u_p non-zero in the internal and reaction regions.

Pong & Austern's model took the blocking of a neutron transfer to ϕ_n to mean that $u_p \equiv 0$ everywhere, but this cannot be true as then, because $<\phi_n|\phi_d> \neq 0$ at least internally, it would mean that u_d would be zero there. We must therefore omit not the wave function 'u_p', but some other wave function, to model the blocking of neutron transfers to a state such as ϕ_n.

In Chapter 5, we will see that as well as a u_p which multiplies ϕ_n in the expression for Ω_2, there is another proton wave function $U_p(\underline{r}_p)$ which is the projection of Ω_2 onto ϕ_n : $U_p = <\phi_n|\ \Omega_2$. The wave functions u_p & U_p are identical asymptotically, and coupled channels systems can be written down that use exclusively u_p or U_p. With the model above, a channel equation in U_p is to be prefered over one in u_p, because u_p can be non-zero even when the transfer to ϕ_n is blocked, whereas $U_p \equiv 0$ is precisely the Pauli condition $P_2\Omega_2 = 0$, as $\phi_n U_p = |\phi_n><\phi_n|\ \Omega_2$. Therefore to model the effect of antisymmetrisation on deuteron motions, one choice is to first set up a set of equations in $u_d(\underline{R})$ & $U_p(\underline{r}_p)$, and then to model the blocking by core nucleon(s) put $U_p \equiv 0$ everywhere. In this way the Pauli condition $P_2\Omega_2 = 0$ can be fulfilled exactly in the model.

The fact that the Pauli condition is not the 'multiplicative' u_p, but the 'projected' U_p being zero, means that the derivation in treatment (3) of the second-order correction $-<\phi_d|\ P_2 V_{np}|\phi_d>$ is only approximate. An assessment of its accuracy must now wait until Chapters 5 & 6, when the twin problems of antisymmetrisation and of nonorthogonalities between transfer channels are treated together in a unified manner.

Chapter 5 Effects of Channel Non-orthogonalities in Transfer Reactions

5.1 Defining the channel amplitudes

In calculating transition rates for transfer reactions, problems arise because the natural coordinates of the elastic and rearranged channels are not the same. In deuteron stripping, for example, the natural coordinates for the deuteron channels are the proton - neutron c.m. and relative coordinates, $\underline{R}$ and $\underline{r}$ respectively, whereas for the outgoing proton channels it is most natural to use the separate coordinates $\underline{r}_p$ and $\underline{r}_n$, for the distances of the proton to the residual nucleus, and of the neutron to the target nucleus, respectively. In these 'natural coordinates' for each channel, the projectile - nucleus relative wavefields appear simply as functions of the one coordinate ($\underline{R}$ or $\underline{r}_p$), and the 'internal wavefields' - the deuteron internal state $\phi_d(\underline{r})$ or the remaining neutron's state $\phi_n(\underline{r}_n)$ - appear as functions solely of the other coordinate $\underline{r}$ or $\underline{r}_n$.

To find a Schrödinger equation for any of the projectile - nucleus relative wave functions, one has to calculate overlaps of the various internal states, overlaps of the form $\langle \phi_d(\underline{r}) | \phi_n(\underline{r}_n) \rangle$, and in many calculations to date, these are usually assumed to be negligible for distinct internal states ϕ_d & ϕ_n. For transfer reactions, however, this overlap is not at all always zero. In fact, because of the way the coordinates $(\underline{R},\underline{r})$ relate to $(\underline{r}_p,\underline{r}_n)$, it is not even just a number, but an integral operator. In the case of a massive core $\underline{r}_n = \underline{R} - \frac{1}{2}\underline{r}$ and $\underline{r}_p = \underline{R} + \frac{1}{2}\underline{r}$, so the above overlap is the operator form $K_{dp} = \int d\underline{r}\ \phi_d(\underline{r})^*\ \phi_n(\underline{R}-\underline{r}/2)$. This operates on functions of $\underline{r}_p$ e.g. $u_p(\underline{r}_p)$, and gives the function of $\underline{R}$ $\int \phi_d(\underline{r})^*\ \phi_n(\underline{R}-\frac{1}{2}\underline{r})\ u_p(\underline{R}+\frac{1}{2}\underline{r})\ d\underline{r}$

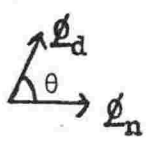
$$= \int K_{dp}(\underline{R},\underline{r}_p)\ u_p(\underline{r}_p)\ d\underline{r}_p$$

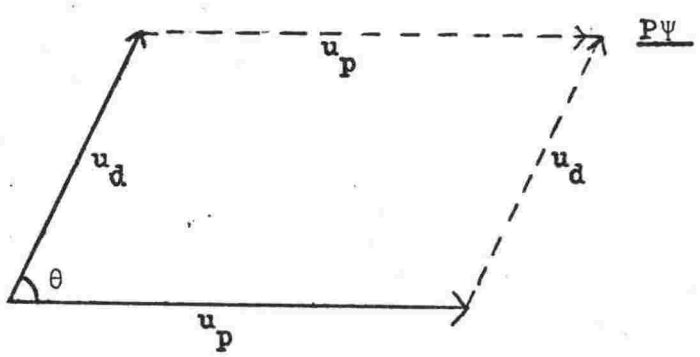
$$= K_{dp}\ u_p .$$

Although the internal wavefields ϕ_d and ϕ_n may not be orthogonal when K_{dp} (or its transpose K_{pd}) is not zero, in general they will not be linearly dependent either. That is, they are not collinear, so any state-vector has a unique expansion in terms of them, and it is possible to use a model subspace of the total three-body wavefunction Ψ of the form $P\Psi = u_d(R)\,\phi_d(\underline{r}) + u_p(\underline{r}_p)\,\phi_n(\underline{r}_n)$ for variable channel wavefunctions u_d & u_p. (As yet we consider only one deuteron and one stripping channel, and treat the target nucleus as a massive inert core.) (1)

This expansion of $P\Psi$ in terms of a basis set of the two normalised states $|\phi_d\rangle$ & $|\phi_n\rangle$, with variable channel functions u_d and u_p, is formally analogous to the expansion of an arbitary two-dimensional vector $\underline{P\Psi}$ in terms of a basis set of two unit vectors $\underline{\phi}_d$ & $\underline{\phi}_n$, with variable coefficients u_d & u_p. The non-orthogonality of $|\phi_d\rangle$ & $|\phi_n\rangle$ is analogous to the vectors $\underline{\phi}_d$ & $\underline{\phi}_n$ not being mutually perpendicular in the plane.

unit directions





Vectorially, $\underline{P\Psi} = u_p\,\underline{\phi}_n + u_d\,\underline{\phi}_d$

and $\cos\theta = \underline{\phi}_n \cdot \underline{\phi}_d$.

From the definition $K_{dp} = \langle \phi_d | \phi_n \rangle$,

the analogy is $K_{dp} \sim \cos\theta \sim K_{pd}$.

Although $\underline{\phi}_d$ and $\underline{\phi}_n$ may be non-orthogonal ($\theta \neq 90^\circ$), in general they are not collinear either ($\theta \neq 0^\circ$). Thus although the basis is non-orthogonal, there are still unique coefficients u_d & u_p in the expansion of $\underline{P\Psi}$.

There is a second method of defining channel amplitudes in $\underline{R}$ or $\underline{r}_p$ that can be used e.g. by Cox(1965), Döhnert(1971) & Brieva(1976). This is to project the total model wavefunction $P\Psi$ onto the various internal states ϕ_d or ϕ_n, and to denote the resulting wavefunctions by $U_d(\underline{R})$ & $U_p(\underline{r}_p)$ respectively. Using the previous expansion (1) for $P\Psi$ as a sum of products of the u_d & u_p wavefunctions (which I call henceforth "multiplicative" functions because they multiply their respective basis vectors), we can express the "projected" U_d & U_p in terms of them:

$$U_d(\underline{R}) = \langle \phi_d(\underline{r}) \, | u_d(\underline{R}) \, \phi_d(\underline{r}) + u_p(\underline{r}_p) \, \phi_n(\underline{r}_n) \rangle$$

ie. $$U_d = u_d + K_{dp} \, u_p, \qquad (2a)$$

and similarly

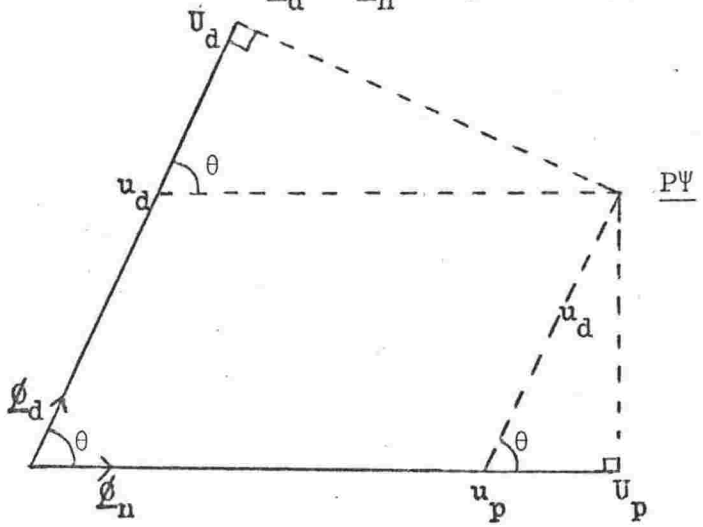
$$U_p(\underline{r}_p) = \langle \phi_n(\underline{r}_n) | \, P\Psi \rangle$$

$$= u_p(\underline{r}_p) + \langle \phi_n(\underline{r}_n) | \, \phi_d(\underline{r}) \rangle \, u_d(\underline{R})$$

ie. $$U_p = u_p + K_{pd} \, u_d. \qquad (2b)$$

The non-orthogonality problem arises when the overlap operators K_{dp} & K_{pd} are non-zero, and hence the multiplicative and the projected wavefunctions are distinct.

The analogy with planar vectors continues with the projected wavefunctions U_d & U_p: they are simply the projection of the total vector $\underline{P\Psi}$ in the directions $\underline{\phi}_d$ & $\underline{\phi}_n$ respectively.



Vectorially $U_p = u_p + u_d \cos\theta$ cf. $U_p = u_p + K_{pd}u_d$

& $U_d = u_d + u_p \cos\theta$ cf. $U_d = u_d + K_{dp}u_p$.

Note that $P\Psi \neq U_p\phi_n + U_d\phi_d$, so a new basis is required if the amplitudes U_p & U_d are to be multiplicative expansion coefficients. This new basis may be found first by inverting the above equations, to find the u's in terms of the U's:

$$u_d = (1 - K_{dp}K_{pd})^{-1} (U_d - K_{dp}U_p) \tag{3a}$$

$$\& \quad u_p = (1 - K_{pd}K_{dp})^{-1} (U_p - K_{pd}U_d), \tag{3b}$$

and then substituting these expressions in $P\Psi = u_d\phi_d + u_p\phi_n$:

$$P\Psi = (\phi_d - \phi_n K_{pd}) (1 - K_{dp}K_{pd})^{-1} U_d + (\phi_n - \phi_d K_{dp}) (1 - K_{pd}K_{dp})^{-1} U_p. \tag{4}$$

Now for convenience I define the Hermitian operators $K_d = K_{dp}K_{pd}$ and $K_p = K_{pd}K_{dp}$. Thus the new basis expansion is

$$P\Psi = B_d U_d + B_n U_p , \tag{5a}$$

defining the new basis 'vectors' B_d & B_n (they are really operators)

$$B_d = (\phi_d - \phi_n K_{pd}) (1 - K_d)^{-1}, \tag{5b}$$

$$\& \quad B_n = (\phi_n - \phi_d K_{dp}) (1 - K_p)^{-1}. \tag{5c}$$

Note that the B_d and B_n are neither orthogonal

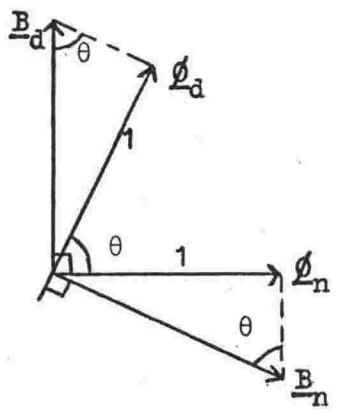
$$\langle B_n | B_d \rangle = -(1-K_p)^{-1}K_{pd} = -K_{pd}(1-K_d)^{-1} \neq 0 \tag{6a}$$

nor normalised

$$\| B_d\|^2 = \langle B_d | B_d \rangle = (1-K_d)^{-1} \neq 1 \quad \& \quad \|B_n\|^2 = (1-K_p)^{-1} \neq 1. \tag{6b}$$

In fact, though, B_d is orthogonal to ϕ_n and B_n to ϕ_d, since B_d, for example, may be rewritten $(1 - |\phi_n\rangle\langle\phi_n|)|\phi_d\rangle (1-K_d)^{-1}$ and thus starts with a projection operator to the subspace orthogonal to ϕ_n.

That is, $\underline{B}_d$ & $\underline{B}_n$ define new directions in the plane, perpendicular to $\underline{\phi}_n$ & $\underline{\phi}_d$ respectively:



$\|B_d\|^2 \neq 1$,

but with $K_{dp} \sim \cos\theta \sim K_{pd}$,

$\|B_d\| = (1 - K_{dp}K_{pd})^{-\frac{1}{2}} \sim (\sin\theta)^{-1} \geq 1$.

Hence $\underline{B}_n$ & $\underline{B}_d$ are longer than the unit vectors $\underline{\phi}_n$ & $\underline{\phi}_d$ by a factor of cosec θ.

If we want an orthogonal basis, we should therefore not use B_d & B_n together (as Döhnert & others have tried), but use a mixed pair of vectors that <u>are</u> orthogonal e.g. ϕ_d & B_n, or else the pair ϕ_n & B_d together. We choose the second basis set to investigate in more detail. It may be made orthonormal by defining $\hat{B}_d$ as a unit vector in the direction of B_d :

$$\hat{B}_d = B_d / \|B_d\| = (\phi_d - \phi_n K_{pd})(1-K_d)^{-\frac{1}{2}}$$
$$= (1 - P_n)\phi_d (1-K_d)^{-\frac{1}{2}} \qquad (7)$$

where $P_n = |\phi_n\rangle\langle\phi_n|$ is a projection operator.

A third vector in the same direction may also be defined (it is the simplest, but is not normalised) : $(1 - P_n)\phi_d$.

These three deuteron basis vectors, (along with ϕ_n, to which they are all orthogonal) lead to three orthogonal expansions for $P\Psi$:

1. $B_d \ (1-K_d)u_d(R) + \phi_n U_p(r_p)$ (8)

2. $\hat{B}_d \ \Omega_d(R) + \phi_n U_p(r_p)$ (9)

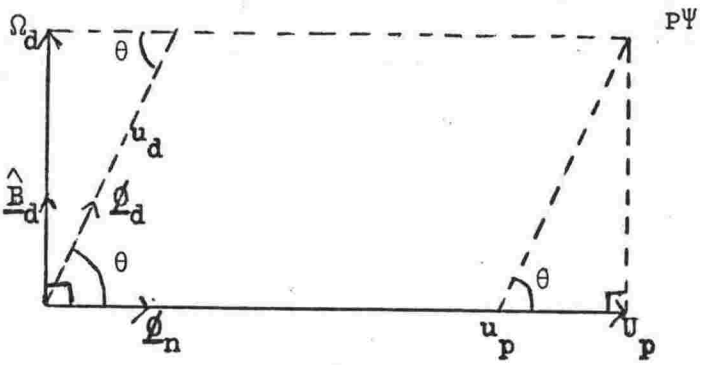
3. $(1-P_n)\phi_d \ u_d(R) + \phi_n U_p(r_p)$ (10)

where $\Omega_d(R) = (1-K_d)^{\frac{1}{2}} u_d(R)$ is a new deuteron channel wave function,

$$= \langle \hat{B}_d | P\Psi \qquad (9b)$$

These expansions have the geometric representation

$$\Omega_d = \sin\theta\ u_d$$
$$= (1-K_d)^{\frac{1}{2}}\ u_d$$
$$= \|B_d\|(1-K_d)\ u_d$$



The decision on which of the three basis sets to use will have to depend on whether the advantages of a normalised basis outweigh the complications of the $(1-K)^{-\frac{1}{2}}$ factors, and on whether the advantages of a simple form maintain when there is no normalisation. It turns out however, as will be seen in section 5.5, that there is a specific $(1-K)^{\frac{1}{2}}$ approximation for the deuteron-channel Hamiltonian, so there can be a cancellation $(1-K)^{\frac{1}{2}}\ (1-K)^{-\frac{1}{2}} = 1$, and the resulting channel operator can be remarkably simple. (Note how already we have methods analogous to those used in the antisymmetrisation problem, with $(1-K)^{\frac{1}{2}}$ factors appearing both in the basis and in the effective Hamiltonian. This similarity will be exploited in the next chapter to unify the treatment of the two problems.)

The third expansion of the model wavefunction has a simple physical explanation. Because in the internal region ϕ_n and ϕ_d are not orthogonal, there is some component of $\phi_d u_d$ in the ϕ_n direction: $\langle \phi_n | \phi_d \rangle u_d \cdot \phi_n$. The redefinition above takes this component away from the deuteron form $\phi_d u_d$, and adds it to the proton form $\phi_n u_p$. Thus the deuteron part becomes $(1 - |\phi_n\rangle\langle\phi_n|)\ \phi_d\ u_d$, which is $\phi_d u_d$ orthogonalised to the ϕ_n-direction. That is, all parts of the deuteron-core wave function are removed which look like a proton against a

neutron bound in a ϕ_n state. Conversely, the proton-channel wavefunction is 'increased' from u_p to U_p, so now $\phi_n U_p$ includes <u>any</u> part of the total state that looks like a proton + ϕ_n-bound-neutron : $U_p = \langle \phi_n | P\Psi \rangle$.

To end this section, I wish to discuss what happens when the various operator reciprocals have zero denominators. Such expressions occur in both the nonorthogonality and antisymmetrisation problems: in both we are given formulae for the 'projected' amplitudes 'U' in terms of the 'multiplicative' amplitudes 'u', and often have to invert them. The question is now over the physical significance of the denominators of $(1-K_d)^{-1}$, $(1-K_p)^{-1}$, and $(1-K)^{-1}$ being zero - the case of K_d, K_p & K having unit eigenvalues.

Feshbach(1968) showed in the antisymmetrisation problem that this corresponds to the possible existence of spurious components of the amplitudes 'u', which, with $U = (1-K)u$, can occur even though 'U' is always well defined. These spurious components are just all those removed from the relative wavefunction by Pauli Principle blocking by the core nucleons. By simply stipulating the the 'u' state is to have no overlap with any spurious components(which are the eigenvectors of K with unit eigenvalues), Feshbach was able to carry out the inversion $u = (1-K)^{-1}U$ and define 'u' uniquely. This is mathematically achieved by factoring $(1-K) = (1-K')(1-P)$, where 'P' has all the unit eigenvalue and K' the non-unit eigenvalue parts of K. Any reciprocal forms $(1-K)^{-n}$ are then replaced by $(1-K')^{-n}$, and the orthogonality condition $PU = 0$ generated.

In the non-orthogonality problem, a unit eigenvalue of $K_d = K_{dp}K_{pd}$ or $K_p = K_{pd}K_{dp}$ has a related meaning. The mathematical details are summarised in Dohnert(1971): the result is that in this case the internal

states ϕ_n & ϕ_d would be linearly dependent. That is, there would be non-zero channel amplitudes u_d^1 & u_p^1 such that $\phi_d u_d^1 + \phi_n u_p^1 = 0$. These amplitudes could be added in arbitary amounts to u_d & u_p in $P\Psi = \phi_d u_d + \phi_n u_p$ without affecting the system state $p\Psi$, so there would be no unique expansion into distinct deuteron & proton channels, as one channel is a linear combination of the others.

The solution is again to stipulate that that channel have no amount of the spurious component u_d^1. With such an orthogonality condition, $\langle u_d^1 | U_d \rangle = 0$, the channel expansion becomes well-defined.

5.2 Calculation of the Overlap Operators K_{dp} and K_{pd}

An overlap operator such as K_{dp} is defined in the model space $P\Psi = u_d(R)\,\phi_d(r) + u_p(r_p)\,\phi_n(r_n)$ as that operator which, when acting on an arbitary function of r_p such as $u_p(r_p)$, produces

$$K_{dp}u_p = \langle \phi_d(r) | \phi_n(r_n) \rangle\ u_p(r_p)$$
$$= \int \phi_d(r)^*\ \phi_n(R-\tfrac{1}{2}r)\ u_p(R+\tfrac{1}{2}r)\ \underline{d^3r},$$

a function of 'R' the deuteron channel variable. It would be more convenient if the variable of integration were changed to r_p, so that

$$K_{dp}u_p = \int K_{dp}(R,r_p)\ u_p(r_p)\ \underline{dr}_p$$

for some function $K_{dp}(R,r_p)$ called the kernel of the integral operator K_{dp}. We therefore change the independent variables from the pair (R,r) to the pair (R,r_p). Let J_{dp} be the Jacobean of this transformation, so

$$K_{dp}(R,r_p) = J_{dp}\ \phi_d(\ r(R,r_p)\ )^*\ \phi_n(\ r_n(R,r_p)\ )$$

and $K_{pd}(r_p,R) = J_{pd}\ \phi_n(r_n)^*\ \phi_d(r)$ similarly.

The Jacobeans are both 8 for deuteron stripping on heavy nuclei, and $(13/7)^3 = 6.41$ on carbon-12. Because the Jacobeans are equal, $K_{dp}(R,r_p) = K_{pd}(r_p,R)$, so K_{dp} & K_{pd} are simply Hermitian transposes.

A much more general model subspace for $P\Psi$ is now adopted: the model described in detail in section 2.1. The overlap kernel function between the deuteron channel $(L_a s_a)J_a I$ and the proton channel $(L_b s_b)J_b J_B$, with the total angular momentum 'J' in both channels, is

$$K^{J}_{(L_a s_a)J_a I\,:\,(L_b s_b)J_b J_B}(R,r_p) = R \cdot \sum_{\substack{M_a\ m_a\ \mu \\ M_b\ m_b\ M_B}} \int d\underline{d} \int d\hat{\underline{r}} \int r^2 dr \iint d\underline{r}_1 .. d\underline{r}_A \int d\hat{R}\ \ i^{-L_a}\, Y^{M_a}_{L_a}(\hat{\underline{R}})^*\, \psi^{m_a}_{s_a}(\underline{d})^*\, \frac{1}{(4\pi)^{\frac{1}{2}}}\, \phi_d(r)^*$$

$$\psi^{\mu}_{I}(\underline{r}_1 .. \underline{r}_A)^* \cdot \psi^{m_b}_{s_b}(\underline{p})\, \psi^{M_B}_{J_B}(\underline{r}_n, \underline{r}_1 .. \underline{r}_A)\, i^{L_b}\, Y^{M_b}_{L_b}(\hat{\underline{r}}_p)\ \ \frac{1}{r_p}$$

$$C^{L_a s_a J_a}_{M_a m_a M_a+m_a}\ C^{J_a\ \ I\ J}_{M_a+m_a\ \mu M}\ C^{L_b s_b J_b}_{M_b m_b M_b+m_b}\ C^{J_b\ \ J_B J}_{M_b+m_b M_B M}$$

We now change the variable of integration from $\underline{r}$ to $\underline{r}_p$, where

$$\underline{r} = p\underline{R} + q\underline{r}_p \quad \text{and} \quad \underline{r}_n = a\underline{R} + b\underline{r}_p$$

with constants $a = \frac{2\,M_B}{M_B+1}$, $b = -\frac{M_A+1}{M_A+2}$, $p = -\frac{2\,M_A}{M_A+2}$, and $q = a$ for deuteron reactions on a target of mass M_A leaving a residual nucleus of mass $M_B = M_A + 1$. The Jacobeans $J_{dp}=q^3$ and $J_{pd}= a^3$ are equal.

The calculations are now closely analogous to those for the usual transfer coupling $V_{dp} = \langle \phi_d \phi_A \mid V_{np}(\underline{r}) \mid \phi_B \rangle$, but we no longer have the very convenient zero-range approximation, whereby $\underline{r} = 0$ and the three vectors $\underline{R}$, $\underline{r}_p$ & $\underline{r}_n$ are all collinear. Instead, $R_{lsj}(r_n)$, the neutron's radial wavefunction, is dependent on the angular variables $\hat{\underline{R}}$ & $\hat{\underline{r}}_p$:

$$r = (p^2R^2 + q^2r_p^{\,2} + 2pq\ R\ r_p \cos\theta\ )^{\frac{1}{2}}$$

and $$r_n = (a^2R^2 + b^2r_p^{\,2} + 2ab\ R\ r_p \cos\theta\ )^{\frac{1}{2}}$$

where θ is the angle between $\underline{R}$ & $\underline{r}_p$: $\cos\theta = \hat{\underline{R}}.\hat{\underline{r}}_p = \frac{\underline{R}.\underline{r}_p}{R\ r_p}$.

First $Y_l^{m'}(\hat{\underline{r}}_n)$ is expanded in terms of the spherical harmonics of $\hat{\underline{R}}$ and $\hat{\underline{r}}_p$, using $\underline{r}_n = a\underline{R} + b\underline{r}_p$:

$$Y_l^{m'}(\hat{\underline{r}}_n) = \sum_{n=0}^{+n} \sum_{\lambda=-n} \left(\frac{4\pi}{2n+1}\right)^{\frac{1}{2}} \binom{2l+1}{2n}^{\frac{1}{2}} \frac{(aR)^{l-n}\,(br_p)^n}{r_n^{\,l}} \; C^{l-n\ n\ l}_{m'-\lambda\ \lambda\ m'}$$

$$\cdot\ Y_{l-n}^{m'-\lambda}(\underline{R})\ \ Y_n^{\lambda}(\underline{r}_p)$$

where $\binom{x}{y} = \frac{x!}{y!(x-y)!}$.

(see Ohmura et al.(1970) eqn 3.8a, or Austern et al.(1964) eqn 26.)

Second, $r_n^{-l}\, R_{lsj}(r_n)\, \phi_d(r)$ is expanded in terms of the Legendre polynomials $P_L(u)$, where $u = \cos\theta$, so $r_n = (a^2R^2 + b^2r_p^2 + 2abRr_p\,u)^{\frac{1}{2}}$ and $r = (p^2R^2 + q^2r_p^2 + 2pqRr_p\,u)^{\frac{1}{2}}$.

Thus $$r_n^{-l}\, R_{lsj}(r_n)\, \phi_d(r) = \sum_L \frac{2L+1}{2}\, q^L_{lj}(R,r_p)\, P_L(u)$$

where $$q^L_{lj}(R,r_p) = \int_{-1}^{+1} \frac{1}{r_n^{\,l}}\, R_{lsj}(r_n)\, \phi_d(r) \cdot P_L(u)\, du$$

are the R & r_p - dependent expansion coefficients.

We then use $$P_L(u) = \frac{4\pi}{2L+1} \sum_{\nu} Y_L^{\nu}(\hat{\underline{R}})^*\ Y_L^{\nu}(\hat{\underline{r}}_p)$$

$$\text{so } r_n^{-l} R_{lsj}(r_n)\phi_d(r) = 2\pi \sum_L q^L_{lj}(R,r_p)\ Y_L^{\nu}(\hat{\underline{R}})^*\, Y_L^{\nu}(\hat{\underline{r}}_p),$$

and we can then proceed with the integrals over $\hat{\underline{R}}$ and $\hat{\underline{r}}_p$.

After considerable Racah algebra, though in part this is similar to that for V_{dp}, the following result for K_{dp} is obtained :

$$K^J_{(L_a s_a)J_a I\ :\ (L_b s_b)J_b J_B}(R,r_p) = \sum_{lj} A^{jIJ_B}_{lsj}\, i^{L_b+1-L_a}\, \hat{J}_B \hat{J}_a W(IjJJ_b;\ J_B J_a)$$

$$\begin{bmatrix} L_b & s_b & J_b \\ l & s & j \\ L_a & s_a & J_a \end{bmatrix} \times \sum_{Ln} \tfrac{1}{2}\, J_{dp}\, R\, r_p\, q^L_{lj}(R,r_p)\, (aR)^{l-n}\, (b\,r_p)^n$$

$$\times \left(\frac{2L+1}{2n}\right)^{\frac{1}{2}} (L_a\, l-nL\, L)(L_b\, nL\, L)\ \hat{l}\ \hat{1-n}\ (2L+1)(-1)^{l-n} \hat{L}_b W(lnL_aL;\ 1-n\ L_b)$$

This should be compared with the expression for the zero-range coupling V_{dp} in the same model:

$$V^{J\,(dp)}_{(L_a s_a)J_a I\,:\,(L_b s_b)J_b J_B}(R)$$

$$= \sum_{lj} A^{jIJ_B}_{lsj}\; i^{L_b+l-L_a}\,\hat{J_B}\,\hat{J_a}\,W(IjJJ_b;\,J_B J_a) \begin{bmatrix} L_b & s_b & J_b \\ l & s & j \\ L_a & s_a & J_a \end{bmatrix}$$

$$\times\, D_o\,\frac{1}{\hat{L_a}}\,(-1)^{L_b-l}\,\frac{\hat{l}\,\hat{L}_a\,\hat{L}_b}{(4\pi)^{\frac{1}{2}}}\,\begin{pmatrix} l & L_a & L_b \\ o & o & o \end{pmatrix}\,R_{lsj}(R)$$

Note how the first lines of the two expressions are the same. This means that if, for reasons of small coefficients of fractional parentage $A^{jIJ_B}_{lsj}$ or of unfavourable angular momentum coupling of certain kinds, it should result that V_{dp} is small, then K_{dp} will be similarly reduced. There are other cases too, in which V_{dp} and K_{dp} can be small or zero for the same reasons. The zero-range coupling V_{dp} is zero for 'unnatural' parity stripping processes ($L_a + l + L_b$ odd), because of the Wigner 3-j coefficient $\begin{pmatrix} l & La & Lb \\ o & o & o \end{pmatrix}$. For such processes, it can be shown either $L_a+l-n+L$ or L_b+n+L must be odd, so, for these 'unnatural parity' reactions, K_{dp} is also zero.

5.3 Systems of Schrodinger equations for transfer reactions

The Schrodinger equation for the whole system, for total energy 'E', is $[H - E]\, P\Psi = 0$. We now form deuteron and proton channel equations by pre-operating by $\langle \phi_d \phi_A |$ and by $\langle \phi_B |$, respectively, in the framework of a 3-particle neutron+proton+core model defined by the expansion $P\Psi = u_d(R)\, \phi_d \phi_A + u_p(r_p)\, \phi_B$ (where $\phi_B(r_n, r_1 .. r_A)$ is a linear combination of $\phi_n(r_n)\phi_A(r_1 .. r_A)$).

The total Hamiltonian 'H' may be written in two forms, H_i & H_f, called the 'prior' and 'post' forms, which most naturally suit the deuteron and proton channels respectively. The details of H_i & H_f are given in section 2.2, but here we have a choice as to which to use in the two places in each of the two equations

$$\langle \phi_d \phi_A | H - E | \phi_d \phi_A \rangle u_d + \langle \phi_d \phi_A | H - E | \phi_B \rangle u_p = 0$$

and $$\langle \phi_B | H - E | \phi_B \rangle u_p + \langle \phi_B | H - E | \phi_d \phi_A \rangle u_d = 0 .$$

We have further choices as to whether we prefer the 'multiplicative' channel wavefunctions u_d & u_p, or the 'projected' functions U_d & U_p, or some hybrid combination of basis expansions. As explained in section 5.1, the total model wavefunction $P\Psi$ can be expanded in any combination of channels, provided the combination spans the model space and its parts are not linearly dependent.

Exercising the choices above, a variety ('A' to 'D') of coupled-channel systems may be obtained, and it is instructive to compare their uses.

(A) Using only the 'multiplicative' u_d & u_p, and using H_i throughout the deuteron channel & H_f for the proton channel:

$$[H_d - E_d]\, u_d(R) + [H_d - E_d]\, K_{dp}\, u_p + V^i_{dp}\, u_p = 0$$

and $$[H_p - E_p]\, u_p(r_p) + [H_p - E_p]\, K_{pd}\, u_d + V^f_{pd}\, u_d = 0,$$

where $E_d = E - e_d - e_A$ & $E_p = E - e_B$

e_d, e_A, & e_B are binding energies of the deuteron ϕ_d, target nucleus ϕ_A, & residual nucleus ϕ_B states,

$V^i_{dp} = \langle \phi_d \phi_A | \mathcal{V}_i | \phi_B \rangle$, and $V^f_{pd} = \langle \phi_B | \mathcal{V}_f | \phi_d \phi_A \rangle$.

The second terms in the two equations are non-orthogonality effects, and have usually been ignored. In their above forms, however, they are not the easiest to evaluate as $H_d(R)$ and $H_p(r_p)$ must be applied to complicated functions of their 'opposite' channels : u_p & u_d respectively. An improvement would be to at least have H_i operating on deuteron channel functions, etc., as in the next scheme.

(B) Using the multiplicative u_d & u_p, but using H_i on all deuteron wavefunctions, and H_f on all the proton ones.

$$[H_d - E_d]\, u_d(R) + K_{dp}\, [H_p - E_p]\, u_p + V^f_{dp}\, u_p = 0$$

and $$[H_p - E_p]\, u_p(r_p) + K_{pd}\, [H_d - E_d]\, u_d + V^i_{pd}\, u_d = 0.$$

These equations, though, still suffer from the difficulty, shared with scheme 'A', of involving the prior coupling potential $\mathcal{V}_i(\underline{R},\underline{r}) = V_p(\underline{R}+\tfrac{1}{2}\underline{r}) + V_n(\underline{R}-\tfrac{1}{2}\underline{r}) - W_d(R)$. This coupling is not as convenient to use as $\mathcal{V}_f(\underline{r}_p,\underline{r}_n) = V_{np}(\underline{r}_p - \underline{r}_n) + V_p(r_p) - W_p(r_p)$, in that the later has a good zero-range approximation.

Given such schemes as above, the question now arises whether the DWBA is the correct limit of the full coupled equations as the transfer coupling becomes small. The DWBA assumption is that u_d can be calculated independently of the other channels by solving $(H_d-E_d)u_d=0$; the u_p is then derived from that u_d solution. From the equations above, it is seen that assuming $(H_d-E_d)u_d=0$ is only reasonable if both the non-orthogonality term and the $\mathcal{V}_f$ or $\mathcal{V}_i$ coupling terms are small.

Ohmura et al.(1969) stated that the "present method is not equivalent to the DWBA because of the non-orthogonality term, even in the weak coupling limit in the sense that either $\mathcal{V}_f$ or $\mathcal{V}_i$ is very weak... The power series expansion in terms of $\mathcal{V}_f$ or $\mathcal{V}_i$ alone, therefore, does not correspond to an iterative solution of the basic coupled equations even in its first order expansion".

This would cast doubt on the validity of the DWBA for transfer reactions, were it not that the $\mathcal{V}_f$-small or $\mathcal{V}_i$-small limits are not the best weak coupling limits, even were they the same limit. It is more appropriate, I argue, to leave $\mathcal{V}_f$ and $\mathcal{V}_i$ fixed at their physical values, and take the weak coupling limit as the case of small spectroscopic factor (i.e. small coefficient of fractional parentage $A^{jIJ_B}_{lsj}$), or of unfavourable angular-momentum couplings. As explained in section 5.2, in such cases the expressions

$$K_{dp} = \langle \phi_d \phi_A \mid \phi_B \rangle ,$$
$$V^f_{dp} = \langle \phi_d \phi_A \mid \mathcal{V}_f \mid \phi_B \rangle ,$$
and $$V^i_{dp} = \langle \phi_d \phi_A \mid \mathcal{V}_i \mid \phi_B \rangle .$$

are all small, on similar grounds. Therefore, in this new defintion of the weak coupling limit, the non-orthogonality and $\mathcal{V}_f$ & $\mathcal{V}_i$ terms <u>are</u> small, and the DWBA should then be reasonably accurate.

(C) Using the 'projected' wavefunctions U_d & U_p (i.e. the basis expansion $P\Psi = B_d U_d + B_n U_p$), and using H_i in the deuteron channel & H_f in the proton channel.

This is effectively the method of Brieva(1976) & Döhnert(1971).

Start with equations of (A) factorised using $U_d = u_d + K_{dp} u_p$ & $U_p = u_p + K_{pd} u_d$:

$$[H_d - E_d]U_d + V^i_{dp} u_p = 0$$

and $$[H_p - E_p]U_p + V^f_{pd} u_d = 0,$$

then substitute the expression in section 5.1 for the u's in terms of the U's ($u_d = (1-K_d)^{-1}(U_d - K_{dp}U_p)$ etc.). We get

$$[H_d - E_d]U_d + \bar{V}_{dd} U_d + \bar{V}_{dp} U_p = 0$$

& $$[H_p - E_p]U_p + \bar{V}_{pp} U_p + \bar{V}_{pd} U_d = 0,$$

where the $\bar{V}$ are new non-local potentials and couplings :

$$\bar{V}_{dp} = V^i_{dp}(1 - K_p)^{-1} \quad \& \quad \bar{V}_{dd} = - V^i_{dp}(1-K_p)^{-1} K_{pd},$$

$$\bar{V}_{pd} = V^f_{pd}(1 - K_d)^{-1} \quad \& \quad \bar{V}_{pp} = - \bar{V}_{pd} K_{dp} .$$

The chosen model space had only one deuteron and one proton channel, so finding the u_i in terms of the U_i by inverting a system of equations of the form $U_i = u_i + \sum_{j \neq i} K_{ij} u_j$ (for integral operators K_{ij}) is a relatively easy task. With many channels u_i, the inversion is more difficult, but, Brieva observes "it is a general result that we can eliminate the non-orthogonality terms in any coupled channels approach if we accept some more complicated effective interaction taking these effects into account." Dohnert states that "the correct treatment of stripping reactions that considers explicitly the coupling between elastic and rearranged channels, without taking into account antisymmetry, introduces nonlocal .. potentials not only into the potentials characterising each channel ($\bar{V}_{dd}$ & $\bar{V}_{pp}$ in my scheme above), but also into the coupling potentials ($\bar{V}_{dp}$ & $\bar{V}_{pd}$ here)."

(D) Using u_d & U_p in the hybrid expansion $P\Psi = (1-|\phi_n><\phi_n|)\phi_d u_d + \phi_n U_p$ (orthogonal expansion no. 3 of section 5.1), and using H_f wherever possible (because v_f is well known).

Starting with

$$[H_{i,f} - E]\,(\,(1-P_n)\phi_d\,u_d + \phi_n\,U_p\,) = 0,$$

we get the proton channel equation if we pre-operate by $<\phi_n|$:

$$[H_p - E_p]\,U_p(r_p) + V^f_{pd}\,u_d = 0,$$

and we get the deuteron channel equation by pre-operating by $<\phi_d|(1-P_n)$:

$$<\phi_d|(1-P_n)[H_{i,f} - E](1-P_n)|\phi_d>u_d + V^f_{dp}\,U_p = 0.$$

The first term is expanded to give as the final deuteron equation

$$([H_d-E_d] - K_{dp}[H_p-E_p]K_{pd} - K_{dp}V^f_{pd} - V^f_{dp}K_{pd})\,u_d + V^f_{dp}\,U_p = 0.$$

If a non-local Hermitian operator F_{dd} is defined by

$$+F_{dd} = K_{dp}[H_p-E_p]K_{pd} + K_{dp}V^f_{pd} + V^f_{dp}K_{pd},$$

the deuteron and proton equations become respectively

$$[H_d - E_d]u_d - F_{dd}u_d + V^f_{dp}\,U_p = 0$$

and $$[H_p - E_p]U_p + V^f_{pd}\,u_d = 0.$$

This is a set of coupled channel equations with no extra deuteron-proton coupling terms, only with extra Hermitian but non-local coupling potentials among the deuteron channel(s). The proton channel equation is formally unchanged by the inclusion of non-orthogonality effects, but has a different physical interpretation as it is an equation for the 'projected' U_p rather than for the usual 'multiplicative' u_p. The only effect of non-orthogonality is the addition of the F_{dd} potential in the deuteron equation. That F_{dd} acts to cancel the channel operator $[H_d-E_d]$ reflects the non-normalisation of the deuteron basis vector $(1-P_n)\phi_d$.

The scheme 'D' has the advantage over scheme 'C' in that the non-local potentials can be written down explicitly in matrix form, given a matrix representation of K_{dp}, and require only matrix multiplications and additions: there is now no need to invert any integral operators or solve systems of linear operator equations.

The above definition of F_{dd} was for a model space with only one deuteron and one proton equation. When there are many channels of each type, the 'non-orthogonality potential' $F_{d_i d_j}$ coupling deuteron channels i & j is in full

$$F_{d_i d_j} = \sum_k \Big(K_{d_i p_k} \big[H_{p_k} - E_{p_k} \big] K_{p_k d_j} + K_{d_i p_k} V^f_{p_k d_j} + V^f_{d_i p_k} K_{p_k d_j} - \sum_l K_{d_i p_l} V_{p_l p_k} K_{p_k d_j} \Big)$$

When there are several channels as here, new definitions replacing $K_d = K_{dp} K_{pd}$ are

$$K_{d_i d_j} = \sum_k K_{d_i p_k} K_{p_k d_j} \quad \& \quad K_{d_i} = K_{d_i d_i} .$$

There are still no additional couplings among the proton channels, or between the deuteron and proton channels.

It is this hybrid scheme 'D', based on an orthogonal expansion, which I have chosen to investigate in more detail and with reference to a specific deuteron stripping reaction.

5.4 Numerical Calculations

To find the actual effect of the non-orthogonality between the deuteron and the transfer channels, the overlap kernels $K_{d_i p_k}(R,r_p)$ are calculated for the deuteron - ^{12}C system described in section 2.4. Stamp(1974) showed that the deuteron incoming partial wave that contributes predominantly to the E_d = 2.71 Mev(lab) resonance is $L_a=2$, $J_a=3$, and that the bound deuteron state around the excited $^{12}C_{2^+}$ core with the largest amplitude has quantum numbers $L_a'=0$, & $J_a'=1$. For that reason, the overlap kernels K_{dp} and the non-orthogonality potentials F_{dd} were calculated in detail for initially just these two deuteron channels, with respect to proton channels up to $L_b=3$, $J_b=7/2$.

The magnitudes relative to unity of the eigenvalues of $K_d = \sum_p K_{dp}K_{pd}$ are instructive as they indicate the fractional non-orthogonality of a deuteron channel relative to the combined proton channels. If the eigenvalues of K_d are small, the channels are nearly orthogonal, but if they are near unity then orthogonalising will have a large effect: $(1-K_d)^{-1}$, which normalises the vectors after orthogonalising, will be large. The dynamic effect on the wave-functions is determined by the non-local potentials F_{dd}, not by K_d directly. They are related, however, as $1-K_d$ measures kinematically the deuteron wavefunction remaining after orthogonalising, whereas F_{dd} is an energy operator which acts to cancel the local channel operator $[H_d-E_d]$ as much as the channels are non-orthogonal.

The magnitudes of the kinematic effects of orthogonalising are indicated by the numerical eigenvalues of the operator $K_d = \sum_p K_{dp}K_{pd}$ summed over all the transfer channels 'p', and hence depend on which transfer channels are included in the coupled channels calculation.

With the $^{12}C(d,p)^{13}C$ reaction, at energies below 3 Mev., only the first four $^{13}C_{J_B}$ states ($J_B = \frac{1}{2}^-, \frac{1}{2}^+, \frac{3}{2}^-$, and $\frac{5}{2}^+$) lead to outgoing proton states : the energies of the second $5/2^+$ and the $3/2^+$ states are sufficiently high to bring the proton below its scattering threshold. Provided these sub-threshold channels are not near any resonance, as they absorb no nett particle flux it should be reasonable to omit them. However, the possibility of resonances in these channels is a delicate question, tied up with the occurence of similar resonances in the inelastic deuteron channels that are below threshold (see section 6.5 for further discussion).

Furthermore, since the Pauli Principle is not yet taken into account, we should strictly take as an open channel the configuration of a proton or neutron entering the deeply-bound $0s_{\frac{1}{2}}$ core eigenstate, and the remaining nucleon having a large positive energy in the scattering continuum. In Chapter 6, however, it will be seen that the Pauli Principle simply means that such channels <u>should</u> be included in the orthogonalising operators K_d & F_{dd}, but (as blocked channels) excluded from the reaction channel calculations. Anticipating this result, they are included in Tables 5.4.1 & 5.4.2 for the sake of completeness only: they will not be included in any coupled channels calculations until Chapter 6.

Table 5.4.1 gives the eigenvalues of the terms $K_{d_2 p_k} K_{p_k d_2}$ for different proton channels 'k' driven from the incoming deuteron partial wave $L_a = 2$ & $J_a = 3$. The eigenvalues are further classified by $n = 0,1,2,..$, the number of radial nodes (excluding the origin) of the associated eigenvector. Also given are the eigenvalues of the total K_{d_2}; these are not exactly the sum of the individual eigenvalues because even for the same n value, the eigenvectors for different k may vary slightly.

Table 5.4.1

Eigenvalues for the $L_a=2$, $J_a=3$ elastic deuteron channel

^{13}C state J_B	proton state L_bJ_b	neutron state nlj	c.f.p $A^{jIJ_B}_{lsj}$	angular momentum & cfp. factor	eigenvalues λ_n of K_{d_2} (with estimate in sho. model) λ_0 (n=0, ρ=2)	λ_1 (n=1, ρ=4)
open channels						
$\frac{1}{2}^-$	$f_{5/2}$	$0p_{\frac{1}{2}}$	-.7090	-.0755		.00055 (.00042)
	$f_{7/2}$	$0p_{\frac{1}{2}}$	"	-.5230		.02637 (.02053)
$\frac{1}{2}^+$	$d_{5/2}$	$1s_{\frac{1}{2}}$	-.9454	-.9454		.16438 (.12974)
$\frac{3}{2}^-$	$p_{3/2}$	$0p_{3/2}$	-.8918	-.8918	.37495 (.3976)	.12781 (.13896)
	$f_{5/2}$	$0p_{3/2}$	"	.1698		.00278 (.00216)
	$f_{7/2}$	$0p_{3/2}$	"	.5696		.03130 (.02435)
$\frac{5}{2}^+$	$s_{\frac{1}{2}}$	$0d_{5/2}$	-.9261	-.9261	.24815 (.2915)	.14145 (.12449)
	$d_{3/2}$	$0d_{5/2}$	"	.3960		.01735 (.01309)
	$d_{5/2}$	$0d_{5/2}$	"	.7275		.05855 (.04420)
					.62869	.48399
channels below threshold at E_d less than 3 Mev.						
$\frac{5}{2}^+$	$s_{\frac{1}{2}}$	$0d_{5/2}$	.0623	.0623	.00112 (.0019)	.00064 (.00056)
	$d_{3/2}$	$0d_{5/2}$	"	-.0266		.00008 (.00006)
	$d_{5/2}$	$0d_{5/2}$	"	-.0489		.00026 (.00020)
$\frac{3}{2}^+$	$d_{3/2}$	$0d_{3/2}$	.0464			.00001
	$d_{5/2}$	$0d_{3/2}$	"			.00004
					.6300	.4850
Pauli blocked channels						
$\frac{1}{2}^+$	$d_{5/2}$	$0s_{\frac{1}{2}}$	1	1	.21767 (.25)	.05811 (.0625)

The 'angular momentum & c.f.p. factor' is a factor common to both V_{dp} & K_{dp} :

$$A^{jIJ_B}_{lsj}\ i^{L_b+l-L_a}\ \hat{J}_B\ \hat{J}_a\ W(IjJJ_b;\ J_BJ_a)\ \begin{bmatrix} L_b & s_b & J_b \\ l & s & j \\ L_a & s_a & J_a \end{bmatrix}.$$

The fact that the eigenvalues of K_{d_2} are as large as 0.629 and 0.484 for only the first four ^{13}C states, and are at least approximately the sum of the individual $K_{dp_k} K_{p_k d}$ eigenvalues, indicates that the effects of orthogonalising a deuteron to many proton channels are mostly cumulative, and can amount to a large fraction of unity when there are many proton channels. Individually the proton channels only have a small orthogonalising effect, but in a reaction model as here with up to 15 proton channels, their combined effect can be large. This is why in section 5.1 we chose the method of orthogonalising the deuteron channel to the proton channels, rather than vice-versa. If each proton channel were orthogonalised to the deuteron channels, then because there are usually many more of the former than of the latter, the non-orthogonality effects would be small corrections to each proton channel, as Goldfarb & Takeuchi(1974) found, rather than a larger effect on a few channels that can perhaps be replaced by some definite approximation. The alternative would be computationally more difficult, even though the overall effects would be the same. Another reason for the choice will be seen in Chapter 6: by it, treating deuteron - core antisymmetrisation becomes simpler.

Table 5.4.2 gives the eigenvalues of K_{d_o} for the $L'_a=0$, $J'_a=1$, $I=2$ deuteron channel, which is coupled to the incoming channel by the rotational excitation of the ^{12}C core from $I = 0^+$ to 2^+. At incoming energies below 4.4 Mev, the deuteron energy in this inelastic channel is negative, and hence the deuteron is trapped around the core until further reactions occur. On the E_d=2.71 Mev resonance, Stamp (1974) shows that the inelastic channel has a large amplitude, and it might be expected that the orthogonalising effects would then be large. The table shows however that this inelastic deuteron channel is more nearly

Table 5.4.2

Eigen-values of K_d for the $L_a J_a = 0,1$ & $I = 2$ inelastic deuteron channel

^{13}C state	proton state	neutron state	c.f.p.	angular momentum & cfp. factor	eigenvalues λ_n with $\rho_n = 2n + L_a$		
J_B	$L_b J_b$	nlj	$A^{jIJ_B}_{lsj}$		λ_0	λ_1	λ_2
					$\rho_n=0$,	2,	& 4.
open channels							
$\frac{1}{2}^-$	$f_{5/2}$	$0f_{5/2}$	.1003	.0031		.00001	
	$f_{7/2}$	$0f_{5/2}$	.1003	.0217		.00013	.00006
$\frac{1}{2}^+$	$d_{5/2}$	$0d_{5/2}$	.3062	.0158 }			.00057
		$0d_{3/2}$	.1118	.0283 }			
$\frac{3}{2}^-$	$p_{3/2}$	$0p_{3/2}$	.2619	-.0552 }		.01608	.00865
		$0p_{\frac{1}{2}}$	.2921	-.1232 }			
	$f_{5/2}$	$0f_{7/2}$	.2186	-.0056 }		.00003	.00001
		$0f_{5/2}$	.0546	-.0046 }			
	$f_{7/2}$	$0f_{7/2}$	.2186	-.0189 }		.00033	.00016
		$0f_{5/2}$	.0546	-.0154			
$\frac{5}{2}^+$	$s_{\frac{1}{2}}$	$1s_{\frac{1}{2}}$	.1410	.1410		.00865	.00341
	$d_{3/2}$	$0d_{5/2}$	.3433	.0440 }			.00091
		$0d_{3/2}$	.0686	.0117			
	$d_{5/2}$	$0d_{5/2}$	.3433	.0809 }			.00306
		$0d_{3/2}$	.0686	.0216			
					0	.0250	.0168

continued...

Table 5.4.2 continued

proton channels below threshold at 3 Mev.							
$\frac{5}{2}^+$	$s_{\frac{1}{2}}$	$1s_{\frac{1}{2}}$	-.8556	-.8556		.31842	.12568
	$d_{3/2}$	$0d_{5/2}$	.5130	.0658	}		.00149
		$0d_{3/2}$	.0324	.0055			
	$d_{5/2}$	$0d_{5/2}$	.5130	.1209	}		.00501
		$0d_{3/2}$	.0324	.0102			
$\frac{3}{2}^+$	$d_{3/2}$	$0d_{5/2}$	.5327	-.0228	}		.00001
		$0d_{3/2}$	-.2026	.0199			
	$d_{5/2}$	$0d_{5/2}$	.5327	-.0744	}		.00002
		$0d_{3/2}$	-.2026	.0648			
					0	.3425	.1610
Pauli-blocked channels							
$\frac{5}{2}^+$	$s_{\frac{1}{2}}$	$0s_{\frac{1}{2}}$	1	1	.89581	.21508	.0564
					.94165	.45782	.23568

orthogonal to the proton channels than is the elastic channel, as the eigenvalues of K_{d_o} are smaller fractions of unity. If the proton channels below threshold are included, the eigenvalues are still less than a third.

For incident deuteron energies of several Mev., it is the K_{d_o} eigen-value for the n = 2, $\rho = 4$ eigenstate ($\rho = 2n+1$) that is relevant, because the approximate energy levels in potential well 'B' (of Table 2.4.3) of the n = 0,1,2,3 K_{d_o} eigenstates are -58.5, -22.8, -1.6, & +43.2 Mev. respectively. For the incoming channel orthogonalised to the first four ^{13}C states, the $\rho = 4$ eigenvalue is 0.484, whereas for the inelastic channel the relevant eigenvalue is the very small 0.0168. If the proton channels below threshold should be included, the two eigenvalues would be 0.6300 and 0.161. The difference between the two channels stems from the distribution of parentage of the first four ^{13}C states. As seen from Table 2.4.1, these first four states have largely I = 0 parentage (the lowest states of ^{13}C could be expected to have large parentage from the ground state of ^{12}C), and (except for $A^{\frac{3}{2}\ 2\ \frac{1}{2}^-}_{1\ \frac{1}{2}\ \frac{3}{2}}$) the amplitudes of I = 2 core states are less the 0.35, a probability of 12%. This means that although the deuteron in the resonant inelastic channel may spend a significant time interval trapped in a doorway state, it is still nearly orthogonal to the first four ^{13}C states, as these states are predominantly I = 0 constitution. Contrary to initial expectations, the non-orthogonality fractions are found to be most important for the elastic channel, and hence will be significant even for non-resonant single-step reactions.

This shows that the deuteron's amplitude in the internal region is not a good indication of the fractional significance of non-orthogonality effects. It might have been expected from the arguments of

sections 5.2 & 5.3, that the wave amplitudes and the non-orthogonality effects would at least be correlated, since the transfer couplings $V^{(dp)}$ and the transfer non-orthogonality operators K_{dp} have many common factors. However, the amplitude in the deuteron inelastic channel is determined primarily not by the transfer coupling $V^{(dp)}$ but by the inelastic coupling $V^{(d\text{-}ex)}$ caused by the deformed core. It is possible, as holds here for the I=2 inelastic channel, for the inelastic couplings and inelastic amplitudes to be large, but the transfer couplings and the transfer non-orthogonalities to be small.

An unambiguous estimate of the fractional orthogonalising effects can be obtained in one approximation by calculating the algebraic eigenvalues of the K_d operators using harmonic oscillator radial wavefunctions, in conjunction with the full algebra of angular-momentum couplings and fractional parentage etc. Table 5.4.1 includes a number of eigenvalues estimated this way, and they generally agree to 20 - 30% with the eigenvalues calculated using realistic radial wavefunctions. The eigenvalues in this radial harmonic-oscillator approximation may be calculated directly as algebraic eigenvalues of the matrix $k^J_{i:j'}$ where

$$k^J_{N_a(L_a s_a)J_a I : N'_a(L'_a s_a)J'_a I'}$$

$$= \sum_{n_b L_b J_b J_B} \sum_{nlj} A^{jIJ_B}_{nlsj}\, i^{L_b+l-L_a}\, \hat{J}_B \hat{J}_a\, W(IjJJ_b; J_B J_a) \begin{bmatrix} L_b & s_b & J_b \\ l & s & j \\ L_a & s_a & J_a \end{bmatrix}$$

$$\times \sum_{n'l'j'} A^{j'I'J_B}_{nT's j'}\, i^{L_b+l'-L'_a}\, \hat{J}_B \hat{J}'_a\, W(Ij'JJ_b; J_B J'_a) \begin{bmatrix} L_b & s_b & J_b \\ l' & s & j' \\ L'_a & s_a & J'_a \end{bmatrix}$$

$$\times \langle N_a L_a\ 00, L_a\rho |\, nl\ n_b L_b, L_a\rho \rangle \langle n'l'\ n_b L_b, L'_a\rho' |\, N'_a L'_a\ 00, L'_a\rho' \rangle$$

with $\rho = 2N_a + L_a = 2n+l + 2n_b + L_b$ and $\rho' = 2N'_a + L'_a = 2n'+l' + 2n_b + L_b$

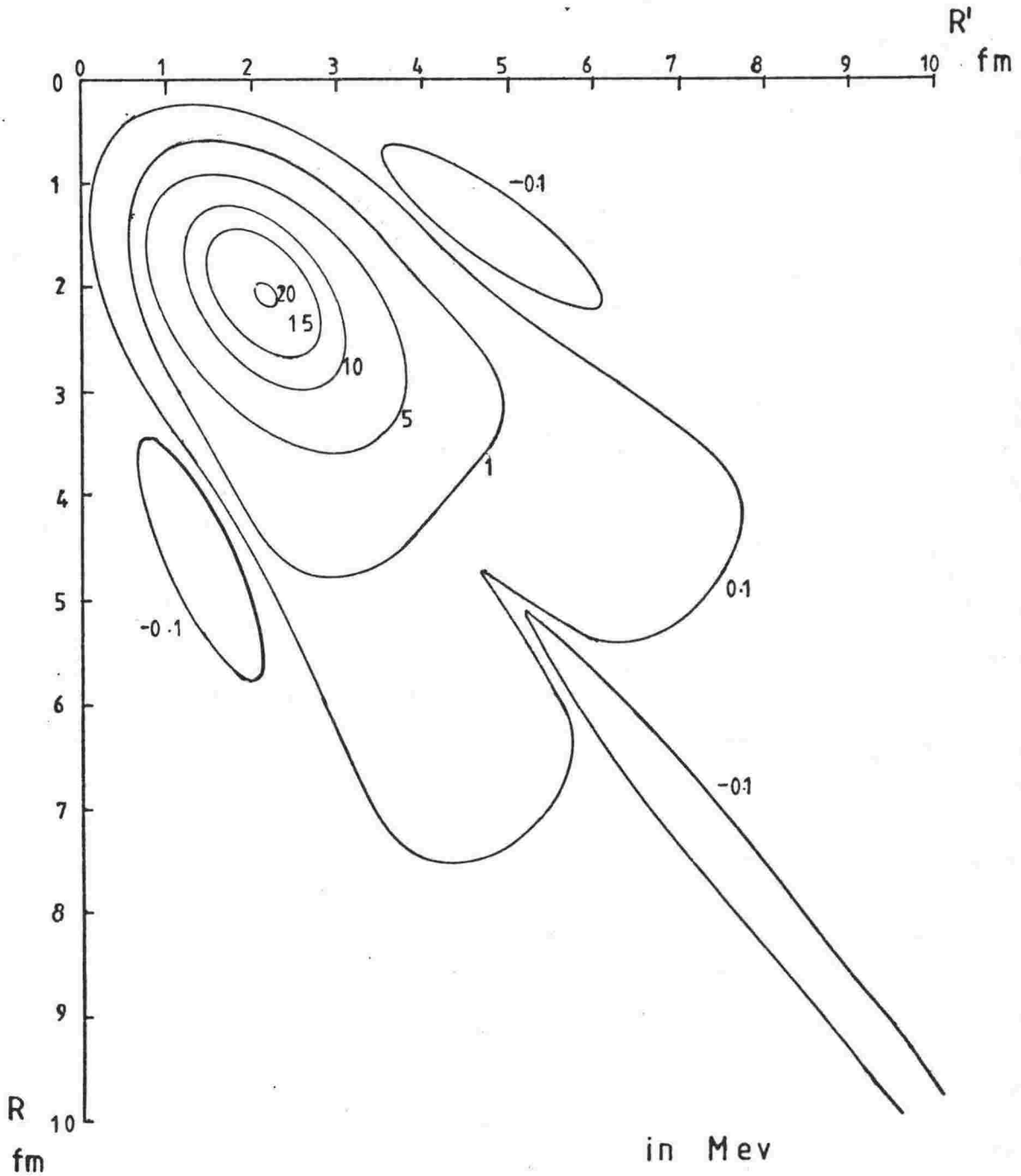
(the last line is a product of Moshinsky brackets).

Figures 5.4.1 & 5.4.2 show the non-local potentials F_{dd} for the $(L_a s_a) J_a I J$ = (21)303 and (01)123 deuteron channels: a contour map of the kernel $F_{dd}(R',R)$ is given. Also included are lists of the coupling magnitudes in a separable expansion of these potentials, as required to include the potentials in the coupled channels system by the method of section 2.6. At incident energies of several Mev., as with the K_d eigenvalues, for the L_a=2 channel the n=1 magnitude is operative; and for L_a=0 it is the n=2 magnitude. That is, the L_a=2 & I=0 elastic channel has a perturbing potential of 9.7 Mev at incident energies of several Mev., and the L_a=0 & I=2 inelastic channel has only 0.3 Mev. This difference correlates with their different K_d eigenvalues discussed earlier.

The effects of the F_{dd} potential on the elastic deuteron channel coupled to the first four transfer states, and on the transfer cross-sections to these states, are shown in Figures 5.4.3 and 5.4.4 . The first figure shows the transfer cross-sections from the 4 incoming deuteron partial waves up to and including L_a=1 & J_a=2, while the effect of the potential F_{dd} of Figure 5.4.1 on the wave function in the L_a=2 & J_a=3 elastic deuteron channel is shown in Figure 5.4.3. Although the wave function in the full coupled channels system that includes the non-local F_{dd} is not expected to be simply 1-K_d times the wave function found with local potentials, the potential F_{dd} is seen to reduce the elastic wave function by about 40% over a wide range of radii. The figures also show the transfer cross-sections and deuteron wave functions that would be found by the CC Born Approximation (CCBA) of Stamp(1974), who does not take the reverse d-from-p coupling of eqn 2.1.24 into account. Fig. 5.4.4 gives finally the wave function orthogonalised by the method of section 6.3. It takes the Pauli Principle into account more accurately, & follows internally if not externally the wave function subject to F_{dd}.

Figure 5·4·1

Potential $F_{dd}(R,R')$ for elastic deuteron channel $L_a = 2$, $J_a = 3$

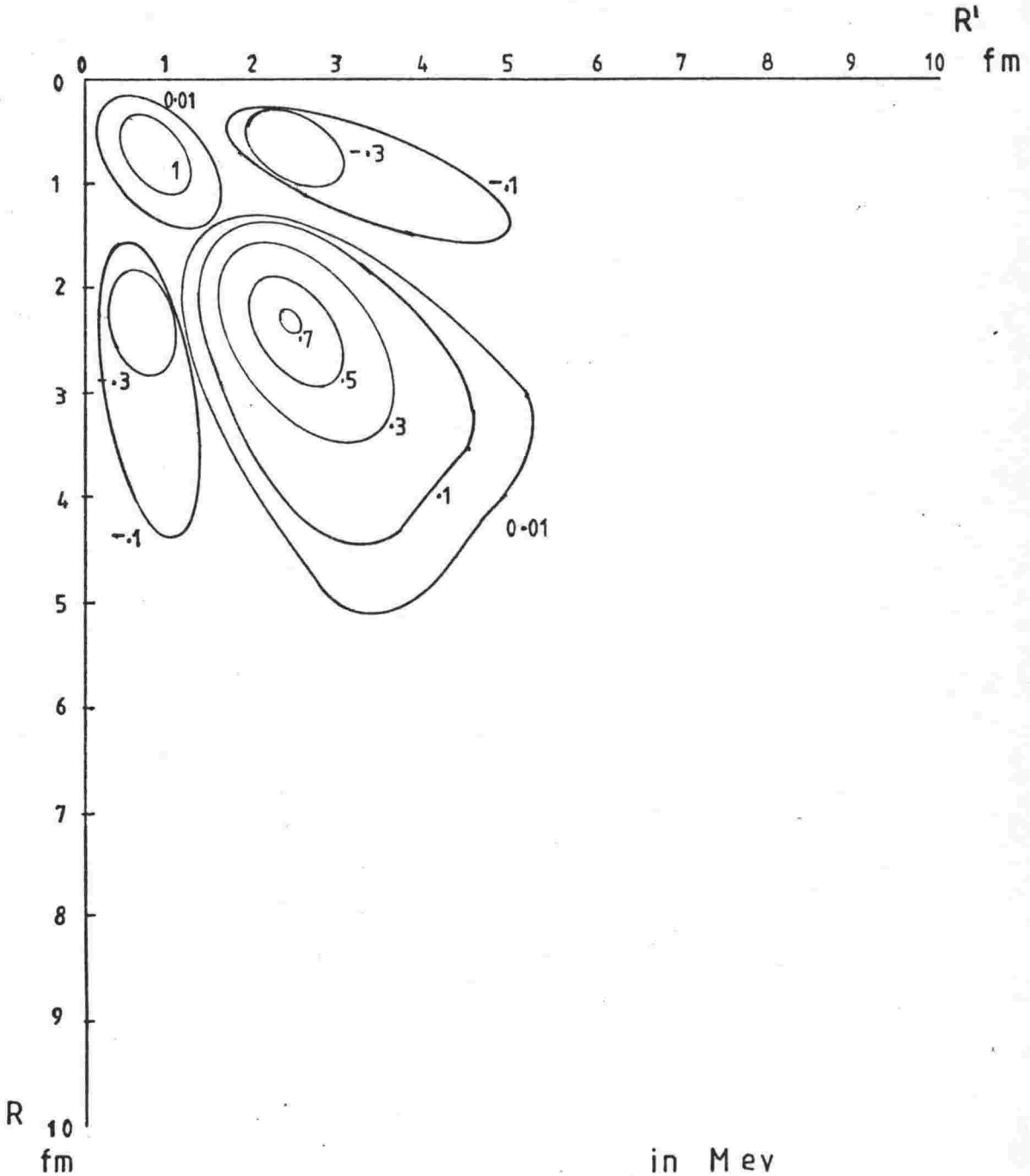


Separable expansion:

		mean level in deuteron well 'B'
n = 0,	magnitude = 29·407 Mev,	−22·4 Mev
1	9·723 Mev	+2·7 Mev
2	1·549 Mev	+25·5 Mev

Figure 5·4·2

Potential $F_{dd}(R,R')$ for inelastic deuteron channel $L_a = 0$, $J_a = 1, I=2$

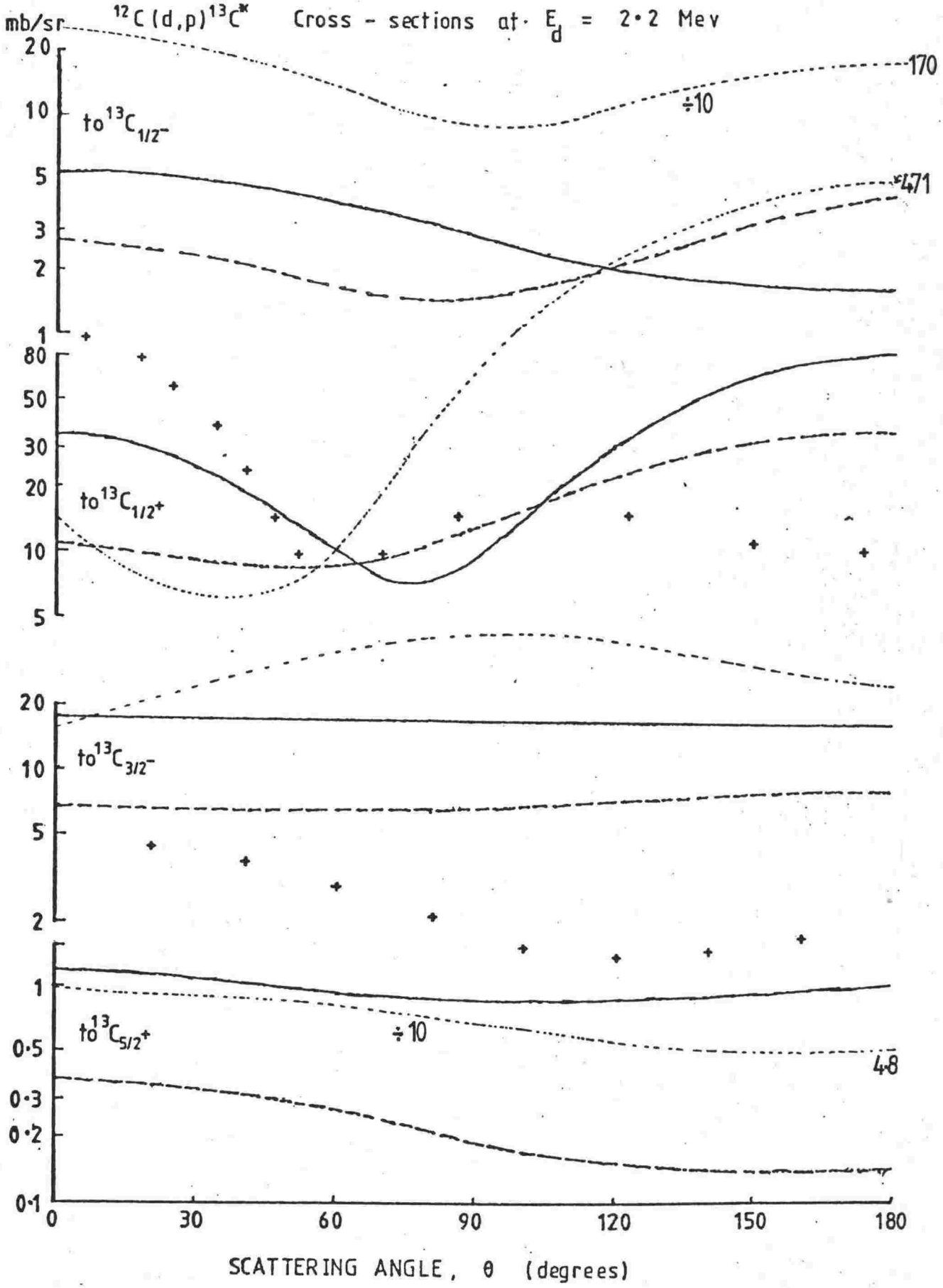


in Mev

Separable expansion:

			mean level in deuteron well 'B'
n = 1,	magnitude = ·980	Mev,	−22·2 Mev
2	·302	Mev	−1·4 Mev
3	·064	Mev	+16·3 Mev.

Figure 5·4·3


mb/sr
$^{12}C(d,p)^{13}C^*$ Cross - sections at E_d = 2·2 Mev
20
10
5
3
2
1
to $^{13}C_{1/2^-}$
170
÷10
471
80
50
30
20
10
5
to $^{13}C_{1/2^+}$
20
10
5
2
to $^{13}C_{3/2^-}$
1
0·5
0·3
0·2
0·1
to $^{13}C_{5/2^+}$
÷10
48
0
30
60
90
120
150
180
SCATTERING ANGLE, θ (degrees)
with non-local potential F_{dd}
observed +
local, simulating the CCBA
local, full coupling

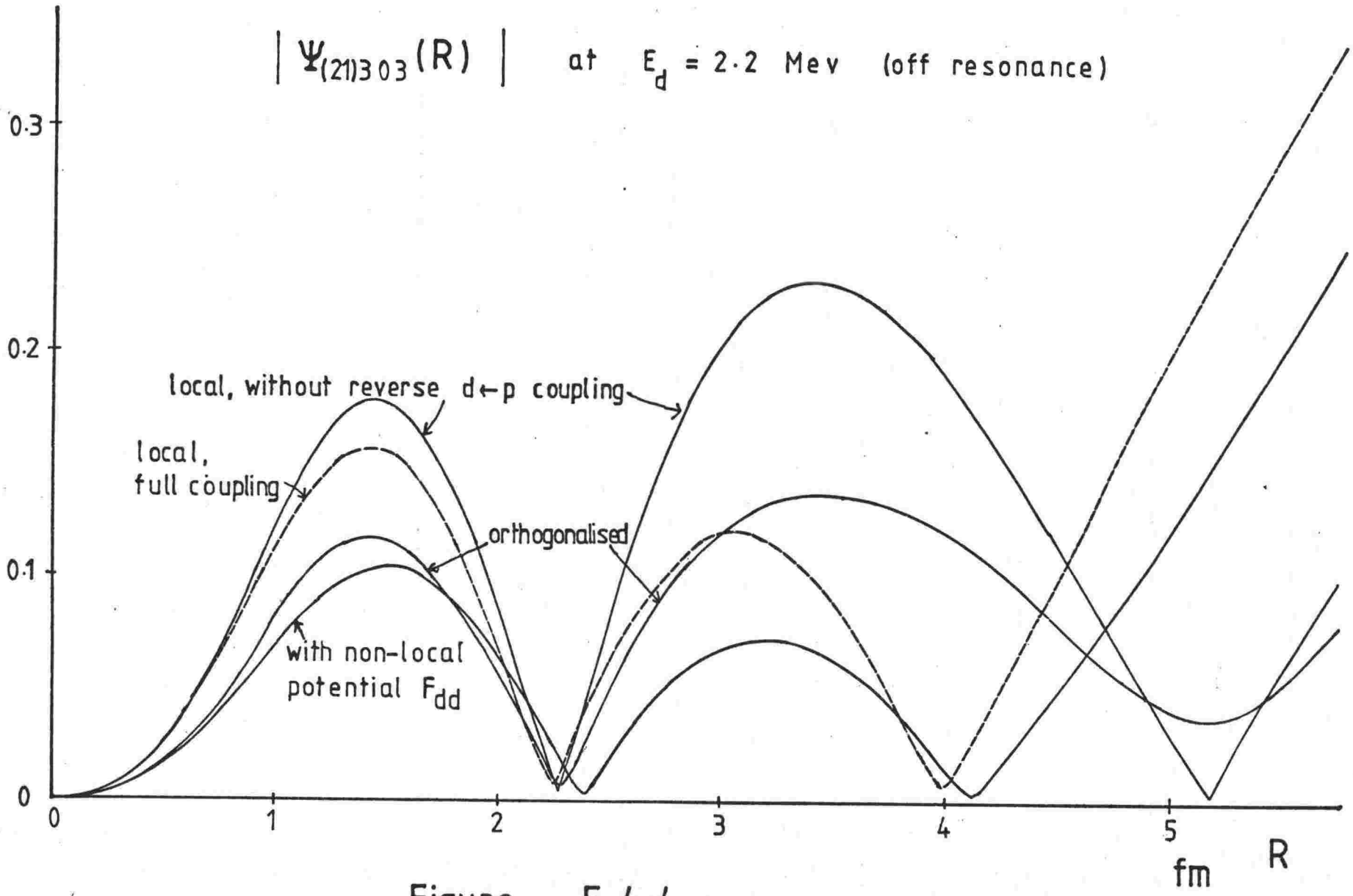

$|\Psi_{(21)303}(R)|$ at E_d = 2·2 Mev (off resonance)
0·3
0·2
0·1
0
local, without reverse d←p coupling
local,
full coupling
orthogonalised
with non-local
potential F_{dd}
0
1
2
3
4
5
fm
R

Figure 5.4.4

5.5 The $(1 - K)^{\frac{1}{2}}$ approximation in the non-orthogonality problem

This section will show the possibility of changing the effect of transfer channels' non-orthogonality from the existence of additional kinds of coupling terms to a modification of the usual transfer coupling terms V_{dp} etc., with a redefinition of the deuteron wavefunctions. This would mean, for example, that in a T - matrix calculation of stripping amplitudes, we do not have an additional 'non-orthogonality matrix element' quite different in form from the usual one, but have instead to take the matrix element of a modified coupling operator. The redefined deuteron wavefunction is asymptotically the same as before, so exactly the same boundary conditions are used, and the same S - matrix elements result.

The primary technique is to use the normalised deuteron basis state $\hat{B}_d$ appearing in orthogonal expansion no. 2 of section 5.1 :

$$\hat{B}_d = (1 - P_n) | \phi_d \rangle (1-K_d)^{-\frac{1}{2}} \quad (\text{where } P_n = |\phi_n\rangle \langle \phi_n|), \qquad (1)$$

and then try to approximate the exact channel Hamiltonian

$$H_{ex} = \langle \phi_d | (1-P_n) [H_{i,f} - E] (1-P_n) | \phi_d \rangle \qquad (2)$$

(appearing in scheme 'D' of section 5.3) by an approximate expression of the form

$$(1-K_d)^{\frac{1}{2}} [H_d - E_d] (1-K_d)^{\frac{1}{2}} \qquad (\text{cf. chap. 4!}) \qquad (3)$$

$$\text{where } 1 - K_d = \langle \phi_d | (1 - P_n) | \phi_d \rangle ,$$

so that the square root factors of (1) & (3) conveniently cancel.

Note that there is an exact equivalence for all scalar parts of the Hamiltonians H_i & H_f, the energy E for example :

$$\langle \phi_d | (1-P_n)\ [E]\ (1-P_n) | \phi_d \rangle$$

$$= E \langle \phi_d | (1-P_n) | \phi_d \rangle \quad \text{as } P_n \text{ is a projection operator}$$

$$= E\ (1-K_d) \quad \text{by the definition of } K_d \text{ ,}$$

and

$$(1-K_d)^{\frac{1}{2}}\ E\ (1-K_d)^{\frac{1}{2}} = E\ (1-K_d) \quad \text{too.}$$

It also turns out that the approximate equivalence (2) ~ (3) holds well for all one-particle parts of the Hamiltonian. Unfortunately the $(1-K_d)^{\frac{1}{2}}$ approximation has to neglect a number of indirect contributions from two-particle parts of the Hamiltonian. This residual will be briefly considered at the end of the section.

Returning to the exact H_{ex} (2), after some algebra this may be rewritten

$$H_{ex} = [H_d-E_d] - \tfrac{1}{2}K_d[H_d-E_d] - \tfrac{1}{2}[H_d-E_d]K_d - H_{res} \qquad (4)$$

where the residual part H_{res} contains matrix elements of the $\mathcal{V}_i$ & $\mathcal{V}_f$ parts of H_i & H_f respectively:

$$H_{res} = \tfrac{1}{2}(K_{dp}V^i_{pd} + K_{dp}V^f_{pd} + V^i_{dp}K_{pd} + V^f_{dp}K_{pd}) \,. \qquad (5)$$

The approximate expression (3) is now expanded using the binomial series (T & K not necessarily commuting)

$$(1-K)^{\frac{1}{2}}T(1-K)^{\frac{1}{2}} = T - \tfrac{1}{2}KT - \tfrac{1}{2}TK$$
$$-1/8\ (K^2T - 2KTK + TK^2)$$
$$-1/16\ (K^3T - K^2TK - KTK^2 + TK^3) - \ldots$$

giving

$$(1-K_d)^{\frac{1}{2}}\ [H_d-E_d]\ (1-K_d)^{\frac{1}{2}}$$

$$= [H_d-E_d] - \tfrac{1}{2}\,K_d\,[H_d-E_d] - \tfrac{1}{2}[H_d-E_d]\,K_d$$

$$- 1/8\ (\,K_d^2\,[H_d-E_d] - 2\,K_d[H_d-E_d]\,K_d + [H_d-E_d]\,K_d^2\,)$$

$$- \text{higher order order terms} \qquad (6)$$

By comparing (4) & (6), the approximate Hamiltonian is found to match the exact one at both the zero and first order. Now $[H_d-E_d]$ and K_d commute only approximately, but it can be seen from (6) that we need only say they commute exactly from second order and up, to justify neglecting these 2nd order and higher terms. Assuming, therefore, that K_d and $[H_d-E_d]$ commute if only from 2nd order on, then the expressions (3)&(6) become virtually equal to the exact results (4)&(2),except for the residual H_{res}.

This remaining H_{res} is in fact of the same order as the commutation product $[H_d,K_d]$ which was above assumed to be zero in all terms 2nd order and up. In detail

$$[K_d,H_d] = K_{dp}\,(V^f_{pd} - V^i_{pd}) - (V^f_{dp} - V^i_{dp})\,K_{pd}$$

and $$H_{res} = \tfrac{1}{2}K_{dp}\,(V^f_{pd} + V^i_{pd}) + \tfrac{1}{2}(V^f_{dp} + V^i_{dp})\,K_{pd}\ .$$

The V^f_{dp} & V^i_{dp} are both matrix elements between $\langle\phi_d|$ and $|\phi_n\rangle$ of negative potentials (of $(V_p+V_n)(1-|\phi_d\rangle\langle\phi_d|)$ & $(1-|\phi_n\rangle\langle\phi_n|)V_{np}$ resp.), but they are not expected to match in detail. Thus $[K_d,H_d]$ and H_{res} may be of the same order, and if one is neglected in a temporary approximation, the other can be too.

Having derived the $(1-K_d)^{\frac{1}{2}}$ approximation to H_{ex}, the deuteron channel equation is now constructed from the orthonormal expansion

$$P\,\Psi = \hat{B}_d\,\Omega_d + \phi_n\,U_p$$

by pre-operating by $\langle\hat{B}_d|$:

$$(1-K_d)^{-\frac{1}{2}}\langle\phi_d|\,(1-P_n)\,[H-E](1-P_n)|\phi_d\rangle\,(1-K_d)^{-\frac{1}{2}}\,\Omega_d + (1-K_d)^{-\frac{1}{2}}V^f_{dp}\,U_p = 0 \quad (7)$$

The $(1-K_d)^{\frac{1}{2}}$ approximation is now used, giving

$$(1-K_d)^{-\frac{1}{2}}\left[(1-K_d)^{\frac{1}{2}}[H_d-E_d]\,(1-K_d)^{\frac{1}{2}}\right](1-K_d)^{-\frac{1}{2}}\,\Omega_d + (1-K_d)^{-\frac{1}{2}}V^f_{dp}\,U_p = 0$$

or $$(1-P_d)\,[H_d-E_d]\,(1-P_d)\,\Omega_d + (1-K_d)^{-\frac{1}{2}}V^f_{dp}\,U_p = 0 \quad (8)$$

where P_d is that part, if any, of K_d with unit eigenvalues.

The residual part H_{res} has been omitted, and this leaves for the deuteron and proton channel equations, respectively

$$(1-P_d)\,[\,H_d - E_d\,]\,(1-P_d)\;\Omega_d(R) \;+\; \tfrac{1}{2}V_{dp}\;U_p(r_p) \;=\; 0 \qquad (9a)$$

$$\&\qquad [\,H_p - E_p\,]\,U_p(r_p) \;+\; \tfrac{1}{2}V_{pd}\;\Omega_d(R) \;=\; 0 \qquad (9b)$$

where $$\tfrac{1}{2}V_{dp} \;=\; (1-K_d)^{-\frac{1}{2}}\;V^f_{dp} \qquad (10a)$$

and $$\tfrac{1}{2}V_{pd} \;=\; \tfrac{1}{2}V_{dp}^{\text{Transpose}} \;=\; V^f_{pd}\;(1-K_d)^{-\frac{1}{2}}\;. \qquad (10b)$$

The channels equations (9a,b) solve the non-orthogonality problem because they result from an orthonormal set of basis vectors ϕ_n & B_d. Their effective channel Hamiltonians $[\,H_d-E_d\,]$ & $[H_p-E_p]$ are just the usual local channel operators (along with perhaps an orthogonality condition $P_d\,\Omega_d = 0$ to remove any spurious solutions : see the discussion at the end of section 5.1), and the channel wavefunctions Ω_d & U_p are asymptotically the same as the usual u_d & u_p, respectively.

There are no additional kinds of d-p coupling terms, as were in the schemes A & B of section 5.3. This means, for example, that the transfer T - matrix element may be simply written as $T_{pd} = \langle U_p^- |\tfrac{1}{2}V_{pd}|\,\Omega_d^+\rangle$ with the new coupling potential $\tfrac{1}{2}V_{pd}$. Further, these new couplings $\tfrac{1}{2}V_{pd}$ & $\tfrac{1}{2}V_{dp}$ are both proportional to V^f, the 'post' form of the deuteron-proton coupling, for which there is a good zero-range local approximation. The only complication is that the $(1-K_d)^{-\frac{1}{2}}$ factors are non-local.

A useful approximation is therefore to consider replacing the non-local

$$\begin{aligned}\tfrac{1}{2}V_{pd} \;&=\; V^f_{pd}\;(1-K_d)^{-\frac{1}{2}} \\ &=\; \langle\phi_n|\;V_{np}(1-P_n)\;|\,\phi_d\rangle / \langle\phi_d\,|1-P_n|\phi_d\rangle^{\frac{1}{2}}\end{aligned}$$

by some kind of local equivalent. One method is to replace $(1-P_n)|\phi_d\rangle$

by another expression which has the correct magnitude even if a different phase. For example, by $|\phi_d\rangle\ (1-K_d)^{\frac{1}{2}}$: the norm of this is $(1-K_d)^{\frac{1}{2}} \langle \phi_d | \phi_d \rangle (1-K_d)^{\frac{1}{2}} = 1-K_d$, the same as $\langle \phi_d | (1-P_n)^2 | \phi_d \rangle$. If this is allowed, then ${}_{\frac{1}{2}}V_{pd}$ is simply $V_{pd} = \langle \phi_n | V_{np} | \phi_d \rangle$, the p - d coupling term usually used in transfer calculations. The coupled equations are then

$$(1-P_d)\ [H_d-E_d]\ (1-P_d)\ \Omega_d(R) + V_{dp}U_p(r_p) = 0$$

and

$$[H_p-E_p]\ U_p(r_p) + V_{pd}\ \Omega_d(R) = 0,$$

the usual CC equations except, if $P_d \neq 0$, for the orthogonality condition $P_d\ \Omega_d = 0$.

The approximations sufficient for the accuracy of the ordinary local coupled-channel equations may therefore be listed :

(1) that H_{res} and similar terms may be neglected

(2) that $(1-P_n)\ |\phi_d\rangle$ can be replaced by $|\phi_d\rangle\langle\phi_d\ |\ 1-P_n\ |\ \phi_d\rangle^{\frac{1}{2}}$, i.e. that the non-local ${}_{\frac{1}{2}}V_{pd}$ is replaceable by the local V_{pd}, and

(3) that K_d has no unit eigenvalues.

The validity of the third approximation was examined numerically in the last section, and was found to hold provided there are only a 'few' proton channels coupled to each deuteron channel. In any case, the effect of unit eigenvalues of K_d is the orthogonality condition $P_d\ \Omega_d = 0$, so if the third approximation is the only one disallowed, we generalise the local CC method to the Orthogonality Condition Model (OCM). The OCM was originally derived for Pauli Principle effects, but is necessitated, as described in section 2.5, by any orthogonality conditions.

If the first approximation is disallowed, and H_{res} & similar terms not neglected, there will be additional terms in the channel equation for $\Omega_d(R)$. It is instructive to investigate their magnitude, if only approximately. The effect of the residual H_{res} is increased by the second & higher order terms of the $(1-K_d)^{\frac{1}{2}}(H_d-E_d)(1-K_d)^{\frac{1}{2}}$ expansion. Let the resultant be H'_{res}, say, so $H_{ex} = (1-K_d)^{\frac{1}{2}}(H_d-E_d)(1-K_d)^{\frac{1}{2}} + H'_{res}$. Further, if K_d has a vector u_d^1 with unit eigenvalue, then it can easily be shown that $H'_{res}|u_d^1\rangle = 0$ and $\langle u_d^1|H'_{res} = 0$. That is, $1-P_d$ can be factored out of both sides of $H'_{res} = (1-P_d)\, H'_{res}\, (1-P_d)$. There is no immediate further simplification of the channel equation

$$(1-P_d)\left\{[H_d-E_d]+ (1-K_d)^{-\frac{1}{2}}H'_{res}\,(1-K_d)^{-\frac{1}{2}}\right\}(1-P_d)\,\Omega_d + V_{dp}U_p = 0,$$

but if the tentative assumption is made that $(1-K_d)^{\frac{1}{2}}$ as well as $(1-P_d)^{\frac{1}{2}}$ can be factored out of each side of H'_{res}, we are left with an expression of the order of symmetric-part$(K_{dp}V^f_{pd} + K_{dp}V^f_{pd})$, $= V_{res}$ say. With this approximation, the deuteron channel equation becomes

$$(1-P_d)\,[H_d + V_{res} - E_d]\,(1-P_d)\,\Omega_d + V_{dp}U_p = 0,$$

a usual CC or OCM channel equation with an extra (non-local) potential V_{res}.

Pong and Austern(1975) calculated a local-equivalent potential to the symmetric part of $K_{dp}V_{pd}$, a major part of V_{res}, when the deuteron channel is orthogonalised to many neutron states ϕ_n, and to occupied proton states similarly. From sections 4.4 & 6.1, this is the effect of deuteron-core antisymmetrisation, which Pong & Austern were investigating. As seen in section 5.4, the effects of many non-orthogonalities are mostly cumulative, so they found their correction to be a significant fraction of the deuteron optical potential.

I have already mentioned in section 4.4 that Pong & Austern have found the symmetric part of $K_{dp}V_{pd}$ to reduce the deuteron folded of ^{16}O at 10 Mev by 11 Mev, and by 3 Mev at 100 Mev incident deuteron energy. Pong & Austern saw this as significant, since, as already remarked, Perey & Satchler(1967) showed that the deuteron folded potential for, say, Cr(d,d)Cr reactions was midway between depths of 74 Mev and 108.9 Mev of possible optical potentials at 11.8 Mev incident energy, and attribute the discrepancy to the neglect of higher-order effects.

On the evidence of Perey & Satchler, however, it would seem that the appropriate correction to the folded potential is greater than that calculated by Pong & Austern : up to 15 or 20 Mev of correction would be better. It is hence desireable to find a local equivalent for the remaining part of V_{res} : $K_{dp}V^{i}_{pd}$. Unfortunately $\mathcal{V}_i$ is more complicated than $\mathcal{V}_f$, and the approximations used by Pong & Austern to simplify $K_{dp}V^{f}_{pd}$ are no longer applicable.

Chapter 6 A Unified Treatment of Pauli Principle and Non-orthogonality Effects

The previous two chapters have proposed solutions for two long-standing problems in the theory of deuteron + nucleus reactions. Chapter 4 dealt with the anti-symmetrisation necessary between the deuteron and the nucleus. Section 4.2 began by looking at the more general problem of a proton & a neutron interacting with a core nucleus, and derived a two-particle Hamiltonian for their motion constrained by the Pauli Principle. In section 4.4, the proton and neutron were assumed to move together at all times as a deuteron, and the above effective Hamiltonian was applied to find the collective motion of the deuteron cluster. Subject to certain assumptions about the core state, it was found that by renormalising the deuteron-nucleus relative wave function the effect of antisymmetrisation can be limited to a set of orthogonality conditions on that wavefunction. That is, we have a new derivation of Buck et al.'s (1976) extension of the OCM (the orthogonality condition model of Saito, 1969).

In Chapter 5, more general motion of the two scattering nucleons was allowed. As well as deuteron elastic and inelastic channels, neutron-transfer reactions were treated. This leads to a well-known calculational difficulty, because the deuteron and transfer channels are not orthogonal, but this was solved by finding a new and orthogonal expansion for the total motion of two nucleons around a core. Antisymmetry with the core nucleons, however, was not considered.

This next problem of combining the hitherto-separate treatments of antisymmetrisation and channel nonorthogonalities is solved in the current chapter. It will be found that given the particular orthogonal expansion chosen in Chapter 5, the combined treatment of the two effects is unexpectedly simple.

To show the basic manner in which the two treatments of chapters 4 & 5 may be easily combined, in section 6.1 we will consider the case of only one deuteron and one neutron transfer channel, both antisymmetrised to the core nucleons. A physical explanation for the easy combination will be given. This two-channel case is generalised in section 6.2, to allow an arbitary number of both neutron- and proton-transfer channels, and in section 6.3 an interesting result will be found when there is orthogonality to all transfer channels, and to all nucleon states already occupied in the core, when the system is below its breakup threshold.

This new result emerging in section 6.3 leads to an extremely useful simplification of the whole coupled-channels system, such that the only non-local operators remaining give just orthogonality conditions (which it is shown can be calculated from independent considerations). In the light of this simplification, section 6.4 expands a new view of the deuteron + core system at low energies. A simple and unified model is formulated, one which is complementary to the usual models in that it is most accurate at low energies when the effects of antisymmetrising and of non-orthogonal channels are at their largest.

6.1 A two-channel model with both antisymmetrisation and non-orthogonal channels

In order to find the combined effect of these two requirements, a simple two-channel model of one deuteron and one neutron-transfer channel is considered. The deuteron interacts in a fully antisymmetrised manner with a target nucleus state $\phi_A(\underline{r}_1 \ldots \underline{r}_A)$, and the neutron can transfer to a state $\phi_n(\underline{r}_n)$ around the nucleus 'A' to form a nucleus 'B' with antisymmetrised state $\phi_B(\underline{r}_n,\underline{r}_1\ldots) = \mathcal{A}_{n-A}\, \phi_n(\underline{r}_n)\, \phi_A(\underline{r}_1\ldots)$. The total system wavefunction in the model is therefore

$$P\Psi = \mathcal{A}_{2-A}\left(u_d(R)\, \phi_d(r)\phi_A(r_1\ldots) \right) + \mathcal{A}_{p-A}\left(u_p(r_p)\, \phi_B(r_n,r_1\ldots) \right)$$

$$= | \mathcal{A}_{2-A} \cdot \phi_A > u_2(r_p,r_n)$$

where $u_2 = u_d\, \phi_d + u_p\, \phi_n$.

Since we are interested only in the motion of the two scattering nucleons, we can obtain a $U_2(r_p,r_n)$ by projecting $P\Psi$ onto a fully antisymmetrised $\mathcal{A} \cdot \phi_A$ as in Chapter 4 :

$$U_2(r_p,r_n) = < \mathcal{A}_{2-A} \cdot \phi_A \,|\, \mathcal{A}_{2-A} \cdot \phi_A > u_2$$

$$= (1-K_2)\, u_2$$

where $1 - K_2 = (1-K_n)(1-K_p)$

In Chapter 4, however, it was also shown that the best wave function for the antisymmetrised motion of two nucleons outside a nucleus is neither u_2 nor U_2 but $\Omega_2(r_p,r_n)$, where

$$\Omega_2(r_p,r_n) = (1 - K_2')^{\frac{1}{2}}\, u_2 = (1 - K_2')^{-\frac{1}{2}}\, U_2$$

(It is the Ω_2 for different energies, not u_2 or U_2, that form an orthonormal set, as the effective Hamiltonian for Ω is Hermitian).

The two-channel expansion of u_2 in the model means that

$$\Omega_2 = (1-K_2')^{\frac{1}{2}} (\phi_d u_d + \phi_n u_p)$$
$$= (1-K_2')^{\frac{1}{2}} \phi_d u_d + (1-K_n')^{\frac{1}{2}} \phi_n (1-K_p')^{\frac{1}{2}} u_p .$$

Now ϕ_n is a single-particle bound state, so by the theory of Chapter 3, $\langle \phi_n | 1-K_n | \phi_n \rangle = 1$. It is therefore better to use $\Omega_n = (1-K_n')^{\frac{1}{2}} \phi_n$ as the renormalised neutron bound state : $\langle \Omega_n | \Omega_n \rangle = 1$ is the consequence of $\langle \phi_A | \phi_A \rangle = 1 = \langle \phi_B | \phi_B \rangle$.

A projected proton state 'U_p' is defined next, as in Chapter 5, by projecting the total 2-particle state $\Omega_2(r_p, r_n)$ onto the internal state $\Omega_n(r_n)$ of the transfer channel :

$$U_p(r_p) = \langle \Omega_n(r_n) | \left[(1-K_2')^{\frac{1}{2}} \phi_d u_d + \Omega_n (1-K_p')^{\frac{1}{2}} u_p(r_p) \right]$$
$$= \langle \Omega_n | (1-K_2')^{\frac{1}{2}} \phi_d u_d + (1-K_p')^{\frac{1}{2}} u_p .$$

Substituting $(1-K_p')^{\frac{1}{2}} u_p$ from this expression into the one above for Ω_2, we derive

$$\Omega_2(r_p, r_n) = (1-|\Omega_n\rangle\langle\Omega_n|)(1-K_n')(1-K_p')^{\frac{1}{2}} \phi_d u_d + \Omega_n U_p ,$$ which is

a generalisation of $P\Psi = (1-|\phi_n\rangle\langle\phi_n|) \phi_d u_d + \phi_n U_p$, the orthogonal expansion no. 3 of equation 5.1.10 .

Note that Ω_2 appears in the channel equation of section 4.3 only in the form $(1-P_2)\Omega_2$:

$$(1-P_2)\Omega_2 = (1 - K_2^+)^{\frac{1}{2}} \phi_d u_d + \Omega_n (1-P_p) U_p ,$$

defining $(1-K_2^+) = (1 - |\Omega_n\rangle\langle\Omega_n|)(1-K_n)(1-K_p)$
$= (1 - |\Omega_n\rangle\langle\Omega_n|)(1 - K_2)$

as the product of the two-particle antisymmetrising operator of the Feshbach theory, $(1 - K_2)$,
and a projection operator orthogonalising to Ω_n too : $(1 - |\Omega_n\rangle\langle\Omega_n|)$.

Examination of this expression shows how the antisymmetrisation and non-orthogonality effects have combined. The functions of $1-K_n$ and $1-K_p$ are to remove from the deuteron wavefunction any overlaps with occupied neutron and/or proton states in the core. Now, as there is a neutron-transfer channel $\Omega_n(r_n)\, U_p(r_p)$, treating the channels' non-orthogonality by the method of Chapter 5 requires removing from the deuteron wavefunction any part of the form 'proton + Ω_n-bound-neutron'. The interesting result is that these two operations on the deuteron wavefunction are exactly-analogous orthogonalisation procedures. That is, the two projection operators $(1-K_n)(1-K_p)$ and $1-|\Omega_n><\Omega_n|$ (which orthogonalise to the occupied core states and to the state of the transferred nucleon, respectively) simply multiply. The effect of channel non-orthogonality is therefore to simply add the state of the transfered nucleon to the list of deuteron components already blocked by the Pauli Principle.

Once the wave function expansion $\Omega_2 = (1-K_2^+)^{\frac{1}{2}}\, \phi_d u_d + \Omega_n U_p$ (orthogonal but not normalised) is found, the channel equation is found by applying to $(1-P_2)\,\Omega_2$ the two-particle Hamiltonian of section 4.3 :

$$(1-P_2)\,[H_2 - E]\,(1-P_2)\;\Omega_2(r_p,r_n) = 0$$

$$\text{ie.} < \phi_d|\;(1-K_2^+)^{\frac{1}{2}}\,[H_2 - E]\;\left[\,(1-K_2^+)^{\frac{1}{2}}\,\phi_d u_d + \Omega_n\,(1-P_p)\,U_p\,\right] = 0$$

$$\text{ie.} < \phi_d|\;(1-K_2^+)^{\frac{1}{2}}\,[H_2 - E\,]\,(1-K_2^+)^{\frac{1}{2}}|\,\phi_d>\;u_d(R) +$$

$$< \phi_d|\;(1-K_2^+)^{\frac{1}{2}}\,|\,\Omega_n>\,[\,H_p - E_p\,]\,(1-P_p)\,U_p(r_p) +$$

$$< \phi_d|\;(1-K_2^+)^{\frac{1}{2}}\,\mathcal{V}_f\,|\,\Omega_n>\,(1-P_p)\,U_p(r_p) = 0\,.$$

The second term measures the non-orthogonality of the deuteron and proton channels, but here it is zero by construction : $(1-K_2^+)^{\frac{1}{2}}\,\Omega_n = 0$.

The deuteron channel equation thus becomes

$$\langle \phi_d | (1-K_2^+)^{\frac{1}{2}} [H_2 - E] (1-K_2^+)^{\frac{1}{2}} | \phi_d \rangle u_d(R)$$

$$+ \langle \phi_d | (1-K_2^+)^{\frac{1}{2}} \mathcal{V}_f | \Omega_n \rangle (1-P_p) U_p(r_p) = 0$$

where $\langle \phi_d | (1-K_2^+)^{\frac{1}{2}} \mathcal{V}_f | \Omega_n \rangle$ is the effective d-p coupling coefficient, and $(1-P_p)$, applied to U_p, orthogonalises the scattering proton's state to the occupied proton states in the core.

The deuteron effective operator $\langle \phi_d | (1-K_2^+)^{\frac{1}{2}} [H_2 - E] (1-K_2^+)^{\frac{1}{2}} | \phi_d \rangle$ is in the standard form encountered in the antisymmetry problem of section 4.4, and in the problem of transfer non-orthogonalities, occuring in sections 5.3 (D), and 5.5. There are three basic ways of simplifying this kind of expression. The first is to expand it in full, using eigenvalue expansions of $1-K_2^+$. This will be done in 6.3, and will be seen to produce a large number of terms.

A second treatment leads to a much simpler result, but involves a square-root approximation analogous to that of section 5.5. The above operator is replaced by

$$\langle \phi_d | (1-K_2^+) | \phi_d \rangle^{\frac{1}{2}} [H_d - E_d] \langle \phi_d | (1-K_2^+) | \phi_d \rangle^{\frac{1}{2}} + (1-P_d) H'_{res} (1-P_d) ,$$

where

$1-P_d$ is the fully-blocking part of $1-K_d^+ = \langle \phi_d | 1-K_2^+ | \phi_d \rangle$,
(just as $(1-P_n)(1-P_p)$ is the blocking part of $(1-K_n)(1-K_p)$).

Define

$1-K'_d$ as the partially-blocking part of $1-K_d^+$, so $1-K_d^+ = (1-P_d)(1-K'_d)$,
and $\Omega_d(R) = (1-K'_d)^{\frac{1}{2}} u_d(R)$ as a renormalised channel wavefunction,
so on dividing by $(1-K'_d)^{\frac{1}{2}}$ the deuteron channel equation becomes

$$(1-P_d) [H_d + V_{res} - E_d] (1-P_d) \Omega_d(R) + (1-P_d) Y_{dp} (1-P_p) U_p(r_p) = 0$$

where Y_{dp} is the renormalised effective d-p coupling, including the effects of both antisymmetry & non-orthogonalities:

$$Y_{dp} = (1-K'_d)^{-\frac{1}{2}} \langle \phi_d \mid (1-K_2^+)^{\frac{1}{2}} v_{np} \mid \Omega_n \rangle$$

and V_{res} is the renormalised residual part of the deuteron channel Hamiltonian :

$$V_{res} = (1-K'_d)^{-\frac{1}{2}} H'_{res} (1-K'_d)^{-\frac{1}{2}} .$$

The corresponding proton-channel equation is

$$(1-P_p) [H_p - E_p] (1-P_p) U_p(r_p) + (1-P_p) Y_{pd} (1-P_d) \Omega_d(R) = 0.$$

Because Ω_d and U_p appear only in the contexts $(1-P_d)\Omega_d$ and $(1-P_p)U_p$ respectively, we can impose the orthogonality conditions $P_d \Omega_d = 0$ and $P_p U_p = 0$ without loss of physical significance. As described in section 2.5 this may be done either by a Saito potential or by a numerical constraint when solving the differential equations. Letting "$(P\psi = 0)$" denote a Saito orthogonalising potential, the deuteron and proton channel equations become

$$[H_d + V_{res} - E_d] \Omega_d + Y_{dp} U_p + (P_d \Omega_d = 0) = 0$$

and $$[H_p - E_p] U_p + Y_{pd} \Omega_d + (P_p U_p = 0) = 0.$$

If further we follow Pong & Austern and find a local equivalent to the residual potential V_{res}, and take local approximations for Y_{pd} & Y_{dp} (see section 5.5), the equations above reduce to the OCM : the usual local coupled-channel equations, extended only with orthogonality constraints, and these are easily handled numerically in section 6.5 .

A third treatment of the deuteron effective operator was tried in section 4.4, but was found to be unsatisfactory if transfer channels were also present.

6.2 Neutron and proton transfer channels together

Normally there is no difficulty in including multiple channels to allow alternative neutron- & proton-transfer reactions from deuteron collisions on nuclei. In certain cases, however, possible double-counting has to be avoided. This can occur, for example, in intermediate 'doorway states', when the core is excited and the incoming deuteron goes into a quasi-bound state. As both the neutron and proton are then in negative-energy states, the system could be regarded either as a neutron-transfer channel with the proton below threshold, or vice-versa as a proton-transfer channel with a quasi-bound neutron. That is, not only are those proton and neutron channels not orthogonal, they are linearly dependent, and their expansion coefficients are not unambiguously defined.

The non-orthogonality between the proton and neutron transfer channels is not as complicated as their non-orthogonality with a deuteron channel, as they at least use the same natural coordinates. To resolve the uncertainty of the channels expansion of $u_2(r_p,r_n)$, all we have to do is to arbitarily decide whether the doubly-bound configurations are to be included in what kind of transfer channel, and then remove these configurations from all the other channels by an orthogonalising procedure. We arbitarily decide to favour (d,p) here over (d,n) reaction configurations, wherever a free choice is possible.

The expansion for $u_2(r_p,r_n)$, previously just $\phi_n u_p + \phi_d u_d$, becomes

$$u_2(r_p,r_n) = \sum_i \phi_{n_i}\left(1 - \sum_j |\phi_{p_j}\rangle\langle\phi_{p_j}|\right) u_{p_i}(r_p)$$

$$+ \sum_j \phi_{p_j} u_{n_j}(r_n) + \phi_d(r)\, u_d(R)$$

where $\phi_{n_i}(r_n)$ & $\phi_{p_j}(r_p)$ are orthonormal collections of neutron & proton bound states, respectively,

and where antisymmetrisation is not yet allowed for.

If we define the 'projected' variables $U_{p_i} = \langle \phi_{n_i} | u_2 \rangle$ and $U_{n_j} = \langle \phi_{p_j} | u_2 \rangle$, then we have equivalently

$$u_2(r_p,r_n) = \sum_i \phi_{n_i} U_{p_i}(r_p) + \sum_j (1 - \sum_i |\phi_{n_i}\rangle\langle\phi_{n_i}|) U_{n_j}(r_n) + (1 - \sum_i |\phi_{n_i}\rangle\langle\phi_{n_i}|)(1 - \sum_j |\phi_{p_j}\rangle\langle\phi_{p_j}|) |\phi_d\rangle u_d(R).$$

Observe how double $\phi_{n_i}\phi_{p_j}$ configurations are removed from the $U_{n_j}(r_n)$ term, and how $u_d(R)$ has taken from it all parts that describe either singly or doubly bound nucleons. In this way, all three kinds of channels are orthogonal by construction.

When we include antisymmetrisation with the core nucleons, the ϕ_{n_i} & ϕ_{p_j} bound states are replaced in the model by the orthonormal sets of $\Omega_{n_i} = (1-K_n)^{\frac{1}{2}} \phi_{n_i}$ and $\Omega_{p_j} = (1-K_p)^{\frac{1}{2}} \phi_{p_j}$, respectively. Then, as in the previous section,

$$(1-P_2)\Omega_2(r_p,r_n) = \sum_i \Omega_{n_i} (1-P_p) U_{p_i}(r_p) + \sum_j \Omega_{p_j} (1-P_n^+) U_{n_i}(r_n) + (1 - K_2^+)^{\frac{1}{2}} |\phi_d\rangle u_d(R),$$

where P_n^+ and K_2^+ are operators redefined by

$$1-P_n^+ = (1 - \sum_i |\Omega_{n_i}\rangle\langle\Omega_{n_i}|)(1 - P_n)$$

and $$1-K_2^+ = (1-\textstyle\sum_i |\Omega_{n_i}\rangle\langle\Omega_{n_i}|)(1-K_n) \cdot (1-\sum_j |\Omega_{p_j}\rangle\langle\Omega_{p_j}|)(1-K_p) .$$

The channel equations again follow from $(1-P_2)(H-E)(1-P_2)\,\Omega_2=0$, so that the deuteron channel equation is

$$\langle\phi_d|(1-K_2^+)^{\frac{1}{2}}\,[H-E](1-K_2^+)^{\frac{1}{2}}|\phi_d\rangle\, u_d(R)$$

$$+\sum_i X_{dp_i}\,(1-P_p)\,U_{p_i}(r_p) + \sum_j X_{dn_j}\,(1-P_n^+)\,U_{n_j} = 0$$

where

$$X_{dp_i} = \langle\phi_d|\,(1-K_2^+)^{\frac{1}{2}}\,V_{np}\,|\Omega_{n_i}\rangle$$

& $$X_{dn_j} = \langle\phi_d|\,(1-K_2^+)^{\frac{1}{2}}\,V_{np}\,|\Omega_{p_j}\rangle$$

are the effective (but not renormalised) transfer couplings.

Again as described in the previous section, there are two satisfactory ways of treating this standard form of the deuteron operator. The method using a $(1-K_d)^{\frac{1}{2}}$ square-root approximation was demonstrated then: I will now expand the operator in full, using an eigenvalue expansions for the antisymmetrisation operators K_n & K_p.

Calling 'N' the number of bound but unoccupied neutron states Ω_{n_i}, i=1 .. N (i.e. N residual nuclei for neutron-transfer reactions), and with 'Z' such proton states, define the eigenvalue expansions of K_n & K_p from the forms

$$(1-K_n)^{\frac{1}{2}} = 1 - \sum_{i=N+1} |w_{n_i}\rangle\langle w_{n_i}| \quad \& \quad (1-K_p)^{\frac{1}{2}} = 1 - \sum_{j=Z+1} |w_{p_j}\rangle\langle w_{p_j}| \,.$$

The w's are all orthogonal but not necessarily normalised: the eigenvalues of K_n & K_p are actually $\|w_{n_i}\|^2(2-\|w_{n_i}\|^2)$ and $\|w_{p_j}\|^2(2-\|w_{p_j}\|^2)$, respectively.

Define also $w_{n_i} = \Omega_{n_i}$ for $i = 1, \ldots, N$

& $w_{p_j} = \Omega_{p_j}$ for $j = 1, \ldots, Z$

so $$(1-K_2^+)^{\frac{1}{2}} = \left(1 - \sum_{i=1} |w_{n_i}\rangle\langle w_{n_i}|\right)\left(1 - \sum_{j=1} |w_{p_j}\rangle\langle w_{p_j}|\right).$$

The full expansion of the deuteron operator is therefore

$$\langle \phi_d | (1-K_2^+)^{\frac{1}{2}} [H_2 - E] (1-K_2^+)^{\frac{1}{2}} | \phi_d \rangle =$$

$$[H_d - E_d] - \sum_i K_{d:p_i} [H_p + e_{n_i} + e_A - E] K_{p_i:d} - \sum_j K_{d:n_j} [H_n + e_{p_j} + e_A - E] K_{n_j:d}$$

$$+ \sum_{ij} K_{d:n_j p_i} (e_{n_i} + e_{p_j} - E) K_{n_j p_i:d}$$

$$- \sum_i (K_{d:p_i} V_{p_i:d} + V_{d:p_i} K_{p_i:d}) - \sum_j (K_{d:n_j} V_{n_j:d} + V_{d:n_j} K_{n_j:d})$$

$$+ \sum_{ik} K_{d:p_i} V_{p_i:p_k} K_{p_k:d} + \sum_{jl} K_{d:n_j} V_{n_j:n_l} K_{n_l:d}$$

$$+ \sum_{ij} (K_{d:p_i} V_{p_i:n_j} K_{n_j:d} + K_{d:n_j} V_{n_j:p_i} K_{p_i:d})$$

$$+ \sum_{ij} (K_{d:n_j p_i} V_{n_j p_i:d} + V_{d:n_j p_i} K_{n_j p_i:d})$$

$$- \sum_{ijk} (K_{d:n_j p_i} V_{n_j p_i:p_k} K_{p_k:d} + K_{d:p_k} V_{p_k:n_j p_i} K_{n_j p_i:d})$$

$$- \sum_{ijl} (K_{d:n_j p_i} V_{n_j p_i:n_l} K_{n_l:d} + K_{d:n_l} V_{n_l:n_j p_i} K_{n_j p_i:d})$$

$$+ \sum_{ijkl} K_{d:n_j p_i} V_{n_j p_i:n_l p_k} K_{n_l p_k:d}$$

where

$$K_{d:p_i} = \langle \phi_d(r) | w_{n_i}(r_n) \rangle \quad \& \quad K_{d:n_j} = \langle \phi_d(r) | w_{p_j}(r_p) \rangle$$

$$K_{d:n_j p_i} = \langle \phi_d(r) | w_{n_i}(r_n)\, w_{p_j}(r_p) \rangle ,$$

and w_{n_i} & w_{p_j} are assumed to be eigenvectors of H_n & H_p at energies e_{n_i} & e_{p_j}, respectively.

The 'V' terms are matrix elements of $V_{np}(\underline{r})$

e.g. $V_{n_j p_i:p_k} = \langle w_{n_j}(r_n)\, w_{p_i}(r_p) | V_{np}(r) | w_{p_k}(r_p) \rangle$.

In obtaining the results of section 6.5 that use a non-local potential F_{dd}, the F_{dd} of section 5.3(D) was generalised as indicated in the present section to include the blocked and the open parts of K_2^+. This approximates the above expression by its 1st, 2nd, 5th & 7th terms.

6.3 Complete Nonorthogonality

Consider now the relatively complete model that includes Pauli blocking from all the core nucleons, and that orthogonalises to all transfer channels limited only by total energy and total angular momentum. In a first-order analysis, the occupied states in the core are the lower-energy eigenstates of the collective core potential, and the transfer states are just all the unoccupied states at higher energies, up to some limiting energy such as the breakup threshold. This means that the model's deuteron channel will have to be orthogonalised to all eigenstates of the potential, occupied or not, provided the states have eigen-energies below some limit.

The collection of single-particle negative-energy eigenstates is physically complete for unperturbed nucleons at negative energies: it is now further assumed that the set is still complete for negative-energy nucleons even in the full deuteron + core system. The treatment of the deuteron + core system as a three-body proton + neutron + core system by a full three-body analysis (e.g. Faddeev equations) would allow for the perturbation of a bound neutron by a scattering proton, for example. The current assumption is a kind of 'bound state approximation' (Levin et al.,1978) for the three-body system. It is assumed that whenever a nucleon has negative energy, it is always in an eigenstate (or a linear combination of eigenstates) of the core - nucleon potential. This implies, for example, that virtual transitions to negative energy states off-the-energy-shell are approximated by multistep real transitions to on-shell states. (For a preliminary investigation of off-shell effects in deuteron reactions, see Pantis, 1979.)

This assumption is significant for calculating tha scattering of deuterons below their break-up threshold at $E_{cm} = 2.225$ Mev. At these low energies the sum of the individual proton and neutron energies is less than zero, so that one of them is always in a negative energy state. But since the deuteron-channel wave function is orthogonalised to all such bound states, the wave function in the internal region must therefore vanish. Of course the deuteron channel is still significant asymptotically, as it is orthogonalised only to bound states, which have finite range. In the internal region, though, <u>all</u> the system's wave function is taken by ij combinations of pairs of nucleon states $\phi_{n_i}(\underline{r}_n)\,\phi_{p_j}(\underline{r}_p)$, eigenstates of the core - nucleon potential.

The assumption above therefore declares the set $\{\phi_{n_i}\phi_{p_j}\}$ to be complete for all proton + neutron states of negative total energy: states below the deuteron breakup threshold. They are by construction complete for one-particle states of protons or neutrons separately, but it is now assumed they are complete for the full system.

In the model of section 6.1 that includes both antisymmetrisation and transfer channels, the operator $1-K_d^+ = \langle \phi_d \mid 1 - K_2^+ \mid \phi_d \rangle$ orthogonalises the deuteron wavefunction $u_d(R)$ to all bound states of protons or neutrons, occupied or unoccupied. The $1-K_d^+$ operator is then factorised $1-K_d^+ = (1-P_d)(1-K_d')$ into a fully-blocking part $1-P_d$ and a partially-blocking part $1-K_d'$. The second part renormalises the wavefunction $\Omega_d(R) = (1-K_d')^{\frac{1}{2}}\, u_d(R)$, while the first part of unit eigenvalues produces an orthogonality condition $P_d\,\Omega_d = 0$.

The 'bound state approximation' of above is that $1-K_d^+$ does have a fully-blocking factor $1-P_d$ that blocks deuteron eigenstates at least up to the breakup threshold. The assumption is required because with realistic model parameters, as shown in section 5.4, K_d^+ will only have eigenvalues near but not exactly unity. Now in a model that includes both exactly, there will be only a small effect of changing an eigensolution in K_d^+ from nearly-blocking (in K_d') to fully blocking (in P_d), but it is numerically much easier to deal with P_d and orthogonality conditions than with K_d' and renormalised effective interactions. Thus we now develop a method that includes most of the effects of the K_d^+ operator , without having to calculate it in full, by putting as much of K_d as possible into P_d, and as little into K_d'; even if minor approximations are necessary.

The full deuteron-channel equation for the renormalised $\Omega_d(R)$ is

$$[H_d + V_{res} - E_d]\,\Omega_d + \sum_i Y_{dp_i} U_{p_i} + \sum_j Y_{dn_j} U_{n_j} + (P_d \Omega_d = 0) = 0$$

where Y_{dp_i} & Y_{dn_j} are the renormalised effective transfer couplings

e.g. $Y_{dp_i} = (1-K_d')^{-\frac{1}{2}} \langle \phi_d \,|\, (1-K_2^+)^{\frac{1}{2}} V_{np} |\, \Omega_{n_i} \rangle$,

V_{res} is the renormalised residual Hamiltonian (see section 5.5),

and '$(P_d \Omega_d = 0)$' represents a Saito potential or a numerical condition to ensure that $P_d \Omega_d = 0$.

If K_d' were small compared with P_d, then the transfer couplings Y_{dp_i} etc. would reduce to the usual $\langle \phi_d \,|\, V_{np} \,|\, \Omega_{n_i} \rangle$. Then the only remaining effect of both antisymmetrisation and nonorthogonality will be the simple orthogonality condition $P_d \Omega_d = 0$, and, to a lesser extent, in the residual term V_{res}. The 'bound state assumption' enables P_d to be calculated directly, without having to first calculate the full $K_d^+ = \sum_i \int K_{dp_i}(R', r_p)\, K_{p_i d}(r_p, R)\; d^3 r_p$ as in sections 5.2 & 5.4.

The eigenvectors w_N (N=0,1,..) of the projection operator P_d are the deuteron states fully blocked by the complete collection of all proton & neutron bound states, occupied or not. As explained earlier, the sum of the neutron & proton energies must be negative, so it is now assumed as an extension of the 'bound state approximation' that the $w_N(R)$ are also negative-energy eigenstates of some deuteron Hamiltonian H_N, say, assumed to have potentials with Woods-Saxon forms. Approximate forms for the H_N are now derived from physical arguments.

The four most important properties of the states w_N are

(1) The correct angular dependence,

(2) the number N of radial nodes (excluding origin),

(3) the radial size of the internal oscillations, and

(4) the correct asymptotic decay form.

These are matched as (1) only bound states w_N with same angular momentum quantum numbers $L_a J_a$ as those of the deuteron channel'd' are considered. This means that (2) we need only consider a collection w_N for varying 'N', the number of radial nodes. As the states N=0,1,.. are at progressively higher energies, the series should be stopped after the highest-energy deuteron state that can still be fully constituted by the bound neutron & proton states. This criterion may be judged approximately using a harmonic oscillator expansion. That is, if $\rho_{p-max} = 2n_p + l_p$ and $\rho_{n-max} = 2n_n + l_n$ are the maximum oscillator quantum numbers of the bound p & n states respectively, then the series is $N = 0,1, .. ,N_{d-max}$ where $2.N_{d-max} + L_a$ equals $\rho_{p-max} + \rho_{n-max}$.

Property (3), the radial size of the internal oscillations, is determined by the fact that H_d by itself is at least an approximate Hamiltonian for the deuteron + core system. This means that we can use the same radial form factors for the potentials in H_N as in H_d.

Ensuring (4), the correct asymptotic decay for the radial wavefunctions, is a little more complicated. This is because, although the deuteron's $\phi_d(r)$ has a definite decay rate proportional to $e^{-k_d r}$, $k_d = (\frac{2\, m_d}{\hbar^2}\, e_d)^{\frac{1}{2}}$, $e_d = 2.225$ Mev., the nucleon bound states have varying decay forms $e^{-k_{n_i} r_n}$, $k_{ni} = (\frac{2\, m_n}{\hbar^2}\, e_{n_i})^{\frac{1}{2}}$, as their binding energies, e_{n_i}, vary considerably. Fortunately, the dominant asymptote comes from the least-bound nucleon state that can still contribute to w_N. Let '$e_n(N)$' denote the energy e_{n_i} of this state. Using

$$K_{pd}(\underline{r}_p,\underline{R}) = 8\, \phi_n(2\underline{R}-\underline{r}_p)^*\, \phi_d(2\underline{r}_p-2\underline{R}) = \sum_N k_N^{\frac{1}{2}}\, w_{pN}(\underline{r}_p)\, w_N(\underline{R})^*,$$

the asymptotic form of $w_N(R)$ is proportional to $e^{-k_D R}$ with $k_D = 2\, k_d + 2\, k_n(N)$, and thus w_N must be at an effective binding energy of $e_N = (\, 2^{\frac{1}{2}} e_n(N)^{\frac{1}{2}} + e_d^{\frac{1}{2}})^2$.

The procedure adopted is thus to approximate w_N by eigenstates of a Hamiltonian H_N, which has potentials with the same form factors as those in H_d, but whose depths are adjusted to give at a binding energy of e_N a state of angular momentum $L_a J_a$, and with N radial nodes. The orthogonality requirement $P_d\, \Omega_d = 0$ is then the collection of conditions $\langle w_N |\, \Omega_d \rangle = 0$ for $N = 0, \ldots, N_{d\text{-max}}$. Neither K_d nor even P_d has to be calculated in full.

It is important to have the correct asymptotic form for the w_N's, to have good matching between the asymptotic deuteron form $\phi_d \ \Omega_d$, and the internal expansions $\sum_i \phi_{n_i} U_{p_i}$ etc., that replace it. The w_N forms are removed from the deuteron wavefunction in the internal region, so it is important that what is removed here closely match what can be alternatively expanded in products of proton or neutron bound states.

These considerations will be used in the numerical model of section 6.5, to replace the full non-local potential by a suitable set of orthogonality conditions on the radial wave function.

6.4 A Unified Model

In the previous section, it was shown that when there is 'complete nonorthogonality' between the deuteron channel and the combined transfer channels, by making a 'bound state approximation' the system's equations may be considerably simplified. I want to show now how these simpler equations can be more directly derived from a simple and unified physical model.

The alternative model constructs the total system wavefunction from two parts. The first part is a sum of all possible pairs of neutron and proton motions, such that one of the nucleons has negative energy. The second part appears only far from the nucleus, and describes the asymptotic form of a deuteron as a bound n-p pairs with specific relative motion $\phi_d(\underline{r}_p-\underline{r}_n)$. The matching of the asymptotic form with the internal sum of pairs is not, as in R-matrix theory, at a predetermined radius, but is achieved, as described in section 6.3, by realistic orthogonality conditions on the deuteron's state of collective motion. These orthogonality conditions ensure that the deuteron channel has no unwanted overlap with any deuteron-like forms of the n-p excitations in the first part of the system wavefunction. They also solve the twin problems of non-orthogonalities between transfer channels, and of antisymmetrisation with the core nucleons, because they ensure that the system's state in the internal region is described by the orthogonal neutron plus proton combinations around the nucleus that are not blocked by the Pauli Principle.

The model tries to be complete only at incident deuteron energies below the deuteron breakup threshold. At these energies, the n-p combinations may be accurately treated without a full three-body

treatment, since at least one of the nucleons has negative energy, and by the bound state approximation this nucleon is in a state known from the core's single-particle potential: the negative-energy state is approximated by linear combinations of the negative-energy eigenstates of this potential. This means that each proton & neutron combination looks like a transfer channel, with one nucleon transferred to a bound state of a possible residual nucleus, and the other nucleon either with positive energy in a scattering state, or with negative energy in a quasi-bound 'doorway state'. Thus the original three-body problem of neutron & proton & core can be modelled by sums of two-body channels, because some two of the three bodies are always bound together and at most one body is in a scattering state.

Exactly which two-body channels need to be included is determined by the usual considerations of total energy and total angular momentum, and also by the Pauli Principle. For, when considering n-p components of the total deuteron plus core state, all components not specifically included are blocked. Thus we should specifically include those transfer channels that together give most of the components of deuteron plus core states at energies of interest, but deliberately leave out channels that give neutron plus proton components that should be blocked by the Pauli Principle. This is easy, because such transfer channels are themselves not allowed by the Pauli Principle, because the transfered nucleon cannot share a state with a core nucleon.

There is a consistency requirement in constructing realistic models along the lines above. Because the usual deuteron - core relative state is now replaced in the internal region by n & p combinations, the interactions between these combinations must be consistent with what is expected from the deuteron - core interactions, and vice versa. For

example, if a deuteron - core interaction is used which gives inelastic excitations, and/or resonances, or intermediate doorway states, or even simply spin-orbit couplings, then if the same effects are desired the same total Hamiltonian should be applied to all the transfer channels. Thus there should be couplings between transfer channels generated by core (de)excitations. The potentials used in the transfer channels should be adjusted to give any deuteron resonances at the required energies. To model doorway resonances that are induced by inelastic core excitations and the scattering nucleons going into quasi-bound states, there must be transfer channels in which the 'free' nucleon is trapped below threshold in some resonant eigenstate. There should be consistent spin-orbit couplings for both nucleons separately, bound or unbound. Finally, since a deuteron cluster state so naturally includes the effect of $V_{np}(r_p-r_n)$ in correlating the neutron & proton motions, if this is important in the internal region we should include between transfer channels the couplings induced by the V_{np} term of the Hamiltonian (the coupling given by equation 2.1.27).

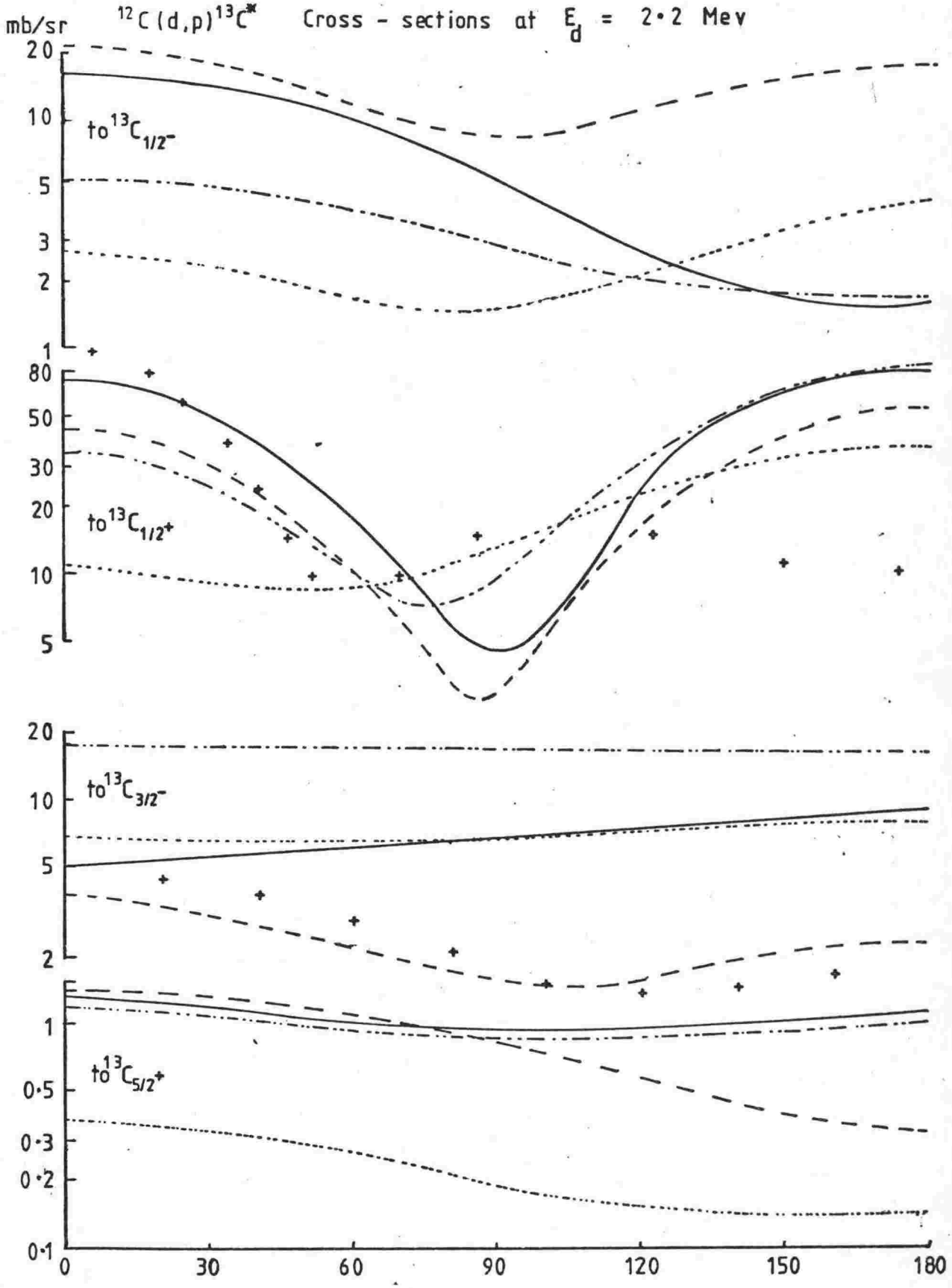
Once these consistency requirements are sorted out, the handling of deuteron - core reactions by this model predicts further phenomena more accurately. Since modelling by combinations of single-nucleon states is more microscopic than by modelling by clusters, it should allow for more 'intermediate structure' in the predicted cross-sections. Again, the possible deformation and polarisation of the deuteron's internal state by the core's potential is now automatically taken into account, as in the internal region the neutron-proton relative state is no longer restricted to a predetermined $\phi_d(r_p-r_n)$.

6.5 Numerical Calculations

In section 6.1, it was found that the antisymmetrisation between the deuteron's and the core's nucleons can be treated as additional terms in the deuteron's orthogonalising operator K_d^+ (p117). This is because each core nucleon blocks an otherwise-feasible transfer channel, and therefore requiring the deuteron channel to be orthogonalised to all transfer channels (open or blocked) is equivalent to orthogonalising as required by the Pauli Principle. It means that in a particular reaction calculation, 'dummy channels' are set up that are blocked by the Pauli Principle, and hence not included in the set of coupled differential equations to be solved, but are still included in the orthogonalising operator K_d (giving K_d^+), & the nonlocal potential F_{dd} of section 5.3(D) as generalised in section 6.2 .

For this reason, in the $^{12}C(d,p)^{13}C^*$ reaction modelled in section 5.4, two dummy channels are now included, corresponding to the transferred neutron entering the 0s eigenstate of the core collective potential, with the ^{12}C core either in its 0^+ ground state or in its 2^+ first excited state. The contribution of these channels to the eigenvalues of K_d^+ has already been given in Tables 5.4.1 & 5.4.2 of section 5.4. Their effects on the calculated cross-sections are now illustrated, for single-step direct reactions to the first four states of ^{13}C, at a non-resonant energy of 2.2 Mev. Figure 6.5.1 reproduces the local and transfer-orthogonalised calculations of 5.4, & adds a further set of curves that result when the 0s dummy transfer channels are included in the nonlocal potential F_{dd}. The eigenvalues of F_{dd} for the $L_a=1$, $J_a=2$ deuteron channel, previously 25.2 Mev & 17.1 Mev for the 0p & 1p eigenvectors respectively, are now increased to 44.8 & 19.9 Mev.

Figure 6·5·1


mb/sr
$^{12}C(d,p)^{13}C^*$ Cross - sections at E_d = 2·2 Mev
to $^{13}C_{1/2^-}$
to $^{13}C_{1/2^+}$
to $^{13}C_{3/2^-}$
to $^{13}C_{5/2^+}$
20
10
5
3
2
1
80
50
30
20
10
5
20
10
5
2
1
0·5
0·3
0·2
0·1
0
30
60
90
120
150
180
SCATTERING ANGLE, θ (degrees)
local
with non-local potential F_{dd}
non-local F_{dd}, with Pauli-blocked channels
orthogonality conditions replacing F_{dd}
observed +

It is seen that orthogonalising to the Os state, as required by the Pauli Principle, increases again, in three of the four curves, the effect of orthogonalising to open transfer channels. Since the 'transfer' of a proton to the Os proton state is isotopically analogous, this change should be doubled to show the effect of both neutron and proton antisymmetrising.

The question of Pauli blocking to the 8 nucleons of ^{12}C in the Op shell needs to be considered. Strictly, since this Op shell is two-thirds filled, there should be additional dummy channels for the occupied Op sub-states, and we should reduce the contributions to K_d^+ & F_{dd} of the $\frac{1}{2}^-$ and $3/2^-$ states of ^{13}C, which involve Op-shell neutrons around the ^{12}C core, to various amplitudes $A^{jI\frac{1}{2}^-}_{1\frac{1}{2}j}$ & $A^{jI3/2^-}_{1\frac{1}{2}j}$, and which therefore involve neutrons partly blocked by the Op core nucleons.

The analysis of section 6.1 in fact allows for arbitary overlaps between the transferred neutron and core neutrons, since their states are all described in their $\Omega_n = (1-K_n)^{\frac{1}{2}} u_n = (1-K'_n)^{-\frac{1}{2}} U_n$ form, and however large the antisymmetrisation operator K_n may be, all the Ω_{ni} form an orthonormal set complete for a specific nuclear shell. Now, all the Ω_i, occupied or not, are combined as required in section 6.1 to form $K_d^+ = \sum_i \langle \phi_d | \Omega_i \rangle \langle \Omega_i | \phi_d \rangle$. The same K_d^+ would hence result from any other complete and orthonormal set of neutron states, such as that set from the simplified model which took the Os shell as all occupied, and all the Op states as unoccupied and open to transferring neutrons. This simplified model is just that numerically solved above. It gives the exact K_d^+ operator, and is therefore used as giving a good approximation to F_{dd}. Thus provided the correct coefficients $A^{jIJ_B}_{lsj}$ are calculated in a properly antisymmetrised ^{12}C-plus-neutron

model(see e.g. Friedman, 1967, or a shell model calculation such as in Cohen & Kurath, 1967), a good approximation to F_{dd} can be found by assuming full shells, without including in detail the antisymmetrisation effects of the 0p shell nucleons of the core.

In section 6.3, it was shown that when all transfer channels are included, and the Pauli Principle fully accounted for, at incident energies below the breakup threshold the eigenvalues of K_d^+ approach unity, to a good approximation the orthogonalising of the deuteron channels may be accomplished by conditions of 'complete orthogonality', instead of by the nonlocal potentials F_{dd}. This approximation, and the 'bound state assumption' on which it is based, may now be tested numerically.

The $^{12}C(d,p)^{13}C^*$ reaction at 2.2 Mev is chosen again : the approximation should hold well at deuteron lab. energies below 2.60 Mev, the threshold for deuteron breakup (d,np). Initially, only the first four ^{13}C states are allowed residual nuclei. Table 6.5.1 lists the eigenvalues of K_d^+ for the deuteron elastic channel, for partial waves up to $L_a=3$, $J_a=3$, calculated by summation as illustrated in Table 5.4.1 for the $L_a=2$, $J_a=3$ channel. The contribution of the 0s dummy channels has been included twice to show the effect of the Pauli Principle for both neutrons and protons, as explained above. The K_d^+ eigenvalues in the table measure the effects not only of orthogonalising to the first four ^{13}C states, therefore, but also of orthogonalising to the 'Pauli blocked' dummy channels. As shown earlier, K_d^+ already includes orthogonalising to the 0p states, occupied or unoccupied, so the eigenvalues in Table 6.5.1 include in full the effects of both transfer-channel and Pauli Principle orthogonalising.

Table 6.5.1 Numerical K_d^+ eigenvalues,
for the elastic deuteron channel,
relative to the first 4 ^{13}C states,
with the required Pauli-blocked channels.

Elastic partial wave		K_d^+ eigenvalues, @ $\rho = 2N + L_a$ level.			
L_a	J_a	N=0	N=1	N=2	N=3
0'	1	1.002 @ 0	.812 @ 2	.612 @ 4	.295 @ 6
1	0	.707 @ 1	.643 @ 3	.323 @ 5	.131 @ 7
1	1	.985 @ 1	.734 "	.390 "	.172 "
1	2	.975 "	.848 "	.465 "	.204 "
2	1	.816 @ 2	.467 @ 4	.198 @ 6	.110 @ 8
2	2	.934 @ 2	.537 @ 4	.261 @ 6	.133 @ 8
2	3	.848 @ 2	.632 @ 4	.323 @ 6	.136 @ 8
3	3	.781 @ 3	.348 @ 5	.235 @ 7	.080 @ 9

(N.B. the 'N' here and in section 4.1
is identical to the 'n' of section 5.4)

Inspection of Table 6.5.1 shows that for values of ρ less than four, the eigenvalues of K_d^+ are all greater than 0.466. The value of $\rho = 4$ is the ρ_{d-max} of section 6.3, and corresponds, using the harmonic oscillator approximation, to the eigenvector having an expected energy level in the ^{12}C - deuteron potential well (113.5 Mev deep) of $\pm$ 3 Mev. Thus the $\rho = 4$ eigenvalues are those relevant to deuteron - ^{12}C scattering at several Mev. Because these are nearly all greater than 0.5, when the nonlocal potentials are replaced by orthogonality conditions, it is more accurate to approximate the eigenvalues by unity (the effect of making its eigenvector into an orthogonality condition) than by zero (the effect of ignoring that eigenvector). It is time-consuming to calculate and take into account the full nonlocal potentials F_{dd} for each energy and each partial wave, whereas as explained in section 6.3, the orthogonality conditions required may be calculated more directly from simpler and independent considerations.

Hence the decision is made to approximate the effect of the nonlocal potentials by orthogonality conditions, that orthogonalise the deuteron elastic channel to eigenvectors of the deuteron optical potential, with quantum numbers $\rho = 2N + L_a$ from 0 to 4 inclusive. The transfer cross-sections now predicted are also shown in Figure 6.5.1; these are found by solving (subject to the orthogonality conditions just described) the simplified local coupled-channel equations of page 118. The residual potential V_{res} has been incorporated into the potential well seen by the deuteron, by using the optical potential 'B' of Table 2.4.3 . This potential reproduces elastic scattering data, and hence includes a local equivalent to a major part of V_{res} : that part (calculated by Pong & Austern, 1975) derived by orthogonalising to at least those bound states that are occupied (and hence blocked by the Pauli Principle).

Modelling the $^{12}C(d,p)^{13}C^*$ reactions on the E_d = 2.71 Mev resonance, the starting point of the present investigations, has proved to be quite complicated. Although the fit to experiment has not been dramatically improved over that shown in Figure 2.4.3, the consideration of this multi-step reaction has always been instructive for estimating the effects of channel nonorthogonalities and of the Pauli Principle. Indeed, as explained in section 5.4, the fractional non-orthogonality effects are expected to be no larger over the resonance than elsewhere, since they are largest for the elastic deuteron channel, and small for the inelastic deuteron channel responsible for the resonance. Nevertheless, taking the channel nonorthogonalities into account has a minor but definite effect on the resonance calculation, so this will now be considered in detail.

To model the resonance, we must first decide which target and which transfer states to include in the coupled channels system. Since it is time-consuming to recalculate the nonlocal potentials F_{dd} for each incident energy and partial wave (especially when looking for the resonance in the first place), we try to choose a channel set in which the channels are all nearly orthogonal, or are nearly 'completely nonorthogonal' and require numerical orthogonality conditions as described earlier in this section. The choice of the channel set may be accomplished by leaving out the second $5/2^+$ and the $3/2^+$ ^{13}C states and their transfer channels, so that the I=2 inelastic deuteron channels are nearly orthogonal to the remaining transfer channels for the reasons given in section 5.4. (If these two transfer states were to be included, there would be large non-orthogonality effects irreducibly between them and the inelastic

channels. Resonances and complicated resonance interactions would be possible in both kinds of channels, since at E_d = 2.71 Mev all these deuteron and proton channels are below the scattering threshold.)

Therefore, the only nonorthogonality effects are numerical orthogonality conditions on the deuteron's elastic channels, just as described earlier in this section for non-resonant direct reactions. The effects of these conditions here are to reduce the amplitude of the elastic channel in the internal region, and hence to reduce the coupling of the inelastic channels to the scattering continuum. This coupling is in fact reduced to a more realistic level, considering the extra transfer couplings from the inelastic deuteron channel to the proton transfer channels. It is precisely this additional coupling to the transfer channels that is superfluous in usual models, since to some extent the deuteron and transfer channels are non-orthogonal and describe the same physical configurations.

The effect of the orthogonality conditions over the E_d = 2.71 Mev resonance is to reduce the coupling between the elastic and inelastic deuteron channels, and to sharpen the inelastic resonance[1]. Figure 2.4.1 showed how the resonance was broadened by the proper inclusion of the reverse transfer couplings. The effect of the orthogonality conditions is to reduce some of this broadening, since part of this coupling was already present as coupling to the elastic channel, because that channel has considerable overlap with the combined transfer channels.

[1] reducing its width from 34 to 22 kev.

On the inelastic resonance, the wave functions ψ in the elastic channel are significantly affected by their orthogonality conditions. This is seen in Figure 6.5.2, which shows the effect of the one orthogonality condition $\langle 1d_3|\psi\rangle = 0$ on the wave functions ψ, which on the system resonance are purely imaginary. Because its binding energy is nearest to the continuum, the $1d_3$ eigenstate of the deuteron potential-well is at $\rho = 4$ the most influential of the orthogonality conditions determined previously. Without the $\langle 1d_3|\psi\rangle = 0$ condition, the resonance appears at $E_d = 3.025$ Mev, whereas once the condition is enforced, the change in coupling (see below) shifts the resonance to 2.725 Mev. (For this reason, although the phase shifts of the 'local' and 'orthogonalised' ψ-functions in Fig. 6.5.2 are identical, the functions themselves do not asymptotically coincide.) Their significant differences are in the internal region. Compared with the off-resonance wave functions shown in Figure 5.4.4 (note the change of scale), the resonant functions here are large internally. However, the original local ψ-function and the $1d_3$ bound state each has 1 internal node at about 2.5 fm, and when they are required to be mutually orthogonal, the ψ-function is forced to have 2 internal nodes, at 2.3 & 4.5 fm. This will typically imply more cancellation in radial integrals over the internal region, and hence reduced couplings to other channels as was also found earlier.

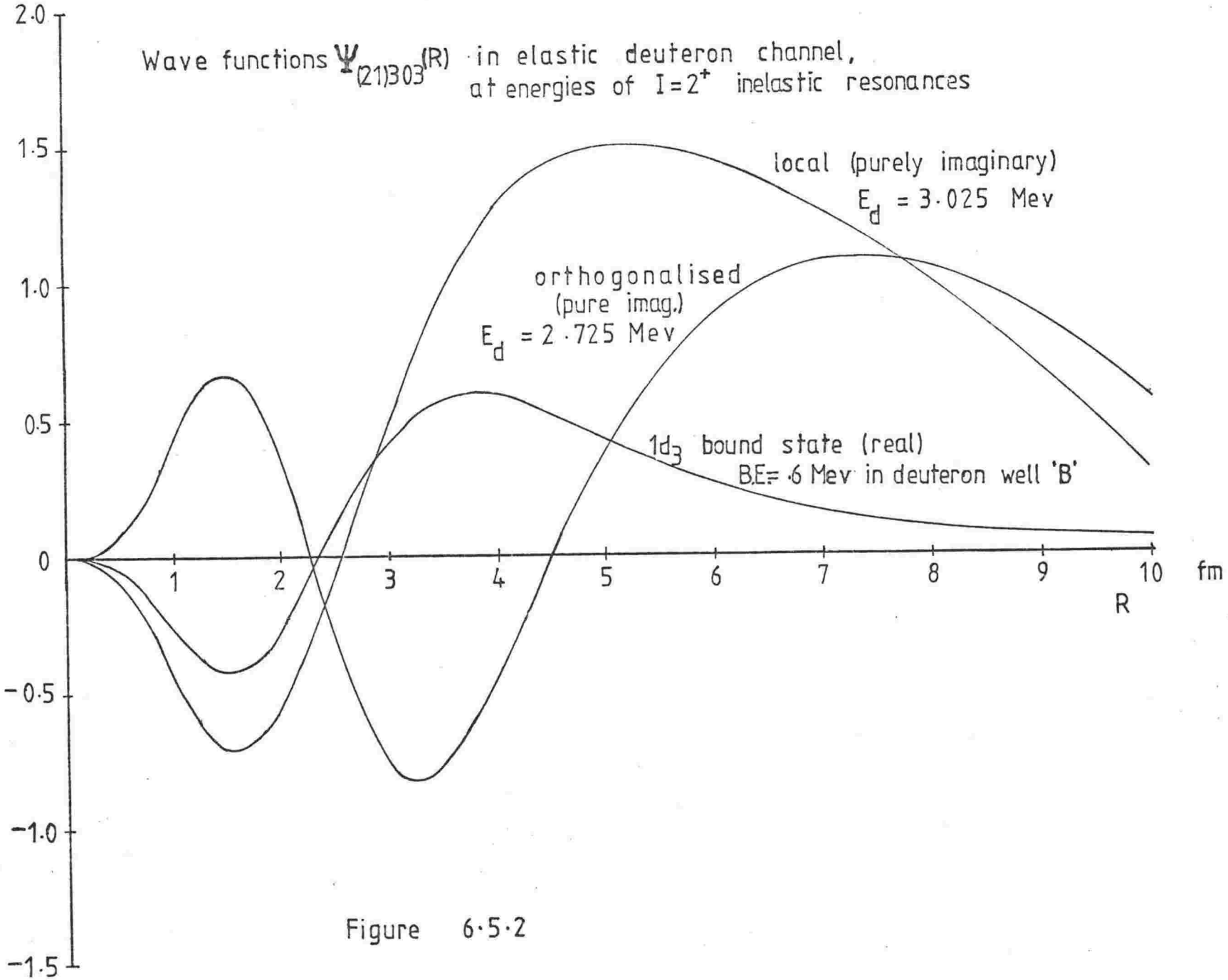

Wave functions $\Psi_{(21)303}(R)$ in elastic deuteron channel,
at energies of $I=2^+$ inelastic resonances
local (purely imaginary)
E_d = 3·025 Mev
orthogonalised
(pure imag.)
E_d = 2·725 Mev
$1d_3$ bound state (real)
B.E= ·6 Mev in deuteron well 'B'
2·0
1·5
1·0
0·5
0
−0·5
−1·0
−1·5
1
2
3
4
5
6
7
8
9
10
fm
R

Figure 6·5·2

Chapter 7 Conclusions

In this short chapter, I summarise the main conclusions of the thesis, and give some indication how they relate to previous work.

The principal conclusions in the theory of cluster interactions between deuterons and a nucleus, when transfer channels and the Pauli Principle are taken into account, are

i) the effect of orthogonalising a deuteron channel to transfer channels is additive on the number of transfer channels,

ii) the effects of the Pauli Principle on the deuteron channel are additive in the same manner,

iii) if the cumulative effects of i) & ii) are less than a threshold (ie. if the eigenvalues of K_d^+ are less than unity) then they can largely be absorbed in a renormalisation of the deuteron-to-nucleus relative wave function, as suggested by Buck et al.(1977),

iv) if the cumulative effects are at the threshold (ie. if K_d^+ has unit eigenvalues) then the relative wave function is subject to orthogonality conditions as in the OCM. These conditions require the wave function to have a minimum number of nodes in the internal region,

v) if all transfer channels and all Pauli Principle effects are included, then the number of unit eigenvalues is increased.

The orthogonality conditions implied by iv) may be found directly using a simplified model.

The orthogonality conditions affect the relative wave function mainly at small radii in the internal region, tending to make it small and oscillatory there. This reduces the effective coupling from the elastic channel, as calculated for example by a T-matrix integral using the wave function. This effect goes part way to explaining the improvement found in the DWBA when the inner region is not included in the radial integrals.

A further effect of the increased number of internal oscillations is to make the cluster-cluster potential well look deeper, while if a deeper well was already used in the model, the orthogonality conditions would be less important. This explains why the deuteron-^{12}C model of the thesis used a well depth of 115 not 80 Mev, and still obtained reasonable results for the E_d=2.71 Mev resonance (see section 2.4), even though preliminary calculations by Pong & Austern of the second-order effects on the well depths favoured the shallower well (see section 4.4). It would appear that the orthogonality conditions and the second-order potentials V_{res} have opposite effects on the depth of an optical potential required, and that the orthogonality conditions have an overriding influence.

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Appendix 1 The operator 'K' with core correlations

Start with the core correlations expressed by the core state $\phi_A(\underline{r}_1,..,\underline{r}_A)$ being written as a linear combination of anti-symmetrised product wave functions:

$$\phi_A(\underline{r}_1,..,\underline{r}_A) = \sum_\lambda a_\lambda \Phi_\lambda(\underline{r}_1,..,\underline{r}_A)$$

where Φ_λ is a Slater-determinant function of size A * A,

and λ describes all the quantum numbers of the 'A' single-particle wave functions : $\lambda = (\lambda_1,\lambda_2,..,\lambda_A)$.

For example, $\lambda = ((j_1 m_1), (j_2 m_2), .. , (j_A m_A))$

and $\Phi_\lambda = (A!)^{-\frac{1}{2}} \det(w_{j_1 m_1}, .. , w_{j_A m_A})$.

Note (i) a_λ is antisymmetric for particle exchanges, i.e. if for some A:A permutation σ we have $\lambda' = \sigma\lambda$, then $a_{\lambda'} = (-1)^\sigma a_\lambda$

(ii) $\sum_\lambda |a_\lambda|^2 = (A!)^{-1}$

The Pauli operator 'K' is defined by its kernel function

$$k(\underline{r}_0,\underline{r}_1) = A < \phi_A(\underline{r}_1,\underline{r}_2,..,\underline{r}_A) \mid \phi_A(\underline{r}_0,\underline{r}_2,..,\underline{r}_A) >$$

$$= A \sum_{\lambda\lambda'} a_\lambda a_{\lambda'} <\Phi_\lambda(\underline{r}_1,..,\underline{r}_A) \mid \Phi_{\lambda'}(\underline{r}_1,..,\underline{r}_A)>$$

Now $\Phi_\lambda = (A!)^{-\frac{1}{2}} \det(w_{j_1 m_1}, .. , w_{j_A m_A})$ so

$$<\Phi_\lambda(\underline{r}_1,..)|\Phi_{\lambda'}(\underline{r}_0,..)> = \frac{1}{A!}\sum_{k=1}^{A} (-1)^{k+1} <w_{j_k m_k}| <Minor_{\lambda,k}|$$

$$* \sum_{\ell=1}^{A} (-1)^{\ell+1} |w_{j'_\ell m'_\ell}> |Minor_{\lambda',\ell}>$$

and as $\langle \text{Minor}_{\lambda,k}(\underline{r}_2,..,\underline{r}_A) \mid \text{Minor}_{\lambda',\ell}(\underline{r}_2,..,\underline{r}_A)\rangle$

$$= \begin{cases} (-1)^{\sigma}\ (A-1)! & \text{if } \lambda=\sigma\lambda' \text{ except perhaps } j_k m_k \neq j'_\ell m'_\ell \\ 0 & \text{otherwise} \end{cases}$$

we get

$$k(\underline{r}_0,\underline{r}_1) = \sum_{\lambda\lambda'} a^*_\lambda a_{\lambda'} \sum_{k\ell} F(\lambda,k;\lambda',\ell)\ |w_{j'_\ell m'_\ell}(\underline{r}_0)\rangle\langle w_{j_k m_k}(\underline{r}_1)|$$

$$\text{where } F(\lambda,k;\lambda',\ell) = \begin{cases} (-1)^{\sigma} & \text{if } \lambda-\{\lambda_k \equiv j_k m_k\} \overset{\sigma}{=} \lambda'-\{\lambda_{\ell'} \equiv j_{\ell'} m_{\ell'}\} \\ 0 & \text{otherwise} \end{cases}$$

In the λ' summation, all the $(A-1)!$ sums over $\lambda'_1 .. \lambda'_A$, except for λ_ℓ, are just different permutations in $\lambda - \{\lambda_k\} = \lambda' - \{\lambda_{\ell'}\}$, so

$$k(\underline{r}_0,\underline{r}_1) = \sum_{k\ell=1}^{A} \sum_{\substack{\lambda \\ \lambda'=\lambda-\{\lambda_k\}+\{\lambda_\ell\}}} (A-1)!\ a^*_\lambda a_{\lambda'}\ |w_{\lambda'_\ell}(\underline{r}_0)\rangle\langle w_{\lambda_k}(\underline{r}_1)|$$

$$= \sum_{\lambda_1\lambda'_1} A.A \sum_{\substack{\lambda \\ \lambda'=\lambda-\{\lambda_k\}+\{\lambda_\ell\}}} (A-1)!\ a^*_\lambda a_{\lambda'}\ |w_{\lambda'_\ell}(\underline{r}_0)\rangle\langle w_{\lambda_k}(\underline{r}_1)|$$

$$= A.A! \sum_{\lambda_1\lambda'_1} \sum_{\overline{\lambda}} a^*_{\lambda_1\overline{\lambda}}\ a_{\lambda'_1\overline{\lambda}}\ |w_{\lambda'_\ell}\rangle\langle w_{\lambda_k}|$$

where $\overline{\lambda} = (\lambda_2,..,\lambda_A)$ so $\lambda = (\lambda_1,\overline{\lambda})$

or

$$K = A.A! \sum_{\substack{j_1 m_1 \\ j'_1 m'_1}} \sum_{\substack{j_2 m_2 \\ \cdots \\ j_A m_A}} a^*_{j_1 m_1 j_2 m_2 ..}\ a_{j'_1 m'_1 j_2 m_2 ..}\ |w_{j'_1 m'_1}\rangle\langle w_{j_1 m_1}|$$

if each λ_k is a jm pair.

Appendix 2 Core Excitations

Here we construct an operator K with kernel function $k(r_0,r_1)$ which acts only on the radial part of the wave function $u(r_0)$. The effects of the angular momenta of the particle, of the core, and of their mutual couplings are all included in the operator 'K'.

If the total particle - core system has angular momentum JM, then we can expand this into products of the core states ϕ^{μ}_{I} and single-particle states $u^{m}_{ljI}(\underline{r}_0) = Y^{m}_{lj}(\hat{\underline{r}}_0)\, u_{ljI}(r_0)$:

$$\Psi^{JM}(\underline{r}_0,\underline{r}_1,\cdots,\underline{r}_A) = \sum_{ljI} \sum_{m\mu} C^{jIJ}_{m\mu M}\, \mathcal{A}\left(u^{m}_{ljI}(\underline{r}_0)\ \phi^{\mu}_{I}(\underline{r}_1,\cdots,\underline{r}_A) \right)$$

$$= \sum_{ljI} \mathcal{A}\left(u_{ljI}(r_0)\ \Phi^{JM}_{ljI}(\hat{\underline{r}}_0,\underline{r}_1,\cdots,\underline{r}_A) \right)$$

where $\Phi^{JM}_{ljI}(\hat{\underline{r}}_0,\underline{r}_1,\cdots) = \sum_{m\mu} C^{jIJ}_{m\mu M}\ Y^{m}_{lj}(\hat{\underline{r}}_0)\ \phi^{\mu}_{I}(\underline{r}_1,\cdots,\underline{r}_A)$

collects the angular, core, and coupling effects.

As usual, we define another single-particle wave function $U_{ljI}(r_0)$ as the projection of the total state Ψ^{JM} onto all the internal states, which are here collected into Φ^{JM}_{ljI}. The 'U' function is

$$U_{l'j'I'}(r_0) = \langle \Phi^{JM}_{l'j'I'}(\hat{\underline{r}}_0,\underline{r}_1,\cdots,\underline{r}_A) \mid \Psi^{JM}(\underline{r}_0,\underline{r}_1,\cdots,\underline{r}_A) \rangle$$

$$= \sum_{ljI} (1 - K^{l'j'I'}_{ljI})\, u_{ljI}$$

where

$$K^{l'j'I'}_{ljI}(r_0,r_1) = \sum_{\substack{m\mu \\ m'\mu'}} C^{j'I'J}_{m'\mu'M}\ C^{jIJ}_{m\mu M}$$

$$\cdot\ A\langle Y^{m'}_{l'j'}(\hat{\underline{r}}_0)\phi^{\mu}_{I}(\underline{r}_1\cdots) \mid Y^{m}_{lj}(\hat{\underline{r}}_1)\phi^{\mu}_{I}(\underline{r}_0,\cdots)\rangle$$

The core states ϕ_I^μ are now expanded into sums of Slater-determinant wave functions, as in Appendix 1 :

$$\phi_I^\mu(\underline{r}_1,..,\underline{r}_A) = \sum_{\substack{j_1 m_1 \\ \cdots \\ j_A m_A}} a_{I\mu:j_1 m_1 .. j_A m_A} \; \Phi_{j_1 m_1 .. j_A m_A}(\underline{r}_1,..,\underline{r}_A)$$

Thus

$$A\langle \Phi_{I'}^{\mu'}(\underline{r}_1,..) \mid \Phi_I^\mu(\underline{r}_0,..) \rangle$$

$$= \sum_{\substack{j_1 m_1 \\ j_1' m_1'}} \mid w_{j_1 m_1}(\underline{r}_0)\rangle \; \kappa_{I\mu:j_1 m_1}^{I'\mu':j_1' m_1'} \; \langle w_{j_1' m_1'}(\underline{r}_1)\mid$$

with

$$\kappa_{I\mu:j_1 m_1}^{I'\mu':j_1' m_1'} = A.A! \sum_{jm_{2-A}} a^*_{I'\mu':j_1' m_1' jm_{2-A}} \; a_{I\mu:j_1 m_1 jm_{2-A}}$$

so

$$K_{\ell j I}^{\ell' j' I'} = \sum_{\substack{m\mu \\ m'\mu'}} C^{j'I'J}_{m'\mu'M} \; C^{jIJ}_{m\mu M} \sum_{\substack{j_1 m_1 \\ j_1' m_1'}} \kappa_{I\mu:j_1 m_1}^{I'\mu':j_1' m_1'}$$

$$\cdot \langle Y^{m'}_{\ell' j'}(\hat{\underline{r}}_0) \mid w_{j_1 m_1}(\underline{r}_0)\rangle \; \langle w_{j_1' m_1'}(\underline{r}_1) \mid Y^m_{\ell j}(\hat{\underline{r}}_1)\rangle \; .$$

Since $\langle Y^{m'}_{\ell' j'}(\hat{\underline{r}}_0) \mid w_{j_1 m_1}(\underline{r}_0)\rangle = \delta_{j_1 j'} \; \delta_{m_1 m'} \; w_{\ell' j'}(r_0)$

we have more simply

$$K_{\ell j I}^{\ell' j' I'} = \mid w_{\ell' j'}\rangle \; k_{\ell j I}^{\ell' j' I'} \; \langle w_{\ell j}\mid$$

with

$$k_{\ell j I}^{\ell' j' I'} = A.A! \sum_{jm_{2-A}} \sum_{\substack{m'\mu' \\ m\mu}} a^*_{I'\mu':jm,jm_{2-A}} \; C^{j'I'J}_{m'\mu'M} \; C^{jIJ}_{m\mu M} \; a_{I\mu:j'm',jm_{2-A}}$$