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Introduction to R-matrix Theory

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Disclaimer

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Contents

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1 Calculable R-matrix methods

1.1 The Problem

We want to describe the cross sections for particles scattering on nuclei, including any known resonances. With that description, we could then predict scattering at any energy, at any outgoing angle, in any of the described channels.

The R-matrix method is the best method we know to describe resonances, even the very many compound-nucleus resonances.

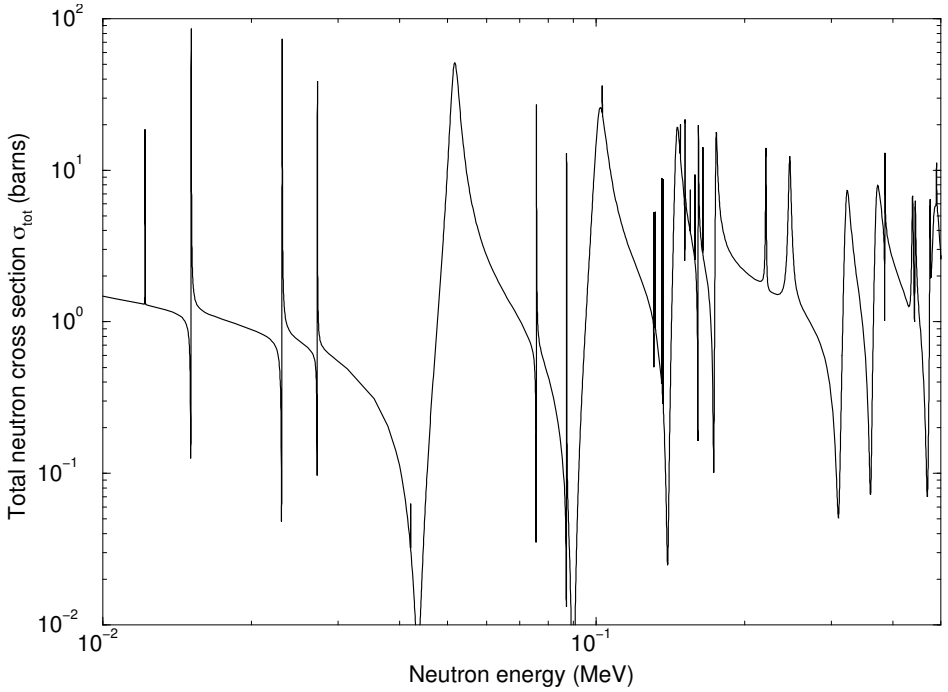

Figure 1: Numerous compound-nucleus resonances can be seen in this plot of the total cross section $\sigma_{\rm tot}(E)$ for neutrons incident on ^{44}Ca. At all energies, individual resonances can be distinguished. Note that ^{44}Ca is near a closed shell: most heavier nuclei have resonances too numerous to be seen on a plot with this scale.

We begin by describing how to solve the one-channel Schrödinger equation with a new kind of expansion, and then introduce the R-matrix method.

1.2 One-channel case

For each partial wave L, we need to numerically solve the one-channel radial Schrödinger equation

$$[\hat{T} + V(R) - E]\chi(R) = 0, \tag{1}$$

where the kinetic operator $\hat{T}$ is

$$\hat{T} = -\frac{\hbar^2}{2\mu}\left(\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \frac{L(L+1)}{R^2}\right) \ . \tag{2}$$

We have scattering boundary conditions

$$\begin{aligned} \chi(0) &= 0 \\ \chi(a) &= \tfrac{\mathrm{i}}{2}\left[H_L^-(\eta, ka) - \mathbf{S}_L H_L^+(\eta, ka)\right] \\ \chi'(a) &= \tfrac{\mathrm{i}}{2}\left[H_L^{-\prime}(\eta, ka) - \mathbf{S}_L H_L^{+\prime}(\eta, ka)\right] \end{aligned} \tag{3}$$

for matching radius a. The derivatives H' are with respect to R, and the $H_L^{+\prime}(\eta, ka)$ are the Coulomb wave functions. The μ is the reduced mass, E is the center-of-mass energy, k is the wave number $k^2 = 2\mu E/\hbar^2$, and η is the Sommerfeld Coulomb parameter $\eta = Z_1 Z_2 e^2 \mu/(\hbar k)$ for colliding particles with charges Z_1 and Z_2.

This equation (1) has a solution for all scattering energies E, giving the wave function $\chi(R)$ and the S-matrix element $\mathbf{S}_L$. The last two boundary conditions above may be combined, and solved to give $\mathbf{S}_L$ in terms of the ratio we call the R-matrix (see Appendix A),

$$\mathbf{R}_L = \frac{\chi(a)}{a\chi'(a)} \ , \tag{4}$$

a dimensionless inverse logarithmic derivative. We end up with

$$\mathbf{S}_L = \frac{H_L^- - a\mathbf{R}_L H_L'^-}{H_L^+ - a\mathbf{R}_L H_L'^+}. \tag{5}$$

The scattering cross sections are determined by the S-matrix element, a complex number. In this one-channel case, the scattering phase shifts satisfy $\mathbf{S}_L = \exp(2\mathrm{i}\delta_L)$.

The cross section $\sigma(\theta) = |f(\theta)|^2$ where the scattering amplitude is

$$f(\theta) = \frac{1}{2\mathrm{i}k}\sum_{L=0}^{\infty}(2L+1)P_L(\cos\theta)(\mathbf{S}_L - 1). \tag{6}$$

1.2.1 R-matrix expansions

The R-matrix method was proposed by Wigner and Eisenbud [1] and promulgated in detail by Lane and Thomas [2]. It uses an orthonormal basis expansion in the interior of some 'R-matrix radius' a, employing eigenfunctions of the diagonal parts of the Hamiltonian as basis states. With the diagonalized interior wave functions it constructs the R matrix to join on to the asymptotic Coulomb functions.

The plan to construct the scattering solution $\chi(R)$ of Eq. (1) at general energy E as the linear combination of N states $w_n(R)$

$$\chi(R) = \sum_{n=1}^{N} A_n w_n(R) \ , \tag{7}$$

where the basis states satisfy $w(0) = 0$, and are solutions of

$$\left[\hat{T} + V(R)\right] w_n(R) = \varepsilon_n \ w_n(R) \tag{8}$$

for some eigen-energies ε_n, $n = 1, 2, \ldots,$. We assume that the $V(R)$ is real.

Ideally, the states $\{w_n\}$ would an orthonormal set on $[0, a]$:

$$\int_0^a w_n(R) w_m(R) \mathrm{d}R = \delta_{mn}, \tag{9}$$

so we may easily make the coefficients $A_n = \int_0^a w_n(R)\chi(R)dR$ to satisfy the scattering boundary conditions of Eq. (3). We expect to progressive convergence as the basis size N increases.

However, it is not that simple. First: the equation Eq. (8) has a scattering solution at *any* energy ε_n, not for discrete n. Secondly, those scattering solutions are *not* orthonormal!

To see why, suppose $w_n(R)$ and $w_m(R)$ are two solutions of Eq. (8) with eigenenergies $\varepsilon_n \neq \varepsilon_m$. If we multiply the w_n equation by w_m, and subtract from the exchanged equation, we obtain

$$-\frac{\hbar^2}{2\mu}[w_m w_n'' - w_n w_m''] + (\varepsilon_m - \varepsilon_n) w_n w_m = 0. \tag{10}$$

Integrating this equation by parts[1] with limits $R = 0$ to a gives

$$-\frac{\hbar^2}{2\mu}[w_m(a)w_n'(a) - w_n(a)w_m'(a)] + (\varepsilon_m - \varepsilon_n) \int_0^a w_n w_m \mathrm{d}R = 0. \tag{11}$$

[1] Or use $\frac{d}{dR}(w_m w_n' - w_n w_m') = w_m' w_n' + w_m w_n'' - w_n' w_m' - w_n w_m'' = w_m w_n'' - w_n w_m''$.

Distinct eigenstates ($\varepsilon_n \neq \varepsilon_m$) are only orthonormal ($\int_0^a w_n w_m \mathrm{d}R = 0$), if the first term $w_m(a)w'_n(a) - w_n(a)w'_m(a)$ is zero! And that term is not zero for ordinary scattering states like $\sin(kR)$.

That is, scattering wave functions over a *finite* range $[0, a]$ are not orthogonal to each other, and they cannot be used as orthonormal basis states for an eigenvalue expansion.

The trick of the R-matrix method is to arbitrarily set some fixed energy-independent and real logarithmic derivative at the R-matrix radius a for all the basis states:

$$\frac{\mathrm{d}}{\mathrm{d}R} \ln w(R)\Big|_{R=a} \equiv \frac{w'(a)}{w(a)} = \beta. \tag{12}$$

In that case at $R = a$, for a fixed β for all eigenstates n,

$$w_m w'_n - w_n w'_m \equiv w_m w_n \left[\frac{w'_n}{w_n} - \frac{w'_m}{w_m}\right] = 0. \tag{13}$$

If we substitute this result in Eq. (11), we see that the R-matrix basis states satisfying Eq. (12) *are* orthogonal for $\varepsilon_n \neq \varepsilon_m$. We scale the w_n basis states to make them all normalized to unity, and then they *do* form a discrete orthonormal set on the finite interval $[0, a]$.

At present β and a are both free input parameters, and the same results should be obtained on convergence for any value of β, and for any matching radius outside the potentials. A dimensionless *boundary condition number* $B = \beta a$ may be defined equivalently to β.

Expansion of the scattering wave function

Unfortunately we can not simply match the wave functions and derivatives of each side of Eq. (7), as might be expected from elementary quantum theory. If we did do this, then, since all the $w_n(R)$ have the same logarithmic derivative β, so will their sum on the right side of the equation. A scattering wave function $\chi(R)$ certainly does not have a fixed logarithmic derivative! This discrepancy comes about from the manner of convergence of the sum (7) as a function of N. The convergence is only with respect to the values of the wave functions, and *not* their derivatives. Exactly how this convergence proceeds will be illustrated in Fig. 2 below. The lack of convergence of derivatives means that we must instead use an integral expression to find the expansion coefficients.

If we repeat the integration by parts with now the pair of solutions $w_n(R)$ and $\chi(R)$, then in place of Eq. (11) we have

$$-\frac{\hbar^2}{2\mu}\left[\chi(a)w_n'(a)-w_n(a)\chi'(a)\right]+(E-\varepsilon_n)A_n=0, \tag{14}$$

which gives

$$\begin{aligned} A_n &= \frac{\hbar^2}{2\mu}\frac{1}{E-\varepsilon_n}[\chi(a)w_n'(a)-w_n(a)\chi'(a)] \\ &= \frac{\hbar^2}{2\mu}\frac{w_n(a)}{\varepsilon_n-E}[\chi'(a)-\beta\chi(a)]. \end{aligned} \tag{15}$$

If we use these expressions in Eq. (7) evaluated at $R=a$, we obtain useful information about the logarithmic derivative of the unknown solution $\chi(R)$. We get

$$\chi(a)=\sum_{n=1}^{N}\frac{\hbar^2}{2\mu}\frac{w_n(a)}{\varepsilon_n-E}[\chi'(a)-\beta\chi(a)]w_n(a), \tag{16}$$

so

$$\frac{\chi(a)}{\chi'(a)-\beta\chi(a)}=\sum_{n=1}^{N}\frac{\hbar^2}{2\mu}\frac{w_n(a)^2}{\varepsilon_n-E}. \tag{17}$$

If β were zero here, the left side would be just $\chi(a)/\chi'(a)$, which is exactly the R matrix defined in Eq. (4). Because we now want freedom to choose β for other reasons, we now define a slightly different R matrix (from Eq. (110)) for a wave function as

$$\mathsf{R}=\frac{1}{a}\frac{\chi(R)}{\chi'(R)-\beta\chi(R)}, \tag{18}$$

in which case the S matrix is now

$$\mathsf{S}=\frac{H^- - a\mathsf{R}(H'^- - \beta H^-)}{H^+ - a\mathsf{R}(H'^+ - \beta H^+)}. \tag{19}$$

This is the equation, therefore, into which we substitute the R-matrix

$$\mathsf{R}=\sum_{n=1}^{N}\frac{\hbar^2}{2\mu a}\frac{w_n(a)^2}{\varepsilon_n-E}. \tag{20}$$

We now define for each pole n the *reduced width amplitudes*

$$\gamma_n = \sqrt{\frac{\hbar^2}{2\mu a}}\, w_n(a), \tag{21}$$

in terms of which the R matrix has the familiar simple form

$$\mathbf{R} = \sum_{n=1}^{N} \frac{\gamma_n^2}{\varepsilon_n - E}. \tag{22}$$

The γ_n^2 are called the *reduced widths*.

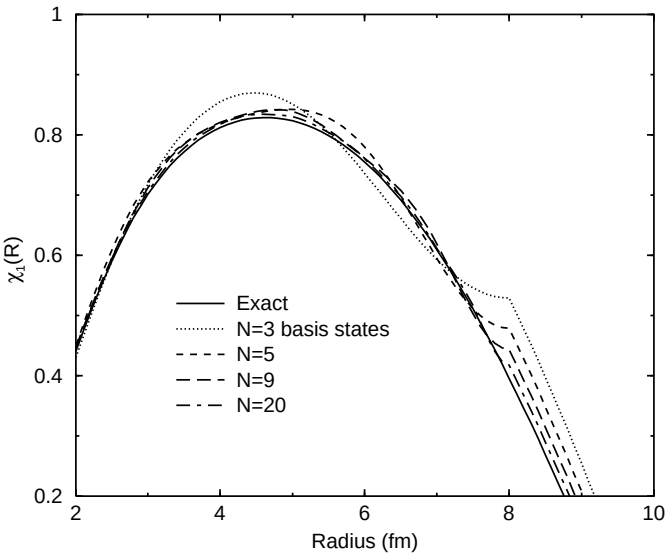

Figure 2: Convergence of the one-channel scattering wave function with varying numbers of basis states, for $a = 8$ fm and $\beta = 0$. We plot the real part of $p_{1/2}$ neutron scattering wave function on ^{4}He at 5 MeV.

The scattering wave function in the same approximation is, using Eq. (3),

$$\chi(R) = \sum_{n=1}^{N} \frac{\hbar^2}{2\mu a} \frac{w_n(a)}{\varepsilon_n - E} [\chi'(a) - \beta\chi(a)] w_n(R). \tag{23}$$

The convergence with N of this wave function is illustrated in Fig. 2. We see that even though the function of (23) has $\beta = 0$ derivative at the matching radius, it still converges closer and closer to the correct wave function with non-zero derivative.

1.2.2 Interpretation for s-wave neutrons

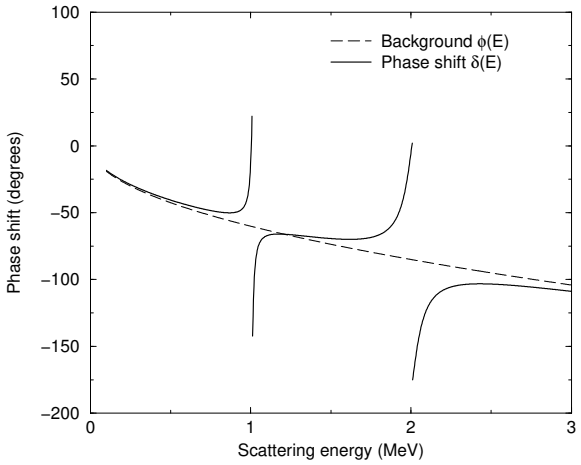

Figure 3: Background phase shifts ϕ (dashed line) and phase shifts δ for 2 R-matrix poles (solid line).

Let us consider the simple case of neutrons scattering on a target in the $L = 0$ partial wave (s-waves). Neutrons have no charge, so the Coulomb functions are simply $H_L^{\pm}(0, ka) = \cos(ka) \pm \mathrm{i}\sin(ka) = \mathrm{e}^{\pm \mathrm{i}ka}$. Let us choose $B = 0 = \beta$, so Eq. (24) becomes

$$\mathbf{S} = \frac{H^- - a\mathbf{R}H'^-}{H^+ - a\mathbf{R}H'^+} = \frac{\mathrm{e}^{-\mathrm{i}ka} + aik\mathbf{R}\ \mathrm{e}^{-\mathrm{i}ka}}{\mathrm{e}^{\mathrm{i}ka} - aik\mathbf{R}\ \mathrm{e}^{\mathrm{i}ka}} = \mathrm{e}^{-2\mathrm{i}ka}\frac{1 + aik\mathbf{R}}{1 - aik\mathbf{R}}\ . \tag{24}$$

If we define phase shifts ϕ and δ_R by $\phi = -ka$ and $\tan\delta_R = ka\mathbf{R}$ respectively, then $\mathbf{S} \equiv \exp(2\mathrm{i}\delta) = \mathrm{e}^{2\mathrm{i}\phi}\mathrm{e}^{-2\mathrm{i}\delta_R}$, so

$$\delta \quad = \phi + \delta_R \tag{25}$$

If there are no R-matrix terms ($\mathbf{R} = 0$) then we have phase shift just ϕ just as a background like the dashed line in Figure 3.

Let us try a simple case of two poles, at $\varepsilon = 1$ and 2 MeV, with reduced width amplitudes $\gamma = 0.1$ and 0.2 respectively. This results in the phase shifts of the solid lines in the figure. We see rapid increases of phase just around the R-matrix poles, so *each pole describes a resonance in the scattering*. From $\tan\delta_R = ka\gamma^2/(\varepsilon - E)$, using a later Eq. (65) for the width of the resonances we find widths $\Gamma = 2\gamma^2 ka$. That is why we connect the γ values with the widths of those resonances.

1.3 Multi-channel R-matrix

Coupled equations, with radial coordinates R_α, are of the form

$$[E_\alpha - H_\alpha]\,\psi_\alpha(R_\alpha) = \sum_{\beta(\neq\alpha)}^{M} \langle\phi_\alpha|H-E|\phi_\beta\rangle\,\psi_\beta(R_\beta). \tag{26}$$

The method for multi-channel problems uses as basis states the eigenfunctions of the real part of the diagonal potential in each partial-wave channel $\alpha = 1..M$. If the boundary condition of Eq. (12) is used, these form an orthonormal basis set. In that way, diagonal real potentials within the coupled-channels set are treated more accurately, while off-diagonal and all imaginary potentials are treated via their matrix elements in this basis.

The basis functions are now written as $w_\alpha^n(R_\alpha)$ for the n'th basis state in channel α. It is most convenient to take them as all the eigensolutions of the diagonal real potential U_α in each separate channel:

$$\Big[T_{\alpha L}(R_\alpha) + U_\alpha(R_\alpha) - \varepsilon_{n\alpha}\Big] w_\alpha^n(R_\alpha) = 0 \tag{27}$$

for eigenenergies $\varepsilon_{n\alpha}$, with the basis functions again all having fixed logarithmic derivatives $\beta = \mathrm{d}\ln w_\alpha^n(R_\alpha)/\mathrm{d}R_\alpha$ at a.

The wave functions of the coupled problem (26) can now be solved completely over the interior range $[0,a]$, by using the orthonormal basis set of the $\{w_\alpha^n(R_\alpha)\}$ with coefficients to be determined. The coefficients are found in two stages: first by finding all the eigensolutions $g_\alpha^p(R_\alpha)$ of the equations (26) using the above orthonormal basis, and then expanding the scattering wave functions in terms of these $g_\alpha^p(R_\alpha)$.

In the traditional R-matrix method, the diagonalization of the M-channel Hamiltonian in equation (26) proceeds by finding the radial wave eigenfunctions $g_\alpha(R_\alpha)$ in that basis. This is to solve

$$[T_{\alpha L} + U_\alpha + \epsilon_\alpha]\,g_\alpha(R_\alpha) + \sum_{\alpha'\neq\alpha} \hat{V}_{\alpha\alpha'}\; g_{\alpha'}(R_{\alpha'}) = e\; g_\alpha(R_\alpha), \tag{28}$$

where $\hat{V}_{\alpha\alpha'}$ refers to all the *off*-diagonal couplings, local or non-local, since the diagonal real potentials U_α already appear, and the energies ϵ_α are the core excitation energies in each channel. This yields $P = NM$ eigenenergies e_p with corresponding multi-channel eigenstates

$$g_\alpha^p(R_\alpha) = \sum_{n=1}^{N} c_\alpha^{pn} w_\alpha^n(R_\alpha). \tag{29}$$

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 $g^p_\alpha(R_\alpha)$ form another orthonormal basis in the interior region if the Hamiltonian is Hermitian.

The coefficients c^{pn}_α and energies e_p in Eq. (29) satisfy matrix equations

$$(\varepsilon_{n\alpha} + \epsilon_\alpha)c^{pn}_\alpha + \sum_{n'\alpha'} \langle w^n_\alpha \mid \hat{V}_{\alpha\alpha'} \mid w^{n'}_{\alpha'} \rangle c^{pn'}_{\alpha'} = e_p c^{pn}_\alpha \tag{30}$$

for each eigenstate p. These are eigenvalue equations of the matrix form

$$\mathbf{Hc} = e\mathbf{c}. \tag{31}$$

Because our coupled equations may have different reduced masses in different transfer channels, we now define a third form of the R matrix by

$$t^{1/2}_\alpha \psi_\alpha(R_\alpha) = a \sum_{\alpha'} \mathsf{R}_{\alpha\alpha'}(E) \Big[\psi'_{\alpha'}(R_\alpha) - \beta \psi_{\alpha'}(R_\alpha) \Big] t^{1/2}_{\alpha'}. \tag{32}$$

Here the factors $t_\alpha \equiv \hbar^2/2\mu_\alpha$ are placed to render the R matrix symmetric even for transfer channels. The progressively more generalized R-matrix definitions are summarized in Table A.

For scattering states at arbitrary energy E, the coupled solutions are then expanded in terms of the multi-channel eigenstates as $\psi_{\alpha\alpha_i} = \sum_p A^p_{\alpha\alpha_i} g^p_\alpha$. The R matrix for this wave function, using Eq. (32), can be calculated [2, 3] from the $g^p_\alpha(a)$ eigenfunctions by the standard methods, which are similar to that given in detail for the one-channel case leading to Eq. (17). We find

$$\mathsf{R}_{\alpha\alpha'}(E) = \sqrt{\frac{t_\alpha}{a}} \sum_{p=1}^{P} \frac{g^p_\alpha(a) g^p_{\alpha'}(a)}{e_p - E} \sqrt{\frac{t_{\alpha'}}{a}}. \tag{33}$$

The *reduced width amplitudes* for each channel α and pole p,

$$\gamma_{p\alpha} = \sqrt{\frac{t_\alpha}{a}}\ g^p_\alpha(a) = \sqrt{\frac{\hbar^2}{2\mu_\alpha a}}\ g^p_\alpha(a), \tag{34}$$

in terms of which the R matrix has the familiar form

$$\mathsf{R}_{\alpha\alpha'}(E) = \sum_{p=1}^{P} \frac{\gamma_{p\alpha}\gamma_{p\alpha'}}{e_p - E}. \tag{35}$$

Scattering S matrix and wave functions

For incoming partial waves α_i, the multi-channel boundary conditions for $R_x > R_n$ are

$$\psi^{J_{\rm tot}\pi}_{\alpha\alpha_i}(R_x) = \frac{\rm i}{2}\left[H^-_{L_i}(\eta_\alpha, k_\alpha R_x)\ \delta_{\alpha\alpha_i} - H^+_L(\eta_\alpha, k_\alpha R_x)\ \mathsf{S}^{J_{\rm tot}\pi}_{\alpha\alpha_i}\right]. \qquad (36)$$

Using this equation with Eq. (32), and writing the Coulomb functions $\mathsf{H}^\pm$ as diagonal matrices, the scattering S matrix is given in terms of R by

$$\mathsf{S} = [\mathsf{t}^{\frac{1}{2}}\mathsf{H}^+ - a\mathsf{R}\ \mathsf{t}^{\frac{1}{2}}(\mathsf{H}^{+\prime} - \beta\mathsf{H}^+)]^{-1}[\mathsf{t}^{\frac{1}{2}}\mathsf{H}^- - a\mathsf{R}\ \mathsf{t}^{\frac{1}{2}}(\mathsf{H}^{-\prime} - \beta\mathsf{H}^-)]. \qquad (37)$$

The scattering states at the arbitrary energy E and incoming wave in channel α_i are linear combinations of the multi-channel eigenstates of Eq. (29):

$$\psi_{\alpha\alpha_i}(R_\alpha) = \sum_p A^p_{\alpha_i}\ g^p_\alpha(R_\alpha), \qquad (38)$$

with expansion coefficients for each eigenstate p and incoming channel α_i of

$$A^p_{\alpha_i} = \frac{\hbar^2}{2\mu_{\alpha_i}}\frac{1}{e_p - E}\sum_{\alpha'} g^p_{\alpha'}(a)\Big[\delta_{\alpha'\alpha_i}(H^{-\prime}_L(k_{\alpha'}a) - \beta H^-_L(k_{\alpha'}a)) - \mathsf{S}_{\alpha'\alpha_i}(H^{+\prime}_L(k_{\alpha'}a) - \beta H^+_L(k_{\alpha'}a))\Big]. \qquad (39)$$

2 R-matrix phenomenology

In the previous section, we saw how the R-matrix could be constructed from a Hamiltonian and its potentials, using the wave functions of eigenstates in the interior region $R \le a$, the R-matrix radius. For scattering, the only properties of the eigenstates used are their energies, and the values of their wave functions at the R-matrix radius. The energies are the R-matrix *pole energies* e_p, and the surface values of the wave functions $g_\alpha^p(R)$ give the *reduced width amplitudes* $\gamma_{p\alpha} = \sqrt{t_\alpha/a}\; g_\alpha^p(a)$ where $t_\alpha = \hbar^2/2\mu_\alpha$. The R matrix is then easily constructed at any desired scattering energy E by Eq. (35):

$$\mathsf{R}_{\alpha'\alpha}(E) = \sum_{p=1}^{P} \frac{\gamma_{p\alpha}\gamma_{p\alpha'}}{e_p - E}. \tag{40}$$

From this R matrix, the scattering S matrix can be found by Eq. (37):

$$\begin{aligned}
\mathsf{S} &= \frac{\mathsf{t}^{\frac{1}{2}}\mathsf{H}^- - a\mathsf{R}\mathsf{t}^{\frac{1}{2}}(\mathsf{H}^{-\prime} - \beta\mathsf{H}^-)}{\mathsf{t}^{\frac{1}{2}}\mathsf{H}^+ - a\mathsf{R}\mathsf{t}^{\frac{1}{2}}(\mathsf{H}^{+\prime} - \beta\mathsf{H}^+)} && \text{most generally,} && (41a)\\
&= \frac{\mathsf{H}^- - a\mathsf{R}(\mathsf{H}^{-\prime} - \beta\mathsf{H}^-)}{\mathsf{H}^+ - a\mathsf{R}(\mathsf{H}^{+\prime} - \beta\mathsf{H}^+)} && \text{if } \mathsf{t}_\alpha \text{ are all equal,} && (41b)\\
&= \frac{\mathsf{H}^- - a\mathsf{R}\mathsf{H}^{-\prime}}{\mathsf{H}^+ - a\mathsf{R}\mathsf{H}^{+\prime}} && \text{when also } \beta = 0, && (41c)
\end{aligned}$$

and hence all the channel cross sections.

This suggests that, if our aim is not so much to start with a Hamiltonian, but to fit a set of reaction measurements over a range of channels, energies and angles, then all we need to do is to find the reduced width amplitudes $\gamma_{p\alpha}$ and the corresponding pole energies e_p. These parameters are sufficient to describe all asymptotic properties of the scattering wave functions, and hence all cross sections that may be measured. After fitting these parameters, it is comparatively easy to interpolate or extrapolate as desired in energies and angles. This fitting programme is called *R-matrix phenomenology* [2, 4, 5].

The *methods* of fitting data to find reduced widths and pole positions will be described elsewhere. For now, we presume that this fitting has been done, and in the present chapter discuss the interpretation of the results.

To facilitate the understanding of an R-matrix fit, it is useful to modify the derivation in Eq. (41) of the S matrix so that approximations may be

made to give simpler formulae that can be more easily understood. These reformulations will refer in particular to widths, either reduced, partial or total, as well as to shift functions and penetrabilities. We will clarify the connection between R matrix poles and resonances (which are S-matrix poles). To begin with, we examine the one-channel R-matrix theory in more detail, beginning with a simpler derivation of elastic phase shifts δ. Later we will derive a level matrix formulation more suitable for multi-channel modeling.

2.1 Single-channel R matrix

2.1.1 Phase shifts from the one-channel R matrix

In the one-channel case, all the reduced masses in the t_α in Eq. (41) are equal, and matrices are only 1×1, so we find the S-matrix element according to Eq. (24):

$$\begin{aligned} \mathsf{S} &= \frac{H^- - a\mathbf{R}(H^{-\prime} - \beta H^-)}{H^+ - a\mathbf{R}(H^{+\prime} - \beta H^+)} \\ &= \frac{1 - a\mathbf{R}(H^{-\prime}/H^- - \beta)}{1 - a\mathbf{R}(H^{+\prime}/H^+ - \beta)} \, \frac{H^-}{H^+}. \end{aligned} \tag{42}$$

At a given scattering energy E, using the Wronskian $\dot{F}G - \dot{G}F = 1$,

$$\frac{H^{+\prime}}{H^+} = \frac{G' + \mathrm{i}F'}{G + \mathrm{i}F} = k\frac{\dot{G} + \mathrm{i}\dot{F}}{G + \mathrm{i}F} = k\frac{\dot{F}F + \dot{G}G}{F^2 + G^2} + \mathrm{i}k\frac{1}{F^2 + G^2}. \tag{43}$$

The derivatives $\dot{F}(\rho)$ are with respect to $\rho = kR$. Thus we can write

$$a\frac{H^{+\prime}}{H^+} = S + \mathrm{i}P \quad \text{and} \quad a\frac{H^{-\prime}}{H^-} = S - \mathrm{i}P, \tag{44}$$

by defining a *shift function*

$$S(E) = ka\frac{\dot{F}F + \dot{G}G}{F^2 + G^2} \tag{45}$$

and a *penetrability*

$$P(E) = \frac{ka}{F^2 + G^2}, \tag{46}$$

where the Coulomb functions F and G are all evaluated for argument $\rho = ka$. The wave number k and Sommerfeld parameter η have their usual relation to the c.m. scattering energy E.

The final factor in Eq. (42) can be rewritten

$$\frac{H^-}{H^+} = \frac{G - \mathrm{i}F}{G + \mathrm{i}F} = \mathrm{e}^{2\mathrm{i}\phi}, \tag{47}$$

$$\text{where} \quad \phi = -\arctan\frac{F}{G} \tag{48}$$

is called the *hard-sphere phase shift* since this would be the scattering phase shift if the wave function were forced to go to zero at $R = a$.

In terms of the shift function S, penetrability P and hard-sphere phase shift ϕ, the $\mathbf{S}$ matrix is

$$\mathbf{S} = \frac{1 - \mathbf{R}(S - \mathrm{i}P - a\beta)}{1 - \mathbf{R}(S + \mathrm{i}P - a\beta)}\,\mathrm{e}^{2\mathrm{i}\phi} \tag{49}$$

$$= \frac{1 - \mathbf{R}(S - a\beta) + \mathrm{i}\mathbf{R}P}{1 - \mathbf{R}(S - a\beta) - \mathrm{i}\mathbf{R}P}\,\mathrm{e}^{2\mathrm{i}\phi} \tag{50}$$

From $\mathbf{S} = \mathrm{e}^{2\mathrm{i}\delta}$, we see the scattering phase shift is $\delta = \phi + \delta_R$, where the *R-matrix phase* δ_R is

$$\delta_R = \arctan\frac{\mathbf{R}P}{1 - \mathbf{R}(S - a\beta)}. \tag{51}$$

For single-channel scattering, this is a practical formula to calculate the phase shifts. Often we will abbreviate $S^0 \equiv S - a\beta \equiv S - B$, but not forget that S, S^0 and P are all functions of the scattering energy E.

In some special cases:

- For bound states at negative energies E, the penetrability is zero, but the shift function can still be defined as the logarithmic derivative of the Whittaker function.
- For neutrons and photons and $ka \ll L$, the penetrability may be found using the low-ρ limit of the G function, namely $P \propto k^{2L+1}$. For s-wave neutrons, this simplifies to $P_{L=0} = ka$, with the shift function $S_0 = 0$, and the hard-sphere phase shift is $\phi_0 = -\arctan ka$ in this partial wave.
- For charged particles with $ka \ll L$, the penetrability is dominated by the large value of the irregular function G for small ka. We find $P_L \approx (2L+1)^2 (ka)^{2L+1} C_L(\eta)^2$. For s-wave scattering, this simplifies to $P_0 = 2\pi\eta ka/(\exp(2\pi\eta) - 1) \approx 2\pi\eta ka \exp(-2\pi\eta)$ (noting that ηk is energy independent).

2.1.2 Interpretation for isolated poles

The simplest R-matrix fit is for a single pole in a one-channel problem. Suppose that we have found a reduced width amplitude γ and a pole energy e_p such that

$$\mathbf{R} = \gamma^2/(e_p - E) \tag{52}$$

gives a suitable fit to some small range of experimental data. Can we tell if there is a resonance or a bound state? What would be the width of the resonance? Why is γ^2 called the reduced width?

From Eq. (49), the S matrix is now

$$\begin{aligned} \mathbf{S} &= \frac{1-\gamma^2(S^0 - \mathrm{i}P)/(e_p - E)}{1-\gamma^2(S^0 + \mathrm{i}P)/(e_p - E)}\ \mathrm{e}^{2\mathrm{i}\phi} \\ &= \left[1 - \frac{2\mathrm{i}\gamma^2 P}{E - (e_p - \gamma^2 S^0 - \mathrm{i}\gamma^2 P)}\right]\ \mathrm{e}^{2\mathrm{i}\phi} \qquad (53) \\ &= \frac{E - [e_p - \gamma^2 S^0 + \mathrm{i}\gamma^2 P]}{E - [e_p - \gamma^2 S^0 - \mathrm{i}\gamma^2 P]}\ \mathrm{e}^{2\mathrm{i}\phi} \qquad (54) \end{aligned}$$

which, at first glance, appears to be a resonance of Breit-Wigner form

$$\mathbf{S}(E) = \mathrm{e}^{2\mathrm{i}\delta_{\mathrm{bg}}(E)}\frac{E - E_r - \mathrm{i}\Gamma/2}{E - E_r + \mathrm{i}\Gamma/2} \tag{55}$$

for a pole at $E = E_r - \mathrm{i}\Gamma/2$ having parameters

$$\begin{aligned} E_r^f &= e_p - \gamma^2 S^0 = e_p - \gamma^2(S - a\beta) \\ \Gamma^f &= 2\gamma^2 P. \end{aligned} \tag{56}$$

These values are called the *formal* resonance position and width, hence the superscripts f. We can see why γ^2 is called the 'reduced width', since it is the result of removing (twice) the penetrability factor from Γ. We can see why $S(E)$ is called a 'shift function', as it contributes to the shift from the R-matrix pole at e_p towards the S-matrix pole at E_r^f.

As $S^0 = S - a\beta$, we will see below that it might be useful to choose $\beta = S(E)/a$ (i.e. $S = B$) in advance in order to fix that $S^0(E) = 0$ for some predetermined energy E of interest. This is called the *natural boundary condition* for β. The R-matrix theory works for *any* set of β values for each channel, as long as they are independent of energy.

These 'formal' values would be exact if the shifts S and penetrabilities P were constants independent of energy, but they are not, so the true position is more complicated. The *true* resonance position is taken as the complex energy where the S matrix has a pole. That is, we should solve for complex energy E the equation

$$\begin{aligned} E &= e_p - \gamma^2 S^0(E) - \mathrm{i}\gamma^2 P(E) \\ \text{or} \quad E_r - \mathrm{i}\tfrac{\Gamma}{2} &= e_p - \gamma^2 S^0(E_r - \mathrm{i}\Gamma/2) - \mathrm{i}\gamma^2 P(E_r - \mathrm{i}\tfrac{\Gamma}{2}). \end{aligned} \tag{57}$$

If we are unwilling to directly evaluate these right-hand sides for complex E, we may use Taylor series to extrapolate off the real axis as $S^0(E_r - \mathrm{i}\Gamma/2) = S^0(E_r) - \mathrm{i}S'(E_r)\Gamma/2$, etc. The *Thomas approximation* [6] assumes that the shift function is locally linear, and this appears to be generally quite accurate. That is, we solve instead the linearized form

$$E_r - \mathrm{i}\tfrac{\Gamma}{2} = e_p - \gamma^2[S^0(E_r) - \mathrm{i}S'(E_r)\tfrac{\Gamma}{2}] - \mathrm{i}\gamma^2[P(E_r) - \mathrm{i}P'(E_r)\tfrac{\Gamma}{2}]. \tag{58}$$

Equating the real and imaginary parts gives

$$E_r = e_p - \gamma^2 S^0(E_r) - \tfrac{1}{2}\gamma^2\Gamma P'(E_r) \tag{59}$$

$$\text{and} \quad -\Gamma = \gamma^2\Gamma S'(E_r) - 2\gamma^2 P(E_r),$$

$$\text{so} \quad \Gamma = \frac{2\gamma^2 P(E_r)}{1 + \gamma^2 S'(E_r)} \tag{60}$$

$$\text{and} \quad E_r = e_p - \gamma^2 S^0(E_r) - \frac{\gamma^4 P(E_r) P'(E_r)}{1 + \gamma^2 S'(E_r)}. \tag{61}$$

Usually the third term in the E_r expression is neglected, along with all higher-order terms, and the solutions are now called the *observed* resonance energy and width. These satisfy

$$E_r^{\mathrm{obs}} = e_p - \gamma^2 S^0(E_r^{\mathrm{obs}}) \tag{62}$$

$$\Gamma^{\mathrm{obs}} = \frac{2\gamma^2 P(E_r^{\mathrm{obs}})}{1 + \gamma^2 S'(E_r^{\mathrm{obs}})}. \tag{63}$$

A further simplification, still in the spirit of the Thomas approximation, is to evaluate $S^0(E)$ not at E_r^{obs} but at the R-matrix pole energy e_p. The Eq. (62) becomes now an explicit rather than an implicit equation for E_r^{obs}. Because the penetrability is extremely dependent on energy, Eq. (63) must still use E_r^{obs} rather than e_p.

The 'observed' resonance energy $E = E_r^{\mathrm{obs}}$ on the real axis has the great virtue that in Eq. (54) the first fraction $\mathbf{S}\mathrm{e}^{-2\mathrm{i}\phi} = -1$, showing that the R-matrix phase shift $\delta_R = \pi/2$. Examples of δ_R plots are shown in Fig. 4.

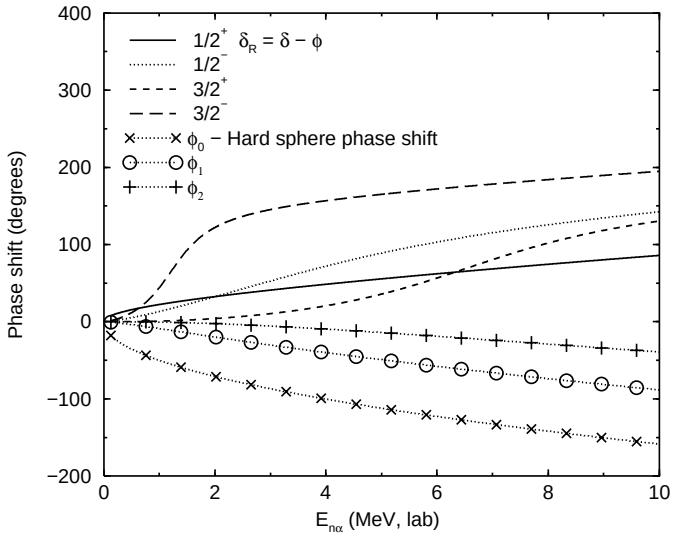

Figure 4: Examples of R-matrix phase shifts δ_R for low-energy n–α scattering, along with the hard-sphere phase shifts ϕ_L in the s, p and d-waves that have been subtracted. The resonance in the $p_{1/2}$ channel is now much more visible than in in a plot of δ alone.

For these reasons, the 'observed' resonance position is often *defined* as the energy where $\delta_R = \pi/2$. This implies from Eq. (51) that the 'observed' energy is in general where

$$R(E_r^{\rm obs})S^0(E_r^{\rm obs}) = 1, \tag{64}$$

an expression which can be used with any number of R-matrix poles to find one-channel resonance positions. The 'observed' width $\Gamma^{\rm obs}$ can in the general case be obtained from

$$\Gamma^{\rm obs} = 2\left[\frac{{\rm d}\delta_R}{{\rm d}E}\right]^{-1}_{E=E_r}, \tag{65}$$

using again the Thomas approximation. As definitions of a resonance energy, however, the equations (62, 64) have residual dependence on the R-matrix radius a which enters into the evaluation of the hard sphere phase shift ϕ.

2.2 Multi-channel R matrix

To facilitate the understanding of a multi-channel R-matrix fit, it is again useful to modify the derivation of Eq. (41) of the S matrix from the R matrix, so various approximations allow simple formulae to be derived that may be easier to understand.

2.3 Another derivation of the scattering S matrix

We start as before with the matrix expression of Eq. (37). We follow the pattern of the derivation giving Eq. (42), but remember that these terms are all matrices:

$$\begin{aligned}\mathbf{S} &= [\mathsf{t}^{\frac{1}{2}}\mathbf{H}^{+} - a\mathbf{R}\,\mathsf{t}^{\frac{1}{2}}(\mathbf{H}^{+\prime}-\beta\mathbf{H}^{+})]^{-1}[\mathsf{t}^{\frac{1}{2}}\mathsf{H}^{-} - a\mathbf{R}\,\mathsf{t}^{\frac{1}{2}}(\mathbf{H}^{-\prime}-\beta\mathbf{H}^{-})] \\ &= (\mathsf{t}^{\frac{1}{2}}\mathbf{H}^{+})^{-1}[1-a\mathbf{R}(\mathbf{H}^{+\prime}/\mathbf{H}^{+}-\beta)]^{-1}[1-a\mathbf{R}(\mathbf{H}^{-\prime}/\mathbf{H}^{-}-\beta)](\mathsf{t}^{\frac{1}{2}}\mathbf{H}^{-}) \qquad (66)\end{aligned}$$

where for matrices $A/B \equiv AB^{-1}$. We have assumed that the asymptotic Coulomb wave functions $\mathbf{H}$ have no off-diagonal terms when the diagonal elements of $\mathsf{t} = \hbar^2/2\mu$ vary for different mass partitions, which is normally the case. Following now the previous pattern of subsection 2.1.1, we now define a 'logarithmic' matrix

$$L = \mathbf{H}^{+\prime}/\mathbf{H}^{+} - \beta = \frac{1}{a}(S + \mathrm{i}P - a\beta) \equiv \frac{1}{a}(S - B + \mathrm{i}P) \qquad (67)$$

where P, S are taken as matrices with diagonal elements

$$\begin{aligned}P_\alpha &= k_\alpha a/(F_\alpha^2 + G_\alpha^2) \qquad (68)\\ \text{and}\quad S_\alpha &= (\dot{F}_\alpha F_\alpha + \dot{G}_\alpha G_\alpha)P_\alpha. \qquad (69)\end{aligned}$$

Since $\mathbf{H}^{-\prime}/\mathbf{H}^{-} = L^*$ also, we have

$$\begin{aligned}\mathbf{S} &= (\mathsf{t}^{\frac{1}{2}}\mathbf{H}^{+})^{-1}[1 - a\mathbf{R}L]^{-1}[1 - a\mathbf{R}L^*](\mathsf{t}^{\frac{1}{2}}\mathbf{H}^{-}) \\ &= \sqrt{\frac{\mathbf{H}^{-}}{\mathbf{H}^{+}}}\frac{1}{\sqrt{\mathsf{t}\mathbf{H}^{-}\mathbf{H}^{+}}}[1 - a\mathbf{R}L]^{-1}[1 - a\mathbf{R}L^*]\sqrt{\mathsf{t}\mathbf{H}^{-}\mathbf{H}^{+}}\sqrt{\frac{\mathbf{H}^{-}}{\mathbf{H}^{+}}} \\ &= \Omega\frac{1}{\sqrt{\mathsf{t}\mathbf{H}^{-}\mathbf{H}^{+}}}[1 - a\mathbf{R}L]^{-1}[1 - a\mathbf{R}L^*]\sqrt{\mathsf{t}\mathbf{H}^{-}\mathbf{H}^{+}}\;\Omega \qquad (70)\end{aligned}$$

where Ω is the matrix with diagonal elements $\mathrm{e}^{\mathrm{i}\phi_\alpha}$ for hard-sphere phase shifts $\tan\phi_\alpha = -F_\alpha/G_\alpha$. The matrix product $(\mathsf{t}\mathbf{H}^{-}\mathbf{H}^{+})$ is diagonal, with elements

$$\mathbf{H}_\alpha^{-}\mathbf{H}_\alpha^{+}\mathsf{t}_\alpha = (F_\alpha^2 + G_\alpha^2)\frac{\hbar^2}{2\mu_\alpha} = \frac{k_\alpha a}{P_\alpha}\frac{\hbar^2}{2\mu_\alpha} = \frac{\hbar v_\alpha a}{2P_\alpha} \qquad (71)$$

in terms of the penetrability defined above in Eq. (68), and channel velocities $v = \hbar k/\mu$.

The symmetric $\tilde{\mathbf{S}}$ matrix is constructed from the above $\mathbf{S}$ by $\tilde{\mathbf{S}} = \mathbf{v}^{\frac{1}{2}}\mathbf{S}\mathbf{v}^{-\frac{1}{2}}$, using the same velocity factors put into a diagonal matrix $\mathbf{v}$. This means that we have the simpler form for

$$\begin{aligned}\tilde{\mathbf{S}} &= \mathbf{v}^{\frac{1}{2}}\Omega\frac{1}{\sqrt{\frac{1}{2}\hbar\mathbf{v}a/P}}[1-a\mathbf{R}L]^{-1}[1-a\mathbf{R}L^*]\sqrt{\tfrac{1}{2}\hbar\mathbf{v}a/P}\;\Omega\mathbf{v}^{-\frac{1}{2}} \\ &= \Omega P^{\frac{1}{2}}[1-a\mathbf{R}\;L]^{-1}[1-a\mathbf{R}\;L^*]P^{-\frac{1}{2}}\Omega. \qquad (72)\end{aligned}$$

We now use the matrix identity

$$[1-RA]^{-1}[1-RB] = 1+[1-RA]^{-1}R(A-B) \qquad (73)$$

to find

$$\begin{aligned}\tilde{\mathbf{S}} &= \Omega P^{\frac{1}{2}}[1+(1-a\mathbf{R}L)^{-1}a\mathbf{R}\;(L-L^*)]P^{-\frac{1}{2}}\Omega \qquad (74)\\ &= \Omega P^{\frac{1}{2}}[1+(1-a\mathbf{R}L)^{-1}a\mathbf{R}\;2\mathrm{i}P/a]P^{-\frac{1}{2}}\Omega \qquad (75)\\ &= \Omega[1+2\mathrm{i}P^{\frac{1}{2}}(1-a\mathbf{R}L)^{-1}\mathbf{R}P^{\frac{1}{2}}]\Omega. \qquad (76)\end{aligned}$$

This is the main result: a derivation of the S matrix from the R matrix, using the penetrabilities and shifts, with $aL = S^0 + \mathrm{i}P \equiv S - B + \mathrm{i}P$.

2.3.1 Two-channel one-level case

In the *one*-channel case, the Eq. (76) reduces to the equations of subsection 2.1.1. In the *two*-channel case, we can perform the matrix inversion by hand, yielding the 2×2 $\tilde{\mathbf{S}}$ matrix

$$\tilde{\mathbf{S}}_{11} = \mathrm{e}^{2\mathrm{i}\phi_1}[1+2\mathrm{i}P_1[\mathbf{R}_{11}-aL_2(\mathbf{R}_{11}\mathbf{R}_{22}-\mathbf{R}_{12}^2)]d^{-1}] \qquad (77a)$$

$$\tilde{\mathbf{S}}_{22} = \mathrm{e}^{2\mathrm{i}\phi_2}[1+2\mathrm{i}P_2[\mathbf{R}_{22}-aL_1(\mathbf{R}_{11}\mathbf{R}_{22}-\mathbf{R}_{12}^2)]d^{-1}] \qquad (77b)$$

$$\tilde{\mathbf{S}}_{12} = \tilde{\mathbf{S}}_{21} = \mathrm{e}^{\mathrm{i}(\phi_1+\phi_2)}2\mathrm{i}P_1^{1/2}\mathbf{R}_{12}^2P_2^{1/2}d^{-1}, \qquad (77c)$$

where the determinant is

$$d = (1-a\mathbf{R}_{11}L_1)(1-a\mathbf{R}_{22}L_2) - a^2L_1\mathbf{R}_{12}^2L_2. \qquad (77d)$$

These equations have a very simple form if there is one isolated level e_p, as here $\mathbf{R}_{\alpha'\alpha} = \gamma_\alpha\gamma_{\alpha'}/(e_p - E)$ and hence $\mathbf{R}_{11}\mathbf{R}_{22} = \mathbf{R}_{12}^2$. In this one-pole case all the elements have the general form

$$\begin{aligned}\tilde{\mathbf{S}}_{\alpha'\alpha} &= \mathrm{e}^{\mathrm{i}\phi_\alpha}\left[\delta_{\alpha'\alpha} + \frac{2\mathrm{i}P_\alpha^{1/2}\gamma_\alpha\gamma_{\alpha'}P_{\alpha'}^{1/2}}{(e_p - E)(1 - a\mathbf{R}_{11}L_1 - a\mathbf{R}_{22}L_2)}\right]\mathrm{e}^{\mathrm{i}\phi_{\alpha'}} \\ &= \mathrm{e}^{\mathrm{i}\phi_\alpha}\left[\delta_{\alpha'\alpha} + \frac{\mathrm{i}\Gamma_\alpha^{1/2}\Gamma_{\alpha'}^{1/2}}{e_p - E - \gamma_1^2 S_1^0 - \mathrm{i}\gamma_1^2 P_1 - \gamma_2^2 S_2^0 - \mathrm{i}\gamma_2^2 P_2}\right]\mathrm{e}^{\mathrm{i}\phi_{\alpha'}}, \qquad (78)\end{aligned}$$

since the formal widths of Eq. (56) are $\Gamma_\alpha = 2\gamma_\alpha^2 P_\alpha$. We have used the shifts and penetrabilities defined in Eq. (67), with $S^0 = S - a\beta$ as before.

This formula suggests we define a *total formal width*

$$\Gamma_{\mathrm{tot}} = 2\gamma_1^2 P_1 + 2\gamma_2^2 P_2 = \Gamma_1 + \Gamma_2, \qquad (79)$$

in terms of which the two-channel one-pole $\tilde{\mathbf{S}}$ matrix begins to look like an isolated Breit-Wigner resonance:

$$\tilde{\mathbf{S}}_{\alpha'\alpha} = \mathrm{e}^{\mathrm{i}\phi_\alpha}\left[\delta_{\alpha'\alpha} - \frac{\mathrm{i}\Gamma_\alpha^{1/2}\Gamma_{\alpha'}^{1/2}}{E - (e_p - \gamma_1^2 S_1^0 - \gamma_2^2 S_2^0) + \mathrm{i}\Gamma_{\mathrm{tot}}/2}\right]\mathrm{e}^{\mathrm{i}\phi_{\alpha'}} \qquad (80)$$

with formal resonance energy $E_r^f = e_p - \gamma_1^2 S_1^0 - \gamma_2^2 S_2^0$. We see that the shift contributions from the individual channels are added together to produce the shift for the coupled-channels resonance.

2.3.2 Cross sections

The non-elastic cross section contribution from a specific coupled-channels set J_{tot}^π to the cross section for scattering to channel α from α_i is

$$\begin{aligned}\sigma_{\alpha\alpha_i}(J_{\mathrm{tot}}^\pi) &= \frac{\pi}{k_i^2}\, g_{J_{\mathrm{tot}}}\, |\tilde{\mathbf{S}}_{\alpha\alpha_i}|^2 \\ &= \frac{\pi}{k_i^2}\, g_{J_{\mathrm{tot}}}\, \frac{\Gamma_\alpha\Gamma_{\alpha_i}}{|E - E_r^f - \mathrm{i}\Gamma_{\mathrm{tot}}/2|^2} \\ &= \frac{\pi}{k_i^2}\, g_{J_{\mathrm{tot}}}\, \frac{\Gamma_\alpha\Gamma_{\alpha_i}}{(E - E_r^f)^2 + \Gamma_{\mathrm{tot}}^2/4}, \qquad (81)\end{aligned}$$

which is exactly the form of an isolated Breit-Wigner resonance with a strong peak at $E \approx E_r^f$ and fwhm of Γ_{tot}. Here we use the spin weighting factor g_{tot}

$$g_{J_{\mathrm{tot}}} \equiv \frac{2J_{\mathrm{tot}} + 1}{(2I_{p_i}+1)(2I_{t_i}+1)}. \qquad (82)$$

The individual Γ_α are called the *partial widths*, because they are ($\hbar$ times) the decay rates of a resonance through specific exit channels. The total (formal) width $\Gamma_{\rm tot} = \sum_\alpha \Gamma_\alpha$ is the sum of all the partial widths, and describes the resonance's overall decay rate. Note that, by time-reversal invariance, the same width applies to the *entrance* channel as to the exit channels, and hence Γ_{α_i} measures also the rate at which a resonance could be populated from a given initial scattering configuration α_i.

This summation of partial widths and shifts has been proved for the two-channel one-pole case. To see how partial widths add together in the multi-channel case, we first need to present the level-matrix formulation of R-matrix theory.

2.3.3 Interpretation for multiple poles

For isolated poles, if we know the energy of the peak $E^{\rm obs}$, we can easily generalized the 'observed' R-matrix parameters of Eq. (63) to give, for each channel α,

$$\Gamma_\alpha^{\rm obs} = \frac{2\gamma_\alpha^2 P_\alpha(E^{\rm obs})}{1 + \sum_{\alpha'} \gamma_{\alpha'}^2 S'_{\alpha'}(E^{\rm obs})}. \tag{83}$$

This formula can be readily inverted to give the γ_α in terms of the $\Gamma_\alpha^{\rm obs}$.

For multiple poles, however, solving for each $E_p^{\rm obs}$ equations like Eq. (62),

$$E_p^{\rm obs} = e_p - \sum_\alpha \gamma_{p\alpha}^2 (S_\alpha(E_p^{\rm obs}) - B), \tag{84}$$

does *not* give the correct peak positions. Several proposals have been made to get physically better results.

1. The code SAMMY allows fits to be made with the boundary condition number B not constant in each channel, but *varying* with energy and channel according to $B_\alpha(E) = S_\alpha(E)$. Using this B=S approximation everywhere means that Eq. (84) is then simply $E_p^{\rm obs} = e_p$: the R-matrix poles e_p are now *exactly* the resonance positions! Very convenient. If only the B=S approximation were properly based on some R-matrix theory as in Section 1.

2. Brune [7] suggest that Eq. (84) should be generalized to eigenvalue matrix equations in the number of poles P. He constructs the $P \times P$

matrix

$$\mathcal{E}_{pq} = e_p \delta_{pq} - \sum_\alpha \gamma_{p\alpha}\gamma_{q\alpha}(S_\alpha(E) - B_\alpha) \tag{85}$$

and then solves for $\tilde{E}_p$ the eigenvalue equation

$$\mathcal{E}\mathbf{a}_p = \tilde{E}_p \mathbf{a}_p \qquad \text{i.e.} \quad \sum_q \mathcal{E}_{p'q} a_{qp} = \tilde{E}_p a_{p'p} \ . \tag{86}$$

Since $\mathcal{E}$ depends on energy E via the shift function $S_\alpha(E)$, this eigenvalue problem has to be solved iteratively for each p using $E = \tilde{E}_p$ from each successive solution. Still, this method does work. Brune also shows how to reverse the process: to obtain the e_p from the $\tilde{E}_p$ once the boundary conditions B_α are specified for each channel (independently of energy).

In numerical tests with two fits of the same data, Brune's $\tilde{E}_p$ are found close to the pole energies fitted in the B=S approximation, but the calculated R-matrix cross sections between resonances are not identical.

3 Level-matrix formulation

All the matrix operations so far in this chapter involve inversion of a matrix with the dimensionality M of the number of *partial-wave channels* in a coupled-channels set for a specific overall spin and parity $J^\pi_{\rm tot}$. Sometimes, however, it is more convenient to reformulate the theory so that the inversion is only needed of a matrix with dimensions P of the number of *levels* e_p. In R-matrix phenomenology, this is often a smaller number. So we now show how to construct a $P\times P$ symmetric level matrix A with elements A_{pq} for level indices p, q, such that the $\tilde{\mathbf{S}}$ matrix depends on calculating the inverse A^{-1}.

3.1 Derivation of level matrix

To simplify the derivation of A, we write the previous theory as much as possible in matrix form. We write the initial $M\times M$ R matrix of Eq. (40) as

$$\mathbf{R} = \gamma^T F \gamma \tag{87}$$

where γ is the $P\times M$ rectangular matrix with elements $\gamma_{p\alpha}$, and F is the matrix of diagonal reciprocals $1/(e_p - E)$. From the previous matrix form Eq. (76), we have

$$\tilde{\mathbf{S}} = \Omega[1 + 2\mathrm{i}P^{\frac{1}{2}}(1 - \gamma^T F\gamma(S^0 + \mathrm{i}P))^{-1}\gamma^T F\gamma]P^{\frac{1}{2}}\Omega. \tag{88}$$

We now try to find a matrix $\mathbf{A}$ so that this can be rewritten

$$\tilde{\mathbf{S}} = \Omega[1 + 2\mathrm{i}P^{\frac{1}{2}}\gamma^T\mathbf{A}\gamma P^{\frac{1}{2}}]\Omega, \tag{89}$$

for which we need to satisfy the identity

$$(1 - \gamma^T F\gamma(S^0 + iP))^{-1}\gamma^T F\gamma = \gamma^T\mathbf{A}\gamma, \tag{90}$$

which is

$$\begin{aligned} \gamma^T F\gamma &= (1 - \gamma^T F\gamma(S^0 + \mathrm{i}P))\gamma^T\mathbf{A}\gamma \\ &= \gamma^T\mathbf{A}\gamma - \gamma^T F\gamma(S^0 + \mathrm{i}P)\gamma^T\mathbf{A}\gamma, \\ \text{or} \qquad & \gamma^T\left[F - \mathbf{A} - F\gamma(S^0 + \mathrm{i}P)\gamma^T\mathbf{A}\right]\gamma = 0. \end{aligned} \tag{91}$$

This condition will always be satisfied if we can choose $\mathbf{A}$ such that

$$F - \mathbf{A} - F\gamma(S^0 + \mathrm{i}P)\gamma^T\mathbf{A} = 0 \tag{92}$$

$$\text{or} \quad \mathbf{A}^{-1} = F^{-1} - \gamma S^0\gamma^T - \mathrm{i}\gamma P\gamma^T. \tag{93}$$

This last equation is the defining equation we are looking for. If we construct diagonal and symmetric off-diagonal shift and width *level matrices* as

$$\hat{\Delta}_{pq} = (\gamma S^0\gamma^T)_{pq} = \sum_\alpha \gamma_{p\alpha}S^0_\alpha\gamma_{q\alpha} \tag{94}$$

$$\text{and} \quad \hat{\Gamma}_{pq} = 2(\gamma P\gamma^T)_{pq} = 2\sum_\alpha \gamma_{p\alpha}P_\alpha\gamma_{q\alpha}, \tag{95}$$

then the defining equation for the symmetric level matrix $\mathbf{A}$ is

$$(\mathbf{A}^{-1})_{pq} = \delta_{pq}(e_p - E) - \hat{\Delta}_{pq} - \tfrac{\mathrm{i}}{2}\hat{\Gamma}_{pq} \tag{96}$$

$$\text{or} \quad -(\mathbf{A}^{-1})_{pq} = E\delta_{pq} - (e_p\delta_{pq} - \hat{\Delta}_{pq} - \tfrac{\mathrm{i}}{2}\hat{\Gamma}_{pq}). \tag{97}$$

The $\hat{\Delta}_{pq}$ and $\hat{\Gamma}_{pq}$ are generalized shifts and widths that now have off-diagonal as well as diagonal effects on the levels. Their signs are now important, and reflect the interference between levels, as they enter into the matrix inversion

$$\mathbf{A} = -\begin{pmatrix} E - e_1 + \hat{\Delta}_{11} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{11} & \hat{\Delta}_{12} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{12} & \dots \\ \hat{\Delta}_{21} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{21} & E - e_2 + \hat{\Delta}_{22} + \frac{\mathrm{i}}{2}\hat{\Gamma}_{22} & \dots \\ \dots & & \end{pmatrix}^{-1}, \tag{98}$$

remembering the symmetry of the $\hat{\Gamma}$ and $\hat{\Delta}$ matrices. From Eq. (89), the full multi-channel multi-level $\tilde{\mathbf{S}}$ matrix is constructed in terms of this matrix inverse $\mathbf{A}$ as

$$\tilde{\mathbf{S}}_{\alpha'\alpha} = \Omega_\alpha \left[\delta_{\alpha'\alpha} + \mathrm{i} \sum_{\lambda\lambda'} \Gamma^{1/2}_{\alpha\lambda} \mathbf{A}_{\lambda\lambda'} \Gamma^{1/2}_{\alpha'\lambda'} \right] \Omega_{\alpha'}, \tag{99}$$

where we define $\Gamma^{1/2}_{\alpha\lambda} = \gamma_{\alpha\lambda}(2P_\alpha)^{1/2}$ to preserve the signs of the $\gamma_{\alpha\lambda}$.

3.2 One-level case

The coupled-channels case with just one level $p = q = 1$ is now particularly easy, as the level matrix $\mathbf{A}$ is then a number. Using

$$\hat{\Delta}_{11} = \sum_\alpha \gamma^2_{1\alpha} S^0_\alpha \tag{100}$$

$$\text{and} \quad \Gamma_{\rm tot} \equiv \hat{\Gamma}_{11} = \sum_\alpha 2\gamma^2_{1\alpha} P_\alpha \equiv \sum_\alpha \Gamma_\alpha, \tag{101}$$

the $\mathbf{A}$ is now

$$-\mathbf{A}^{-1} = E - (e_1 - \hat{\Delta}_{11} - \tfrac{\mathrm{i}}{2}\Gamma_{\rm tot}) \equiv E - E_p, \tag{102}$$

where $E_p = e_1 - \hat{\Delta}_{11} - \frac{\mathrm{i}}{2}\Gamma_{\rm tot}$ is the complex resonance pole position. Thus the matrix of scattering from this isolated pole is

$$\tilde{\mathbf{S}}_{\alpha'\alpha} = \Omega_\alpha \left[\delta_{\alpha'\alpha} - \frac{\mathrm{i}\Gamma^{1/2}_\alpha \Gamma^{1/2}_{\alpha'}}{E - E_p} \right] \Omega_{\alpha'} \ . \tag{103}$$

Elastic scattering: The contributing part to an *elastic* cross section ($\alpha = \alpha'$) is therefore identical to Eq. (53),

$$\tilde{\mathbf{S}}_{\alpha\alpha} = \Omega^2_\alpha \left[1 - \frac{\mathrm{i}\Gamma_\alpha}{E - E_p} \right]. \tag{104}$$

A function of $\tilde{\mathbf{S}}$ which appears in the elastic amplitude $f(\theta)$ is =

$$\tilde{\mathbf{S}}_{\alpha\alpha} - 1 = 2i\mathrm{e}^{\mathrm{i}\phi} \left[\sin\phi - \frac{\mathrm{i}}{2} \frac{\mathrm{e}^{\mathrm{i}\phi}\Gamma_\alpha}{E - E_p} \right] \tag{105}$$

using $\Omega_\alpha = \mathrm{e}^{2\mathrm{i}\phi}$. The scattering arising from the first term $\sin\phi$ is sometimes called in R-matrix theory the 'potential scattering', and that from

the $\Gamma/(E - E_p)$ term the 'resonance scattering', and there will also be an interference term. However, the 'potential' under discussion here is just the 'hard sphere' at radius $R = a$, and should not be mistaken for the attractive optical-potential well, more commonly called the scattering potential.

Non-elastic reactions: The contributing part to a *inelastic* cross section ($\alpha \neq \alpha'$) is analogously

$$\sigma_{\alpha\alpha_i}(J^\pi_{\rm tot}) = \frac{\pi}{k_i^2}\ g_{J_{\rm tot}}\ \frac{\Gamma_\alpha \Gamma_{\alpha_i}}{(E - e_1 + \hat{\Delta}_{11})^2 + \Gamma^2_{\rm tot}/4} \tag{106}$$

which is a Breit-Wigner form that is similar to Eq. (81), but now established for any number of partial-wave channels. The total (formal) width $\Gamma_{\rm tot} = \sum_\alpha \Gamma_\alpha$ is again the sum over all the partial widths for each coupled channel. Because, strictly, the shifts and widths are energy dependent:

$$\sigma_{\alpha\alpha_i}(J^\pi_{\rm tot}; E) = \frac{\pi}{k_i^2}\ g_{J_{\rm tot}}\ \frac{\Gamma_\alpha(E) \Gamma_{\alpha_i}(E)}{(E - e_1 + \hat{\Delta}_{11}(E))^2 + \Gamma_{\rm tot}(E)^2/4}, \tag{107}$$

the observed and true resonance widths will be as usual slightly different from the formal value $\Gamma_{\rm tot}$.

A Progressively more flexible definitions of the R matrix

For partial wave L, the simplest definition of Eq. (4) at radius a defines the matrix element

$$\mathsf{R}_L = \frac{1}{a}\frac{\chi_L(a)}{\chi'_L(a)}. \tag{108}$$

For a matrix of coupled-channels solutions, this comes to require a matrix inversion

$$\mathsf{R} = \frac{1}{a}\mathsf{Y}(a)[\mathsf{Y}'(a)]^{-1}. \tag{109}$$

For one channel, with logarithmic boundary condition β, Eq. (18) we choose instead the more general matrix element

$$\mathsf{R} = \frac{1}{a}\frac{\chi(a)}{\chi'(a) - \beta\chi(a)}. \tag{110}$$

For coupled transfer channels, with $\beta \neq 0$ and variable reduced masses μ_α, Eq. (32) leads us to define the matrix $\mathbf{R}_{\alpha\alpha'}$ by

$$t_\alpha^{1/2}\psi_\alpha(a) = a\sum_{\alpha'}\mathbf{R}_{\alpha\alpha'}\Big[\psi'_{\alpha'}(a) - \beta\psi_{\alpha'}(a)\Big]t_{\alpha'}^{1/2}, \tag{111}$$

using $t_\alpha \equiv \hbar^2/2\mu_\alpha$. In matrix form with t as a matrix of diagonal elements t_α,

$$\mathsf{t}^{\frac{1}{2}}\ \mathsf{Y}(a) = a\ \mathbf{R}\ [\mathsf{Y}'(a) - \beta\mathsf{Y}(a)]\ \mathsf{t}^{\frac{1}{2}}, \tag{112}$$

so

$$\mathbf{R} = \frac{1}{a}\ \mathsf{t}^{\frac{1}{2}}\ \mathsf{Y}(a)\ \mathsf{t}^{-\frac{1}{2}}\ [\mathsf{Y}'(a) - \beta\mathsf{Y}(a)]^{-1}. \tag{113}$$

References

[1] E. P. Wigner and L. Eisenbud, *Phys. Rev.* **72** (1947) 29.

[2] A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30** (1958) 257.

[3] P. G. Burke and M. J. Seaton, *J. Phys. B* **17** (1984) L683.

[4] E. W. Vogt, *Rev. Mod. Phys.* **34** (1962) 723.

[5] P. Descouvemont 2004, *Theoretical Models for Nuclear Astrophysics*, Hauppauge NY: Nova Science Publishers.

[6] R. G. Thomas, *Phys. Rev.* **81** (1951) 148.

[7] C.R. Brune, *Phys. Rev. C* **66** (2002) 044611