

Chapter 3.2

METHODS OF DIRECT REACTION THEORIES

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PART 3 SCATTERING IN NUCLEAR PHYSICS

Topic 3.1 Nuclear Physics

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In this chapter we see how scattering in nuclear physics gives amplitudes and cross sections not only for elastic scattering, but also inelastic and rearrangement reactions. We build on the standard approaches of Austern¹ and Satchler², but place more emphasis on the non-perturbative methods which are now more widely used³.

3.2.1. Direct Reaction Model Space

Direct reaction theory attempts to solve the Schrödinger equation for a specific model of the components thought to be important in a reaction, with the component interaction potentials. In direct reaction theories, the phases describing the superposition of all parts of the wave function are coherently maintained, and the potentials typically include imaginary components to model how flux is lost from the channels of the model to other channels. Direct reactions are connected directly or via several steps with the elastic entrance channel, and therefore have cross sections that depend on the exit angles relative to the initial beam direction.

The intermediate states in theories of direct reactions are the discrete states of *two interacting nuclei* and the relative motion of these nuclei. These two nuclei will be the projectile and target nuclei, the excited states of one or both of these, and those subsequent pairs of nuclei that may be obtained by transferring one or more nucleons between them. All the nuclei derived from the projectile will be referred to as the ‘projectile-like fragment’ p , and the ‘target-like fragment’ t similarly, with pairs of states ϕ_{pi} and

ϕ_{ti} , and masses m_{pi} and m_{ti} , respectively. If these nuclei are at positions \mathbf{R}_{pi} and \mathbf{R}_{ti} , we form a relative coordinate vector $\mathbf{R}_i = \mathbf{R}_{pi} - \mathbf{R}_{ti}$. The direct reaction model space is then taken as the product of the pairs of nuclear states and wave function $\psi(\mathbf{R}_i)$ for the relative motion:

$$\Psi_{\text{model}} = \sum_i^N \phi_{pi} \phi_{ti} \psi_i(\mathbf{R}_i). \quad (1)$$

The states can be in different mass partitions (m_{pi} depending on i), or they can be different excited states of the projectile and/or the target in any one of the partitions. The basis states ϕ_{pi} and ϕ_{ti} can be bound states of their respective nuclei, or they may be discrete representations of continuum levels. In the former case we have a ‘bound state approximation’, and in the second case we have a ‘coupled discrete continuum channels’ (CDCC) approximation^{4, 5, 6}. What is essential to the direct reaction framework is that they form a finite set (N say) of square-integrable basis functions, as then we can derive a finite set of equations coupling the channel wave functions $\psi_i(\mathbf{R}_i)$ as unknowns.

The physical Hamiltonian H contains the kinetic energy of projectile–target relative motion $T_i = -\hbar^2/2\mu_i \nabla_{\mathbf{R}}^2$ with reduced mass $\mu_i = m_{pi}m_{ti}/(m_{pi} + m_{ti})$, and the separate internal nuclear Hamiltonians for the projectile- and target-like fragments are h_{ni} for $n = p, t$ respectively, of which the ϕ_{ni} are eigenstates: $h_{ni}\phi_{ni} = e_{ni}\phi_{ni}$, each of which is assumed to be fully antisymmetric under the exchange of any internal pair of identical nucleons. The total Hamiltonian H also contains the potential energy terms between the nucleons the p and t nuclei, that couple together all the transfer and inelastic states, whether single-particle, collective or compound.

We do not explicitly treat compound nuclear states, where all the interacting nucleons form a single excited nucleus, and hence all states that are produced consequently to compound intermediate states. The effects of the compound nuclear states will be only included in some average manner, as described in the next section.

3.2.2. Elimination of the Compound Nucleus States

Because the model space in direct reaction theory is not the whole physical range, we need to define a division of the full Hilbert space by means of projection operators. Following Feshbach⁷ we define P as the projection operator onto the model space, including the entrance channels, and Q as projecting on to the remaining space.

Such operators must obey $P^2 = P$, $Q^2 = Q$, $PQ = QP = 0$ and $P+Q = I$, where I is the identity operator. With these operators we divide the physical wave function Ψ of the system as $\Psi = \Psi_P + \Psi_Q$ where $\Psi_P = P\Psi$ and $\Psi_Q = Q\Psi$. The Ψ_P component, includes the elastic channel and just those channels ‘directly’ related to it that we choose to include in our direct reaction model. The Ψ_P contains the same reaction channels as the model wave function Ψ_{model} , but the wave functions are not identical since the model Hamiltonian is obtained by some energy-averaging procedure to be discussed below.

The physical Hamiltonian H governs the full wave function Ψ at energy E by the Schrödinger equation $(H - E)\Psi = 0$. This equation is now separated into two coupled equations for Ψ_P and Ψ_Q :

$$(E - H_{PP})\Psi_P = H_{PQ}\Psi_Q \quad (2)$$

$$(E - H_{QQ})\Psi_Q = H_{QP}\Psi_P \quad (3)$$

where $H_{PP} \equiv PHP$, $H_{PQ} \equiv PHQ$ and so on.

The Eq. (2) has an incoming wave boundary condition in the elastic channel, and there are outgoing waves in all other channels of this and Eq. (3) too. We may therefore formally solve Eq. (3) as

$$\Psi_Q = (E + i\varepsilon - H_{QQ})^{-1} H_{QP}\Psi_P \quad (4)$$

and substitute this into Eq. (2) to obtain a formally exact uncoupled equation for Ψ_P :

$$\left(E - H_{PP} - H_{PQ}(E + i\varepsilon - H_{QQ})^{-1} H_{QP} \right) \Psi_P = 0.$$

Optical Operator

The Feshbach procedure therefore gives an effective Hamiltonian H_{eff} for the direct-reaction model space $P\Psi$:

$$H_{\text{eff}}(E) = H_{PP} + H_{PQ}(E + i\varepsilon - H_{QQ})^{-1} H_{QP}. \quad (5)$$

This is an exact expression, and describes precisely the effect on the model space all variations and resonances (for example) in the eliminated space. The effective Hamiltonian however, is non-local and

energy-dependent even when the potential interactions in H are local and energy-independent.

The contributions of distinct compound-nucleus state to the effective Hamiltonian may be seen by expanding over a complete set of such states:

$$H_{QQ}|Q_\lambda(E')\rangle = E'|Q_\lambda(E')\rangle$$

where λ distinguishes among degenerate states. Then the second term on the r.h.s of Eq. (5) becomes

$$H_{PQ}(E + i\varepsilon - H_{QQ})^{-1} H_{QP} = \sum_\lambda \int dE' \frac{H_{PQ}|Q_\lambda(E')\rangle \langle Q_\lambda(E')| H_{QP}}{(E - E') + i\varepsilon}. \quad (6)$$

This term, from coupling to the Q channels, has Hermitian and anti-Hermitian parts,

$$H_{PQ}(E + i\varepsilon - H_{QQ})^{-1} H_{QP} = \mathcal{H}_R - i\mathcal{H}_I \quad (7)$$

where

$$\mathcal{H}_R = \sum_\lambda \int dE' \frac{H_{PQ}|Q_\lambda(E')\rangle \langle Q_\lambda(E')| H_{QP}}{(E - E')^2 + \varepsilon^2} \quad (8)$$

$$\mathcal{H}_I = \sum_\lambda H_{PQ}|Q_\lambda(E)\rangle \rho(E) \langle Q_\lambda(E)| H_{QP} \times \int \frac{\varepsilon dE'}{(E - E')^2 + \varepsilon^2} \quad (9)$$

$$= \pi \sum_\lambda H_{PQ}|Q_\lambda(E)\rangle \rho(E) \langle Q_\lambda(E)| H_{QP} \quad (10)$$

with $\rho(E)$ the density of states of H_{QQ} at energy E . The anti-Hermitian part \mathcal{H}_I is positive definite, and arises because the compound-nucleus Ψ_Q channels act, asymmetrically, only to *remove* flux from the the model-space channels that are in Ψ_P .

Energy Averaging

In direct reaction calculations, the precise compound nuclear resonances are not needed in all their fluctuations, but only the average effect of these and similar channels. This is most easily accomplished by averaging $H_{\text{eff}}(E)$ over small energy intervals, giving \bar{H}_{eff} as

$$\bar{H}_{\text{eff}}(E) = \int dE' f(E - E') H_{\text{eff}}(E') \quad (11)$$

where $f(E - E')$ is some distribution function of unit integral and width of the order ΔE . If ΔE is significantly larger than the average spacing of the compound nucleus levels ($\rho(E)\Delta E \gg 1$), then the resulting $\bar{H}_{\text{eff}}(E)$ has Hermitian and anti-Hermitian components that vary rather slowly with energy E .

Optical Model

In order to formulate an Optical Model, we further assume that the energy-averaged effective Hamiltonian $\overline{H}_{\text{eff}}$ can be approximated by a *local* potential that depends only on the coordinate degrees of freedom that are explicitly treated in the model wave function. That is, we approximate $\overline{H}_{\text{eff}}(E) \approx H_{\text{opt}}$, which depends only on the collective and/or single-particle degrees of freedom that distinguish the particular N nuclei eigenstates ϕ_{pi} and ϕ_{ti} .

If the model space contains only the elastic channel ($N = 1$), we thereby reduce the effective Hamiltonian to contain a *local optical potential* $U_i(\mathbf{R}_i)$ that depends only on the radial separation of the pair of interacting nuclei. This gives a single-channel Hamiltonian operator

$$H_{\text{opt}}(\mathbf{R}_i) = H_i \equiv T_i + h_{pi} + h_{ti} + U_i^{(1)}(\mathbf{R}_i) \quad (12)$$

for the pair i of the interacting nuclei. The ⁽¹⁾ superscript indicates the size of the model space.

If there are more than 1 channel ($N \geq 2$), then the same optical model Hamiltonian may be written with different partitioning of the kinetic and internal energies that are appropriate for the different mass partitions. Thus, there will be a way of writing the optical channel Hamiltonian for each channel:

$$\overline{H}_{\text{opt}}(E) = H_i \equiv T_i(\mathbf{R}_i) + h_{pi} + h_{ti} + V_i \quad (13)$$

each with some effective potential V_i . This last term can always be separated into diagonal and off-diagonal parts as $V_i = U_i^{(N)}(\mathbf{R}_i) + \mathcal{V}_i$, where \mathcal{V}_i is the term that couples together the different channels. The separation is often made unique by requiring that \mathcal{V}_i has zero diagonal matrix element.

The optical potentials (their sum labelled V_i in general) give rise to the elastic scattering cross section, and the Optical Model procedure uses this causality in reverse, to determine them as those local potentials which fit elastic scattering. We typically look for optical potentials that vary only smoothly and slowly with energy, as appropriate to averaging over some energy scale ΔE , and is most often found just for the one channel case ($N = 1$).

Note that in the coupled channels case ($N > 1$) the diagonal potentials $U_i^{(N)}(\mathbf{R}_i)$ do not *by themselves* reproduce the elastic scattering without the work of the off-diagonal couplings \mathcal{V}_i . We therefore call the diagonal $U_i^{(N)}$ the *bare* potentials, because, even though they are optical potentials which include the effects of $Q\Psi$ channels not in the model space, they do not include the dressing effects of the inter-channel couplings *within* the model space $P\Psi$. Only

the potential in the one-channel model space $U_i^{(1)}$ is supposed to reproduce the elastic scattering by itself.

Because $H_{\text{eff}}(E)$ has Hermitian and anti-Hermitian parts, the optical potentials will have real and imaginary terms, and because \mathcal{H}_I is positive definite the imaginary parts will be negative and absorptive.

3.2.3. Model Schrödinger Equation

The Schrödinger equation for the model wave function Ψ_{model} at total energy E is

$$[E - H_{\text{opt}}(E)]\Psi_{\text{model}} = 0 \quad (14)$$

We use the expansion of Eq. (1) in square-integrable states ϕ of the participating nuclei. Using for each pair i of nuclei the ‘channel optical Hamiltonians’ H_i defined above (Eqs. 12 or 13), Eq. (14) becomes

$$\sum_i^N [T_i(\mathbf{R}_i) + V_i - E_i] \phi_{pi} \phi_{ti} \psi_i(\mathbf{R}_i) = 0 \quad (15)$$

where in each channel there is an asymptotic kinetic energy $E_i = E - e_{pi} - e_{ti}$, corresponding to momentum $\mathbf{k}_i = (2\mu_i E_i / \hbar^2)^{1/2}$. Operating on Eq. (15) to the left by $\langle \phi_{pj} \phi_{tj} |$, we obtain (after swapping the i and j indices)

$$[T_i + U_i - E_i] \psi_i(\mathbf{R}_i) + \sum_j V_{ij} \psi_j(\mathbf{R}_j) = 0 \quad (16)$$

$$\text{with } V_{ij} \equiv \langle \phi_{pi} \phi_{ti} | H_m - E | \phi_{pj} \phi_{tj} \rangle$$

Here, the Hamiltonian H_m in the coupling operator V_{ij} takes one of the forms of Eq. (13): choosing $m = i$ is called the *post* form, and choosing $m = j$ the *prior* form; the two alternatives should give the same results. (If i and j describe different inelastic states of the same nuclei, then $\mathbf{R}_i \equiv \mathbf{R}_j$, we can use orthogonality of ϕ_{ni} and ϕ_{nj} , and the coupling V_{ij} is just a local function of \mathbf{R}_i :

$$V_{ij}(\mathbf{R}_i) = \langle \phi_{pi} \phi_{ti} | V_i | \phi_{pj} \phi_{tj} \rangle \quad (17)$$

This set of coupled equations (16) must be solved with boundary conditions at large radii consisting of an incoming plane wave in channel (say) i_0 , and outgoing spherical waves in all other channels:

$$\psi_{ii_0}(\mathbf{R}_i) = R_i \rightarrow \infty \delta_{i_0 i} e^{i\mathbf{k}_{i_0} \cdot \mathbf{R}_i} + f_{ii_0}(\theta) e^{ik_i R_i} \quad (18)$$

Since ϕ_{pi} , ϕ_{ti} , ϕ_{pj} and ϕ_{tj} are all antisymmetrised internally, the cross section depends on the number of identical nucleons (or nucleonic clusters) that may be transferred in the reaction (see Austern¹, §3.5 or Satchler², §2.11.3.2). If we define n_{pi} and n_{ti} as the numbers of nucleons (or clusters) within respectively the projectile and target states i that are identical to the transferred set, then the scattering amplitude

$f_{i i_0}$ for each channel i directly gives the cross section in that channel as

$$\frac{d\sigma_i(\theta)}{d\Omega} = \frac{k_i}{\mu_i} \frac{\mu_{i_0}}{k_{i_0}} \frac{n_{p i_0}! n_{t i_0}!}{n_{p i}! n_{t i}!} |f_{i i_0}(\theta)|^2 \quad (19)$$

(neglecting a possible elastic Coulomb amplitude in the incoming channel i_0). Partial wave expansions for the Ψ_i , and corresponding expressions for the $f_{i i_0}(\theta)$ will be presented in section 3.2.6.

3.2.4. Transition Amplitudes

Greens function methods may also be used to solve the coupled equations, and furthermore suggest various approximations which simplify the solution methods in many special cases of interest. First, therefore, we present in this section several exact results using T -matrix integrals derived from Greens function analysis. In the following section 3.2.5 we examine various consequent approximations that are often still accurate.

If the full wave function Ψ were known, then the scattering amplitude f_i for the $i_0 \rightarrow i$ reaction may be found from the T -matrix by the equivalence

$$T_{i_0 i} = -\frac{2\pi\hbar^2}{\mu_i} f_i \quad (20)$$

so that, written in terms of the transition amplitudes, the expression for the cross section becomes

$$d\sigma_i(\theta_i)/d\Omega = \frac{\mu_i \mu_{i_0}}{(2\pi\hbar^2)^2} \frac{k_i}{k_{i_0}} \frac{n_{p i_0}! n_{t i_0}!}{n_{p i}! n_{t i}!} |T_{i_0 i}|^2 \quad (21)$$

Expressions for the T transition amplitudes may be derived by using either plane waves or distorted waves in the exit channel.

In addition, for transfer reactions where the channel Hamiltonians are different in the initial and final channels, we have a further choice of using either post or prior forms of the coupling. The post form uses the form of H_i for the exit channel, and the prior form the H_{i_0} from the entrance channel. The plane-wave post matrix element is

$$T_{i_0 i} = \langle \phi_{p i} \phi_{t i} e^{i\mathbf{k}_i \cdot \mathbf{R}_i} | H_i - E | \sum_j \phi_{p j} \phi_{t j} \psi_j^{(+)} \rangle \quad (22)$$

$$= \langle \phi_{p i} \phi_{t i} e^{i\mathbf{k}_i \cdot \mathbf{R}_i} | V_i | \sum_j \phi_{p j} \phi_{t j} \psi_j^{(+)} \rangle \quad (23)$$

where the $(+)$ superscript in $\psi_j^{(+)}$ indicates that they are found with plane incoming waves in the i_0 channel. A prior matrix element uses the Hamiltonian H_{i_0} of the initial channel. Direct substitution in Eq. (22), however, affords no simplifications, so we insert it in the matrix element for the time-reversed reaction, and derive

$$T_{i_0 i} = \langle \sum_j \phi_{p j} \phi_{t j} \psi_j^{(-)} | V_{i_0} | \phi_{p i_0} \phi_{t i_0} e^{i\mathbf{k}_{i_0} \cdot \mathbf{R}_{i_0}} \rangle \quad (24)$$

where the $(-)$ superscript in $\psi_j^{(-)}$ indicates that it has an incident plane wave along \mathbf{k}_{i_0} and incoming spherical waves $e^{-i\mathbf{k}_i \cdot \mathbf{R}_i}$ in all channels.

Distorted-wave expressions may be found by replacing the exponential factors on the left sides by one-channel scattering waves ($\chi_i^{(+)}(\mathbf{R}_i)$ on the right sides and $\chi_i^{(-)}(\mathbf{R}_i)$ on the left), found with some distorting potential W_i by $[T_i + W_i - E_i] \chi_i(\mathbf{R}_i) = 0$. The distorted-wave post matrix element is then

$$T_{i_0 i} = \langle \phi_{p i} \phi_{t i} \chi_i^{(-)} | V_i - W_i | \sum_j \phi_{p j} \phi_{t j} \psi_j^{(+)} \rangle \quad (25)$$

and the equivalent prior form is

$$T_{i_0 i} = \langle \sum_j \phi_{p j} \phi_{t j} \psi_j^{(-)} | V_{i_0} - W_{i_0} | \phi_{p i_0} \phi_{t i_0} \chi_i^{(+)} \rangle \quad (26)$$

The distorting potential W_i may be real or complex without affecting the validity of these matrix elements.

All these four expressions are so far identical, and exactly equivalent to solving the coupled equations directly and using Eq. (20).

3.2.5. Distorted Wave Born Approximation

Various approximate transition amplitudes may be derived by different approximations for the model wave function $\Psi_{\text{model}} = \sum_i \phi_{p i} \phi_{t i} \psi_i(\mathbf{R}_i)$ in the expressions (23,24,25,26). One approach is to emphasize the role of the entrance channel in the model wave function, and consider only those more direct reactions that proceed immediately from the entrance channel. Furthermore, we use in that entrance channel the wave function derived from the optical potential, not the full coupled equations (16).

One-step Born approximation

The first approximation here is to neglect the explicit calculation of multistep effects that proceed from the entrance channel i_0 via some intermediate channel(s) j to the final channel i . This will be more accurate when the intermediate channels are only weakly excited in the reaction, or when the final channel does not couple strongly to those intermediate channels that are populated.

The Born approximation (BA) to the post distorted wave transition amplitude (25) is therefore

$$T_{i_0 i} = \langle \phi_{p i} \phi_{t i} \chi_i^{(-)} | V_i - W_i | \phi_{p i_0} \phi_{t i_0} \psi_{i_0}^{(+)} \rangle \quad (27)$$

with similar one-step Born approximations to the other three transition matrix elements. These approximate DWBA forms are not invariant under the choice of distorting potential W_i , and therefore only

yield useful results if this potential is chosen correctly.

Optical potential

The conventional Distorted Waves Born Approximation (DWBA) makes the second assumption that both the entrance and exit channel wave functions use the corresponding one-channel optical potentials $U_i^{(1)}$ that fitted the elastic scattering (energy-averaged in some way, if necessary). It also uses the coupling potential \mathcal{V}_i from $V_i = U_i^{(2)} + \mathcal{V}_i$. The post-form and prior-form DWBA transition amplitudes, are then

$$T_{i_0 i}^{\text{postDWBA}} = \langle \phi_{p_i} \phi_{t_i} \chi_i^{(-)} | \mathcal{V}_i | \phi_{p_{i_0}} \phi_{t_{i_0}} \chi_{i_0}^{(+)} \rangle \quad (28)$$

$$T_{i_0 i}^{\text{priorDWBA}} = \langle \phi_{p_i} \phi_{t_i} \chi_i^{(-)} | \mathcal{V}_{i_0} | \phi_{p_{i_0}} \phi_{t_{i_0}} \chi_{i_0}^{(+)} \rangle \quad (29)$$

The matrix elements use optical potentials $U_i^{(1)}$ as distorting potentials which depend only on the channel radii \mathbf{R}_i , and coupling interactions \mathcal{V}_i will depend on coordinates of both the channels and the internal structure of the interacting nuclei. Although the prior and post DWBA expressions (28,29) are consistently equal to each other, this equality holds for *any* choice of distorting potentials, and does not guarantee any physical accuracy.

Possible reasons for choosing different exit-channel distorting potentials W_i are discussed in §4.5 of Austern¹.

3.2.6. Partial-wave expansions

The total wave function is expanded in partial waves using a coupling order such as

$$\mathbf{L} + \mathbf{J}_p = \mathbf{J}; \quad \mathbf{J} + \mathbf{J}_t = \mathbf{J}_T, \quad (30)$$

which may be defined by writing

$$\psi_{i J_T}^{M_T} = |(L J_p) J, J_t; J_T\rangle \quad (31)$$

where J_p = projectile spin, J_t = target spin, L = orbital partial wave, and J_T = total system angular momentum.

The set $\{i, (L J_p) J, J_t; J_T\}$ will be abbreviated by the single variable α . Thus, in each partition the partial wave expansion of the wave function is

$$\psi_{i J_T}^{M_T}(\mathbf{R}_i, \xi_p, \xi_t) = \sum_{L J_p J J_t} \phi_{J_p}(\xi_p) \phi_{J_t}(\xi_t) i^L Y_L^M(\hat{\mathbf{R}}_i) \\ M \mu_p M_J \mu_t \\ f_{(L J_p) J, J_t}^{i J_T}(R_i) / R_i \langle L M J_p \mu_p | J M_J \rangle \langle J M_J J_t \mu_t | J_T M_T \rangle \quad (32)$$

here ξ_p and ξ_t are the internal coordinates of the projectile and target, and

$$f_{(L J_p) J, J_t}^{i J_T}(R) \equiv f_\alpha(R) \quad (33)$$

are the radial wave functions. The (optional) i^L factors are included to simplify the spherical Bessel expansion of the incoming plane wave.

The wave function ψ could also have been defined using the ‘channel spin’ representation $\psi = |L, (J_p J_t) S; J_T\rangle$, which is symmetric upon projectile \rightarrow target interchange except for a phase factor $(-1)^{S-J_p-J_t}$.

The coupled partial-wave equations are of the form

$$[E_i - T_{iL}(R_i) - U_i(R_i)] f_\alpha(R_i) = \\ \sum_{\alpha', \Gamma > 0} i^{L'-L} V_{\alpha: \alpha'}^\Gamma(R_i) f_{\alpha'}(R_i) \\ + \sum_{\alpha', i' \neq i} i^{L'-L} \int_0^{R_m} V_{\alpha: \alpha'}(R_i, R_{i'}) f_{\alpha'}(R_{i'}) dR_{i'} \quad (34)$$

where the partial-wave kinetic energy operator is

$$T_{iL}(R_i) = -\frac{\hbar^2}{2\mu_i} \left(\frac{d^2}{dR_i^2} - \frac{L(L+1)}{R_i^2} \right), \quad (35)$$

$U_i(R_i)$ is the diagonal optical potential with nuclear and Coulomb components, and R_m is a radius limit larger than the ranges of $U_i(R_i)$ and of the coupling terms.

The $V_{\alpha: \alpha'}^\Gamma(R_{i'})$ are the local coupling interactions of multipolarity Γ , and the $V_{\alpha: \alpha'}(R_i, R_{i'})$ are the non-local couplings between mass partitions that arise from particle transfers. The equations (34) are in their most common form; they become more complicated when non-orthogonalities are included by the method of section 3.2.8.

For incoming channel α_0 , the solutions $f_\alpha(R_i)$ satisfy the boundary conditions when $R_i > R_m$ of

$$f_\alpha(R_i) = \frac{i}{2} \left[\delta_{\alpha \alpha_0} H_{L \eta_i}^{(-)}(k_i R_i) - S_{\alpha \alpha_0} H_{L \eta_i}^{(+)}(k_i R_i) \right] \quad (36)$$

where $H_{L \eta}^{(-)}$ and $H_{L \eta}^{(+)}$ are the Coulomb functions with incoming and outgoing boundary conditions respectively, and

$$\eta_i = \frac{2\mu_i}{\hbar^2} \frac{Z_{p_i} Z_{t_i} e^2}{2k_i} \quad (37)$$

is the Sommerfeld parameter for the Coulomb wave functions.

In terms of the S -matrix elements $S_{\alpha \alpha_0}$, and for coupling order of Eq. (30), the scattering amplitudes for transitions to projectile & target m -states of m , M to m' , M' are

$$f_{m' M'; m M}^{i i_0}(\theta) = \delta_{\alpha \alpha_0} F_c(\theta) + \\ \sum_{L L' J J' J_T} \langle L O J_p m | J m \rangle \langle J m J_t M | J_T M_T \rangle \\ \langle L' M_{L'} J'_p m' | J' M_{L'} + m' \rangle \langle J' M_{L'} + m' J'_t M' | J_T M_T \rangle$$

$$\frac{4\pi}{k_{i0}} e^{i(\sigma_L - \sigma_0)} e^{i(\sigma'_{L'} - \sigma'_0)} \sqrt{\frac{2L+1}{4\pi}} \left(\frac{i}{2}\right) [\delta_{\alpha', \alpha} - S_{\alpha' \alpha}^{JT}] Y_{L'}^{m'+M'-m-M}(\theta, 0) \quad (38)$$

where

$$\sigma_L = \arg \Gamma(1 + L + i\eta_i) \quad (39)$$

are the Coulomb phase shifts and the Coulomb amplitude F_c is

$$F_c(\theta) = -\frac{\eta_{i0}}{2k_{i0}} \frac{\exp(-2i\eta_{i0} \ln(\sin \theta/2))}{\sin^2 \theta/2}. \quad (40)$$

The corresponding differential cross section is

$$\frac{d\sigma_{ii_0}(\theta)}{d\Omega} = \frac{k_i \mu_{i0} n_{pi_0}! n_{ti_0}!}{\mu_i k_{i0} n_{pi}! n_{ti}!} \frac{1}{(2J_p + 1)(2J_t + 1)} \times \sum_{m'M'mM} |f_{m'M':mM}^{ii_0}(\theta)|^2. \quad (41)$$

The spherical tensor analysing powers T_{kq} describe how the outgoing cross section depends on the incoming polarisation state of the projectile. If the spherical tensor τ_{kq} is an operator with matrix elements

$$(\tau_{kq})_{mm''} = \sqrt{2k+1} \langle J_p m k q | J_p m'' \rangle,$$

we have

$$\begin{aligned} T_{kq}(\theta) &= \frac{\text{Tr}(\mathbf{f} \tau_{kq} \mathbf{f}^+)}{\text{Tr}(\mathbf{f} \mathbf{f}^+)} \\ &= \hat{k} \sum_{m'M'mM} f_{m'M':mM}^*(\theta) \langle J_p m k q | J_p m'' \rangle f_{m'M':m''M}(\theta) \\ &\div \sum_{m'M'mM} |f_{m'M':mM}(\theta)|^2 \end{aligned}$$

3.2.7. Channel couplings

The coupling terms V_{ij} need to be determined for common reaction mechanisms such as inelastic excitations of nuclei, or particle transfers from the projectile to/from the target.

Nuclear Rotational Model

Consider one deformed nucleus with deformation lengths δ_λ , (the fractional deformation β_λ times some average radius R_c). The effect of these deformations can be expressed as a change in the radius at which we evaluate the optical potentials, the change depending on the relative orientations of the radius vector to the intrinsic orientation of the nucleus. When $U(R)$ is the potential shape to be deformed, the coupling interaction is

$$\mathbf{V}(\xi, \mathbf{R}) = U(R - \delta(\hat{\mathbf{R}}, \xi)) \quad (42)$$

where the ‘shift function’ has the multipole expansion

$$\delta(\hat{\mathbf{R}}') = \sum_{\lambda \neq 0} \delta_\lambda Y_\lambda^0(\hat{\mathbf{R}}') \quad (43)$$

($\hat{\mathbf{R}}'$ is the vector $\hat{\mathbf{R}}$ rotated to the body-centred frame of coordinates defined by ξ). Transforming to the space-fixed frame of reference, and projecting onto the spherical harmonics, the multipole expansion becomes

$$\mathbf{V}(\xi, \mathbf{R}) = \sum_{\lambda \mu} \mathbf{V}_\lambda^N(R) D_{\mu 0}^\lambda Y_\lambda^\mu(\hat{\mathbf{R}})$$

$$\text{where } \mathbf{V}_\lambda^N(R) = 2\pi \int_{-1}^{+1} U(r(R, \cos \theta)) Y_\lambda^\mu(\theta, 0) d(\cos \theta)$$

$$\text{and } r(R, u) = R - \sum_\lambda \sqrt{\frac{2\lambda+1}{4\pi}} P_\lambda(u) \delta_\lambda + \epsilon$$

$$\text{with } \epsilon = \sum_\lambda \delta_\lambda^2 / (4\pi R_c)$$

The correction ϵ is designed⁽⁸⁾ to ensure that the volume integral of the nuclear monopole potential $\mathbf{V}_0^N(R)$ is the same as that of $U(R)$, and is correct to second order in the $\{\delta_\lambda\}$.

When the $\{\delta_\lambda\}$ are small, the above multipole functions are simply the first derivatives of the $U(R)$ function:

$$\mathbf{V}_\lambda^N(R) = -\frac{\delta_\lambda}{\sqrt{4\pi}} \frac{dU(R)}{dR}, \quad (44)$$

with the same shape for all nuclear multipoles $\lambda > 0$.

The deformations of the Coulomb potential can also be defined by the δ_λ , but more accurately by means of the Coulomb reduced matrix element $\langle I' || E\lambda || I \rangle$ that is directly related to electromagnetic decay strengths as $\pm \sqrt{(2I+1)B(E\lambda, I \rightarrow I')}$. The reduced matrix element defined by the Wigner-Eckart theorem of the form.

$$\langle j_f m_f | \hat{O}_{jm} | j_i m_i \rangle = \hat{j}_f^{-1} \langle j_i m_i j m | j_f m_f \rangle \langle j_f || \hat{O}_j || j_i \rangle \quad (45)$$

For a rotational model of the nucleus, the matrix element is determined to first order in δ_λ by

$$\langle I' || E\lambda || I \rangle = \frac{3Z\delta_\lambda R_c^{\lambda-1}}{4\pi} \sqrt{2I+1} \langle IK\lambda 0 | I'K \rangle \quad (46)$$

for transitions from a state of spin I to one of spin I' in a rotational band of projection K in a nucleus of charge Z .

The radial form factors for Coulomb inelastic processes are derived from the multipole expansion of $|\mathbf{r} - \mathbf{r}'|^{-1}$, giving for interactions with the other nucleus (charge Z') of

$$\mathbf{V}_\lambda^C(R) = \langle I' || E\lambda || I \rangle \frac{\sqrt{4\pi e^2 Z'}}{2\lambda+1} \begin{cases} R^\lambda / R_c^{2\lambda+1} & (R \leq R_c) \\ 1/R^{\lambda+1} & (R > R_c) \end{cases} \quad (47)$$

Note that, especially for dipole and quadrupole couplings ($\lambda = 1, 2$), these Coulomb couplings have a long range that is much larger than the sum of the radii of the interacting nuclei. Any method for numerically solving the coupled equations with these couplings has to include some particular treatment of these couplings at large distances as discussed in ref. 16.

For projectile inelastic excitations, the coupling matrix elements between different partial waves defined with Eq. (30) are

$$\langle (LJ_p)J, J_t; J_T | \mathbf{V}_\lambda | (L'J'_p)J, J_t; J_T \rangle = \mathbf{X}_{LJ_p, L'J'_p}^{J\lambda}(R) \quad (48)$$

whereas for target excitations,

$$\begin{aligned} \langle (LJ_p)J, J_t; J_T | \mathbf{V}_\lambda | (L'J'_p)J', J'_t; J_T \rangle &= (-1)^{J-J'-L+L'} \hat{j} \hat{j}' \\ &\times \sum_{J_2} (2J_2 + 1) W(J_p L J_T J_t; J J_2) W(J_p L' J_T J'_t; J' J_2) \\ &\times \mathbf{X}_{LJ_t, L'J'_t}^{J_2\lambda}(R) \end{aligned}$$

having defined the ‘spatial’ couplings as

$$\begin{aligned} \mathbf{X}_{LI, L'I'}^{J\lambda}(R) &= \hat{L} \hat{L}' (-1)^{J-I'-L+L'} W(LL'II'; \lambda J) \langle L0L'0 | \lambda 0 \rangle \\ &[\mathbf{V}_\lambda^C(R) + \hat{I}' \langle I'K\lambda 0 | IK \rangle \mathbf{V}_\lambda^N(R)] \end{aligned} \quad (49)$$

The rotational model factor $\hat{I}' \langle I'K\lambda 0 | IK \rangle$ has been built into the definition of the Coulomb reduced matrix element.

Rearrangement Reactions

Spectroscopic amplitudes and factors If the nuclear state ϕ_{pi} is transformed into state ϕ_{pj} by removal of some nucleon(s), then we can define an overlap wave function

$$\chi_{j,i}^p(\mathbf{r}) = \langle \phi_{pj}(\xi_{pj}) | \phi_{pi}(\xi_{pj}, \mathbf{r}) \rangle \quad (50)$$

The partial wave components of this overlap can be written as the sum of some amplitudes A times normalised wave functions φ . The coefficients A are called spectroscopic amplitudes (or coefficients of fractional parentage), and their square moduli $|A|^2$ the spectroscopic factors. If a coupling order $|(\ell s)j, I; JM\rangle$ is used, the composite nucleus wave function is

$$\phi_{JM}(\xi_{pj}, \mathbf{r}) = \frac{1}{\sqrt{n_{pi}}} \sum_{\ell j I} A_{\ell s j}^{j I J} [\phi_I(\xi_{pj}) \varphi_{\ell s j}(\mathbf{r})]_{JM}, \quad (51)$$

and

$$S_{\ell s j}^{j I J} = |A_{\ell s j}^{j I J}|^2 \quad (52)$$

is the spectroscopic factor. The n_{pi} is again the number of nucleons (or clusters) in the composite system ϕ_{pi} that are identical to that transferred, and the $n_{pi}^{-1/2}$ factor arises because of the normalisation

of antisymmetrised wave functions for the core and composite nuclei. (In many common reactions with or near closed shell nuclei, the $n_{pi}^{-1/2}$ factor cancels some of the $n!$ terms in eqs. (19,21)).

Similar target overlap wave functions can also be defined.

Transfer couplings To calculate the coupling term that arises when a particle is transferred, for example from a target bound state to being bound in the projectile, we need to evaluate matrix elements where the initial (primed) state has a composite target with internal coordinates $\xi'_t \equiv \{\xi'_t, \mathbf{r}'\}$: $\phi_{J'_t}(\xi'_t, \mathbf{r}') = |(\ell' s)j', J_t; J'_t\rangle$ and the final (unprimed) state has a composite projectile with internal coordinates $\xi_p \equiv \{\xi_p, \mathbf{r}\}$: $\phi_{J_p}(\xi_p, \mathbf{r}) = |(\ell s)j, J_p; J_p\rangle$.

Let \mathbf{V} be the interaction potential, of which the prior form is

$$\mathbf{V} = V_{\ell s j}(\mathbf{r}) + U_{cc}(R_c) - U_{\alpha'}(\mathbf{R}') \quad (53)$$

and the post form is

$$\mathbf{V} = V_{\ell' s j'}(\mathbf{r}') + U_{cc}(R_c) - U_{\alpha}(\mathbf{R}) \quad (54)$$

where $V_{\beta}(\mathbf{r})$ is the potential which binds $\varphi_{\beta}(\mathbf{r})$, $U_{\alpha}(\mathbf{R})$ are the optical potentials, and $U_{cc}(\mathbf{R}_c)$ is the ‘core-core’ potential, here between the p' and the t nuclei. The V_{β} will be real, but the U_{α} and U_{cc} will typically have both real and imaginary components.

The matrix element is now a non-local integral operator, as it operates on the function $f_{\alpha'}(R')$ to produce a function of R . This section therefore derives the non-local kernel $V_{\alpha, \alpha'}(R, R')$ so that the matrix element operation on a wave function, which initially involves a five dimensional integral over \mathbf{r} and $\hat{\mathbf{R}}$, may be calculated by means of a one-dimensional integral over R' :

$$\int_0^{R_m} V_{\alpha, \alpha'}(R, R') f_{\alpha'}(R') dR'. \quad (55)$$

Note that when the initial and final single-particle states are real, then the kernel function is symmetric

$$V_{\alpha, \alpha'}(R, R') = V_{\alpha', \alpha}(R', R). \quad (56)$$

When the potential \mathbf{V} contains only scalar potentials, the kernel calculation can be reduced to the problem of finding the spatial part $\mathbf{X}_{\ell L, \ell' L'}^{\Lambda}(R, R')$ defined so that, given

$$\begin{aligned} &\langle (LJ_p)J, J_t; J_T | \mathbf{V} | (L'J'_p)J', J'_t; J_T \rangle \\ &= \sum_{\Lambda F} (-1)^{s+J'_p-F} \hat{J} \hat{J}'_t \hat{J} \hat{F} \hat{J}_p \hat{\Lambda} \left\{ \begin{array}{ccc} L' & J'_p & J' \\ \ell' & s' & j' \\ \Lambda & F & J \end{array} \right\} \\ &W(J_t j' J_T J'; J'_t J) W(\ell s J_p J_p; j F) W(L \ell J F; \Lambda J_p) \\ &\langle \ell L; \Lambda | \mathbf{V} | \ell' L'; \Lambda \rangle, \end{aligned} \quad (57)$$

the integral operator $\langle \ell L; \Lambda | \mathbf{V} | \ell' L'; \Lambda \rangle$ has the kernel function $\mathbf{X}_{\ell L: \ell' L'}^{\Lambda}(R, R')$.

Now the \mathbf{r} and \mathbf{r}' are linear combinations of the channel vectors \mathbf{R} and \mathbf{R}' : $\mathbf{r} = a\mathbf{R} + b\mathbf{R}'$ and $\mathbf{r}' = a'\mathbf{R} + b'\mathbf{R}'$ where, when $\varphi_{\ell}(\mathbf{r})$ is the projectile bound state,

$$a = \nu_t \omega, b = -\omega, a' = \omega, b' = -\nu_p \omega, \quad (58)$$

with $\nu_p \equiv m_{pi}/m_{pi'}$, $\nu_t \equiv m_{ti}/m_{ti'}$, and $\omega = (1 - \nu_p \nu_t)^{-1}$. When $\varphi_{\ell}(\mathbf{r})$ is the target bound state

$$a = -\nu_p \omega, b = \omega, a' = -\omega, b' = \nu_t \omega, \quad (59)$$

with $\nu_p \equiv m_{pi}/m_{pi'}$, $\nu_t \equiv m_{ti}/m_{ti'}$, and $\omega = (1 - \nu_p \nu_t)^{-1}$. The 'core-core' vector is always $\mathbf{R}_c = \mathbf{r}' - \mathbf{r} = (a' - a)\mathbf{R} + (b' - b)\mathbf{R}'$.

Thus the spherical harmonics $Y_{\ell}(\hat{\mathbf{r}})$ and $Y_{\ell'}(\hat{\mathbf{r}}')$ can be given in terms of the spherical harmonics $Y_n(\hat{\mathbf{R}})$ and $Y_{n'}(\hat{\mathbf{R}}')$ by means of the Moshinsky⁹ solid-harmonic expansion (see also refs. ^{10, 11})

$$Y_{\ell}^m(\hat{\mathbf{r}}) = \sqrt{4\pi} \sum_{n\lambda} c(\ell, n) \frac{(aR)^{\ell-n} (bR')^n}{r^{\ell}} \quad (60)$$

$$Y_{\ell-n}^{m-\lambda}(\hat{\mathbf{R}}) Y_n^{\lambda}(\hat{\mathbf{R}}') \langle \ell - nm - \lambda n \lambda | \ell m \rangle \quad (61)$$

from $\mathbf{r} = a\mathbf{R} + b\mathbf{R}'$, where

$$c(\ell, n) = \left(\frac{(2\ell + 1)!}{(2n + 1)! (2(\ell - n) + 1)!} \right)^{1/2}.$$

We now perform the Legendre expansion

$$\mathbf{V} \frac{u_{\ell sj}(r)}{r^{\ell+1}} \frac{u_{\ell' sj'}(r')}{r'^{\ell'+1}} = \sum_T (2T + 1) \mathbf{q}_{\ell, \ell'}^T(R, R') P_T(u) \quad (62)$$

where the Legendre polynomials $P_T(u)$ are functions of u , the cosine of the angle between \mathbf{R} and \mathbf{R}' , by using $r = (a^2 R^2 + b^2 R'^2 + 2abRR'u)^{1/2}$ (with r' analogously) in the numerical quadrature of the integral

$$\mathbf{q}_{\ell, \ell'}^T(R, R') = \frac{1}{2} \int_{-1}^{+1} \mathbf{V} \frac{u_{\ell sj}(r)}{r^{\ell+1}} \frac{u_{\ell' sj'}(r')}{r'^{\ell'+1}} P_T(u) du \quad (63)$$

Using the Legendre expansion, the radial kernel function

$$\begin{aligned} \mathbf{X}_{\ell L: \ell' L'}^{\Lambda}(R, R') &= \frac{|b|^3}{2} \sum_{nn'} c(\ell, n) c(\ell', n') \\ &\times RR' (aR)^{\ell-n} (bR')^n (a'R)^{\ell'-n'} (b'R')^{n'} \\ &\times \sum_T (2T + 1) (-1)^{\Lambda+T+L+L'} \hat{\ell} \hat{\ell}' (\ell - n) (\ell' - n') \hat{n} \hat{n}' \hat{L} \hat{L}' \\ &\times \sum_{KK'} (2K + 1) (2K' + 1) \begin{pmatrix} \ell - n & n' & K \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \begin{pmatrix} \ell' - n' & n & K' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} K & L & T \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} K' & L' & T \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \sum_Q (2Q + 1) W(\ell L \ell' L'; \Lambda Q) W(K L K' L'; T Q) \quad (64) \\ &\times \begin{pmatrix} \ell' & Q & \ell \\ n' & K & \ell - n \\ \ell' - n' & K' & n \end{pmatrix} \mathbf{q}_{\ell, \ell'}^T(R, R') \end{aligned}$$

These formulae can also be used with $\mathbf{V} \equiv 1$ to calculate the kernel functions $K_{\ell L: \ell' L'}^{\Lambda}(R, R')$ for the wave function overlap operators $K_{ij} \equiv \langle \Phi_i | \Phi_j \rangle$ needed in evaluating the non-orthogonality terms of section 3.2.8.

Zero Range Transfers When the projectile wave functions $\varphi_{\ell}(\mathbf{r})$ are all s -states ($\ell = 0$ and the interaction potential is of zero-range ($\mathbf{V}\varphi(\mathbf{r}) \sim D_0\delta(\mathbf{r})$), then the form factor $\mathbf{X}_{\ell L: \ell' L'}^{\Lambda}(R, R')$ of equation (64) can be simplified to

$$\begin{aligned} \mathbf{X}_{0L: \ell' L'}^L(R, R') &= D_0 \frac{(-1)^{L'-\ell'}}{\hat{L}} \frac{\hat{\ell}' \hat{L} \hat{L}'}{\sqrt{4\pi}} \begin{pmatrix} \ell' & L & L' \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \frac{1}{R} u_{\ell' sj'}(R) \frac{b^2}{a} \delta(aR + bR'). \quad (65) \end{aligned}$$

This can be made local by defining a new step size $h' = -ah/b \equiv \nu_t h$ in the stripping channel α' .

Local Energy Approximation If the interaction potential is of small range, though not zero, and the projectile still contains only s -states, then a first-order correction may be made to the above form factor. This correction will depend on the rate of oscillation of the source wave function $f_{(L' J'_p), J', J'_t}^{JT}(R')$ within a 'finite-range effective radius' ρ . The rate of oscillation is estimated from the local energy in the entrance and exit channels, and the result¹² is to multiply $u_{\ell' sj'}(R)$ in the previous section by a factor

$$\left[1 + \rho^2 \frac{2\mu_{\alpha}^{(p)}}{\hbar^2} (U_{\alpha'}(R) + V_{\ell' sj'}(R) - U_{\alpha}(R) + \epsilon_{\alpha}) \right] \quad (66)$$

where the $U(R)$ are the optical potentials, with $V_{\ell' sj'}(r)$ the single-particle binding potential in the target. The $\mu_{\alpha}^{(p)}$ is the reduced mass of the particle in the projectile, and ϵ_{α} its binding energy.

At sub-Coulomb incident energies¹³, the details of the nuclear potentials in equation (66) become invisible, and as the longer-ranged Coulomb potentials cancel by charge conservation, the form factor can be simplified to

$$u_{\ell' sj'}(R) D_0 \left[1 + \rho^2 \frac{2\mu_{\alpha}^{(p)}}{\hbar^2} \epsilon_{\alpha} \right] = D u_{\ell' sj'}(R) \quad (67)$$

where

$$D = D_0 \left[1 + \left(\rho k_{\alpha}^{(p)} \right)^2 \right] \quad (68)$$

is the effective zero-range coupling constant for sub-Coulomb transfers.

The parameters D_0 and D can be derived from the details of the projectile bound state $\varphi_{0ss}(\mathbf{r})$. The zero-range constant D_0 may be defined as

$$D_0 = \sqrt{4\pi} \int_0^\infty r V_{0ss}(r) u_{0ss}(r) dr. \quad (69)$$

The parameter D , on the other hand, reflects the asymptotic strength of the wave function $u_{0ss}(r)$ as $r \rightarrow \infty$, as it is the magnitude of this tail which is important in sub-Coulomb reactions:

$$u_{0ss}(r) =_{r \rightarrow \infty} \frac{2\mu_\alpha^{(p)}}{\hbar^2} \frac{1}{\sqrt{4\pi}} D e^{-k_\alpha^{(p)} r}. \quad (70)$$

It may be also found, using Schrödinger's equation, from the integral

$$D = \sqrt{4\pi} \int_0^\infty \frac{\sinh(k_\alpha^{(p)} r)}{k_\alpha^{(p)}} V_{0ss}(r) u_{0ss}(r) dr. \quad (71)$$

From this equation we can see that as the range of the potential becomes smaller, D approaches D_0 . The 'finite-range effective radius' ρ of equation (68) is thus some measure of the mean radius of the potential $V_{0ss}(r)$.

3.2.8. Coupled Channels Methods

Coupled Reaction Channels

The numerical solution of Eqs. (16) is straightforward if the inter-channel couplings V_{ij} are local, as is the case for inelastic excitations of one or both nuclei. These are called 'coupled channels' (CC) cases. Transfer couplings, however, couple different \mathbf{R}_i and \mathbf{R}_j values, giving what are called 'coupled reaction channels' (CRC). The non-locality from a 'finite range' treatment of recoil means that the coupled reaction equations must be solved either iteratively, or by a R-matrix treatment using square-integrable basis functions in an interior region. Local and iterative solution methods are presented in ref.³, while the R-matrix methods presented in section 3.2.8, are common in atomic and molecular scattering research, but not so widely used in nuclear scattering problems.

A variety of standard computer programs are available for evaluation of the couplings described above, and for solution of the coupled equations by the methods described below. The program PTOLEMY¹⁷ can find coupled-channels solutions for local couplings or one-step non-local couplings from transfers, and ECIS¹⁵ also solves coupled-channels equations. Both pay particular attention to the long-range couplings of Eq. (47) that arise from inelastic Coulomb excitations. The program FRESKO³ includes these capabilities, as well as the iterative so-

lutions of coupled equations with non-local couplings by all the methods to be now described.

With non-local couplings from transfer channels, the Eqs. (16) may be solved iteratively, and the successive iterations amount to n -th DWBA solutions. As explained in section 3.2.3, the coupling matrix element $V_{ij} = \langle \phi_{pi} \phi_{ti} | H_m - E | \phi_{pj} \phi_{tj} \rangle$ has two different forms, depending on whether we use $H_m = H_i$ (post form) or $H_m = H_j$ (prior form). If we abbreviate $\Phi_i \equiv \phi_{pi} \phi_{ti}$, these give rise to the respective matrix elements

$$\begin{aligned} \langle \Phi_i | H_m - E | \Phi_j \rangle &= V_{ij}^{\text{post}} + [T_i + U_i - E_i] K_{ij} \\ \text{and} &= V_{ij}^{\text{prior}} + K_{ij} [T_j + U_j - E_j] \end{aligned} \quad (72)$$

$$\begin{aligned} \text{where } V_{ij}^{\text{post}} &= \langle \Phi_i | V_i | \Phi_j \rangle, V_{ij}^{\text{prior}} = \langle \Phi_i | V_j | \Phi_j \rangle, \\ \text{and } K_{ij} &= \langle \Phi_i | \Phi_j \rangle. \end{aligned}$$

The wave function overlap operator K_{ij} in equation (72) arises from the non-orthogonality between the transfer basis states defined around different centres in different mass partitions. We will see below that this term disappears in first-order DWBA, and can be made to disappear in second-order DWBA, if the first and second steps use the prior and post interactions respectively.

Multistep Born Approximations

If the coupling interactions V_i in Eq. (72) are weak, or if the back coupling effects of these interactions are already included in the optical potentials of the prior channel, then it becomes reasonable to use a n -step distorted wave Born approximation (DWBA). This approximation always feeds flux 'forwards' in the sequence $1 \rightarrow 2 \rightarrow \dots \rightarrow n + 1$ neglecting the back couplings. In the elastic channel the wave function is governed by the optical potential defined there, and the wave function in the i 'th channel is governed by the equation

$$[E_i - T_i - U_i] \psi_i(\mathbf{R}_i) = \sum_{j=1}^{j=i-1} \langle \Phi_i | \mathcal{H} - E | \Phi_j \rangle \psi_j(\mathbf{R}_j) \quad (73)$$

Initial channel:

$$[E_1 - T_1 - U_1] \psi_1(\mathbf{R}_1) = 0$$

Second channel:

$$[E_2 - T_2 - U_2] \psi_2(\mathbf{R}_2) = \langle \Phi_2 | H_m - E | \Phi_1 \rangle \psi_1(\mathbf{R}_1) \quad (74)$$

If the *prior* interaction is used, the right hand side can be simplified to

$$\begin{aligned} &= \langle \Phi_2 | V_1 | \Phi_1 \rangle \psi_1 + \langle \Phi_2 | \Phi_1 \rangle [T_1 + U_1 - E_1] \psi_1 \\ &= \langle \Phi_2 | V_1 | \Phi_1 \rangle \psi_1 \text{ as } \psi_1 \text{ is on-shell.} \\ &= V_{21}^{\text{prior}} \psi_1 \end{aligned}$$

Final channel: $c = n + 1$

$$[E_c - T_c - U_c] \psi_c(\mathbf{R}_c) = \sum_{j=1}^{j=c-1} \langle \Phi_c | H_m - E | \Phi_j \rangle \psi_j(\mathbf{R}_j) \quad (75)$$

If the *post* interaction had been used for all the couplings to this last channel, then there is again a simplification:

$$\begin{aligned} & [E_c - T_c - U_c] \psi_c(\mathbf{R}_c) \\ &= \sum_{j=1}^{j=c-1} \langle \Phi_c | \mathcal{V}_c | \Phi_j \rangle \psi_j + [T_c + U_c - E_c] \sum_{j=1}^{j=c-1} \langle \Phi_c | \Phi_j \rangle \psi_j \end{aligned}$$

so

$$[E_c - T_c - U_c] \chi_c(\mathbf{R}_c) = \sum_{j=1}^{j=c-1} V_{nj}^{\text{post}} \psi_j \quad (76)$$

where

$$\chi_c(\mathbf{R}_c) = \psi_c + \sum_{j=1}^{j=c-1} \langle \Phi_c | \Phi_j \rangle \psi_j = \langle \Phi_c | \Psi \rangle$$

Note that, as all the $\Phi_i \equiv \phi_{pi} \phi_{ti}$ are square-integrable and hence decay faster than r^{-1} at large radii, the ψ_c and χ_c are the same asymptotically. They differ only by an ‘off-shell transformation’, and hence yield the same (on-shell) scattering amplitudes. The equation for χ_c has no non-orthogonality terms once the *post* interaction is used in the final channel: this is what is meant by saying that the final channel is ‘effectively on-shell’.

These results imply that in n -step DWBA, some non-orthogonality terms can be made to disappear if ‘prior’ interactions are used for the first step, and/or if ‘post’ interactions are used for the final step. This means that the non-orthogonality term never appears in the first-order DWBA, irrespective of the choice of prior or post forms. In second-order DWBA, the prior-post combination must be chosen¹⁴ to avoid the non-orthogonality terms. It is clear that non-orthogonality terms will have to be evaluated if the DWBA is continued beyond second order.

Iterative Solutions

The iterative method of solving the CRC equations (16) proceeds by analogy with the n -step DWBA iterations until the series converges. Convergence is readily obtained if the couplings are sufficiently small, and different iterative strategies may be employed¹⁷. The procedure will however diverge if the the couplings are too large, or if the system is too near a resonance or a bound state pole. On divergence, the successive wave functions $\psi_i^{(n)}$ will become

larger and larger as n increases, and not converge to any fixed limit. Unitarity will of course be violated as the S-matrix elements will become much larger than unity. In this case we may use Padé approximants to accelerate the convergence of the sequence $S_\alpha^{(n)}$ of S-matrix elements^{15, 17}.

A given sequence $S^{(0)}, S^{(1)}, \dots$ of S-matrix elements that result from iterating the coupled equations can be regarded as the successive partial sums of a ‘vector valued’ polynomial

$$f(\lambda) = S^{(0)} + (S^{(1)} - S^{(0)})\lambda + (S^{(2)} - S^{(1)})\lambda^2 + \dots \quad (77)$$

evaluated at $\lambda=1$. This polynomial will clearly converge for λ sufficiently small, but will necessarily diverge if the analytic continuation of the $f(\lambda)$ function has any pole or singularities inside the circle $|\lambda| < 1$ in the complex λ -plane. The problem that Padé approximants solve is that of finding a computable approximation to the analytic continuation of the $f(\lambda)$ function to $\lambda=1$. This is accomplished by finding a rational approximation

$$P_{[N,M]}(\lambda) = \frac{p_0 + p_1\lambda + p_2\lambda^2 + \dots + p_N\lambda^N}{1 + q_1\lambda + q_2\lambda^2 + \dots + q_M\lambda^M} \quad (78)$$

which agrees with the $f(\lambda)$ function in the region where the latter does converge, as tested by matching the coefficients in the polynomial expansion of $P_{[N,M]}(\lambda)$ up to and including the coefficient of λ^n for $n = N + M$.

There are many different ways¹⁸ of evaluating the coefficients p_i, q_j , but for the present problem we can use Wynn’s ϵ -algorithm^{19, 20}, which is a method of evaluating the upper right half of the Padé table at $\lambda=1$ directly in terms of the original sequence $S^{(0)}, S^{(1)}, \dots$. Experience has shown that for typical sequences the most accurate Padé approximants are those near the diagonal of the Padé table. We use $\overline{S^{(n)}} \equiv P_{[N,M]}(1)$ for $N = [(n+1)/2]$ and $M = [n/2]$ in calculating the Padé-resummed cross sections.

R-matrix Solutions

The radial stepping methods of solving the coupled equations only allow local couplings to be treated properly, and non-local couplings from transfers have to be included iteratively. The R -matrix method²¹ is an equivalent way of solving the coupled equations, and has the advantages of being more stable numerically, and also allowing non-local components of the Hamiltonian in an interior region to be included to all orders. It has recently been revived in nuclear physics applications^{22, 23} for these reasons. Both transfer and non-orthogonality non-localities may be included non-perturbatively, and resonances and bound states may be described without difficulty.

This method uses a basis set of ‘energy eigenstates’ of the *diagonal* parts of Eqs. (34):

$$\left(T_{iL}(R_i) + U_i(R_i) + e_{pi} + e_{ti} - \varepsilon_q\right)w_i^q(R_i) = 0 \quad (79)$$

for eigenenergies ε_q , with the basis functions all having fixed logarithmic derivatives $\beta = d \ln w_i^q(R_i)/dR_i$ at R_m . The constancy of the logarithmic derivatives β means that (for each i channel separately) the w_i^q form an orthogonal basis set over the interval $[0, R_m]$, and *over this range* they can be normalised to unity. Without this constancy, a Bloch operator must be added to the kinetic energy to make it Hermitian.

The wave functions of the coupled problem (34) can now be solved completely over the interior range $[0, R_m]$, by using the orthonormal basis set of the $\{w_i^q(R_i)\}$ with coefficients to be determined. The coefficients are found in two stages: first by finding all the eigensolutions $g_i^p(R_i)$ of the equations (34) using the above orthonormal basis, and then expanding the scattering wave functions in terms of these $g_i^p(R_i)$.

In the traditional R -matrix method, the diagonalisation of the N -channel Hamiltonian in equation (34) yields $P = QN$ eigenenergies e_p with corresponding multichannel eigenstates

$$g_i^p(R_i) = \sum_{q=1}^Q c_i^{pq} w_i^q(R_i) \quad (80)$$

Eigenstates here with $e_p < 0$ are close to the bound states, while solutions with $e_p > 0$ contribute to the scattering solutions. Certain of the $e_p > 0$ solutions may correspond to low-lying resonances if those are present, but the majority of the positive eigenenergies have no simple physical interpretation. These $g_i^p(R_i)$ form of course another orthonormal basis in the interior region.

For scattering states at arbitrary energy E , the coupled solutions are then expanded in terms of the multichannel eigenstates as $\psi_{ii_0} = \sum_p A_{ii_0}^p g_i^p$. If we define an R -matrix at energy E by

$$\psi_i(R_i) = \sum_{i'} R_{ii'}(E) \left[\psi'_{i'}(R_i) - \beta \psi_{i'}(R_i) \right] \quad (81)$$

in the limit of $R_i \rightarrow R_m$ from above, then the R -matrix \mathbf{R} can be calculated from the eigenstates by standard methods^{21, 24}

$$R_{ii'}(E) = \frac{\hbar^2}{2\mu_i'} \sum_{p=1}^P \frac{g_i^p(R_m) g_{i'}^p(R_m)}{e_p - E}. \quad (82)$$

The coefficients c_i^{pq} and energies e_p in Eq. (80) satisfy matrix equations

$$\varepsilon_q c_i^{pq} + \sum_{q'} \langle w_i^q | V_{ii'} | w_{i'}^{q'} \rangle c_{i'}^{pq'} = e_p c_i^{pq} \quad (83)$$

for each eigenstate p , where $V_{ii'}$ refers to all the off-diagonal couplings. These equations are of the matrix form

$$\mathbf{H}\mathbf{c} = e\mathbf{c}. \quad (84)$$

There is an alternative method^{25, 23} for finding the $R_{ii'}$, which does not diagonalise the matrix on the left side of Eq. (84), but solves a set of linear equations. We need the solution of $(\mathbf{H} - E)\mathbf{x} = \mathbf{w}(R_m)$ for the right hand side consisting of the values of the basis functions at the R -matrix boundary. Then we can solve directly

$$\mathbf{R} = \frac{\hbar^2}{2\mu_i} \mathbf{w}^T(R_m) (\mathbf{H} - E)^{-1} \mathbf{w}(R_m). \quad (85)$$

This has the advantage of naturally continuing the R -matrix method to complex potentials, avoiding the diagonalisation of non-Hermitian matrices.

Using Eqs. (36) and (81), and writing the Coulomb functions \mathbf{H}^\pm as diagonal matrices, the scattering S -matrix is given in terms of \mathbf{R} by

$$\mathbf{S} = [\mathbf{H}^+ - \mathbf{R}(\mathbf{H}^+ - \beta\mathbf{H}^+)]^{-1} [\mathbf{H}^- - \mathbf{R}(\mathbf{H}^- - \beta\mathbf{H}^-)] \quad (86)$$

and the expansion coefficients for the wave functions are

$$A_{ii_0}^p = -\frac{\hbar^2}{2\mu_i'} \frac{1}{e_p - E} \sum_{i'} g_{i'}^p(R_m) \left[\delta_{ii_0} (H_L^-(k_i R_m) - \beta H_L^-(k_i R_m)) - S_{ii_0} (H_L^+(k_i R_m) - \beta H_L^+(k_i R_m)) \right]. \quad (87)$$

Buttle Correction The R -matrix calculated by Eq. (82) is only exact when the sum over p extends to all energies e_p . To improve the accuracy of calculations with finite Q (and hence finite P), the Buttle correction²⁶ is added to the right hand side of Eqs. (82,85). This modifies the diagonal terms $R_{ii}(E)$ to reproduce for each uncoupled problem the exact scattering solution $\chi_i(R_i)$ after this has been integrated separately. From the definition of the energy eigenstates $w_i^q(R_i)$, the R -matrix sum from (82) for each uncoupled channel is

$$R_{ii}^u(E) = \frac{\hbar^2}{2\mu_i} \sum_{q=1}^Q \frac{w_i^q(R_m)^2}{\varepsilon_q - E} \quad (88)$$

and the exact one-channel R -matrix is $R_i^0(E) = \chi_i(R_m)/(\chi_i'(R_m) - \beta\chi_i(R_m))$. The Buttle-corrected full R -matrix to be used in Eq. (86) is then

$$R_{ii'}^c(E) = R_{ii'}(E) + \delta_{ii'} \left[R_i^0(\tilde{E}) - R_{ii}^u(\tilde{E}) \right]. \quad (89)$$

The energy \tilde{E} can be equal to E , or chosen just near to it if necessary to avoid the poles in Eq. (88), since the Buttle correction varies smoothly with energy.

CRC matrix elements The solution of the CRC equations (16) with all the non-orthogonality terms in Eq. (72) requires in Eq. (83) the matrix element integrals of the form

$$\langle w_i^q | V_{i i'} | w_{i'}^{q'} \rangle = \langle w_i^q | \langle \Phi_i | H_m - E | \Phi_{i'} \rangle | w_{i'}^{q'} \rangle \quad (90)$$

for $m = i$ (post) or $m = i'$ (prior). In the post form, H_m contains $T_i + U_i$, and since w_i^q is just the eigenfunction of this operator with eigenvalue ε_q , we can operate to the left to obtain

$$\langle w_i^q | V_{i i'} | w_{i'}^{q'} \rangle_{\text{post}} = \langle w_i^q \Phi_i | V_i | \Phi_{i'} w_{i'}^{q'} \rangle + (\varepsilon_q - E_i) \langle w_i^q \Phi_i | \Phi_{i'} w_{i'}^{q'} \rangle \quad (91)$$

with the similar prior form

$$\langle w_i^q | V_{i i'} | w_{i'}^{q'} \rangle_{\text{prior}} = \langle w_i^q \Phi_i | V_{i'} | \Phi_{i'} w_{i'}^{q'} \rangle + (\varepsilon_{q'} - E_{i'}) \langle w_i^q \Phi_i | \Phi_{i'} w_{i'}^{q'} \rangle \quad (92)$$

The wave function overlaps in the second term $\langle \Phi_i | \Phi_{i'} \rangle$ go to zero asymptotically, and may be assumed small when $R_i, R_{i'} > R_m$. The standard R -matrix theory therefore still applies in the asymptotic region.

3.2.9. Conclusion

In this chapter, the theory of direct reactions from Austern¹ and Satchler² has been developed for two interacting nuclei. By considering a model subset of the states of these nuclei, and finding effective optical potentials for their interactions, the theory solves the Schrödinger equation to predict the relevant amplitudes and cross sections to those particular states.

The potential interactions are taken to be local optical potentials, and Feshbach⁷ showed how to formally relate these to the energy average of the effective interactions derived by eliminating the states, such as compound nuclear states, which are outside the model space. This introduces imaginary parts to the optical potentials, to represent the fact that flux leaves the model space, and the resulting complex potentials are discussed in Satchler^{2, ch11, 12, 15}.

Within a well defined model space with specific interactions, 'direct reaction theory'^{2, ch3, 5} attempts to solve the Schrödinger equation as accurately as possible. In such a theory, the phases describing the coherence of all components of the wave function are consistently maintained, and all quantum interference effects are taken into account.

The scattering amplitudes to a specific final state is shown to be related to the T -matrix between the entrance channel and that exit channel, and various expressions are given for the T -matrix. Alternatively, the exit scattering amplitudes for all channels together may be found by solving a full coupled-channels set of equations, as discussed in Tamura^{27, 28}, Taylor^{29, ch17-20} and Satchler^{2, ch5, 7, 16}.

Expressions are given for the couplings between channels in such a set, for inelastic excitation of a single nucleus, and for transfer of a nucleon or nucleonic cluster from one nucleus to another. The spectroscopy of transfer overlaps is discussed further in Austern^{1, ch8} and Satchler^{2, ch17}.

Finally, a selection of methods for solving the coupled equations are discussed. For weak couplings, iterative solutions give progressively the first-order and multistep Born approximations^{1, ch5, 10, 2, ch6}. For strong couplings, either Padé acceleration is necessary to resum a diverging sequence, or an all-order method is necessary such as the R -matrix method detailed in Lane and Thomas²¹. The R -matrix method includes all couplings within a finite radius R_m , and then determines the scattering amplitudes by matching to asymptotic scattering wave functions. This approach has the advantage that the non-local couplings from transfer and exchange processes can be easily included, as otherwise they force iterative methods to be used.

Direct reaction theory as presented here deals with a finite set of bound states of the participating nuclei by means of partial wave expansions. For breakup processes more detailed theories are necessary, and at high incident energies eikonal and Glauber approximations become competitive as discussed in the following chapter on few-body models of nuclear reactions.

See also: Few-body models of nuclear reactions

References

1. N. Austern 1970 *Direct Nuclear Reaction Theories*, New York: Wiley-Interscience.
2. G.R. Satchler 1983 *Direct Nuclear Reactions*, Oxford: Clarendon.
3. I.J. Thompson, *Comput. Phys. Rep.* **7**, 167 (1988)
4. G.H. Rawitscher, *Phys. Rev.* **C9** (1974) 2210, **C11** (1975) 1152, *Nucl. Phys.* **A241** (1975) 365.
5. M. Yahiro and M. Kamimura, *Prog. Theor. Phys.* **65** (1981) 2046, **65** (1981) 2051.
6. Y. Sakuragi, M. Yahiro and M. Kamimura, *Prog. Theor. Phys. Suppl.* **89** (1986).
7. H. Feshbach, *Ann. Phys.* **5** (1958) 357; **19** (1962) 287
8. J.M. Bang and J.S. Vaagen, *Z. Physik A* **297** (1980) 223.
9. M. Moshinsky, *Nucl. Phys.* **13** (1959) 104.
10. N. Austern, R.M. Drisko, E.C. Halbert and G.R. Satchler, *Phys. Rev.* **133** (1964) B3.
11. T. Ohmura, B. Imanishi, M. Ichimura and M. Kawai, *Prog. Theor. Phys.* **41** (1969) 391, **43** (1970) 347, **44** (1970) 1242.

12. P.J.A. Buttle and L.J.B. Goldfarb, Proc. Phys. Soc. (London) **83** (1964) 701; see also §6.14.1 of Satchler².
13. L.J.B. Goldfarb and E. Parry, Nucl. Phys. **A116** (1968) 309.
14. T. Udagawa, H.H. Wolter and W.R. Coker, Phys. Rev. Letts. **31** (1973) 1507.
15. J. Raynal, *Computing As a Language of Physics*, (IAEA, Vienna, 1972) 281.
16. M. Rhoades-Brown, M.H. Macfarlane and S.C. Pieper, Phys. Rev. C **21** (1980) 2417
17. M. Rhoades-Brown, M.H. Macfarlane and S.C. Pieper, Phys. Rev. C **21** (1980) 2436.
18. P.R. Graves-Morris, *Padé Approximants*, Institute of Physics, London and Bristol, 1973
19. P. Wynn, Numer. Math. **8** (1966) 264
20. A. Genz, p 112 in ⁽¹⁸⁾.
21. A.M. Lane and R.G. Thomas, Rev. Mod. Phys. **30** (1958) 257
22. I.J. Thompson, B.V. Danilin, V.D. Efros, J.S. Vaagen, J.M. Bang and M.V. Zhukov, Phys. Rev. C **61** (2000) 24318
23. D. Baye, M. Hesse, J.-M. Sparenberg and M. Vincke, J. Phys. B, **31** (1998) 3439; Nucl. Phys. A **640** (1998) 37
24. P.G. Burke and M.J. Seaton, J. Phys. **B17** (1984) L683
25. D.H. Glass, P.G. Burke, H.W. van der Hart and C.J. Noble, J. Phys. B, **30** (1997) 3801
26. P.J.A. Buttle, Phys. Rev. **160** (1967) 719
27. T. Tamura, Rev. Mod. Phys. **37** (1965) 679.
28. T. Tamura, Phys. Reports **14C** (1974) 59
29. J.R. Taylor 1972 *Scattering Theory*, New York: Wiley.