Nucleon–Nucleon Scattering: R- and S-Matrix Formalism

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1 Introduction

In quantum scattering theory, the evolution of an interacting two-body system is elegantly encoded in the S-matrix, while the R-matrix offers a numerically convenient alternative based on boundary matching. This document reviews the definitions, physical interpretations, and mathematical derivations of both quantities, particularly within the context of nucleon–nucleon scattering.

2 The S-Matrix and R-Matrix: Definitions and Interpretations

2.1 The Scattering Matrix (S-Matrix)

Definition: The S-matrix connects asymptotic incoming and outgoing states:

$$|\text{out}\rangle = S|\text{in}\rangle$$

Physical Role:

- Encodes all observable aspects of scattering: phase shifts, cross sections, and mixing.
- Ensures conservation of probability via unitarity: $S^\dagger S = I$.
- For uncoupled channels: $S_\ell = e^{2i\delta_\ell}$, where δ_ℓ is the phase shift.

2.2 The Reactance Matrix ($\boldsymbol{R}$-Matrix)

Definition: Defined via the logarithmic derivative of the wavefunction at the boundary of the interaction region:

$$R_\ell(E) = \left.\frac{a\, u_\ell'(a)}{u_\ell(a)}\right|_{\text{internal}}$$

Physical Role:

- Arises from dividing configuration space into internal ($r < a$) and external ($r > a$) regions.
- Useful for resonance physics and numerical stability.
- Related to the S-matrix via:
$$S = \frac{1 + iR}{1 - iR}$$

3 From Schrödinger Equation to Scattering Matrices

3.1 Radial Schrödinger Equation

Consider two nucleons interacting via a central potential $V(r)$. The time-independent Schrödinger equation reads:

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Partial Wave Expansion: Using spherical symmetry:

$$\psi(\mathbf{r}) = \sum_{\ell m} \frac{u_\ell(r)}{r} Y_{\ell m}(\hat{r})$$

The radial equation becomes:

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)\right] u_\ell(r) = E u_\ell(r)$$

Asymptotic Behavior: For $r \to \infty$ (free motion), define the wave number $k = \sqrt{2\mu E}/\hbar$. Then:

$$u_\ell(r) \xrightarrow{r\to\infty} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)$$

3.2 Definition of the S-Matrix

Rewriting the asymptotic form as a combination of incoming and outgoing spherical waves:

$$u_\ell(r) \sim \frac{1}{2i}\left[e^{-i(kr-\ell\pi/2)} - S_\ell\, e^{i(kr-\ell\pi/2)}\right]$$

This identifies $S_\ell = e^{2i\delta_\ell}$.

3.3 Definition of the R-Matrix

In the R-matrix framework:

- **Internal region**: $r < a$, where interactions occur.
- **External region**: $r > a$, free-particle motion.

In the external region, the general solution is:

$$\psi_\ell(r) = C_\ell \left[F_\ell(kr)\cos\delta_\ell + G_\ell(kr)\sin\delta_\ell\right] , \tag{1}$$

where C_ℓ is a normalization constant. Matching this with the internal solution at $r = a$, one derives [1]:

$$S_\ell = \frac{1 + iR_\ell}{1 - iR_\ell}$$

4 Matrix Structure: Uncoupled and Coupled Channels

4.1 Summary Table: Key Characteristics

Quantity	**Uncoupled**	**Coupled (Stapp)**	**Coupled (BB)**
S	$e^{2i\delta}$	$\mathrm{diag}(e^{2i\delta_i})\, O(\epsilon)\, \mathrm{diag}(e^{2i\delta_i})$	$O^T(\epsilon)\, \mathrm{diag}(e^{2i\delta_i})\, O(\epsilon)$
R	$\tan\delta$	$\mathrm{diag}(\tan\delta_i)\, O(\epsilon)\, \mathrm{diag}(\tan\delta_i)$	$O^T(\epsilon)\, \mathrm{diag}(\tan\delta_i)\, O(\epsilon)$
O	–	$O(\epsilon) = \begin{pmatrix} \cos 2\epsilon & i\sin 2\epsilon \\ i\sin 2\epsilon & \cos 2\epsilon \end{pmatrix}$	$O(\epsilon) = \begin{pmatrix} \cos\epsilon & \sin\epsilon \\ -\sin\epsilon & \cos\epsilon \end{pmatrix}$

Table 1: Summary of S- and R-matrix structures in uncoupled and coupled cases, using Stapp [2] and Blatt–Biedenharn [3] conventions.

4.2 Remarks

- In coupled channels, the phase shifts δ_i and mixing angles ϵ fully characterize the scattering process.
- The two conventions differ in the placement of rotation matrices but yield the same observables.

5 Variational code

In the variational code the R-matrix is evaluated using Koön principle to second order. Then through the following steps one recovers the phase-shifts and mixing angles for both the Stapp and the Blatt–Biedenharn (BB) conventions.

5.1 BB phase shifts and mixing angle

Using Tab. 1 the R matrix can be written as

$$R = \begin{pmatrix} \tan\delta_1\cos^2\epsilon + \tan\delta_2\sin^2\epsilon & (\tan\delta_1 - \tan\delta_2))\sin\epsilon\,\cos\epsilon \\ (\tan\delta_1 - \tan\delta_2))\sin\epsilon\,\cos\epsilon & \tan\delta_1\sin^2\epsilon + \tan\delta_2\cos^2\epsilon \end{pmatrix} . \tag{2}$$

The combination $R_{11} - R_{22}$ is

$$R_{11} - R_{22} = \cos(2\epsilon)\,(\tan\delta_1 - \tan\delta_2) \ .$$

Therefore

$$\tan(4\epsilon) = \frac{2\,R_{12}}{R_{11} - R_{22}} \qquad \to \qquad \epsilon = \frac{1}{2}\,\mathrm{atan}\left(\frac{2\,R_{12}}{R_{11} - R_{22}}\right) .$$

Once ϵ is known, one can evaluate

$$\tan\delta_1 = \cos^2\epsilon\ R_{11} + \sin^2\epsilon\ R_{22} + 2\cos\epsilon\ \sin\epsilon\, R_{12}$$

and

$$\tan\delta_2 = \sin^2\epsilon\ R_{11} + \cos^2\epsilon\ R_{22} - 2\cos\epsilon\ \sin\epsilon\, R_{12}\,.$$

5.2 Stapp phase shifts and mixing angle

One can then use δ_1, δ_2 and ϵ to evaluate the S-matrix, which is independent from the parametrization,

$$S = S_{\rm BB} = \begin{pmatrix} e^{2i\delta_1}\cos^2\epsilon + e^{2i\delta_2}\sin^2\epsilon & \left(e^{2i\delta_1} - e^{2i\delta_2}\right)\sin\epsilon\cos\epsilon \\ \left(e^{2i\delta_1} - e^{2i\delta_2}\right)\sin\epsilon\cos\epsilon & e^{2i\delta_1}\sin^2\epsilon + e^{2i\delta_2}\cos^2\epsilon \end{pmatrix}.$$

It is possible now to extract the phase shifts and mixing angle in the Stapp parametrization. In this parametrization

$$S = S_{\rm Stapp} = \begin{pmatrix} e^{2i\delta_1}\ \cos(2\epsilon) & i\, e^{i(\delta_1+\delta_2)}\ \sin(2\epsilon) \\ i\, e^{i(\delta_1+\delta_2)}\ \sin(2\epsilon) & e^{2i\delta_2}\cos(2\epsilon) \end{pmatrix}.$$

The determinant in this case is

$$\det S_{\rm Stapp} = e^{2i(\delta_1+\delta_2)}$$

and therefore

$$\sin(2\epsilon) = \sqrt{-\frac{S_{12}^2}{\det S}}$$

and

$$\cos(2\epsilon) = \sqrt{1-\sin^2(2\epsilon)}\,.$$

It is possible to evaluate

$$e^{i\delta_k} = \sqrt{\frac{S_{kk}}{\cos(2\epsilon)}} = \sqrt{e^{2i\delta_k}}\,.$$

Therefore

$$\delta_1 = \ \mathrm{acos}\left[\mathrm{Re}\left(\sqrt{\frac{S_{11}}{\cos(2\epsilon)}}\right)\right] \times \begin{cases} 1 & \text{if } \mathrm{Im}\left(\sqrt{\frac{S_{11}}{\cos(2\epsilon)}}\right) \geq 0 \\ -1 & \text{if } \mathrm{Im}\left(\sqrt{\frac{S_{11}}{\cos(2\epsilon)}}\right) < 0 \end{cases}$$

and

$$\delta_2 = \mathrm{acos}\left[\mathrm{Re}\left(\frac{S_{22}}{\cos(2\epsilon)}\right)\right] \times \begin{cases} 1 & \text{if } \mathrm{Im}\left(\frac{S_{22}}{\cos(2\epsilon)}\right) \geq 0 \\ -1 & \text{if } \mathrm{Im}\left(\frac{S_{22}}{\cos(2\epsilon)}\right) < 0 \end{cases}.$$

6 Conclusion

The S-matrix and R-matrix are central tools in analyzing nucleon–nucleon scattering. While the S-matrix encapsulates the observable content of the interaction, the R-matrix provides a convenient and often more numerically robust intermediate object, especially in resonance or coupled-channel analyses. Their connection through a Möbius transformation reflects deep structural links in scattering theory.

A Asymptotic expansion and scattering length

As seen in Eq. (1) it is possibly to write for non-coupled channels

$$\psi_\ell(r) = A_\ell\ \left(F_\ell + \tan\delta_\ell\, G_\ell\right)\,,$$

where $A_\ell \equiv C_\ell\,\cos\delta_\ell$. In this case $R_{\ell\ell} = \tan\delta_\ell$ and therefore

$$\psi_\ell(r) = A_\ell\ \left(F_\ell + R_{\ell\ell}\, G_\ell\right)\,.$$

Here R_ℓ (G_ℓ) are the regular (irregular) solution to the Schrödinger equation and in the case if the potential is short-range

$$\begin{cases} F_\ell(kr) & \to \quad j_\ell(kr)\,, \\ G_\ell(kr) & \to \quad y_\ell(kr)\,, \end{cases}$$

where j_ℓ (y_ℓ) is the regular (irregular) spherical Bessel function.
In case of a long range potential of the type $\propto 1/r$

$$\begin{cases} F_\ell & \to \quad F_\ell(\eta, kr)\,, \\ G_\ell & \to \quad G_\ell(\eta, kr)\,, \end{cases}$$

where $F_\ell(\eta, kr)$ ($G_\ell(\eta, kr)$) is the regular (irregular) Coulomb function.

A.1 The scattering length

For small energies there are two observables of importance, which depend linearly on the energy, the scattering length a_ℓ and the effective range $r_{e,\ell}$, they are connected to the momentum k and the phase shift δ_ℓ by

$$k^{2\ell+1}\, \cot\delta_\ell = -\frac{1}{a_\ell} + \frac{1}{2}\, r_{e,\ell}\, k^2\,.$$

Specifically, for $E \to 0$

$$k^{2\ell+1}\, \cot\delta_\ell \to -\frac{1}{a_\ell}\,.$$

Since for uncoupled channels $R_{\ell\ell} = \tan\delta_\ell$ it is possible to write

$$R_{\ell\ell} \to -a_\ell\, k^{2\ell+1}\,.$$

A.1.1 Eliminating the energy dependence from the spherical Bessel functions

Focusing on the spherical Bessel function, the asymptotic limit for their argument going to zero is [4]

$$\begin{cases} F_\ell(kr) = j_\ell(x) & \to \quad \dfrac{x^\ell}{(2\ell+1)!!}\,, \\[2ex] G_\ell(kr) = y_\ell(x) & \to \quad -\dfrac{(2\ell-1)!!}{x^{\ell+1}}\,. \end{cases}$$

Using for $E \to 0$ the functions [code]

$$\begin{cases} \tilde{F}_\ell(r) = r^\ell\,, \\ \tilde{G}_\ell(r) = -\dfrac{1}{(2\ell+1)\, r^{\ell+1}}\, \left(1 - e^{-\epsilon r}\right)^{2\ell+1}\,, \end{cases}$$

for $r \to \infty$ it is possible to write

$$\tilde{A}_\ell \left(\tilde{F}_\ell + R\, \tilde{G}_\ell\right) = \tilde{A}_\ell \left(r^\ell - \frac{\tilde{R}_{\ell\ell}}{2\ell+1}\, \frac{1}{r^{\ell+1}}\right)$$

and confronting it with the actual behavior

$$A_\ell\, \left(F_\ell(kr) + R_{\ell\ell}\, G_\ell(kr)\right) \simeq A_\ell \left(\frac{k^\ell r^\ell}{(2\ell+1)!!} - R_{\ell\ell}\, \frac{(2\ell-1)!!}{k^{\ell+1} r^{\ell+1}}\right)$$

it is possible to map

$$\frac{\tilde{R}_{\ell\ell}}{2\ell+1} = \frac{(2\ell+1)!!\,(2\ell-1)!!}{k^{2\ell+1}}\, R_{\ell\ell}$$

and therefore

$$\tilde{R}_{\ell\ell} = -\left[(2\ell+1)!!\right]^2\, a_\ell\,.$$

Coupled case In the case of a coupled channel

$$\begin{cases} A_{\ell_1}\left(F_{\ell_1}(kr) + R_{\ell_1\ell_1}\,G_{\ell_1}(kr) + R_{\ell_1(\ell_2)}\,G_{\ell_2}(kr)\right)\,, \\ A_{\ell_2}\left(F_{\ell_2}(kr) + R_{(\ell_2)\ell_1}\,G_{\ell_1}(kr) + R_{(\ell_2)(\ell_2)}\,G_{\ell_2}(kr)\right) \end{cases}$$

the choice for small energies brings to

$$\begin{cases} \tilde{A}_{\ell_1}\left(r^{\ell_1} - \dfrac{\tilde{R}_{\ell_1\ell_1}}{(2\ell_1+1)}\,\dfrac{1}{r^{\ell_1+1}} - \dfrac{\tilde{R}_{\ell_1\ell_2}}{(2\ell_2+1)}\,\dfrac{1}{r^{\ell_2+1}}\right)\,, \\ \tilde{A}_{\ell_2}\left(r^{\ell_2} - \dfrac{\tilde{R}_{\ell_2\ell_1}}{(2\ell_1+1)}\,\dfrac{1}{r^{\ell_1+1}} - \dfrac{\tilde{R}_{\ell_2\ell_2}}{(2\ell_2+1)}\,\dfrac{1}{r^{\ell_2+1}}\right)\,. \end{cases}$$

Comparing with the actual behavior

$$\begin{cases} A_{\ell_1}\left(\dfrac{k^{\ell_1}\,r^{\ell_1}}{(2\ell_1+1)!!} - \tilde{R}_{\ell_1\ell_1}\,\dfrac{(2\ell_1-1)!!}{k^{\ell_1+1}\,r^{\ell_1+1}} - \tilde{R}_{\ell_1\ell_2}\,\dfrac{(2\ell_2-1)!!}{k^{\ell_2+1}\,r^{\ell_2+1}}\right)\,, \\ A_{\ell_2}\left(\dfrac{k^{\ell_2}\,r^{\ell_2}}{(2\ell_2+1)!!} - \tilde{R}_{\ell_2\ell_1}\,\dfrac{(2\ell_1-1)!!}{k^{\ell_1+1}\,r^{\ell_1+1}} - \tilde{R}_{\ell_2\ell_2}\,\dfrac{(2\ell_2-1)!!}{k^{\ell_2+1}\,r^{\ell_2+1}}\right)\,, \end{cases}$$

it is possible to extract

$$\begin{cases} \tilde{R}_{\ell_1\ell_1} = & [(2\ell_1+1)!!]^2\,\dfrac{R_{\ell_1\ell_1}}{k^{2\ell_1+1}}\,, \\ \tilde{R}_{\ell_1\ell_2} = & (2\ell_1+1)!!\,(2\ell_2+1)!!\,\dfrac{R_{\ell_1\ell_2}}{k^{\ell_1+\ell_2+1}}\,, \\ \tilde{R}_{\ell_2\ell_1} = & (2\ell_1+1)!!\,(2\ell_2+1)!!\,\dfrac{R_{\ell_2\ell_1}}{k^{\ell_1+\ell_2+1}}\,, \\ \tilde{R}_{\ell_2\ell_2} = & [(2\ell_2+1)!!]^2\,\dfrac{R_{\ell_2\ell_2}}{k^{2\ell_2+1}} \end{cases}$$

Since for coupled channels $\ell_2 = \ell + 2$ where $\ell \equiv \ell_1$ it is possible to use Eq. (2) and write

$$\begin{pmatrix} \tilde{R}_{\ell_1\ell_1} & \tilde{R}_{\ell_1\ell_2} \\ \tilde{R}_{\ell_2\ell_1} & \tilde{R}_{\ell_2\ell_2} \end{pmatrix} = \begin{pmatrix} [(2\ell+1)!!]^2\left(\dfrac{\tan\delta_1}{k^{2\ell+1}}\cos^2\epsilon + \dfrac{\tan\delta_2}{k^{2\ell+1}}\sin^2\epsilon\right) & (2\ell+1)!!(2\ell+5)!!\dfrac{\tan\delta_1-\tan\delta_2}{k^{2\ell+3}}\sin\epsilon\cos\epsilon \\ (2\ell+1)!!(2\ell+5)!!\dfrac{\tan\delta_1-\tan\delta_2}{k^{2\ell+3}}\sin\epsilon\cos\epsilon & [(2\ell+5)!!]^2\left(\dfrac{\tan\delta_1}{k^{2\ell+5}}\sin^2\epsilon + \dfrac{\tan\delta_2}{k^{2\ell+5}}\cos^2\epsilon\right) \end{pmatrix}.$$

Simplifying

$$\begin{pmatrix} \tilde{R}_{\ell_1\ell_1} & \tilde{R}_{\ell_1\ell_2} \\ \tilde{R}_{\ell_2\ell_1} & \tilde{R}_{\ell_2\ell_2} \end{pmatrix} = -\begin{pmatrix} [(2\ell+1)!!]^2\left(a_1\,\cos^2\epsilon + a_2\,k^4\sin^2\epsilon\right) & (2\ell+1)!!(2\ell+5)!!\left(a_1 - k^4\,a_2\right)\dfrac{\sin 2\epsilon}{k^2} \\ (2\ell+1)!!(2\ell+5)!!\left(a_1 - k^4\,a_2\right)\dfrac{\sin 2\epsilon}{k^2} & [(2\ell+5)!!]^2\left(a_1\,\dfrac{\sin^2\epsilon}{k^4} + a_2\,\cos^2\epsilon\right) \end{pmatrix}.$$

From this it is possible to infer that, in order for the R matrix to not diverge $\epsilon \simeq k^2$ at least, this is proven in Ref. [3]. Defining

$$e_J = \frac{\epsilon}{k^2}$$

the R matrix becomes

$$\boxed{\begin{pmatrix} \tilde{R}_{\ell_1\ell_1} & \tilde{R}_{\ell_1\ell_2} \\ \tilde{R}_{\ell_2\ell_1} & \tilde{R}_{\ell_2\ell_2} \end{pmatrix} = -\begin{pmatrix} [(2\ell+1)!!]^2\,a_1 & 2(2\ell+1)!!(2\ell+5)!!\,a_1\,e_1 \\ 2(2\ell+1)!!(2\ell+5)!!\,a_1\,e_1 & [(2\ell+5)!!]^2\left(a_1\,e_1^2 + a_2\right) \end{pmatrix}.}$$

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