II. A. EQUATIONS FOR SCATTERING THEORY

In this section, equations for scattering theory are presented but not derived. Specifics for the R-matrix formulation of scattering theory are presented in Section II.A.1, which provides a discussion of an alternative formulation (the A-matrix). Readers interested in the derivation of the equations for scattering theory are referred to the Lane and Thomas article [AL58] for a detailed derivation in the general case, or to Section II.A.2 of this document for a simplified version.

In scattering theory, a channel may be defined by c = (α, l, s, J), where the following definitions apply:

- α represents the two particles making up the channel; α includes mass (m and M), charge (z and Z), spin (i and I) with associated parities, and all other quantum numbers for each of the two particles, plus the Q-value (equivalent to the negative of the threshold energy in the center of momentum system).
- l is the orbital angular momentum of the pair, and the associated parity is given by $(-1)^l$.
- s represents the channel spin (including the associated parity); that is, s is the quantized vector sum of the spins of the two particles of the pair: $\vec{\boldsymbol{s}} = \vec{\boldsymbol{i}} + \vec{\boldsymbol{I}}$.
- J is the total angular momentum (and associated parity); that is, J is the quantized vector sum of l and s: $\vec{\boldsymbol{J}} = \vec{\boldsymbol{l}} + \vec{\boldsymbol{s}}$.

Only J and its associated parity π are conserved for any given interaction. The other quantum numbers may differ from channel to channel, as long as the sum rules for spin and parity are obeyed. Within this document and within the SAMMY code, the set of all channels with the same J and π are called a "spin group."

In all formulae given below, spin quantum numbers (e.g., J) are implicitly assumed to include the associated parity. Quantized vector sum rules are implicitly assumed to be obeyed. Readers unfamiliar with these sum rules are referred to Section II.C.1.a for a mini-tutorial on the subject.

Let the angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J be represented by $\sigma_{cc'}$. This cross section is given in terms of the scattering matrix $U_{cc'}$ as

$$\sigma_{cc'} = \frac{\pi}{k_\alpha^2} g_{J\alpha} \left| e^{2iw_c} \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'} \quad , \tag{II A.1}$$

where k_α is the wave number (and $K_\alpha = \hbar\, k_\alpha$ = center-of-mass momentum) associated with incident particle pair α, $g_{J\alpha}$ is the spin statistical factor, and w_c is the Coulomb phase-shift difference. Note that w_c is zero for non-Coulomb channels. (Details for the charged-particle case are presented in Section II.C.4.) The spin statistical factor g is given by

$$g_{J\alpha} = \frac{2J+1}{(2i+1)\,(2I+1)} \quad , \tag{II A.2}$$

and center-of-mass momentum K_α by

$$K_\alpha^2 = \left(\hbar k_\alpha\right)^2 = \frac{2m\,M^2}{\left(m+M\right)^2} E \quad . \tag{II A.3}$$

Here E is the laboratory kinetic energy of the incident (moving) particle. A derivation of this value for K_α is given in Section II.C.2.

The scattering matrix U can be written in terms of matrix W as

$$U_{cc'} = \Omega_c \, W_{cc'} \, \Omega_{c'} \quad , \tag{II A.4}$$

where Ω is given by

$$\Omega_c = e^{i\,(w_c - \varphi_c)} \quad . \tag{II A.5}$$

Here again, w_c is zero for non-Coulomb channels, and the potential scattering phase shifts for non-Coulomb interactions φ_c are defined in many references (e.g., [AL58]) and shown in Table II A.1. The matrix W in Eq. (II A.4) is related to the R-matrix (in matrix notation with indices suppressed) via

$$W = P^{1/2}(I - RL)^{-1}(I - RL^*)P^{-1/2} \quad . \tag{II A.6}$$

The quantity I in this equation represents the identity matrix. The form of the R-matrix is given in Section II.A.1 in general and in Section II.B for the versions used in SAMMY. The quantity L in Eq. (II A.6) is given by

$$L = (S - B) + iP \quad , \tag{II A.7}$$

with P being the penetration factor (penetrability) S the shift factor, and B the arbitrary boundary constant at the channel radius a_c. P and S are functions of energy E, and also depend on the orbital angular momentum l and the channel radius a_c. Formulae for P and S are found in many references (see, for example, Eq. (2.9) in [JL58]).

For non-Coulomb interactions, the penetrability and shift factor have the form

$$P \rightarrow P_l\left(\rho\right) \quad \text{and} \quad S \rightarrow S_l\left(\rho\right) \quad , \tag{II A.8}$$

where ρ is related to the center-of-mass momentum which in turn is related to the laboratory energy of the incident particle (E). For arbitrary channel c with particle pair α, orbital angular momentum l, and channel radius a_c, ρ has the form

$$\rho = k_\alpha \, a_c = \frac{1}{\hbar}\sqrt{\frac{2m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)} \frac{M}{(m+M)}} \sqrt{\left(E - \Xi_\alpha\right)} \;\; a_c \quad , \tag{II A.9}$$

as shown in Section II.C.2. Here Ξ_α is the energy threshold for particle pair α, m_α and M_α are the masses of the two particles of particle pair α, and m and M are the masses of the incident particle and target nuclide, respectively.

Appropriate formulae for P, S, and φ in the non-Coulomb case are shown in Table IIA.1. For two charged particles, formulae for the penetrabilities are given in Section II.C.4.

The energy dependence of fission and capture widths is negligible over the energy range of these calculations. Therefore, a penetrability of unity may be used.

Table II A.1. Hard-sphere penetrability (penetration factor) *P*, level shift factor *S*, and potential-scattering phase shift φ for orbital angular momentum *l*, wave number *k*, and channel radius a_c, with $\rho = ka_c$

l	P_l	S_l	φ_l
0	ρ	0	ρ
1	$\rho^3/(1+\rho^2)$	$-1/(1+\rho^2)$	$\rho-\tan^{-1}\rho$
2	$\rho^5/(9+3\rho^2+\rho^4)$	$-(18+3\rho^2)/(9+3\rho^2+\rho^4)$	$\rho-\tan^{-1}[3\rho/(3-\rho^2)]$
3	$\rho^7/(225+45\rho^2+6\rho^4+\rho^6)$	$-(675+90\rho^2+6\rho^4)/(225+45\rho^2+6\rho^4+\rho^6)$	$\rho-\tan^{-1}[\rho(15-\rho^2)/(15-6\rho^2)]$
4	$\rho^9/(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8$	$-(44100+4725\rho^2+270\rho^4+10\rho^6)/(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)$	$\rho-\tan^{-1}[\rho(105-10\rho^2)/(105-45\rho^2+\rho^4)]$
l	$\dfrac{\rho^2 P_{l-1}}{(l-S_{l-1})^2+P_{l-1}^2}$	$\dfrac{\rho^2(l-S_{l-1})}{(l-S_{l-1})^2+P_{l-1}^2}-l$	$\varphi_{l-1}-\tan^{-1}\left((P_{l-1}/(l-S_{l-1})\right)$ or $B_l=(B_{l-1}+X_l)/(1-B_{l-1}X_l)$ with $B_l=\tan(\rho-\varphi_l)$ and $X_l=(P_{l-1})/(l-S_{l-1})$

Formulae for a particular cross section type can be derived by summing over the terms in Eq. (II A.1). For the total cross section, the sum over all possible exit channels and all spin groups gives

$$\begin{aligned}\sigma^{total} &= \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \sum_{J} \frac{\pi}{k_\alpha^2} g_\alpha \left|\delta_{cc'} - U_{cc'}\right|^2 \\ &= \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \left(\delta_{cc'} - U_{cc'}\delta_{cc'} - U_{cc'}^*\delta_{cc'} + \left|U_{cc'}\right|^2\right) \qquad \text{(II A.10)} \\ &= \frac{2\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{incident\\channels\\c}} \left(1 - \mathrm{Re}\left(U_{cc}\right)\right) \quad .\end{aligned}$$

For non-charged incident particles, the elastic (or scattering) cross section is given by

$$\sigma_{\alpha\alpha} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=incident\\channel}} \left(1 - 2\,\mathrm{Re}\left(U_{cc}\right) + \sum_{\substack{c'=incident\\channel}} \left|U_{cc'}\right|^2\right) \quad . \qquad \text{(II A.11)}$$

Similarly, the cross section for any non-elastic reaction can be written

$$\sigma_\alpha^{reaction} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=incident\\channel}} \sum_{\substack{c'=reaction\\channel}} \left|U_{cc'}\right|^2 \quad . \qquad \text{(II A.12)}$$

In particular, the capture cross section could be written as the difference between the total and all other cross sections,

$$\sigma^{capture} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=incident\\channel}} \left(1 - \sum_{\substack{c'=all\ channels\\except\ capture}} \left|U_{cc'}\right|^2\right) \quad . \qquad \text{(II A.13)}$$

(This form will be used later, in Section II.B.1.a, when the capture channels are treated in an approximate fashion.)