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:

$$|out\rangle = S|in\rangle$$

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 (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.
- \bullet 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 Schr $\ddot{\imath}_{2}^{\frac{1}{2}}$ dinger 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:

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

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	$e^{2i\delta}$	$\operatorname{diag}(e^{2i\delta_i}) O(\epsilon) \operatorname{diag}(e^{2i\delta_i})$	$O^T(\epsilon)\operatorname{diag}(e^{2i\delta_i})O(\epsilon)$
R	$\tan \delta$	$\operatorname{diag}(\tan \delta_i) O(\epsilon) \operatorname{diag}(\tan \delta_i)$	$O^T(\epsilon) \operatorname{diag}(\tan \delta_i) O(\epsilon)$
О	_	$O(\epsilon) = \begin{pmatrix} \cos 2\epsilon & i \sin 2\epsilon \\ i \sin 2\epsilon & \cos 2\epsilon \end{pmatrix}$	$O(\epsilon) = \begin{pmatrix} \cos \epsilon & \sin \epsilon \\ -\sin \epsilon & \cos \epsilon \end{pmatrix}$

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

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

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

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

Therefore

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

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,

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

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

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

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

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

and

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

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

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