Exercise:

Solving the Lippmann - Schwinger eqn

The R-matrix carries information about a particle scattered off the given potential V. For the S-wave scattering (angular momentum = 0) of a spin-0 particle, $R(q', q)$ is the R-matrix value for incoming momentum q and outgoing momentum q'.

B/c $R(q', q)$ is a two-variable function, it is called R "matrix". $R(q', q)$ satisfies the Lippmann-Schwinger equation, which can be derived from the schrödinger equation (we don't need to know how)

$$R(q', q) = V(q', q) + \mathcal{P} \int_0^\infty dk\, k^2 \frac{M}{q^2 - k^2} V(q', k) R(k, q)$$

$V(q', q)$: potential V in momentum space

$q', q, k \in [0, \infty)$

M : mass of the particle (often can be taken as "1")

$\mathcal{P}\int$ denotes principle-value integral, in order to define the integration near $k=q$.

$V(q', q)$ becomes exponentially small when q' or $q \to \infty$, so the integral can be assumed to converge even though the upper limit is ∞.

Our goal is to solve for $R(q', q)$ for arbitrary q' and q, with $V(q', q)$ as the known input.

The key is to realize that ① upon discretization,

$$q', q, k \to \{q_i'\} = \{q_i\} = \{k_i\}$$

$$0 < q_1 < q_2 < \cdots < q_i < \cdots < q_N < \infty$$

$\{q_i'\}$, $\{q_i\}$ and $\{k_i\}$ are the same set of positive real numbers

(2) discretization turns R and V into matrices

$$R(q', q) \longrightarrow R_{ij} \quad 1 \le i, j \le N$$

$$V(q', q) \longrightarrow V_{ij}$$

The integral equation becomes a matrix equation of the form,

$$\mathbb{R} = \mathbb{V} + \mathbb{V}\,\mathbb{G}\,\mathbb{R}$$

For a fixed j, the matrix equation can be thought of as a linear system of equations

$$R_{ij} = V_{ij} + \sum_{k=1}^{N} V_{ik}\, G(j,k)\, R_{kj}$$

$$\mathbb{X} = \begin{pmatrix} R_{1j} \\ R_{2j} \\ \vdots \\ R_{Nj} \end{pmatrix} \qquad \mathbb{B} = \begin{pmatrix} V_{1j} \\ V_{2j} \\ \vdots \\ V_{Nj} \end{pmatrix} \qquad \mathbb{A} = \begin{pmatrix} a_{ik} \end{pmatrix}$$

$$\Rightarrow \mathbb{X} = \mathbb{B} + \mathbb{A} \cdot \mathbb{X}$$

And $\mathbb{X}$ can be solved for by calling LAPACK routines.

※ More technical detail can be found in Machleidt Section 1.4.2, espesially the following point.

$$\mathcal{P}\int_0^\infty dk \, \frac{k^2}{q^2-k^2} f(k)$$

The integrand has a pole at $k = q$ $(q>0)$. "principle value"

$$\Longrightarrow \int_0^{q-\varepsilon} dk \, \frac{k^2}{q^2-k^2} f(k) + \int_{q+\varepsilon}^{\infty} dk \cdots$$

It is important that the integrands in the neighborhood to the left and to the right of $k=q$ cancel each other out.

$k = q-\varepsilon$ $(\varepsilon>0)$

$$\frac{k^2}{q^2-k^2} f(k) \longrightarrow \frac{q^2}{2q\cdot\varepsilon} f(q)$$

$k = q+\varepsilon$

$$\frac{k^2}{q^2-k^2} f(k) \longrightarrow \frac{q^2}{2q(-\varepsilon)} f(q)$$

How to ensure this cancellation numerically to a satisfactory precision? Read the beginning of section 1.4.2