II.A.2. Derivation of Scattering Theory Equations

Many authors have given derivations of the equations for the scattering matrix in terms of the R-matrix. Sources for the derivation shown here are unpublished lecture notes of Fröhner [FF02], presented at the SAMMY workshop in Paris in 2002, and Foderaro [AF71]. This derivation is valid for only the simple case of spinless projectiles and target nuclei, assuming only elastic scattering and absorption. For the general case, the reader is referred to Lane and Thomas [AL58].

Schrödinger equation

The Schrödinger equation with a complex potential is

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V + iW\right)\psi = E\psi \quad , \tag{II A2.1}$$

in which one can consider that V causes scattering and W causes absorption. The wave function can be expanded in the usual fashion,

$$\psi(r,\cos\theta) \;=\; \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos\theta) \quad , \tag{II A2.2}$$

for which the radial portion obeys the equation

$$\frac{d^2 u_l}{dr^2} \;+\; \left[k^2 - \frac{2m}{\hbar^2}(V + iW) - \frac{l(l+1)}{r^2}\right] u_l \;=\; 0 \quad , \tag{II A2.3}$$

subject to the conditions that $|\psi|^2$ is everywhere finite and that

$$u_l(r=0) = 0 \quad . \tag{II A2.4}$$

In the external region, $r > a$, the nuclear forces are zero ($V = W = 0$), so the solution has the form

$$u_l(r) \;=\; I_l(r) - U_l\, O_l(r) \quad . \tag{II A2.5}$$

I_l represents an incoming free wave, and O_l represents an outgoing free wave. U_l is the "collision function" or "S function" that describes the effects of the nuclear interaction, giving both the attenuation and the phase shift of the outgoing wave:

and

$$\begin{aligned} |U_l|^2 &= 1 \;\text{ for } W = 0 \quad , \\ |U_l|^2 &< 1 \;\text{ for } W \neq 0 \quad . \end{aligned} \tag{II A2.6}$$

Our goal is to determine an appropriate analytic form for U_l.

Orthogonal eigenvectors in interior region

For the interior region $r < a$, we define eigenfunctions $w_{\lambda l}(r)$ and eigenvalues E_λ,

$$E_\lambda = \frac{\hbar^2 k_\lambda^2}{2m} \quad , \tag{II A2.7}$$

for the wave equation without absorption (W = 0),

$$\frac{d^2 w_{\lambda l}}{dr^2} + \left[k_\lambda{}^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} = 0 \quad , \tag{II A2.8}$$

for which the boundary conditions are

$$w_{\lambda l}(r=0) = 0 \qquad \text{and} \qquad \frac{a}{w_{\lambda l}(a)} \left. \frac{d\, w_{\lambda l}}{d\, r} \right|_{r=a} = B_l \quad . \tag{II A2.9}$$

Note that $w_{\lambda l}(r)$ is real if the boundary parameter B_l is chosen to be real. The eigenfunctions are orthogonal, since

$$\begin{aligned}
\int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr &= \int_0^a \frac{d}{dr} \left(\frac{d\, w_{\lambda l}}{d\, r} w_{\mu l} - w_{\lambda l} \frac{d\, w_{\mu l}}{d\, r} \right) dr \\
&= \left[\frac{d\, w_{\lambda l}}{d\, r} w_{\mu l} - w_{\lambda l} \frac{d\, w_{\mu l}}{d\, r} \right]_0^a \\
&= \left. \frac{d\, w_{\lambda l}}{d\, r} \right|_{r=a} w_{\mu l}(a) \; - \; w_{\lambda l}(a) \left. \frac{d\, w_{\mu l}}{d\, r} \right|_{r=a} - [0] \\
&= \frac{B_l}{a} \left[w_{\lambda l}(a) w_{\mu l}(a) - w_{\lambda l}(a) w_{\mu l}(a) \right] = 0 \quad ,
\end{aligned} \tag{II A2.10}$$

in which both equations of (II A2.9) have been invoked. The integral in Eq. (II A2.10) can also be evaluated using Eq. (II A2.8), giving

$$\begin{aligned}
&\int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr \\
&\quad = \int_0^a \left(\left[-k_\lambda^2 - \frac{2mV}{\hbar^2} \right] w_{\lambda l} w_{\mu l} - w_{\lambda l} \left[-k_\mu^2 - \frac{2mV}{\hbar^2} \right] w_{\lambda l} \right) dr \\
&\quad = \int_0^a \left(-k_\lambda^2 w_{\lambda l} w_{\mu l} + k_\mu^2 w_{\lambda l} w_{\mu l} \right) dr \\
&\quad = -\left(k_\lambda^2 - k_\mu^2 \right) \int_0^a w_{\lambda l} w_{\mu l} \, dr \quad .
\end{aligned} \tag{II A2.11}$$

Equating Eq. (II A2.10) to Eq. (II A2.11) gives

$$\left(k_\lambda^2 - k_\mu^2 \right) \int_0^a w_{\lambda l} w_{\mu l} \, dr = 0 \quad . \tag{II A2.12}$$

For $\lambda \neq \mu$, assuming no degenerate states, it therefore follows that

$$\int_0^a w_{\lambda l} w_{\mu l} \, dr = 0 \;\; \text{if } \lambda \neq \mu \quad . \tag{II A2.13}$$

The orthogonality of the eigenvectors is therefore established. We assume that these wave functions are normalized such that

$$\int_0^a w_{\lambda l} \, w_{\mu l} \;\, dr \;=\; \delta_{\lambda \mu} \quad . \tag{II A2.14}$$

Matching at the surface

The internal wave function for the true potential (including the imaginary part iW) can be expanded in terms of the eigenfunctions as

$$u_l\left(r\right) = \sum_\lambda c_{\lambda l} \, w_{\lambda l}\left(r\right) \quad \text{for } r \leq a \quad , \tag{II A2.15}$$

with

$$c_{\lambda l} = \int_0^a u_l \, w_{\lambda l} \;\, dr \quad . \tag{II A2.16}$$

This equation for $c_{\lambda l}$ is derived by multiplying Eq. (II A2.15) by $u_{\lambda l}\left(r\right)$, integrating, and applying Eq. (II A2.14).

Consider now the integral

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \quad , \tag{II A2.17}$$

which can be expanded by use of Eqs. (II A2.3) and (II A2.8) to give

$$\begin{aligned} &\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \\ &= \int_0^a \left(-\left[k^2 - \frac{2m}{\hbar^2}(V + iW) - \frac{l(l+1)}{r^2} \right] u_l \, w_{\lambda l} + u_l \left[k_\lambda{}^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} \right) dr \qquad \text{(II A2.18)} \\ &= \left(k_\lambda{}^2 - k^2 \right) \int_0^a u_l w_{\lambda l} \, dr \;\; + \;\; \frac{2m}{\hbar^2} \int_0^a W \, u_l w_{\lambda l} \, dr \quad . \end{aligned}$$

Defining $\overline{W}_{\lambda l}$ as

$$\overline{W}_{\lambda l} \;\; = \;\; \int_0^a W \, u_l \, w_{\lambda l} \, dr \bigg/ \int_0^a u_l \, w_{\lambda l} \, dr \tag{II A2.19}$$

permits rewriting Eq. (II A2.18) in the form

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr = \left(k_\lambda{}^2 - k^2 + i \frac{2m}{\hbar^2} \overline{W}_{\lambda l} \right) \int_0^a u_l \, w_{\lambda l} \, dr \quad . \tag{II A2.20}$$

Integrating the left-hand side of this equation gives

$$\begin{aligned} \int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_0^a = \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_{r=a} \\ &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{B_l}{a} w_{\lambda l} \right]_{r=a} = \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \frac{w_{\lambda l}(a)}{a} \quad , \end{aligned} \tag{II A2.21}$$

in which we have again made use of the boundary condition of Eq. (II A2.9). Integrating the right-hand side of Eq. (II A2.20) by applying Eq. (II A2.16) gives

$$\left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\overline{W}_{\lambda l}\right)\int_0^a u_l\, w_{\lambda l}\, dr \;=\; \left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\overline{W}_{\lambda l}\right)c_{\lambda l} \quad . \qquad \text{(II A2.22)}$$

Equating Eqs. (II A2.21) and (II A2.22) therefore gives

$$\begin{aligned} \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \frac{w_{\lambda l}}{a} &= \left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\overline{W}_{\lambda l}\right)c_{\lambda l} \quad , \\ \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \frac{w_{\lambda l}}{a} &= \left(E_\lambda - E + i\overline{W}_{\lambda l}\right)\frac{2m\, c_{\lambda l}}{\hbar^2} \quad , \end{aligned} \qquad \text{(II A2.23)}$$

or

$$c_{\lambda l} = \frac{\hbar^2\, w_{\lambda l}(a)}{2m\, a\left(E_\lambda - E + i\overline{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad . \qquad \text{(II A2.24)}$$

Inserting this into Eq. (II A2.15) gives

$$u_l(r) = \sum_\lambda w_{\lambda l}(r)\frac{\hbar^2 w_{\lambda l}(a)}{2m\, a\left(E_\lambda - E + i\overline{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad , \qquad \text{(II A2.25)}$$

which, when evaluated at $r = a$, becomes

$$u_l(a) = \sum_\lambda \frac{\hbar^2 w_{\lambda l}^2(a)}{2m\, a\left(E_\lambda - E + i\overline{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad . \qquad \text{(II A2.26)}$$

Rearranging, this becomes

$$\begin{aligned} u_l(a) &= \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \sum_\lambda \frac{\left[\hbar^2 w_{\lambda l}^2(a)/2m\, a\right]}{\left(E_\lambda - E + i\overline{W}_{\lambda l}\right)} \\ &= \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)} \quad , \end{aligned} \qquad \text{(II A2.27)}$$

in which the decay amplitude $\gamma_{\lambda l}$ is defined as

$$\gamma_{\lambda l} \equiv \sqrt{\frac{\hbar^2 w_{\lambda l}^2(a)}{2m\, a}} \qquad \text{(II A2.28)}$$

and the absorption width $\Gamma_{\lambda l}$ as

$$\Gamma_{\lambda l} \equiv 2W_{\lambda l} \quad . \qquad \text{(II A2.29)}$$

If we then define the R-function as

$$R_l = \sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)} \quad , \tag{II A2.30}$$

then Eq. (II A2.27) can be written in the form

$$u_l = \left(a \frac{d u_l}{d r} - u_l B_l \right) R_l \quad , \tag{II A2.31}$$

in which everything is evaluated at the matching radius *a*.

Scattering matrix in terms of R-matrix (neutrons only)

Equation (II A2.31) can be converted into the usual R-matrix formulae by inserting Eq. (II A2.5),

$$u_l = I_l - U_l O_l \quad , \tag{II A2.32}$$

yielding

$$I_l - U_l O_l = \left[a \left(\frac{d I_l}{d r} - U_l \frac{d O_l}{d r} \right) - B_l \left(I_l - U_l O_l \right) \right] R_l \quad , \tag{II A2.33}$$

in which everything is again evaluated at the matching radius *a*. Solving Eq. (II A2.33) for *U* gives

$$U_l \left[-O_l + R_l \left(a \frac{d O_l}{d r} - B_l O_l \right) \right] = I_l - R_l \left(a \frac{d I_l}{d r} - B_l I_l \right) \quad , \tag{II A2.34}$$

or

$$U_l = \frac{I_l - R_l \left(a \frac{d I_l}{d r} - B_l I_l \right)}{\left[-O_l + R_l \left(a \frac{d O_l}{d r} - B_l O_l \right) \right]} \;=\; \frac{I_l}{O_l} \; \frac{1 - R_l \left(\frac{a}{I_l} \frac{d I_l}{d r} - B_l \right)}{1 - R_l \left(\frac{a}{O_l} \frac{d O_l}{d r} - B_l \right)} \quad . \tag{II A2.35}$$

We define L_l as

$$L_l \;\equiv\; \frac{a}{O_l(a)} \frac{d O_l}{d r}\bigg|_{r=a} \;\equiv\; S_l + i\,P_l \quad . \tag{II A2.36}$$

For spinless particles, $I_l^* = O_l$, so that

$$\frac{a}{I_l(a)} \frac{d\,I_l}{d\,r}\bigg|_{r=a} = L_l^* = S_l - iP_l \tag{II A2.37}$$

and

$$\frac{I_l}{O_l} = \frac{O_l^*}{O_l} = \frac{|O|e^{-i\varphi}}{|O|e^{i\varphi}} = e^{-2i\varphi} \quad . \tag{II A2.38}$$

Therefore Eq. (II A2.34) becomes

$$U_l \;=\; e^{-2i\varphi}\,\frac{1 - R_l\left(L_l^* - B_l\right)}{1 - R_l\left(L_l - B_l\right)} \quad , \tag{II A2.39}$$

which is the usual form for the scattering matrix in terms of the R-matrix in this simple case.