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

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Contents

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,

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

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

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

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

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

and

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

6 Asymptotic expansion at low energies

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

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

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

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

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]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{cases} a_1 & = -\dfrac{\tilde{R}_{\ell_1\ell_1}}{[(2\ell+1)!!]^2}\,, \\ e_J & = \dfrac{(2\ell+1)!!\,\tilde{R}_{\ell_1\ell_2}}{(2(\ell+\Delta\ell)+1)!!\,\tilde{R}_{\ell_1\ell_1}}\,, \\ a_2 & = \dfrac{\tilde{R}^2_{\ell_1\ell_2} - \tilde{R}_{\ell_1\ell_1}\tilde{R}_{\ell_2\ell_2}}{(2(\ell+\Delta\ell)+1)!!\,\tilde{R}_{\ell_1\ell_1}}\,, \end{cases} \qquad \text{and} \qquad \begin{cases} \delta_1 & \simeq -a_1\,k^{2\ell_1+1}\,, \\ \epsilon & \simeq e_J\,k^{\Delta\ell} \\ \delta_2 & \simeq -a_2\,k^{2\ell_2+1}\,. \end{cases} \tag{6}$$

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)

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

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

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

6.4 The effective range

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

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

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

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

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

$$\mathcal{R}(k) = -\frac{2\cancel{f^2}}{k^2}\, \frac{\cancel{f^2}\left(\dfrac{1}{-\frac{1}{a} + \frac{1}{2}\, r_0\, k^2 + b\, k^4} - \dfrac{1}{-\frac{1}{a}}\right)}{\cancel{f^4}\, a^2} = -\frac{2}{a^2\, k^2}\left(\frac{1}{-\frac{1}{a} + \frac{1}{2}\, r_0\, k^2 + b\, k^4} + a\right)\,.$$

This can be further simplified to

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

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

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

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

$$e^{2i\tilde{\delta}_1} = \frac{e^{2i\delta_1}\cos^2\epsilon + e^{2i\delta_2}\sin^2\epsilon}{\cos\left[-\cancel{2}\frac{1}{\cancel{2}}\arcsin\left(-i\frac{(e^{2i\delta_1}-e^{2i\delta_2})\sin\epsilon\cos\epsilon}{e^{i(\delta_1+\delta_2)}}\right)\right]}\,.$$

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

$$
\begin{aligned}
1 + 2i\tilde{\delta}_2 &\simeq (1 + 2i\delta_1)\,\epsilon^2 + (1 + 2i\delta_2)\left(1 - \frac{\epsilon^2}{2}\right)^2 , \\
1 + 2i\tilde{\delta}_2 &\simeq \epsilon^2 + 2i\delta_1\,\epsilon^2 + (1 + 2i\delta_2)\left(1 - \epsilon^2\right) , \\
\cancel{1} + 2i\tilde{\delta}_2 &\simeq \cancel{\epsilon^2} + 2i\delta_1\,\epsilon^2 + \cancel{1} + 2i\delta_2 - \cancel{\epsilon^2} , \\
\tilde{\delta}_2 &\simeq \delta_2 + \delta_1\,\epsilon^2 .
\end{aligned}
$$

Using the expansion for small energies

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

Therefore finally

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

References

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