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Computing the Phase Shift

Eller noe slikt

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Abstract

GitHub repository: https://github.com/ErlendLima/NuclearForces

Contents

1 Introduction

The interactions between nucleons is [fullfør] In contrast to the electromagnetic force, there is no fundamental theory of the strong force. As the quarks and gluons dance together within nuclei, their strong interaction leaks out as the residual nuclear force, binding the nucleons together. As such, the nucleon-nucleon interaction must be described by approximations and phenomenological models.

The phase shift is a useful proxy for understanding nucleon-nucleon interaction, acting as a bridge between empirically obtained cross sections and theoretical models. Among these theoretical tools to compute the phase section are the K-matrix theory and the variable phase approach (VPA). Both of these are herein investigated by applying them to a two-nucleon system, implemented in the https://julialang.org/.

2 Theory

Quantum scattering is a very complicated process, behaving so differently from the classical case of billiard balls that our intuition breaks down. Fortunately, the intricacies of the scattering process itself can be conveniently omitted by instead focusing on the relationship between the initial and resulting states, illustrated in FIGURE. Specifically, the true state $|\psi\rangle$ is related to the asymptotic incoming and outgoing states $|\psi_{\text{in}}\rangle$ and $|\psi_{\text{out}}\rangle$ through the so-called Møller operators $\Omega_{\pm}$:

$$|\psi\rangle = \Omega_{+} |\psi_{\text{in}}\rangle = |\phi+\rangle$$
$$|\psi\rangle = \Omega_{-} |\psi_{\text{out}}\rangle = |\phi-\rangle .$$

[Add some history of Møller]

If time dependence is added, the Møller operations allows one to move between the asymptotic states and the actual state at time t. Combining them, the outgoing state is related to the incoming state by

$$|\psi_{\text{out}}\rangle = \Omega_{-}^{\dagger} \Omega_{+} |\psi_{\text{in}}\rangle = \mathcal{S} |\psi_{\text{in}}\rangle$$

giving the definition of the scattering operator $\mathcal{S}$. In the general case let $|\chi-\rangle$ and $|\Phi+\rangle$ by any arbitrary orbits. The probability of the process $|\chi-\rangle \leftarrow |\Phi+\rangle$ occurring is then the square of the matrix element of $\mathcal{S}$:

$$w(\chi \leftarrow \Phi) = |\langle \chi - | \Phi + \rangle|^2 = |\langle \chi | \mathcal{S} | \Phi \rangle|^2 .$$

The probability w is itself not observable, however, the related quantity cross-section $\sigma(\chi \leftarrow \Phi)$ is. The outgoing particle can scatter in a solid angle $d\Omega$, oriented in the direction of momentum $\vec{p}$. Likewise, the incoming particle can be described as wave packets with narrowly defined momentum $\vec{p_0}$. It can then be shown that[CITE] the differential cross section is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\vec{p} \leftarrow \vec{p_0})|^2$$

with $f(\vec{p} \leftarrow \vec{p_0})$ being the scattering amplitude, as known from elementary scattering theory. Note that only the magnitude of f can be obtained through the cross-section.

The next step is to relate cross-section to the scattering operator. It can be shown that $\mathcal{S}$ commutes with the free Hamiltonian$\mathcal{H}_0$

$$\mathcal{H} = \mathcal{H}_0 + V \qquad [\mathcal{H}_0, \mathcal{S}] = 0$$

Letting $|\mathrm{p}\rangle$ be the eigenvectors of $\mathcal{H}_0$ in momentum basis, we have

$$\langle \mathrm{p}'|[\mathcal{H}_0, \mathcal{S}]|\mathrm{p}\rangle = (E_{p'} - E_p)\langle \mathrm{p}'|\mathcal{S}|\mathrm{p}\rangle = 0$$

implying that $\langle \mathrm{p}'|\mathcal{S}|\mathrm{p}\rangle$ is zero except for $E_{p'} = E_p$. This leads to the form

$$\langle \mathrm{p}'|\mathcal{S}|\mathrm{p}\rangle = \delta(E_{p'} - E_p) \times \text{remainder}$$

At this point it is fruitful to define a new operator $\mathcal{R} \equiv 1 - \mathcal{S}$. $\mathcal{R}$ is the difference between the case of scattering and no scattering. It too commutes with $\mathcal{H}_0$, and so has the form

$$\langle \mathrm{p}'|\mathcal{R}|\mathrm{p}\rangle = -2\pi i \delta(E_{p'} - E_p) t(\mathrm{p}' \leftarrow \mathrm{p})$$

with the factors $-2\pi i$ and $t(\mathrm{p}' \leftarrow \mathrm{p})$ introduced for future convenience. The elements of $\mathcal{S}$ can therefore be written

$$\langle \mathrm{p}'|\mathcal{S}|\mathrm{p}\rangle = \delta(\mathrm{p}' - \mathrm{p}) - 2\pi i \delta(E_{p'} - E_p) t(\mathrm{p}' \leftarrow \mathrm{p}).$$

The first term describes the situation where no scattering occurs, while the second is the amplitude when the wave is actually scattered. The function $t(\mathrm{p}' \leftarrow \mathrm{p})$ is continuous for most potentials and analytic for many, but only defined for the "shell" $\mathrm{p}'^2 = \mathrm{p}^2$. However unphysical, it is computationally beneficial to define an operator $\mathcal{T}$ whose matrix elements $\langle \mathrm{p}'|T|\mathrm{p}\rangle$ are defined for all p and coincide with the values of t on the shell.

The scattering amplitude can be shown to be related to the on-shell $\mathcal{T}$ matrix elements as[cite]

$$f(\mathrm{p}' \leftarrow \mathrm{p}) = -(2\pi)^2 m t(\mathrm{p}' \leftarrow \mathrm{p}).$$

The elements of the scattering matrix can from this be directly related to the scattering amplitude as

$$\langle \mathrm{p}'|\mathcal{S}|\mathrm{p}\rangle = \delta(\mathrm{p}' - \mathrm{p}) - \frac{i}{2\pi m}\delta(E_{p'} - E_p) f(\mathrm{p}' \leftarrow \mathrm{p}).$$

2.1 The Spherical Case

Introducti

As known from elementary quantum mechanics, $\mathcal{H}^0$ commutes with the angular momentum operator $\mathcal{L}^2$ and z-axis projection $\mathcal{L}_3$. These three operators form a complete set of commuting observables. Since $\mathcal{S}$ commutes with $\mathcal{H}^0$, $\mathcal{S}$ too commutes with the aforementioned operators, and is diagonal in the common basis, namely the basis of spherical waves $\{|Elm\rangle\}$, with $E, l(l+1)$ and m being the eigenvalues for $\mathcal{H}^0$, $\mathcal{L}^2$ and $\mathcal{L}_3$ respectively. Since this basis diagonalizes $\mathcal{S}$, its matrix elements are

$$\langle E'l'm'|\mathcal{S}|Elm\rangle = \delta(E' - E)\delta_{l'l}\delta_{m'm} s_l(E).$$

$\mathcal{S}$ can be shown to be unitary, implying the eigenvalues $s_l(E)$ must have modulus one, justifying the form

$$\langle E'l'm'|\mathcal{S}|Elm\rangle = \delta(E'-E)\delta_{l'l}\delta_{m'm}\exp(2i\delta_l(E))$$

The quantity $\delta_l(E)$ is the important phase shift, an observable obtainable from both experiment and numerical calculations. It is purely real with an inherent ambiguity modulo π, as seen from

$$\exp(2i[\delta_l + n\pi]) = \exp(2i\delta_l)\exp(2in\pi) = \exp(2i\delta_l).$$

The decomposition of $f(\mathrm{p}' \leftarrow \mathrm{p})$ into partial waves can be obtained by exploiting the relation

$$\langle \mathrm{p}'|(\mathcal{S}-1)|\mathrm{p}\rangle = \frac{i}{2\pi m}\delta(E'-E)f(\mathrm{p}' \leftarrow \mathrm{p}). \tag{2.1}$$

Inserting a complete set of states of the left hand side gives

$$\begin{aligned}
\langle \mathrm{p}'|(\mathcal{S}-1)|\mathrm{p}\rangle &= \int \mathrm{d}E \sum_{l,m} \langle \mathrm{p}'|(\mathcal{S}-1)|Elm\rangle \langle Elm|\mathrm{p}\rangle \\
&= \int \mathrm{d}E \sum_{l,m} (s_l(E)-1) \langle \mathrm{p}'|Elm\rangle \langle Elm|\mathrm{p}\rangle \\
&= \frac{1}{mp}\delta(E_{p'}-E_p)\sum_{l,m} Y_l^m(\hat{\mathrm{p}}')[s_l(E_p)-1]Y_l^m(\hat{\mathrm{p}})^*
\end{aligned}$$

where Y_l^m is the spherical harmonical and hat denotes unit vector. Combining this with (2.1), the amplitude can be decomposed to

$$f(\mathrm{p}' \leftarrow \mathrm{p}) = \frac{2\pi}{ip}\sum_{l,m} Y_l^m(\hat{\mathrm{p}}')[s_l(E_p)-1]Y_l^m(\hat{\mathrm{p}})^*$$

Letting $\hat{\mathrm{p}}$ lie along z and noting independence of m [WHY], we define

$$f(E_p,\theta) \equiv f(\mathrm{p}' \leftarrow \mathrm{p}) = \frac{1}{2ip}\sum_l (2l+1)[s_l(E_p)-1]P_l(\cos\theta)$$

This leads to the natural definition of the partial wave amplitude as

$$f_l(E) \equiv \frac{s_l(E)-1}{2ip} = \frac{\exp[2i\delta_l(\theta)]-1}{2ip} = \frac{\exp[2i\delta_l(E)]\sin\delta_l(E)}{p}$$

Analogously the total cross-section can be decomposed into partial wave cross-sections, giving

$$\sigma(p) = \sum_l \sigma_l(p) = \sum_l 4\pi(2l+1)\left|f_l(p)\right|^2 = \sum_l 4\pi(2l+1)\frac{\sin^2\delta_l}{p^2}$$

The magnitude of each partial wave cross-section is from this constrained by the so called unitary bound:

$$|\sigma_l| \leq 4\pi\frac{2l+1}{p^2}.$$

The maximal value is only reached if δ_l is an odd multiple of $\pi/2$

2.2 Green's Function

[Introduce motivation for free and full Green]

[Trivially derive LS]

2.3 Lippman Schwinger

[Use LS for G to derive it for T]

2.4 The K-Matrix

[This section was written before I understood the connection between K and T. Use it to motivate the introduction and resulting computation of K]

To actually obtain the phase shifts numerically, we turn to yet another matrix, the K-matrix[*]. Its associated operator $\mathcal{M}$ is the Caley transform of $\mathcal{S}$, ensuring $\mathcal{M}$ is Hermitian:

$$\mathcal{M} = i\frac{1-\mathcal{S}}{1+\mathcal{S}}.$$

The K-matrix is defined as the matrix elements of $\mathcal{M}$

$$\langle \mathrm{p}'|\mathcal{M}|\mathrm{p}\rangle = \delta(E_{p'} - E_p)k(\mathrm{p}' \leftarrow \mathrm{p}).$$

When $\mathcal{S}$ is symmetric, $\mathcal{M}$ is both Hermitian and symmetric, implying its matrix elements are real. As with $\mathcal{S}$ and $\mathcal{R}$, $\mathcal{M}$ becomes diagonal in the basis $\{|Elm\rangle\}$:

$$\begin{aligned}
\langle E'l'm'|\mathcal{S}|Elm\rangle &= \delta(E_{p'} - E_p)\delta_{l',l}\delta_{m',m}s_l(E) \\
\langle E'l'm'|\mathcal{R}|Elm\rangle &= \delta(E_{p'} - E_p)\delta_{l',l}\delta_{m',m}2ipf_l(E) \\
\langle E'l'm'|\mathcal{M}|Elm\rangle &= \delta(E_{p'} - E_p)\delta_{l',l}\delta_{m',m}k_l(E).
\end{aligned}$$

The elements $k_l(E)$ will in this case be real, and are directly related to the phase shifts:

$$k_l = i\frac{1-s_l}{1+s_l} = \tan\delta_l.$$

[fix factor 1/p]

It can be shown that in the same way as $\mathcal{S}$ is related to expansion into plane wave stationary states $|\mathrm{p}\pm\rangle$, $\mathcal{M}$ is related to expansion into standing waves $|\mathrm{p}s\rangle$

[Expand a bit on standing waves]

[Derive Heitler's equation]

2.5 Bound States and Levinson's Theorem

[The Jost function] [Poles of S] [Levinson]

[*] The nomenclature of the K-matrix is a mess. It is also called the R-matrix, the T-matrix, the reaction matrix, the reactance matrix, the dampening matrix, the distortion matrix, and Heitler's matrix. To avoid overworking any of the other letters, I follow the style of Taylor.

2.6 Potentials

2.6.1 The Square Well

Near and dear to everyone is the square well potential; a simple discontinuous potential with value V_0 in the interacting region and zero everywhere else:

$$V(r) = \begin{cases} V_0 & \text{for } 0 \leq r \leq R \\ 0 & \text{for } r > R \end{cases}$$

The potential is plotted in Fig. 2.1

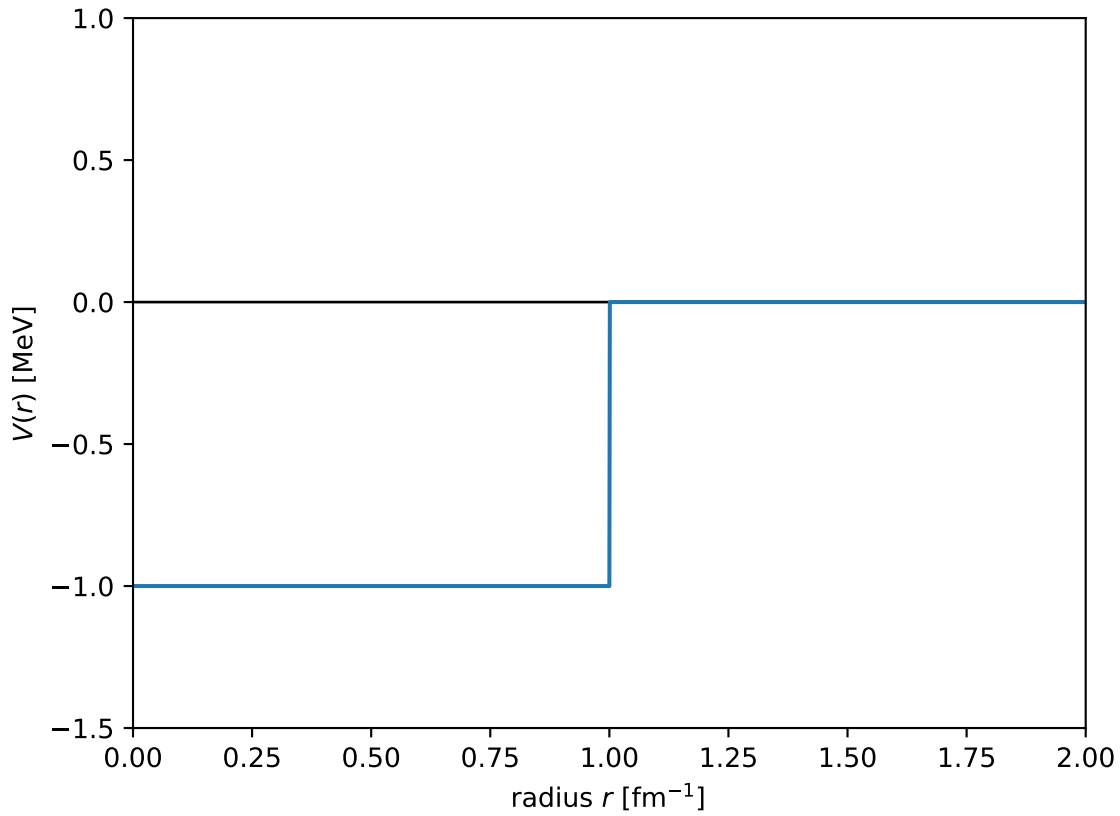

Figure 2.1: An attractive square well potential with $V_0 = -1$ MeV.

[Analytical Solutions]

2.6.2 The Yukawa Potential

[HISTORY]

The Yukawa potential was later generalized into a class of generalized Yukawa potentials. They are potentials build on superpositions of Yukawa potentials:

$$V(r) = \sum_{i=1}^{N} C_i \frac{e^{-\eta_i r}}{r}$$

for some coefficients C_i and η_i.

A specific instance of a generalized Yukawa potential is the Reid potential. It is a parameterized potential between a proton and a neutron for the partial wave ${}^1S_0$, consisting of three terms:

$$V(r) = V_a \frac{e^{-ax}}{x} + V_b \frac{e^{-bx}}{x} + V_c \frac{e^{-cx}}{x}$$

where $x = \mu r$, $\mu = 0.7$ MeV, $V_a = -10.463$ MeV, $V_b = -1650.6$ MeV, $V_c = 6484.3$ MeV, and $a = 1$, $b = 4$ and $c = 7$. [History of Reid].

2.6.3 Momentum Basis

Going from position basis to momentum space requires a change of basis, achieved through a Fourier transform. The problem is multidimensional, requiring a generalized Fourier transform. As we are only dealing with spherically symmetric and central potentials, the more suitable Hankel transform[†] can be used. For s-waves, it takes the form:

$$V_l(k, k') = \int_0^\infty j_0(kr) V(r) j_0(k'r) r^2 \mathrm{d}r.$$

[Square well in momentum basis]

[Reid in momentum basis]

3 Method

3.1 Discretizing Lippman-Schwinger

The equation [REF] can be solved numerically by iteration. To this end it is discretized through a series of steps. The principal value poses a problem due to the limited precision of computers. To step around this, the integral is rewritten. The function $\frac{1}{k-k_0}$ is even about k_0, hence having parts of the curve above and below the x-axis, meaning

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}k}{k - k_0} = 0.$$

Breaking the integral into its positive and negative parts and performing the substitution $k \to -k$ in the negative part then yields

$$\int_0^\infty \frac{\mathrm{d}k}{k^2 - k_0^2} = 0$$

The principal value can now be expressed as

$$\mathcal{P} \int_0^\infty \frac{f(k)}{k^2 - k_0^2} \mathrm{d}k = \int_0^\infty \frac{f(k) - f(k_0)}{k^2 - k_0} \mathrm{d}k$$

[†]The Hankel transform can be regarded as the Fourier transform in hyperspherical coordinates, expanding the function in Bessel functions instead of sines and cosines.

The integral is no longer singular at k_0, instead being proportional to $\frac{\mathrm{d}f}{\mathrm{d}k}$, allowing it to be computed numerically.

In particular, [REF] can be recast to the form

$$K(k,k') = V(k,k') + \frac{2}{\pi}\int_0^\infty \mathrm{d}q \frac{q^2 V(k,q)K(q,k' - k_0^2 V(k,k_0)K(k_0,k')}{(k_0^2 - q^2)/m}$$

The integral is approximated through

$$\int_{-1}^{1} f(x)\mathrm{d}x \approx \sum_{i=1}^{N} f(x_i)w_i$$

for N lattice points through the corresponding weights w_i and points $x_i \in [-1,1]$. This is done through Gaussian-Legendre quadrature, using Legendre polynomials to construct the weights and corresponding points. To map the integral from $[-1,1]$ to $[0,\mathrm{inf}]$, the points and weights are transformed by

$$k_i = C \times \tan\frac{\pi}{4}(1+x_i)$$
$$w_i = C \times \frac{\pi}{4}\frac{w_i}{\cos^2\left(\frac{\pi}{4}(1-x_i)\right)}$$

where C is a constant to fix the units.

Applied to our problem, it is discretized into

$$K(k,k') = V(k,k') + \frac{2}{\pi}\sum_{i=1}^{N}\frac{w_j k_j^2 V(k,k_j)K(k_j,k')}{(k_0^2 - k_j^2)/m} - \frac{2}{\pi}k_0^2 V(k,k_0)K(k_0,k')\sum_{n=1}^{N}\frac{w_n}{(k_0^2 - k_n^2)/m}.$$

There are $N \times N$ unknowns for $K(k,k')$, plus 1 for $K(k_0,k_0)$, for a total of $N+1$ unknowns. They can be described by a single extended K-matrix. Defining another matrix A as

$$A_{i,j} = \delta_{i,j} - V(k_i,k_j)u_k$$

with

$$u_j = \frac{2}{\pi}\frac{w_j k_j^2}{(k_0^2 - k_j^2)/m} \qquad \text{for } j = 1,2,\ldots,N$$
$$u_{N+1} = -\frac{2}{\pi}\sum_{j=1}^{N}\frac{k_0^2 w_j}{(k_0^2 - k_j^2)/m}.$$

The implementation of this main loop is shown in Section 3.1

The equation can now be rendered as the matrix equation

Listing 1 The main loop of the K-matrix method.

```
function createA(V, k,  , m)
    N = length(k)-1
    k  = k[end]
    A = diagm(0 => repeat([1.0,], N+1))
    u  = 0.0

    @inbounds for j in 1:N+1
        u  = 0.0
        if j   N+1
            u  = 2/  *  [j]*k[j]^2/((k ^2 - k[j]^2)/m)
        else
            for n in 1:N
            u  +=  [n]*k ^2/((k ^2 - k[n]^2)/m)
            end
            u  *= -2/
        end

        for i in 1:N+1
            A[i, j] -= V[i, j] * u
        end
    end
    return A
end
```

$$AK = V.$$

Solving for K then simply amounts to inverting A and computing the product

$$K = A^{-1}V. \tag{3.1}$$

As known from [REF], the diagonal of K is proportional to the phase shift

$$K(k_{N+1}, k_{N+1}) = K(k_0, k_0) = -\frac{1}{mk_0}\tan\delta_0(k_0)$$

The number of mesh points N controls both the accuracy and the computation resources, demanding more memory and time as N increases. Running over the $(N+1)\times(N+1)$ matrices scales as roughly $\mathcal{O}(N+1)^2$ in both time and memory allocation. This is the expected behavior to compare to when measuring its actual resource usage.

3.2 Variable Phase Approach

In contrast to the LS approach, implementing the variable phase approach is straightforward. Julia has a very good differential equations solver DifferentialEq.jl[1], which is used for the actual computation. Since the limit in the relation $\delta(k) = \lim_{\rho\to\infty}\delta(k,\rho)$ can not be taken to infinity on a computer, ρ is instead substituted with a very large number, like 5. There

Listing 2 Implementation of VPA in Julia [Fix stupid UTF8]

```
struct VPA <: Method
  rspan::Tuple{Float64, Float64}  # Range of the interaction
end
VPA() = VPA((1e-4, 15.0))


function (vpa::VPA)(k, m, V::Potential)
    m = m/2

    function d dr( , p, r)
      -1.0/k * 2.0m * V(r) * sin(k*r +  )^2
    end

     0 = 0.0

    prob = ODEProblem(d dr,  0, vpa.rspan)
    sol = solve(prob, maxiters=10000, reltol=1e-8)

      = sol.u[end]
end
```

is a trade-off between accuracy and computation time, with smaller ρ giving lesser accuracy while taking shorter time to compute, assuming the same step length is being used. To find the optimal ρ, several values were tried and the result compared to a high ρ.

The code implementation is shown in Listing 2

3.3 The Potentials

Two potentials are examined: the square well and the Reid potential. The former has analytical solutions and is relatively simple to understand, and will be used as a check on the implementation of the methods and to illustrate concepts discussed in the theory. The latter is more complicated, being a sum of three Yukawa potentials with the intent on modeling NN-interactions, with coefficients fitted to data.

Their precise implementation is not interesting, but is available in the file potentials.jl.

4 Results and Discussion

4.1 The Square Well Potential

4.2 The Reid Potential

4.2.1 K-Matrix

4.2.2 VPA

5 Conclusion

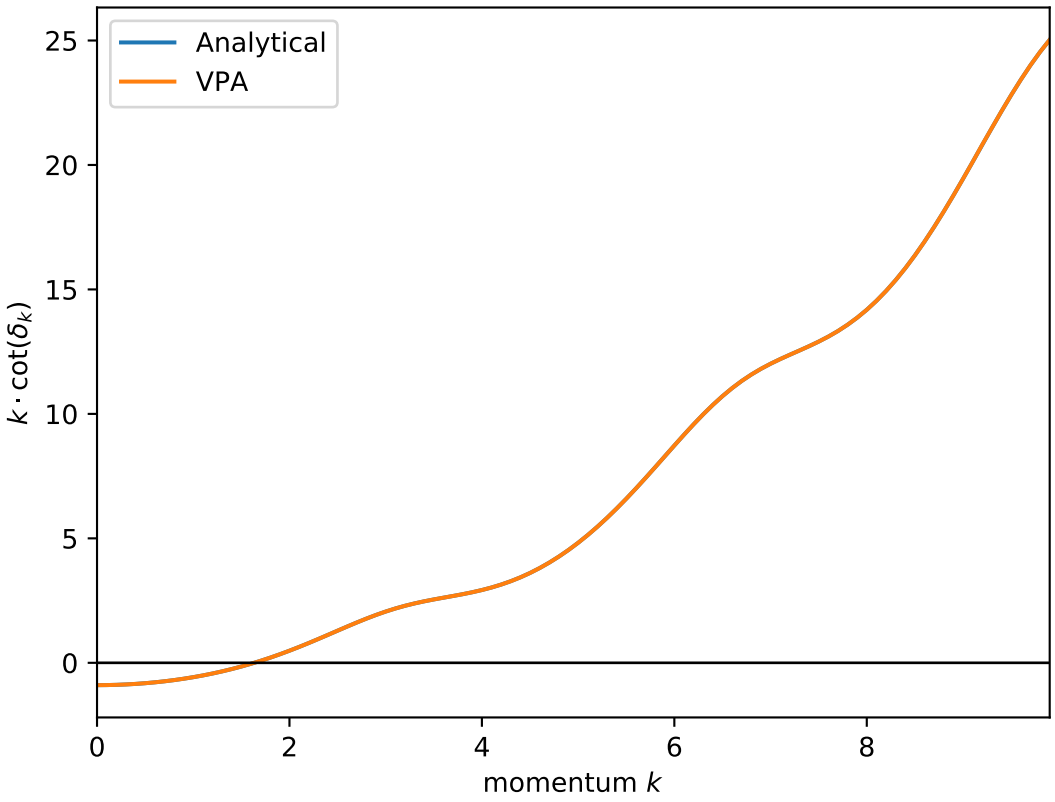

Figure 4.1

References

[1] Christopher Rackauckas and Qing Nie. "Differentialequations.jl–a performant and feature-rich ecosystem for solving differential equations in julia". In: Journal of Open Research Software 5.1 (2017) (cit. on p. 8).