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)

 $\textbf{Definition:} \quad \text{The S-matrix connects asymptotic incoming and outgoing states:} \\$

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

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 (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	$e^{2i\delta}$	$\operatorname{diag}(e^{2i\delta_i}) O(\epsilon) \operatorname{diag}(e^{2i\delta_i})$	$O^T(\epsilon)\operatorname{diag}(e^{2i\delta_i})O(\epsilon)$
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

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

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

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

Therefore

$$\tan(4\epsilon) = \frac{2R_{12}}{R_{11} - R_{22}} \longrightarrow \epsilon = \frac{1}{2} \arctan\left(\frac{2R_{12}}{R_{11} - R_{22}}\right).$$

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,

$$S = S_{\rm BB} = \begin{pmatrix} e^{2i\delta_1}\cos^2\epsilon + e^{2i\delta_2}\sin^2\epsilon & (e^{2i\delta_1} - e^{2i\delta_2})\sin\epsilon\cos\epsilon \\ (e^{2i\delta_1} - e^{2i\delta_2})\sin\epsilon\cos\epsilon & e^{2i\delta_1}\sin^2\epsilon + e^{2i\delta_2}\cos^2\epsilon \end{pmatrix}.$$
(3)

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

$$\sin(2\epsilon) = \sqrt{-\frac{S_{12}^2}{\det S}} \tag{4}$$

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

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

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 Asymptotic expansion at low energies

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

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

where j_{ℓ} (y_{ℓ}) is the regular (irregular) spherical Bessel function. In case of a long range potential of the type $\propto 1/r$

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

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

6.1 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

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

6.1.1 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]

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

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

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

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

$$\frac{\tilde{R}_{\ell\ell}}{2\ell+1} = \frac{(2\ell+1)!! (2\ell-1)!!}{k^{2\ell+1}} R_{\ell\ell}$$
 (5)

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

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

Comparing with the actual behavior

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

it is possible to extract

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

It is possible to use Eq. (2) and write

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

Simplifying using $\ell_2 = \ell + \Delta \ell$ where $\ell \equiv \ell_1$

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

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

$$e_J \equiv \frac{\epsilon}{k^{\Delta \ell}}$$

the R matrix becomes

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

Notice that these results are in the BB parametrization!

6.2 BB scattering lengths a_i and mixing constant e_J

In this case it is possible to solve for a_1 , a_2 and e_J

$$\begin{cases}
a_{1} = -\frac{R_{\ell_{1}\ell_{1}}}{[(2\ell+1)!!]^{2}}, \\
e_{J} = \frac{(2\ell+1)!! \,\tilde{R}_{\ell_{1}\ell_{2}}}{(2(\ell+\Delta\ell)+1)!! \,\tilde{R}_{\ell_{1}\ell_{1}}}, \quad \text{and} \quad
\begin{cases}
\delta_{1} \simeq -a_{1} \,k^{2\ell_{1}+1}, \\
\epsilon \simeq e_{J} \,k^{\Delta\ell}, \\
\delta_{2} \simeq -a_{2} \,k^{2\ell_{2}+1}.
\end{cases}$$

$$a_{2} = \frac{\tilde{R}_{\ell_{1}\ell_{2}}^{2} - \tilde{R}_{\ell_{1}\ell_{1}} \tilde{R}_{\ell_{2}\ell_{2}}}{(2(\ell+\Delta\ell)+1)!! \,\tilde{R}_{\ell_{1}\ell_{1}}}, \quad (6)$$

6.3 Stapp scattering lengths \tilde{a}_i and mixing constant \tilde{e}_J

Inserting Eq. (3) into Eq. (4)

$$\sin 2\tilde{\epsilon} = \frac{1}{2} \sqrt{-e^{-2i(\delta_1 + \delta_2)} \left(e^{2i\delta_1} - e^{2i\delta_2}\right)^2 \sin^2(2\epsilon)},$$

where δ_1 , δ_2 and ϵ are respectively the scattering length of the first and second channel, and the mixing angle in the BB parametrization. From now on the quantities in the Stapp parametrization will have a tilde on top of them. Reporting here the solution from Eq. (7) (appendix)

$$\tilde{\epsilon} \simeq -a_1 e_1 k^{\ell_1 + \ell_2 + 1}$$

and defining

$$\tilde{e}_J \equiv \frac{\tilde{\epsilon}}{k^{\ell_1 + \ell_2 + 1}}$$

one finds

$$\tilde{e}_J = -a_1 \, e_J \, .$$

In the appendix it is also proved that

$$\tilde{a}_1 = a_1$$

and

$$\tilde{a}_2 = a_2 + a_1 e_J^2 \,.$$

To summarize

$$\begin{cases} \tilde{a}_1 &= a_1 \,, \\ \tilde{e}_J &= -a_1 \, e_J \,, \\ \tilde{a}_2 &= a_2 + a_1 \, e_J^2 \,, \end{cases} \quad \text{and} \quad \begin{cases} \tilde{\delta}_1 &\simeq -\tilde{a}_1 \, k^{2\ell_1 + 1} \,, \\ \tilde{\epsilon} &\simeq \tilde{e}_J \, k^{\ell_1 + \ell_2 + 1} \,, \\ \tilde{\delta}_2 &\simeq -\tilde{a}_2 \, k^{2\ell_2 + 1} \,. \end{cases}$$

6.4 The effective range

Starting from the uncoupled channel and taking Eq. (5) one can write

$$\tilde{R}_{\ell\ell} = \left[(2\ell+1)!! \right]^2 \, \frac{R_{\ell\ell}}{k^{2\ell+1}} = \left[(2\ell+1)!! \right]^2 \, \frac{1}{k^{2\ell+1} \, \cot \delta_\ell} \, .$$

Recalling the expansion

$$k^{2\ell+1} \cot \delta_{\ell} \simeq -\frac{1}{a} + \frac{1}{2} r_0 k^2 + b k^4 + \mathcal{O}(k^5)$$
,

it is easy to evaluate

$$\mathcal{R}(k) = -2 \left[(2\ell + 1)!! \right]^2 \frac{\tilde{R}_{\ell\ell}(k) - \tilde{R}_{\ell\ell}(0)}{k^2 \, \tilde{R}_{\ell\ell}^2(0)} \,.$$

To make things simpler it is better to define $f \equiv (2\ell + 1)!!$,

$$\mathcal{R}(k) = -\frac{2\cancel{f^{2}}}{k^{2}} \frac{\left(\frac{1}{-\frac{1}{a} + \frac{1}{2} r_{0} k^{2} + b k^{4}} - \frac{1}{-\frac{1}{a}}\right)}{\cancel{f^{2}} a^{2}} = -\frac{2}{a^{2} k^{2}} \left(\frac{1}{-\frac{1}{a} + \frac{1}{2} r_{0} k^{2} + b k^{4}} + a\right).$$

This can be further simplified to

$$\mathcal{R}(k) = \frac{2}{a^2 \, k^2} \, \left(\frac{2a}{-2 + a \, r_0 \, k^2 + 2ab \, k^4} + a \right) = -\frac{2}{\mathbf{z}^2 \, \mathbf{z}^2} \underbrace{\mathbf{z}^2 - \mathbf{z}^2 + \mathbf{z}^2 r_0 \, \mathbf{z}^2 + 2ab \, k^4}_{-2 + a \, r_0 \, k^2 + 2ab \, k^4}$$

or

$$\mathcal{R}(k) = -2 \, \frac{r_0 + 2b \, k^2}{-2 + a \, r_0 \, k^2 + 2ab \, k^4}.$$

For $k \to 0$

$$\mathcal{R}(k) = r_0 \left(1 + \frac{1}{2} \left(a r_0 + \frac{4b}{r_0} \right) k^2 \right) + \mathcal{O}(k^4) = r_0 + \mathcal{O}(E).$$

Unfortunately so far the code seems to unstable to evaluate this or there is a problem with formulas/code.

A Proving Stapp expansions

Another way to calculate $\tilde{\epsilon}$ is

$$\sin 2\tilde{\epsilon} = \frac{S_{12}}{i\sqrt{\det S}}.$$

Using the BB version of the S-matrix

$$\det S = \det \left(O^T(\epsilon) \begin{pmatrix} e^{2i\delta_1} & 0 \\ 0 & e^{2i\delta_2} \end{pmatrix} O(\epsilon) \right) = \det \left(O(\epsilon) \right)^2 \, \det \begin{pmatrix} e^{2i\delta_1} & 0 \\ 0 & e^{2i\delta_2} \end{pmatrix} = e^{2i(\delta_1 + \delta_2)} \, .$$

Therefore

$$\sin 2\tilde{\epsilon} = -i \frac{\left(e^{2i\delta_1} - e^{2i\delta_2}\right) \sin \epsilon \cos \epsilon}{e^{i(\delta_1 + \delta_2)}}.$$

Using Eq. (6), for $k \to 0$, δ_1 , δ_2 and ϵ get to zero and

$$\tilde{\epsilon} \simeq -\frac{1}{2}\arcsin\left(i\frac{(\cancel{1}+2i\delta_1-\cancel{1}-2i\delta_2)\epsilon}{1}\right) \simeq (\delta_1-\delta_2)\epsilon \simeq (-a_1\,k^{2\ell+1}+a_2\,k^{2\ell+1+2\Delta\ell})e_J\,k^{\Delta\ell}\,.$$

Therefore

$$\tilde{\epsilon} \simeq -a_1 e_J k^{2\ell+1+\Delta\ell}$$

and finally

$$\tilde{\epsilon} \simeq -a_1 \, e_J \, k^{\ell_1 + \ell_1 + 1} \,. \tag{7}$$

For $\tilde{\delta}_1$ one can write

$$e^{2i\tilde{\delta}_1} = \frac{S_{11}}{\cos 2\tilde{\epsilon}} \,.$$

Therefore

$$e^{2i\tilde{\delta}_1} = \frac{e^{2i\delta_1}\cos^2\epsilon + e^{2i\delta_2}\sin^2\epsilon}{\cos\left[-2/2 \arctan\left(-i\frac{(e^{2i\delta_1}-e^{2i\delta_2})\sin\epsilon\cos\epsilon}{e^{i(\delta_1+\delta_2)}}\right)\right]}.$$

Using

$$\cos(\arcsin x) = \sqrt{1 - \sin^2(\arcsin x)} = \sqrt{1 - x^2}$$

it simplifies to

$$e^{2i\tilde{\delta}_1} = \frac{e^{2i\delta_1}\cos^2\epsilon + e^{2i\delta_2}\sin^2\epsilon}{\sqrt{1 + e^{-2i(\delta_1 + \delta_2)}(e^{2i\delta_1} - e^{2i\delta_2})^2\sin^2\epsilon\cos^2\epsilon}}.$$

Since $\epsilon \to 0$, and $\delta_i \to 0$ for small energies one finds

$$e^{2i\tilde{\delta}_1} \simeq e^{2i\delta_1}$$

and

$$\tilde{\delta}_1 \simeq \delta_1 \simeq -a_1 \, k^{2\ell_1+1} \, .$$

Here the fact that $\delta_2 = \mathcal{O}(\delta_1)$ has been used. Therefore

$$\tilde{a}_1 = a_1$$
.

Finally one finds $\tilde{\delta}_2$ using

$$e^{2i\tilde{\delta}_2} = \frac{S_{22}}{\cos 2\tilde{\epsilon}} \,.$$

which expands to

$$e^{2i\tilde{\delta}_2} = \frac{e^{2i\delta_1}\sin^2\epsilon + e^{2i\delta_2}\cos^2\epsilon}{\sqrt{1 + e^{-2i(\delta_1 + \delta_2)}(e^{2i\delta_1} - e^{2i\delta_2})^2\sin^2\epsilon\cos^2\epsilon}}.$$

For small energies

$$1 + 2i\tilde{\delta}_2 \simeq (1 + 2i\delta_1) \epsilon^2 + (1 + 2i\delta_2) \left(1 - \frac{\epsilon^2}{2}\right)^2,$$

$$1 + 2i\tilde{\delta}_2 \simeq \epsilon^2 + 2i\delta_1 \epsilon^2 + (1 + 2i\delta_2) \left(1 - \epsilon^2\right),$$

$$1 + 2i\tilde{\delta}_2 \simeq \cancel{e}^2 + 2i\delta_1 \epsilon^2 + \cancel{1} + 2i\delta_2 - \cancel{e}^2,$$

$$\tilde{\delta}_2 \simeq \delta_2 + \delta_1 \epsilon^2.$$

Using the expansion for small energies

$$\begin{split} -\tilde{a}_2 \, k^{2\ell_2+1} &= -a_2 \, k^{2\ell_2+1} - a_1 \, e_J^2 \, k^{2\ell_1+1+2\Delta\ell} \, , \\ \tilde{a}_2 \, k^{2\ell_2+1} &= a_2 \, k^{2\ell_2+1} + a_1 \, e_J^2 \, k^{2\ell_2+1} \, . \end{split}$$

Therefore finally

$$\tilde{a}_2 = a_2 + a_1 e_J^2$$
.

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