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:

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

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:

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

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

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

and

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

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

$$u_\ell(r) = \tilde{A}_\ell\, kr\ \left(F_\ell + \tan\delta_\ell\, G_\ell\right)\,,$$

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

$$u_\ell(r) = \tilde{A}_\ell\, kr\ \left(F_\ell + R_{\ell\ell}\, G_\ell\right)\,.$$

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

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

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

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

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 $E \rightarrow 0$

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

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

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

It is possible to re-define the variational asymptotic functions to

$$\begin{cases} F_\ell(kr) & \rightarrow & \tilde{F}_\ell(kr) = \sqrt{k^{2\ell+1}}\,F_\ell(kr)\,, \\ G_\ell(kr) & \rightarrow & \tilde{G}_\ell(kr) = -f(r)\dfrac{1}{\sqrt{k^{2\ell+1}}}\,G_\ell(kr)\,, \end{cases}$$

where $f(r)$ goes to zero faster than the denominator of $G_\ell(kr)$ for small r, but otherwise is basically one outside the core.
Using this redefinition, outside the core the reduced radial function becomes

$$u_\ell(kr) = \mathcal{A}_\ell\,kr\left(F_\ell(kr) + \tilde{R}_{\ell\ell}\,G_\ell(kr)\right)$$

with

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

and, for $E \rightarrow 0$,

$$\tilde{R}_{\ell\ell} \rightarrow a_\ell\,.$$

The problem with this approach is that for $E \rightarrow 0$ the asymptotic function tend to zero or to infinity.

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]

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

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

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

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

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

Simplifying

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

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

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

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).

[4] M. Abramowitz, and I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Dover Publications Inc., New York (1965), (page 437).