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:

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

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 Schrï¿½dinger 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 $\boldsymbol{S}$-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 $\boldsymbol{R}$-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:

$$u_\ell(r) = A_\ell \left[F_\ell(kr) \cos\delta_\ell + G_\ell(kr) \sin\delta_\ell \right]$$

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 BB conventions.

5.1 BB phase shifts and mixing angle

Using Tab. 1 the R matrix can be written as

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

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,

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

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

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

The determinant in this case is

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

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

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

and

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

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.

References

[1] L.M. Delves, Advances in Nuclear Physics, vol. 5 (1972), Eds. M. Baranger, E. Vögt (Plenum Press, London, New York).

[2] H.P. Stapp, T. Ypsilantis and N. Metropolis, Phys. Rev. **105**, 302 (1957).

[3] J. M. Blatt and L. C. Biedenharn, Phys. Rev. **86**, 399 (1952).