Brief Review of the R-Matrix Theory

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Introduction

Resonance theory deals with the description of the nucleon-nucleus interaction and aims at the prediction of the experimental structure of cross sections. Resonance theory is basically an interaction model which treats the nucleus as a black box, whereas nuclear models are concerned with the description of the nuclear properties based on models of the nuclear forces (nuclear potential). Any theoretical method of calculating the neutron-nucleus interactions or nuclear properties cannot fully describe the nuclear effects inside the nucleus because of the complexity of the nucleus and because the nuclear forces, acting within the nucleus, are not known in detail. Quantities related to internal properties of the nucleus are taken, in this theory, as parameters which can be determined by examining the experimental results.

The general R-matrix theory, introduced by Wigner and Eisenbud in 1947, is a powerful nuclear interaction model. Despite the generality of the theory, it does not require information about the internal structure of the nucleus; instead, the unknown internal properties, appearing as elements in the R-matrix, are treated as parameters and can be determined by examining the measured cross sections.

A brief review of the R-matrix theory will be given here and the interaction models which are specializations of the general R-matrix will be described. The practical aspects of the general R-matrix theory, as well as the relationship between the collision matrix U and the level matrix A with the R-matrix, will be presented.

Overview of the R-Matrix Theory

The general R-matrix theory has been extensively described by Lane and Thomas. An overview is presented here as introduction for the resonance formalisms which will be described later.

To understand the basic points of the general R-matrix theory, we will consider a simple case of neutron collision in which the spin dependence of the constituents of the interactions is neglected. Although the mathematics involved in this special case is over-simplified, it nevertheless contains the essential elements of the general theory.

As mentioned before, the nuclear potential inside the nucleus is not known; therefore, the behavior of the wave function in the internal region of the nucleus cannot be calculated directly from the Schrödinger equation. In the R-matrix analysis the inner wave function of the angular momentum l is expanded in a linear combination of the eigenfunctions of the energy levels in the compound nucleus. Mathematically speaking, if $\phi_l(E,r)$ is the inner wave function at any energy E and $\phi_l(E_\lambda,r)$ is the eigenfunction at the energy eigenvalue $E_{\lambda,}$ the relation becomes

$$\phi_l(E,r) = \sum_\lambda A_{l\lambda}\, \phi_l(E_\lambda,r) \quad . \tag{1}$$

Both $\phi_l(E,r)$ and $\phi_l(E_\lambda,r)$ are solutions of the radial Schrödinger equations in the internal region given by

$$\left\{\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right]\right\}\phi_l(E,r) = 0 \tag{2}$$

and

$$\left\{\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left[E_\lambda - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right]\right\}\phi_l(E_\lambda,r) = 0 \quad . \tag{3}$$

Since all terms in this expression must be finite at $r = 0$, both functions vanish at that point. In addition, the logarithmic derivative of the eigenfunction at the nuclear surface, say at $r = a$, is taken to be constant so that

$$\left[\frac{d\phi_l(E_\lambda,r)}{dr}\right]_{r=a} = a^{-1} B_l \phi_l(E_\lambda,a) \quad , \tag{4}$$

where B_l is an arbitrary boundary constant.

Since we are dealing with eigenfunctions of a real Hamiltonian, $\phi_l(E_\lambda,r)$ are orthogonal. Assuming that $\phi_l(E_\lambda,r)$ are also normalized, we have

$$\int_0^a \phi_l(E_\lambda,r)\,\phi_l(E_{\lambda'},r)\,dr = \delta_{\lambda\lambda'} \quad . \tag{5}$$

From Eq. (xx-1) and the orthogonality condition, we find the coefficients $A_{l\lambda}$,

$$A_{l\lambda} = \int_0^a \phi_l(E_\lambda,r)\; \phi_l(E,r)\,dr \quad . \tag{6}$$

To proceed to the construction of the R-matrix, Eq. (xx-2) is multiplied by $\phi_l(E_\lambda,r)$ and Eq. (xx-3) is multiplied by $\phi(E_\lambda,r)$. Subtracting and integrating the result over the range 0 to a (as in Eq. (xx-6)) produces the expression for the coefficients $A_{l\lambda}$:

$$A_{l\lambda} = \frac{\hbar^2}{2m}(E_\lambda - E)^{-1}\left[\phi_l(E_\lambda,r)\frac{d\phi_l(E,r)}{dr} - \phi_l(E,r)\frac{d\phi_l(E_\lambda,r)}{dr}\right]_{r=a} \quad . \tag{7}$$

Inserting $A_{l\lambda}$ into Eq. (xx-1) for r=a at the surface of the nucleus and using Eq. (xx-4), gives the following expression for the wave function:

$$\phi_l(E,a) = \frac{\hbar^2}{2ma}\sum_\lambda\left[\frac{\phi_l(E_\lambda,a)\,\phi_l(E_\lambda,a)}{E_\lambda - E}\right]\left[r\frac{d\phi_l(E,a)}{dr} - B_l\phi_l(E,r)\right]_{r=a} \quad . \tag{8}$$

Equation (xx-8) relates the value of the inner wave function to its derivative at the surface of the nucleus. The R matrix is defined as

$$R_l = \frac{\hbar^2}{2ma}\sum_\lambda\left[\frac{\phi_l(E_\lambda,a)\,\phi_l(E_\lambda,a)}{E_\lambda - E}\right] \tag{9}$$

or

$$R_l = \sum_\lambda \frac{\gamma_{\lambda l}\,\gamma_{\lambda l}}{E_\lambda - E} \; , \tag{10}$$

where $\gamma_{\lambda l}$, the reduced width amplitude for the level λ and angular momentum l, is defined as

$$\gamma_{\lambda l} = \sqrt{\frac{\hbar^2}{2ma}}\;\phi_l(E_\lambda,a) \quad . \tag{11}$$

The reduced width amplitude depends on the value of the inner wave function at the nuclear surface. Both E_λ and $\gamma_{\lambda l}$ are the unknown parameters of the R matrix which can be evaluated by examining the measured cross sections.

The generalization of Eq. (xx-10) is obtained by including the neutron-nucleus spin dependence and several possibilities in which the reaction process can occur. The concept of channel is introduced to designate a possible pair of nucleus and particle and the spin of the pair. The channel containing the initial state is called the entrance channel (channel c), whereas, the channel containing the final state is the exit channel (channel c'). The elements of the R matrix in the general case are given by

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_{\lambda} - E} \ , \tag{12}$$

where the reduced width amplitude becomes

$$\gamma_{\lambda c} = \sqrt{\frac{\hbar^2}{2 m_c a_c}}\ \phi_c(E_{\lambda}, a_c) \ . \tag{13}$$

The next objective is to relate the R-matrix to the cross-section formalism so that cross sections can be computed once the elements of the R-matrix are known.

Relation between the R-matrix and the Collision Matrix U

The general expressions for the neutron-nucleus cross sections are based on the collision matrix, also known as U-matrix, whose elements can be expressed in terms of the elements of the R-matrix. From basic quantum mechanics theory the cross sections for the neutron-nucleus interaction can be given as a function of the matrix U as follows:

(1) Elastic Cross Section

$$\sigma_n = \pi \lambdabar^2 \sum_{l} (2l+1) |\, 1 - U_l |^2 \ , \tag{14}$$

(2) Reaction Cross Section which includes everything which is not elastic scattering (i.e., reaction=fission, capture, inelastic, ...)

$$\sigma_r = \pi \lambdabar^2 \sum_{l} (2l+1) (\, 1 - |\, U_l |^2) \ , \tag{15}$$

3) Total Cross Section

$$\sigma_t = 2 \pi \lambdabar^2 \sum_{l} (2l+1) (\, 1 - Re |\, U_l |) \ , \tag{16}$$

where $\lambdabar$ is the neutron reduced wavelength given by

$$\lambdabar = \frac{\hbar}{\sqrt{2mE}} \quad . \tag{17}$$

We first derive the relationship between the U and R matrices, for a simple case of spinless neutral particles. The total wave function in the region outside the nuclear potential can be expressed as a linear combination of the incoming and outgoing wave functions. If $\phi_l^{inc}(r)$ and $\phi_l^{out}(r)$ are the incoming and outgoing wave functions for a free particle, respectively, the solution of the radial Schrödinger equation can be written as

$$\phi_l(r) = C_l\left[\phi_l^{inc}(r) - U_l\phi_l^{out}(r)\right] \qquad \text{for } r \geq a \ , \tag{18}$$

where C_l is a normalization constant.

The presence of the U-matrix in Eq. (xx-18) (in this case a matrix of one element) indicates that the amplitudes of the incoming and outgoing wave functions are, in general, different. The case of $| U_l | = 1$ corresponds to pure elastic scattering which means that no reaction has occurred.

The Schrödinger equation for $\phi_l^{inc}(r)$ and $\phi_l^{out}(r)$ is the same as Eq. (xx-2) with $V(r) = 0$ since the potential outside the nucleus is zero. The solution is a combination of the spherical Bessel (j_l) and Neumann (n_l) functions

$$\phi_l^{inc}(r) = kr\left[n_l(kr) + i\, j_l(kr)\right] \ , \tag{19}$$

and

$$\phi_l^{out}(r) = kr\left[n_l(kr) - i\, j_l(kr)\right] \ , \tag{20}$$

where $i = \sqrt{-1}$.

The relation between the U and the R-matrices is obtained by first noting that Eq. (xx-8) can be written as

$$\phi_l(E,a) = \left[r\frac{d\phi_l(E_\lambda,a)}{dr} - B_l\phi_l(E,r)\right]_{r=a} R_l \ , \tag{21}$$

where R_l is given in Eq. (xx-9).

Equation (xx-21), when combined with Eq. (xx-18), provides the relation between R and U-matrices as

$$U_l = \left(\frac{\phi_l^{inc}}{\phi_l^{out}} \right)_{r=a} \frac{1 - \left[\left(\frac{r}{\phi_l^{inc}} \frac{d\phi_l^{inc}}{dr} - B_l \right)_{r=a} \right] R_l}{1 - \left[\left(\frac{r}{\phi_l^{out}} \frac{d\phi_l^{out}}{dr} - B_l \right)_{r=a} \right] R_l} \ . \tag{22}$$

We define the logarithmic derivative as

$$L_l^* = \left(\frac{r}{\phi_l^{out}} \frac{d\phi_l^{out}}{dr} \right)_{r=a} \ . \tag{23}$$

Since from Eqs. (xx-19) and (xx-20), ϕ_l^{inc} and ϕ_l^{out} are complex conjugates,

$$L_l = \left(\frac{r}{\phi_l^{inc}} \frac{d\phi_l^{inc}}{dr} \right)_{r=a} \ . \tag{24}$$

Equation (xx-22) becomes

$$U_l = \left(\frac{\phi_l^{inc}}{\phi_l^{out}} \right)_{r=a} \frac{1 - (L_l^* - B_l)_{r=a} \ R_l}{1 - (L_l - B_l)_{r=a} \ R_l} \ . \tag{25}$$

Equation (xx-25) represents the desired relationship between the collision matrix U and the matrix R.

The representation of the neutron cross sections will depend on the reduced width amplitudes $\gamma_{\lambda c}$ and E_λ which are unknown parameters of Eq. (xx-25). Those parameters are obtained by fitting the experimental cross section.

The general relation between the matrices U and R is similar to Eq. (xx-25) with each term converted to matrix form:

$$\boldsymbol{U} = \rho^{1/2} \phi_{out}^{-1} [\boldsymbol{I} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B})]^{-1} \ [\boldsymbol{I} - \boldsymbol{R}(\bar{\boldsymbol{L}} - \boldsymbol{B})] \ \phi_{inc} \rho^{-1/2} \ . \tag{26}$$

All matrices in Eq. (xx-26) are diagonal except the **R** matrix. The matrix elements of $\boldsymbol{\rho}^{\mathbf{1/2}}$ are given by $(k_c\, a_c)^{1/2}$.

It should be noted that no approximation was used in deriving Eq. (xx-26). That equation represents an exact expression relating **U** and **R**, and leads to the determination of the cross section according to Eqs. (xx-14, xx-15, and xx-16).

To avoid dealing with matrices of large dimensions, several approximations of the R-matrix theory have been introduced. We will discuss various of these cross-section formalisms in the pages to come; we begin by introducing the level matrix A.

Relation between U, R, and A

Another presentation of Eq. (xx-26) may be obtained by introducing the following definitions

$$\boldsymbol{L_0} = \boldsymbol{S_0} + i\boldsymbol{P} \;, \tag{27}$$

$$\boldsymbol{L_0} = \boldsymbol{L} - \boldsymbol{B} \;, \tag{28}$$

and

$$\boldsymbol{S_0} = \boldsymbol{S} - \boldsymbol{B} \;, \tag{29}$$

where **S** and **P** are real matrices which contains the shift and the penetration factors, respectively and $\bar{\boldsymbol{L}}_{\boldsymbol{0}} = \boldsymbol{L} - 2i\boldsymbol{P}$.

From Eqs. (xx-20, xx-23, and xx-27), the penetration factors can be written as $\boldsymbol{P} = \rho\,(\phi_{inc}\,\phi_{out})^{-1}$, and Eq. (xx-26) becomes

$$\boldsymbol{U} = \Omega\,[\boldsymbol{I} + 2i\boldsymbol{P}^{\mathbf{1/2}}(\boldsymbol{I} - \boldsymbol{R}\boldsymbol{L_0})^{-\mathbf{1}}\boldsymbol{R}\boldsymbol{P}^{\mathbf{1/2}}]\,\Omega \;, \tag{30}$$

with $\boldsymbol{\Omega} = \phi_{inc}^{1/2}\,\phi_{out}^{-1/2}$.

It should be realized that the R-matrix is a channel matrix; i.e. it depends on the entrance and outgoing channels c and c’. The level matrix concept introduced by Wigner attempts to relate the U matrix to a matrix in which the indices are the energy levels of the compound nucleus, the level matrix of elements $A_{\mu\lambda}$. In relating the channel matrix to the level matrix we recall that the **R** matrix is defined as

$$\boldsymbol{R} = \sum_{\lambda} \frac{\gamma_\lambda \times \gamma_\lambda}{E_\lambda - E} \;, \tag{31}$$

where $\gamma_\lambda \times \gamma_\lambda$ indicates the direct product between two vectors.

The expression $\boldsymbol{I} - \boldsymbol{RL_0} = \mathbf{1} - \sum_{\lambda} \frac{\gamma_\lambda \times \gamma_\lambda}{E_\lambda - E} \boldsymbol{L_0}$ can be written as

$$\boldsymbol{I} - \boldsymbol{RL_0} = \mathbf{1} - \sum_{\lambda} \frac{\gamma_\lambda \times \beta_\lambda}{E_\lambda - E} \;, \tag{32}$$

where we have defined $\beta_\lambda = \boldsymbol{L_0} \gamma_\lambda$, and $\boldsymbol{L_0}$ is a symmetric matrix. The form of Eq. (xx-32) suggests the following relation

$$(\boldsymbol{I} - \boldsymbol{RL_0})^{-1} = \mathbf{1} + \sum_{\mu\lambda} (\gamma_\mu \times \gamma_\lambda) \boldsymbol{A}_{\mu\lambda} \;, \tag{33}$$

where the indices μ and λ refer to energy levels in the compound nucleus and $\boldsymbol{A}$ is determined as follows:

Multiplying Eqs. (xx-32) and (xx-33) and using the identity $\boldsymbol{(x \times y)(z \times w)} = \boldsymbol{(y.z)(x \times w)}$, we obtain the following expression,

$$\sum_{\lambda\nu} (\gamma_\mu \times \beta_\nu) \boldsymbol{A}_{\mu\nu} - \sum_{\lambda} \frac{\gamma_\lambda \times \beta_\lambda}{E_\lambda - E} - \sum_{\lambda\mu\nu} \frac{\gamma_\lambda \times \beta_\nu}{E_\lambda - E} (\beta_\lambda \cdot \gamma_\mu) \boldsymbol{A}_{\mu\nu} = 0 \;. \tag{34}$$

Factoring the term $\gamma_\lambda \times \beta_\nu$ in the above equation, we find that the level matrix $A_{\mu\lambda}$ satisfies the equation

$$A_{\lambda\nu}(E_\lambda - E) - \sum_{\mu} (L_0 \gamma_\lambda \cdot \gamma_\mu) A_{\mu\nu} = \delta_{\lambda\nu} \;. \tag{35}$$

The evaluation of the matrix $(\boldsymbol{I} - \boldsymbol{RL_0})^{-1} \boldsymbol{R}$ which appears in Eq. (xx-30) is obtained by combining Eqs. (xx-31) and (xx-33) which gives

$$(\boldsymbol{I}-\boldsymbol{R}\boldsymbol{L}_{\mathbf{0}})^{-1}\boldsymbol{R}=\sum_{\lambda}\left[\frac{\gamma_\lambda\times\gamma_\lambda}{E_\lambda-E}+\frac{1}{E_\lambda-E}\sum_{\mu}(\gamma_\mu\times\gamma_\lambda)\sum_{\nu}(\beta_\nu\cdot\gamma_\lambda)\boldsymbol{A}_{\mu\nu}\right]. \qquad \mathbf{(36)}$$

Using Eq. (xx-35) as $\sum_{\nu}(\beta_\nu\cdot\gamma_\lambda)\,\boldsymbol{A}_{\mu\nu}=-\delta_{\lambda\mu}+(E_\lambda-E)\boldsymbol{A}_{\lambda\mu}$ gives

$$(\boldsymbol{I}-\ \boldsymbol{R}\boldsymbol{L}_{\mathbf{0}})^{-1}\boldsymbol{R}=\sum_{\mu\lambda}(\gamma_\mu\times\gamma_\lambda)\boldsymbol{A}_{\mu\lambda}\ . \qquad \mathbf{(37)}$$

Hence, the collision matrix is related to the level matrix as

$$\boldsymbol{U}=\boldsymbol{\Omega}\left[\boldsymbol{I}+2i\,\boldsymbol{P}^{\mathbf{1/2}}\left(\sum_{\mu\lambda}(\gamma_\mu\times\gamma_\lambda)A_{\mu\lambda}\right)\boldsymbol{P}^{\mathbf{1/2}}\right]\boldsymbol{\Omega}\ . \qquad \mathbf{(38)}$$

The elements of the collision matrix for entrance and exit channels c and c’, respectively, are given as

$$U_{cc'}=\Omega_c\left[\delta_{cc'}+i\sum_{\mu\lambda}(\Gamma^{1/2}_{\mu c}A_{\mu\lambda}\,\Gamma^{1/2}_{\lambda c'})\right]\Omega_{c'}\ , \qquad \mathbf{(39)}$$

where

$$\Gamma^{1/2}_{\mu c}=\gamma_{\mu c}\,(2P_c)^{1/2} \qquad \mathbf{(40)}$$

is the level width, and from Eq. (xx-35) the level matrix is

$$A^{-1}_{\mu\lambda}=(E_\lambda-E)\,\delta_{\mu\lambda}-\sum_{c}\ (\gamma_{\mu c}\,L_{0c}\,\gamma_{\lambda c})\ . \qquad \mathbf{(41)}$$

It should be remembered that no approximation has been introduced in the formal derivation of the collision matrix up to this point.

Simplified Models Derived from the General R-Matrix Theory

In this session we will present the approximations introduced to the R-matrix and, likewise, to the level matrix A which leads to various simplified resonance formalisms. The cross section formalisms frequently used are the single-level Breit-Wigner (SLBW), the Multilevel Breit-Wigner (MLBW), the Adler-Adler (AA), and the Reich-Moore (RM) formalism (also known as the reduced R-matrix formalism). A new methodology, called multipole representation of the cross section, was developed at Argonne National Laboratory by R. N. Hwang; in this approach the cross section representation is done in the momentum space ($\sqrt{E}$). We will address the approximations needed to obtain these simplified R-matrix models.

The starting points in deriving these formalisms will be the level matrix A and its relation to the collision matrix U.

The collision matrix is given by

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})}\left[\delta_{cc'} + 2i\,P_c^{1/2}\Big(\sum_{\mu\lambda} \gamma_{\lambda c} A_{\lambda\mu}\, \gamma_{\mu c'}\Big) P_{c'}^{1/2}\right] . \tag{42}$$

The level matrix is represented as

$$A^{-1}_{\lambda\mu} = (E_\lambda - E)\,\delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} L_{0c} \gamma_{\mu c} . \tag{43}$$

1. Multilevel Breit-Wigner (MLBW) Formalism

In the MLBW approximation the level matrix is assumed to be diagonal, which means that the off-diagonal elements of the second term in the matrix given in Eq. (xx-43) are neglected, i.e.,

$$\sum_c (\gamma_{\lambda c} L_{0c} \gamma_{\mu c}) \approx \delta_{\lambda\mu} \sum_c L_{0c} \gamma^2_{\mu c} . \tag{44}$$

Hence Eq. (xx-43) becomes

$$A^{-1}_{\lambda\mu} = (E_\lambda - E - \sum_c L_{0c} \gamma^2_{\lambda c})\,\delta_{\lambda\mu} . \tag{45}$$

From Eqs. (xx-27) and (xx-40) we have $L_{0c} = (S_c - B_c) + i\,P_c$ and $\gamma^2_{\lambda c} = \dfrac{\Gamma_{\lambda c}}{2P_c}$, which leads to

$$A^{-1}_{\lambda\mu} = (E_\lambda - E + \Delta_\lambda - \frac{i}{2}\Gamma_\lambda)\,\delta_{\lambda\mu} , \tag{46}$$

where $\Delta_\lambda = -\sum_c \frac{S_c - B_c}{2P_c}\,\Gamma_{\lambda c}$ (energy shift factor for the MLBW) and $\Gamma_\lambda = \sum_c \Gamma_{\lambda c}$. Redefining

$E_\lambda \rightarrow E_\lambda + \Delta_\lambda$, the level matrix becomes

$$A_{\lambda\mu} = \frac{\delta_{\lambda\mu}}{E_\lambda - E - \frac{i}{2}\Gamma_\lambda} \quad . \tag{47}$$

The collision matrix given by Eq. (xx-42) becomes

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})}\left[\delta_{cc'} + i\sum_\lambda \frac{\Gamma_{\lambda c}^{1/2}\,\Gamma_{\mu c'}^{1/2}}{E_\lambda - E - \frac{i}{2}\Gamma_\lambda}\right] . \tag{48}$$

From this point, we proceed to the derivation of the cross section formalism in the MLBW representation. For a reaction in which $c \neq c'$ (fission, capture, or inelastic scattering channels) the collision matrix and the reaction cross section are given respectively by

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'} - \frac{\pi}{2})}\ \sum_\lambda \frac{\Gamma_{\lambda c}^{1/2}\,\Gamma_{\mu c'}^{1/2}}{E_\lambda - E - \frac{i}{2}\Gamma_\lambda} \ , \tag{49}$$

and

$$\sigma_{cc'} = \pi\,\lambda\!\!\!^{-2}\,|\,U_{cc'}|^2 = \pi\,\lambda\!\!\!^{-2}\,U_{cc'}U_{cc'}^* \tag{50}$$

where we have used the identity $i = e^{i\pi/2}$ in Eq. (xx-49). Inserting Eq. (xx-49) into Eq. (xx-50) gives

$$\sigma_{cc'} = \pi\,\lambda\!\!\!^{-2}\sum_\lambda\sum_{\lambda'} \frac{\Gamma_{\lambda c}^{1/2}\Gamma_{\lambda c'}^{1/2}\,\Gamma_{\lambda' c}^{1/2}\Gamma_{\lambda' c'}^{1/2}}{(\epsilon_\lambda - E)(\epsilon_{\lambda'}^* - E)} \ , \tag{51}$$

where we have made $\epsilon_\lambda = E_\lambda - \frac{i}{2}\Gamma_\lambda$ and $\epsilon_\lambda^* = E_\lambda + \frac{i}{2}\Gamma_\lambda$. This expression can be further modified by using the following identity

$$\frac{1}{(\epsilon_\lambda - E)(\epsilon_{\lambda'}^* - E)} = \frac{1}{(\epsilon_{\lambda'}^* - \epsilon_\lambda)}\left[\frac{1}{(\epsilon_\lambda - E)} - \frac{1}{(\epsilon_{\lambda'}^* - E)}\right] , \qquad \textbf{(52)}$$

which gives

$$\sigma_{cc'} = \pi \lambda\!\!\!^{-2}\left\{\sum_{\lambda\lambda'} \frac{M_{\lambda\lambda'}^{cc'}}{(\epsilon_{\lambda'}^* - \epsilon_\lambda)(\epsilon_\lambda - E)} - \sum_{\lambda\lambda'} \frac{M_{\lambda\lambda'}^{cc'}}{(\epsilon_{\lambda'}^* - \epsilon_\lambda)(\epsilon_{\lambda'}^* - E)}\right\} , \qquad \textbf{(53)}$$

where $M_{\lambda\lambda'}^{cc'} = \Gamma_{\lambda c}^{1/2}\Gamma_{\lambda c'}^{1/2}\Gamma_{\lambda' c}^{1/2}\Gamma_{\lambda' c'}^{1/2}$. The second term in Eq. (xx-53) is the complex conjugate of the first term, hence

$$\sigma_{cc'} = 2\pi \lambda\!\!\!^{-2} Re\left\{\sum_\lambda \frac{1}{\epsilon_\lambda - E} \sum_{\lambda'} \frac{M_{\lambda\lambda'}^{cc'}}{\epsilon_{\lambda'}^* - \epsilon_\lambda}\right\} . \qquad \textbf{(54)}$$

The term in the summation on λ' can be expanded to give

$$\sigma_{cc'} = 4\pi \lambda\!\!\!^{-2}\sum_\lambda \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{\Gamma_\lambda^2} \left[(Re\, C_\lambda^{cc'})\psi_\lambda + (Im\, C_\lambda^{cc'})\chi_\lambda\right] , \qquad \textbf{(55)}$$

where

$$C_\lambda^{cc'} = 1 + \sum_{\lambda \neq \lambda'} \frac{\gamma_{\lambda' c}}{\gamma_{\lambda c}} \frac{i\Gamma_{\lambda c}}{E_{\lambda'} - E + \frac{i}{2}(\Gamma_{\lambda'} + \Gamma_\lambda)} \frac{\gamma_{\lambda' c'}}{\gamma_{\lambda c'}} , \qquad \textbf{(56)}$$

and the line shapes ψ_λ and χ_λ are defined as

$$\psi_\lambda = \frac{\Gamma_\lambda^2/4}{(E_\lambda - E)^2 + \Gamma_\lambda^2/4} , \qquad \textbf{(57)}$$

and

$$\chi_\lambda = \frac{(E_\lambda - E)\Gamma_\lambda/2}{(E_\lambda - E)^2 + \Gamma_\lambda^2/4} \quad . \tag{58}$$

Equation (xx-55) is the MLBW cross section form for the reaction cross section. A similar procedure can be followed to derive the elastic cross section.

2. Single Level Breit-Wigner (SLBW) Formalism

The SLBW cross section formalism is a particular case of Eq. (xx-55) when the second term in Eq. (xx-56) is zero, that is, $C_\lambda^{cc'} = 1$.

3. Adler-Adler (AA) Formalism

The AA approximation consists of applying an orthogonal complex transformation which diagonalizes the level matrix as given in Eq. (xx-43). We are looking for a transformation such that

$$O A^{-1} O^{-1} = \underline{\epsilon} - E \;, \tag{59}$$

or

$$A = O^{-1} (\underline{\epsilon} - E)^{-1} O \;, \tag{60}$$

where $O O^{-1} = O^{-1} O = I$. Here O is a orthogonal complex matrix and $\underline{\epsilon}$ is a diagonal matrix of complex elements. The elements of the matrix in Eq. (xx-60) are given as

$$A_{\lambda\mu} = \sum_\nu \frac{O_{\lambda\nu} O_{\mu\nu}}{\epsilon_\nu - E}. \tag{61}$$

The collision matrix of Eq. (xx-42) then becomes

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})} \left[\delta_{cc'} + i \sum_\nu \frac{g_{\nu c}^{1/2} g_{\nu c'}^{1/2}}{\epsilon_\nu - E} \right] , \tag{62}$$

where $g_{\nu c}^{1/2} = \sum_\lambda O_{\lambda\nu} \Gamma_{\lambda c}^{1/2}$ and $g_{\nu c'}^{1/2} = \sum_\mu O_{\mu\nu} \Gamma_{\mu c'}^{1/2}$. The elements of the O matrix are determined from

$$(E_\lambda - E)\,\delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} L_{0c} \gamma_{\mu c} = \sum_\nu O_{\lambda\nu} \epsilon_\nu O_{\mu\nu} \ , \qquad \textbf{(63)}$$

where Eq. (xx-43) has been used.

Because of the energy dependence of L_{0c} through the penetration factor P_c, the elements $O_{\lambda\nu}$ will, in general, be energy-dependent. In the AA approach, the energy dependence of L_{0c} is neglected. This assumption works very well for fissile isotopes where the resonance region is predominantly described by s-wave resonances (angular momentum corresponding to $l=0$) for which the penetration factor is energy independent. However, the assumption breaks down when p-wave ($l=1$) or other neutron partial wave functions with angular momentum l greater than 1 are present.

The reaction cross section in the AA formalism can be obtained in a similar way to that developed for the MLBW. The result is

$$\sigma_{cc'} = 2\pi\lambdabar^2 \sum_\lambda \frac{\nu_\lambda G_\lambda^{cc'} + (\mu_\lambda - E) H_\lambda^{cc'}}{(\mu_\lambda - E)^2 + \nu_\lambda^2} \ , \qquad \textbf{(64)}$$

where the following definitions were made

$$H_\lambda^{cc'} - i\,G_\lambda^{cc'} = \sum_{\lambda'} \frac{g_{\lambda c} g_{\lambda c'} g_{\lambda' c} g_{\lambda' c'}}{\epsilon^*_{\lambda'} - \epsilon_\lambda} \ , \qquad \textbf{(65)}$$

and

$$\epsilon_\lambda = \mu_\lambda - i\,\nu_\lambda \ . \qquad \textbf{(66)}$$

4. Reich-Moore Formalism

The approach proposed by Reich and Moore for treating the neutron-nucleus cross sections consists of eliminating the off-diagonal contribution of the photon channels. The rationale for this assumption is this: systematic measurements of the resonance widths, mainly in the case of the neutron and fission widths, show strong fluctuations among resonances of the same total angular momentum and parity. It should be expected, from Eq. (xx-40), that these fluctuations are connected either to the reduced widths $\gamma_{\lambda c}$ or to the penetration factors P_c. However, it is improbable that such fluctuations are due to the penetration factors because they are either constant or a smooth function of the energy. Hence, the fluctuations must be related to the reduced widths. Porter and Thomas noted that the reduced widths $\gamma_{\lambda c}$ of Eq. (xx-13) are functions of the channel functions $\phi_c(E_\lambda,a_c)$ which, in turn, are projections of the eigenfunctions of the compound nucleus onto the nuclear surface and exhibit random size variations. Consequently, the large number of gamma channels implies that $\sum_{c\in\gamma} \gamma_{\mu c}\gamma_{\lambda c}$ is very small for $\mu \neq \lambda$. The second term of the level matrix in Eq. (xx-43) is divided in two parts as

$$\sum_{c} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} = \sum_{c\in\gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} + \sum_{c\notin\gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \;, \tag{67}$$

and in the RM approximation

$$\sum_{c\in\gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \approx \delta_{\mu\lambda} \sum_{c\in\gamma} L_{0c} \gamma_{\lambda c}^2 \;. \tag{68}$$

The level matrix becomes

$$A_{\lambda\mu}^{-1} = (E_\lambda - E + \Delta_{\lambda\gamma} - \frac{i}{2}\Gamma_{\lambda\gamma})\,\delta_{\lambda\mu} + \sum_{c\notin\gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \;, \tag{69}$$

where, similarly to the MLBW, the following definitions were made:

$\Delta_{\lambda\gamma} = -\sum_{c\in\gamma} \dfrac{S_c - B_c}{2P_c}\,\Gamma_{\lambda c}$ (Energy shift factor), and $\Gamma_{\lambda\gamma} = \sum_{c\in\gamma} \Gamma_{\lambda c}$. Note that these quantities are different from that in the MLBW formalism. Again, redefining $E_\lambda \to E_\lambda + \Delta_\lambda$ we have

$$A_{\lambda\mu}^{-1} = (E_\lambda - E - \frac{i}{2}\Gamma_{\lambda\gamma})\,\delta_{\lambda\mu} + \sum_{c\notin\gamma} \gamma_{\lambda c} L_{0c} \gamma_{\mu c} \;. \tag{70}$$

From this point we are going to derive a relation between the collision and the level matrix in the RM representation. Multiplying Eq. (xx-70) by $A_{\alpha\lambda}$ and summing over λ gives

$$\frac{\delta_{\alpha\mu}}{(E_\mu - E - \frac{i}{2}\Gamma_{\mu\gamma})} = A_{\alpha\mu} - \sum_{c\notin\gamma} \sum_{\lambda} \frac{A_{\alpha\lambda}\gamma_{\lambda c} L_{0c} \gamma_{\mu c}}{(E_\mu - E - \frac{i}{2}\Gamma_{\mu\gamma})} \;. \tag{71}$$

Multiplying Eq. (xx-71) on the left by $\gamma_{\alpha c'}$ and on the right by $\gamma_{\alpha c''}$ and summing over α and μ gives

$$\sum_{\mu} \frac{\delta_{\mu c'}\delta_{\mu c''}}{E_{\mu} - E - \frac{i}{2}\Gamma_{\mu\gamma}} = \sum_{\mu}\sum_{\alpha} \gamma_{\alpha c'} A_{\alpha\mu} \gamma_{\mu c''} - \sum_{c\notin\gamma}\sum_{\alpha}\sum_{\lambda} \gamma_{\lambda c'} A_{\alpha\lambda} \gamma_{\lambda_{\lambda c}} L_{0c} \sum_{\mu} \frac{\gamma_{\mu c}\gamma_{\mu c''}}{E_{\mu} - E - \frac{i}{2}\Gamma_{\mu\gamma}} \ . \tag{72}$$

If we define

$$R_{c'c''} = \sum_{\mu} \frac{\delta_{\mu c'}\delta_{\mu c''}}{E_{\mu} - E - \frac{i}{2}\Gamma_{\mu\gamma}} \tag{73}$$

and

$$Q_{c'c} = \sum_{\mu}\sum_{\alpha} \gamma_{\alpha c'} A_{\alpha\mu} \gamma_{\mu c''} \ , \tag{74}$$

then Eq. (xx-72) becomes

$$R_{c'c''} = \sum_{c\notin\gamma} Q_{c'c} \, (\delta_{cc''} - L_{0c} \, R_{cc''}) \ . \tag{75}$$

Note that this R matrix is an approximation, not to be confused with the exact R-matrix defined earlier.

Rearranging Eq. (xx-75) gives

$$Q_{cc'} = \sum_{c''\notin\gamma} R_{cc''} \, (\delta_{c''c'} - L_{0c''} \, R_{c''c'})^{-1} \ . \tag{76}$$

Hence, from Eq. (xx-42) the collision matrix in the RM approximation becomes

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})} \left\{ \delta_{cc'} + 2i \, P_c^{1/2} \left[\sum_{c''\notin\gamma} R_{cc''} (\delta_{c''c'} - L_{0c''} R_{c''c'})^{-1} \right] P_{c'}^{1/2} \right\} . \tag{77}$$

Equation (xx-77) relates the collision matrix to the Reich-Moore R-matrix in a form similar to that in the case of the general R-matrix theory. In the general R-matrix, the elements are

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\,\gamma_{\lambda c'}}{E_{\lambda} - E} \ , \tag{78}$$

whereas in the RM approximation they are

$$R_{cc'} = \sum_{\lambda} \frac{\delta_{\lambda c}\,\delta_{\lambda c'}}{E_{\lambda} - E - \dfrac{i}{2}\Gamma_{\lambda\gamma}} \ . \tag{79}$$

Equation (xx-79) is frequently referred to as the reduced R-matrix theory.

We now proceed to obtain a form for the cross section in the RM approximation, by writing Eq. (xx-77) as

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})}\Omega_{cc'} \ , \tag{80}$$

where

$$\Omega_{cc'} = \delta_{cc'} + 2i\,P_c^{1/2}\left[\sum_{c''\notin\gamma} R_{cc''}\,(\delta_{c''c'} - L_{0c''}R_{c''c'})^{-1}\right]P_{c'}^{1/2} \ . \tag{81}$$

It is useful to write the reduced R-matrix as

$$R_{cc'} = \frac{1}{i}\,P_c^{-1/2}\,K_{cc'}\,P_{c'}^{-1/2} \ , \tag{82}$$

in which the elements of K are given by

$$K_{cc'} = i\,P_c^{1/2}\,R_{cc'}\,P_{c'}^{1/2} \ . \tag{83}$$

The explicit form of $K_{cc'}$ is

$$K_{cc'} = \frac{i}{2}\sum_{\lambda} \frac{\Gamma_{\lambda c}^{1/2}\,\Gamma_{\lambda c'}^{1/2}}{E_\lambda - E - \frac{i}{2}\Gamma_{\lambda\gamma}} \quad . \tag{84}$$

Therefore $\Omega_{cc'}$ becomes

$$\Omega_{cc'} = \delta_{cc'} + 2i\,P_c^{1/2} \sum_{c''\notin\gamma} \frac{1}{i} P_c^{-1/2} K_{cc''} P_{c''}^{-1/2} \left(\delta_{c''c'} - L_{0c''} \frac{1}{i} P_{c''}^{-1/2} K_{c''c'} P_{c'}^{-1/2} \right)^{-1} P_{c'}^{1/2} \quad . \tag{85}$$

Recalling that $L_{0c} = (S_c - B_c) + iP_c$ and making $B_c = S_c$, the expression for $\Omega_{cc'}$ becomes

$$\Omega_{cc'} = \delta_{cc'} + 2 \sum_{c''\notin\gamma} K_{cc''} P_{c''}^{-1/2} \left(\delta_{c''c'} - P_{c''}^{1/2} K_{c''c'} P_{c'}^{-1/2} \right)^{-1} P_{c'}^{1/2} \quad . \tag{86}$$

The matrix form of Eq. (xx-86) is

$$\boldsymbol{\Omega} = \boldsymbol{I} + 2\,\boldsymbol{K}\boldsymbol{P}^{-1/2} (\boldsymbol{I} - \boldsymbol{P}^{1/2}\boldsymbol{K}\boldsymbol{P}^{-1/2})^{-1} \boldsymbol{P}^{1/2} \quad . \tag{87}$$

Equation (xx-87) can be further reduced by using the identity $(\boldsymbol{B}+\boldsymbol{C})^{-1} = \boldsymbol{v}(\boldsymbol{wBv}+\boldsymbol{wCv})^{-1}\,\boldsymbol{w}$. Letting $\boldsymbol{B} = \boldsymbol{I}$, $\boldsymbol{C} = -\boldsymbol{P}^{1/2}\boldsymbol{K}\boldsymbol{P}^{-1/2}$, $\boldsymbol{w} = \boldsymbol{P}^{-1/2}$ and $\boldsymbol{v} = \boldsymbol{P}^{1/2}$ we have

$$\boldsymbol{\Omega} = \boldsymbol{I} + 2\,\boldsymbol{K}(\boldsymbol{I} - \boldsymbol{K})^{-1} \quad . \tag{88}$$

If we then add and subtract $2(\boldsymbol{I} - \boldsymbol{K})^{-1}$ the expression becomes,

$$\boldsymbol{\Omega} = 2\,(\boldsymbol{I} - \boldsymbol{K})^{-1} - \boldsymbol{I} \quad , \tag{89}$$

for which the elements are, explicitly,

$$\Omega_{cc'} = 2\,(I - K)_{cc'}^{-1} - \delta_{cc'} \quad . \tag{90}$$

The collision matrix of Eq. (xx-80) then takes the form

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})}[2(I - K)_{cc'}^{-1} - \delta_{cc'}] \quad , \tag{91}$$

where the elements of $(I-K)_{cc'}$ are given as

$$(I-K)_{cc'} = \delta_{cc'} - \frac{i}{2}\sum_{\lambda} \frac{\Gamma_{\lambda c}^{1/2}\,\Gamma_{\lambda c'}^{1/2}}{E_{\lambda} - E - \frac{i}{2}\Gamma_{\lambda\gamma}} \ . \tag{92}$$

The RM cross sections are written in terms of the transmission probability, defined as

$$\rho_{cc'} = \delta_{cc'} - (I-K)^{-1}_{cc'} \ , \tag{93}$$

for which the collision matrix can be written as

$$U_{cc'} = e^{-i(\phi_c + \phi_{c'})}[\delta_{cc'} - 2\rho_{cc'}] \ , \tag{94}$$

The cross sections can then be obtained by using Eqs. (xx-14), (xx-15), and (xx-16) as,

$$\sigma_t = 2\pi\lambda\!\!\!^{-}{}^2 \sum_l (2l+1)\Big[(1-\cos 2\phi_l) + 2Re(\rho_{nn}\, e^{-2i\phi_l})\Big] \ , \tag{95}$$

$$\sigma_{abs} = 4\pi\lambda\!\!\!^{-}{}^2 \sum_l (2l+1)\Big[Re(\rho_{nn}) - |\rho_{nn}|^2)\Big] \ , \tag{96}$$

$$\sigma_f = 4\pi\lambda\!\!\!^{-}{}^2 \sum_l (2l+1)\sum_{c\in f} |\rho_{nc}|^2 \ , \tag{97}$$

and

$$\sigma_\gamma = \sigma_{abs} - \sigma_f \ . \tag{98}$$

5. Conversion of RM parameters into AA parameters

A procedure to convert RM parameters into an equivalent set of AA parameters was developed by DeSaussure and Perez. Their approach consisted of writing the RM transmission probabilities ρ_{nn} and ρ_{nc} as the ratio of polynomials in energy; these polynomials can then be expressed in terms of partial fraction expansions by matching the AA cross sections as:

$$\frac{1}{\sqrt{E}}\,\rho_{nn} = \frac{P_n^{N-1}(E)}{P^N(E)} = \sum_{\lambda=1}^{N} \frac{r_{\lambda n}}{d_\lambda - E} \;, \tag{99}$$

and

$$\frac{1}{\sqrt{E}}\,|\rho_{nc}|^2 = \frac{|P_c^{N-1}(E)|^2}{|P^N(E)|^2} = \sum_{\lambda=1}^{N} \left[\frac{r_{\lambda c}}{d_\lambda - E} + \frac{r_{\lambda c}^*}{d_\lambda^* - E} \right] \qquad c \neq n \;, \tag{100}$$

where

$$P^N = Q\,\Delta \;, \tag{101}$$

$$P_n^{N-1} = Q\,\frac{\Delta - m_{nn}}{\sqrt{E}} \;, \tag{102}$$

$$Q = \prod_\lambda \left(E_\lambda - E - \frac{i}{2}\Gamma_{\lambda\gamma}\right) \;, \tag{104}$$

$$|P_c^{N-1}|^2 = \frac{|Q\,m_{nc}|^2}{\sqrt{E}} \;, \tag{103}$$

and $\Delta = |I - K|$.

Equations (xx-99) and (xx-100) have poles $d_\lambda = \mu_\lambda - i\,\nu_\lambda$ which are roots of the equation

$$P^N(E) = Q\Delta = 0 \ , \tag{105}$$

and are identifiable as the parameters of the Adler-Adler formalism. In deriving this methodology DeSaussure and Perez neglected the energy dependence of the neutron widths, i.e., $\Gamma_n \propto \sqrt{E}$. This assumption limits the application of this methods to s-wave cross section. Hwang has extended the application of the DeSaussure and Perez approach to the calculation of cross sections for any angular momentum. In his approach, instead of using energy space, Hwang noted that the dependence of Γ_n on $\sqrt{E}$ suggests that an expansion in terms of $\sqrt{E}$ would lead to a rigorous representation of the cross section. Since momentum is proportional to $\sqrt{E}$, Hwang calls his methodology a rigorous pole representation in the momentum space or, for short, a multipole representation of the cross sections (MP). The transformation of the RM parameters into the MP parameters is obtained as

$$\rho_{nn} = \frac{P_n^{2M-1}(E)}{P^{2M}(E)} = \sum_{\lambda=1}^{2M} \frac{r_{\lambda n}}{d_\lambda - \sqrt{E}} \ , \tag{106}$$

and

$$|\rho_{nc}|^2 = \frac{|P_c^{2M-1}(E)|^2}{|P^{2M}(E)|^2} = \sum_{\lambda=1}^{2M} \left[\frac{r_{\lambda c}}{d_\lambda - \sqrt{E}} + \frac{r_{\lambda c}^*}{d_\lambda^* - \sqrt{E}} \right] \qquad c \neq n \ , \tag{107}$$

where

$$M = (l+1)N \ , \tag{108}$$

and N is the number of resonance parameters in the RM representation. The factor Q of Eq. (xx-104) becomes

$$Q = \prod_{\lambda=1}^{N} (E_\lambda - E - \frac{i}{2}\Gamma_{\lambda\gamma}) \ q_l(\sqrt{E}) \ , \tag{109}$$

where

$$q_0(\sqrt{E}) = 1, \tag{110}$$

$$q_1(\sqrt{E}) = 1 + (k\,a)^2 \ , \tag{111}$$

and

$$q_2(\sqrt{E}) = 9 + 3\,(k\,a)^2 + (k\,a)^4 \ . \qquad \textbf{(112)}$$

Doppler Broadening and Effective Cross Sections

The Doppler broadening of cross sections is a well-known effect which is caused by the motion of the atoms of the target nuclei. Since the target nuclei are not at rest in the laboratory system, the neutron-nucleus cross section will depend on the relative speed of the neutron and the nucleus. The effective cross section for mono-energetic neutrons of mass m and energy E (laboratory velocity v) is given by the number of neutrons per unit volume, multiplied by the number of target nuclei per unit volume, times the probability that a reaction will occur per unit time at an energy equivalent to the relative velocity $|\,v - W\,|$, integrated over all values of W, the velocity of the nucleus. The relation between the cross section measured in the laboratory and the effective cross section is

$$v\,\bar{\sigma}(mv^2/2) = \int d^3W\ p(\vec{W})\ |\vec{v}-\vec{W}|\ \sigma(m|\vec{v}-\vec{W}|^2/2)\ , \qquad \textbf{(113)}$$

where $\bar{\sigma}(mv^2/2)$ is the effective or Doppler-broadened cross section for incident particles with speed v [laboratory energy $mv^2/2$]. The distribution of velocities of the target nuclei is described by $p(\vec{W})$. A major issue is the choice of the appropriate velocity distribution function of the target nuclei. Let us now assume that the target nuclei have the same velocity distribution as the atoms of an ideal gas; i.e. the Maxwell-Boltzmann distribution,

$$p(\vec{W})\,d^3W \ = \ \frac{1}{\pi^{3/2}}\ \exp\left(-\frac{W^2}{u^2}\right)\ \frac{d^3W}{u^3}\ , \qquad \frac{M}{2}\,u^2 \ = \ k\,T\,, \qquad \textbf{(114)}$$

where M is the nuclear mass and kT the gas temperature in energy units. Combining Eqs. (xx-113) and (xx-114) gives

$$v\bar{\sigma}(mv^2/2) \ = \ \frac{1}{\pi^{3/2}\,u^3}\ \int_{\text{all }\vec{W}} d^3W\ \exp\left(-\frac{W^2}{u^2}\right)\ |\vec{v}-\vec{W}|\ \sigma(m|\vec{v}-\vec{W}|^2/2)\ \ . \qquad \textbf{(115)}$$

Note that, from the above definitions, a *1/v* cross section remains unchanged.

Changing the integration variable from $\vec{W}$ to $\vec{w} = \vec{v} - \vec{W}$ and choosing spherical coordinates simplifies the integral to the following:

$$
\begin{aligned}
v\bar{\sigma}\left(\frac{mv^2}{2}\right) &= \frac{1}{\pi^{3/2}u^3}\int_{\text{all }\bar{w}} d^3w\ \exp\left(-\frac{(v^2-2vw\cos\theta+w^2)}{u^2}\right)\ w\,\sigma\left(\frac{mw^2}{2}\right) \\
&= \frac{1}{\pi^{3/2}u^3}\int_0^{\pi} d\phi\int_0^{\infty} w^2\,dw\int_0^{\pi} d(\cos(\theta)\ \exp\left(-\frac{(v^2-2vw\cos\theta+w^2)}{u^2}\right)\ w\,\sigma\left(\frac{mw^2}{2}\right) \\
&= \frac{1}{\pi^{3/2}u^3}\int_0^{2\pi} d\phi\int_0^{\infty} dw\,w^3\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v^2+w^2)}{u^2}\right)\int_{-1}^{+1} d\mu\ \exp\left(-\frac{2vw\mu}{u^2}\right) \qquad \textbf{(116)} \\
&= \frac{2\pi}{\pi^{3/2}u^3}\int_0^{\infty} dw\,w^3\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v^2+w^2)}{u^2}\right)\left(\frac{-u^2}{2vw}\right)\left[\exp\left(-\frac{2vw}{u^2}\right)-\exp\left(+\frac{2vw}{u^2}\right)\right] \\
&= \frac{1}{v\sqrt{\pi}\,u}\int_0^{\infty} dw\,w^2\,\sigma\left(\frac{mw^2}{2}\right)\left[\exp\left(-\frac{(v-w)^2}{u^2}\right)-\exp\left(-\frac{(v+w)^2}{u^2}\right)\right]\ .
\end{aligned}
$$

This equation, known as the Solbrig's kernel, may be more familiar when written as the sum of two integrals,

$$
\begin{aligned}
\bar{\sigma}\left(E=\frac{mv^2}{2}\right) &= \frac{1}{v^2\sqrt{\pi}\,u}\int_0^{\infty} dw\,w^2\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v-w)^2}{u^2}\right) \\
&\quad -\frac{1}{v^2\sqrt{\pi}\,u}\int_0^{\infty} dw\,w^2\,\sigma\left(\frac{mw^2}{2}\right)\exp\left(-\frac{(v+w)^2}{u^2}\right)\ .
\end{aligned}
\qquad \textbf{(117)}
$$

At sufficiently high energies, the contribution from the second integral may be omitted since the value of the exponential is vanishingly small.

To simplify Eq. (xx-117) further, we make the following definition:

$$
\begin{aligned}
s(w) &= \sigma(\ m(w)^2/2) \qquad \text{for } w>0 \\
&= -\sigma(m(-w)^2/2) \qquad \text{for } w<0\ .
\end{aligned}
\qquad \textbf{(118)}
$$

Equation (xx-117) then becomes

$$\bar{\sigma}\left(\frac{mv^2}{2}\right) = \frac{1}{v^2\sqrt{\pi}\,u} \int_{-\infty}^{\infty} dw\, w^2\, s(w) \exp\left(-\frac{(v-w)^2}{u^2}\right) \quad . \tag{119}$$

For programming convenience, we make a change of variable from velocity to square root of energy. Thus instead of v we use

$$V = \sqrt{E} = v\sqrt{m/2} \quad ; \tag{120}$$

we redefine W to be

$$W = w\sqrt{m/2} \quad , \tag{121}$$

and define U as

$$U = \sqrt{m/2}\,u = \sqrt{mkT/M} \quad . \tag{122}$$

In addition, $S(W)$ is set equal to $s(w)$, or

$$\begin{aligned} S(W) &= \sigma((W)^2) \qquad \text{for } W>0 \\ &= -\sigma((-W)^2) \qquad \text{for } W<0 \; . \end{aligned} \tag{123}$$

These changes give the formulation which is used in SAMMY for the exact monatomic free gas model (FGM):

$$\bar{\sigma}(V^2) = \frac{1}{V^2\sqrt{\pi}\,U} \int_{-\infty}^{\infty} dW\, W^2\, S(W) \exp\left(-\frac{(V-W)^2}{U^2}\right) \quad . \tag{124}$$

These equations hold for $1/v$ cross sections, for constant cross sections, and for cross sections with resonance structure.

To transform to the high-energy Gaussian approximation (hereafter referred to as HEGA) from the FGM, define E as V^2 and E' as W^2. Then Eq. (xx-124) takes the form

$$\bar{\sigma}(E) \cong \frac{1}{E\sqrt{\pi}\,U} \int_{E_{\min}>0}^{\infty} \frac{dE'}{2\sqrt{E'}}\, E'\, \sigma(E') \exp\left(-\frac{\left(\sqrt{E}-\sqrt{E'}\right)^2}{U^2}\right) , \tag{125}$$

in which the lower limit has been changed from -∞ to E_{min}, a number above zero, since the next step involves approximations which are valid only for $E' >> 0$. If we expand the integrand of Eq. (xx-125) in powers of *(E-E')* for values of E'/E close to 1 and set $\delta = E' - E$, then

$$\sqrt{E} - \sqrt{E+\delta} = \sqrt{E}\left(1 - \sqrt{1 + \frac{\delta}{E}}\right)$$

$$\approx \sqrt{E}\left[1 - \left(1 + \frac{1}{2}\frac{\delta}{E}\right)\right] \quad . \qquad \textbf{(126)}$$

$$\approx -\frac{1}{2}\frac{E - E'}{\sqrt{E}}$$

Defining Δ^2 (Doppler width) as

$$\Delta^2 = 4\,E\,U^2$$

$$= \sqrt{\frac{4kTE}{M/m}} \ , \qquad \textbf{(127)}$$

(Note that this quantity is energy-dependent) then the HEGA becomes

$$\bar{\sigma}_{HEGA}(E) \cong \frac{1}{\sqrt{\pi}\,\Delta}\int_{-\infty}^{\infty} dE' \;\; \sigma(E')\exp\left(-\frac{(E-E')^2}{\Delta^2}\right) \quad , \qquad \textbf{(128)}$$

where the lower limit was extended to negative infinity since that portion of the integrand is essentially zero. This is the usual Gaussian formulation of the free gas model.

Other Energy-Dependent Cross Sections

No discussion of Doppler broadening would be complete without an analysis of the effects of Doppler broadening on particular types of cross sections. Here we examine some important types of energy dependencies.

Doppler Broadening of 1/*v* Cross Sections

Doppler broadening is expected to preserve (i.e., leave unchanged) a 1/*v*-cross section. To test whether this is the case with FGM and/or HEGA broadening, we note that a 1/*v*-cross section may be expressed as

$$\sigma(W^2) = \frac{\sigma_0 V_0}{W} \quad , \qquad \textbf{(129)}$$

where the subscript "0" denotes constants. To evaluate the FGM with this type of cross section, note that our function *S* of Eq. (xx-123), combined with Eq. (xx-129), gives

$$\begin{aligned} S(W) &= \frac{\sigma_0 V_0}{W} \quad \text{for } W \geq 0 \\ &= -\frac{\sigma_0 V_0}{-W} = \frac{\sigma_0 V_0}{W} \quad \text{for } W < 0 \quad . \end{aligned} \qquad \textbf{(130)}$$

From Eq. (xx-11) the FGM-broadened form of the 1/*v* cross section is therefore

$$\bar{\sigma}(V^2) = \frac{\sigma_0 V_0}{V^2 \sqrt{\pi}\, U} \int_{-\infty}^{+\infty} W\, dW\, e^{-(V-W)^2/U^2} = \frac{\sigma_0 V_0}{V} \quad , \qquad \textbf{(131)}$$

i.e., in the exact same mathematical form as the original of Eq. (xx-129). In other words, a 1/*v* cross section is conserved under Doppler broadening with the free gas model.

That is not the case for HEGA broadening. With the HEGA from Eq. (xx-128), the Doppler-broadened 1/*v* cross section takes the form

$$\bar{\sigma}_{HEGA}(E) = \frac{1}{\sqrt{\pi}\,\Delta} \int_{-\infty}^{+\infty} dE' \, \frac{\sigma_0 V_0}{\sqrt{E'}} \, e^{-(E-E')^2/\Delta^2} = \frac{\sigma_0 V_0}{\sqrt{\pi}\,\Delta} \int_{-\infty}^{+\infty} \frac{dE'}{\sqrt{E'}} \, e^{-(E-E')^2/\Delta^2} \quad , \qquad \textbf{(132)}$$

which is not readily integrable analytically. What *is* clear is that the result is *not* 1/*v*.

Doppler Broadening of a Constant Cross Section

In contrast to the 1/*v* cross section, a constant cross section is not conserved under Doppler broadening. That it is true experimentally can be seen by examining very low energy capture cross sections, for which the unbroadened cross section is constant (which can be shown by taking the low-energy limit of the Reich-Moore equations, for example) but the experimental cross section rises with decreasing energy. See, for example, the S elastic cross section from 0.01 to 1.0 eV or the Cu elastic cross section below 2.0 eV (on pages 100 and 234, respectively, of [VM88]), which clearly rise with decreasing energy.

To calculate analytically what effect FGM and HEGA broadening have upon a constant cross section, we first note that a constant cross section can be expressed as

$$\sigma(E) = \sigma_0 \quad . \tag{133}$$

The function *S* needed for our formulation of FGM broadening (see Eq. (xx-123)) is found to be

$$\begin{aligned} S(W) &= \sigma_0 \quad \text{for } W \geq 0 \\ &= -\sigma_0 \quad \text{for } W < 0 \quad , \end{aligned} \tag{134}$$

so that Eq. (xx-124) gives, for the FGM-broadened constant cross section,

$$\bar{\sigma}(V^2) = \frac{\sigma_0}{V^2 \sqrt{\pi}\, U} \left[\int_0^\infty dW\, W^2\, e^{-(V-W)^2/U^2} - \int_{-\infty}^0 dW\, W^2\, e^{-(V-W)^2/U^2} \right] \quad . \tag{135}$$

Replacing (*W*-*V*) / *U* by *x* gives

$$
\begin{aligned}
\bar{\sigma}(V^2) &= \frac{\sigma_0\, U^3}{V^2\sqrt{\pi}\, U}\left[\ \int_{-v}^{\infty} dx\ (x^2+2xv+v^2)\ e^{-x^2} \ -\ \int_{-\infty}^{-v} dx\ (x^2+2xv+v^2)\ e^{-x^2}\ \right] \\
&= \frac{\sigma_0}{v^2\sqrt{\pi}}\left[\ \int_0^{\infty} + \int_{-v}^{0} - \int_{-\infty}^{0} + \int_{-v}^{0}\ \right] dx\ (x^2+2xv+v^2)\ e^{-x^2} \\
&= \frac{\sigma_0}{v^2\sqrt{\pi}}\left[\ 2\int_0^{\infty} dx\ (2xv)\ e^{-x^2} + 2\int_{-v}^{0} dx\ (x^2+2xv+v^2)\ e^{-x^2}\ \right] \\
&= \frac{\sigma_0\, 4\, v}{v^2\sqrt{\pi}}\int_0^{\infty} x\, dx\ e^{-x^2} + \frac{2\,\sigma_0}{v^2\sqrt{\pi}}\int_{-v}^{0} x^2\, dx\ e^{-x^2} \\
&\qquad + \frac{4\, v\, \sigma_0}{v^2\sqrt{\pi}}\int_{-v}^{0} x\, dx\ e^{-x^2} + \frac{2\,\sigma_0\, v^2}{v^2\sqrt{\pi}}\int_{-v}^{0} dx\ e^{-x^2} \qquad\qquad \textbf{(136)} \\
&= \frac{\sigma_0\, 4}{v\sqrt{\pi}}\ \frac{1}{2} + \frac{2\,\sigma_0}{v^2\sqrt{\pi}}\left(-\frac{v}{2}\, e^{-v^2} + \frac{\sqrt{\pi}}{4}\Big[\mathrm{erfc}(0) - \mathrm{erfc}(v)\Big]\right) \\
&\qquad + \frac{4\,\sigma_0}{v\sqrt{\pi}}\left(-\frac{1}{2}\Big[1 - e^{-v^2}\Big]\right) + \frac{2\,\sigma_0}{\sqrt{\pi}}\Big[\mathrm{erfc}(0) - \mathrm{erfc}(v)\Big] \\
&= \frac{\sigma_0}{v\sqrt{\pi}}\ e^{-v^2} + \sigma_0\left(\frac{1}{2\, v^2} + 1\right)\Big(\ 1 - \mathrm{erfc}(v)\Big)
\end{aligned}
$$

in which we have replaced *V/U* by *v*.

In the limit of small *v*, the quantity in Eq. (xx-6) becomes

$$
\bar{\sigma}(V^2) \to \sigma_0\left[\ \frac{1}{\sqrt{\pi}\, v} + \frac{1}{2\, v^2}\, \frac{2}{\sqrt{\pi}}\,(v+v^3)\right] \to \frac{\sigma_0}{\sqrt{\pi}\, v}\quad , \qquad \textbf{(137)}
$$

so that the leading term is $1/v$; this is somewhat counterintuitive but is nevertheless observed in measured low-energy cross sections. For large values of *v*, the limiting case is

$$
\bar{\sigma}(V^2) \to \sigma_0\Big[\ 0 + 1\times 1\ \Big] \to \sigma_0\quad ; \qquad \textbf{(138)}
$$

i.e., the broadened cross section is a constant, as expected.

In contrast, HEGA broadening preserves a constant cross section everywhere:

$$\bar{\sigma}_{HEGA}(E) = \frac{\sigma_0}{\sqrt{\pi}\,\Delta}\int_{-\infty}^{\infty} dE'\; e^{-(E-E')^2/\Delta^2} = \sigma_0 \quad ; \tag{139}$$

that is, the Gaussian kernel is normalized to unity, as expected. This result, which may intuitively appear to be correct, is nevertheless unphysical. As discussed above, It is well known that measured (and therefore Doppler-broadened) cross sections exhibit 1/*v* behavior at very low energies.

Doppler Broadening of the Line Shapes ψ and χ

Equations (xx-57) and (xx-58) can be written as

$$\psi(x) = \frac{1}{1+x^2} \;, \tag{140}$$

and

$$\chi = \frac{x}{1+x^2} \;, \tag{141}$$

where $x = \dfrac{2(E_\lambda - E)}{\Gamma_\lambda}$.

The HEGA of these functions are obtained by replacing $\sigma(E)$ in Eq. (xx-128) by ψ and χ, which gives

$$\psi(x,\theta) = \frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{+\infty} dy\; \frac{\exp[-\frac{1}{4}\theta^2(x-y)^2]}{1+y^2} \;, \tag{142}$$

and

$$\chi(x,\theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} dy\ 2y\ \frac{\exp[-\frac{1}{4}\theta^2 (x-y)^2]}{1+y^2} \quad , \tag{143}$$

where $\theta = \frac{\Gamma}{\Delta}$.

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