Phase Shift Calculation with Matlab

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Abstract

Adapted from handwritten notes.

I. PHASE SHIFT CALCULATION

- Let's recall the method from Landau's Quantum Mechanics II book, Section 18.3 [1]:
- This applies directly to uncoupled channels. We'll consider coupled channels separately.
- We solve for the R matrix (known as the K-matrix in other contexts), which has standing wave boundary conditions

$$R_l(k_0, k_0, E_{k0}) = -\frac{\tan\delta_l}{\rho_T} \quad \text{where } \rho_T = 2\mu k_0,\ \mu = \frac{m_N}{2} \tag{1}$$

and R_l satisfies

$$R_l(k', k, E) = V_l(k', k) + \frac{2}{\pi}\mathbb{P}\int_0^\infty dp\, \frac{p^2 V_l(k',\rho) R_l(\rho, k, E)}{E - E_p} \tag{2}$$

- We work in units where $\frac{\hbar^2}{m} = 41.47105$ MeV-fm^2 (for np only)
- Lab energy E_{lab} is related to COM momentum k by

$$E_{lab} = 2\frac{\hbar^2}{m}k^2 \tag{3}$$

but the energy E_p is given by

$$E_p = \frac{\hbar^2}{2\mu}p^2 = \frac{\hbar^2}{m}p^2 \to p^2 \tag{4}$$

- So, in our standard units, R_l and V_l are in fm and ρ in fm^{-1}, so the dimensions in Eqn.(2) work out without any other factors.
- Then

$$\delta_l(E_{k0}) = \tan^{-1}[-k_0 \cdot R_l(k_0, k_0, k_0^2)] \tag{5}$$

To Eqn.(2), we do the standard subtract and add trick to move the $\mathbb{P}$ to an integral we can do

$$\begin{aligned} R_l(k', k) = \quad & V_l(k', k) + \frac{2}{\pi}\int_0^\Lambda dp\, \frac{p^2 V_l(k',\rho)R_l(\rho,k) - k_0^2\, V_l(k',k_0)R_l(k_0,k)}{k_0^2 - p^2} \\ & + \frac{2}{\pi}k_0^2 V_l(k',k_0)R_l(k_0,k)\, \underbrace{\mathbb{P}\int_0^\Lambda dp \frac{1}{k_0^2 - p^2}}_{\frac{1}{k_0}\tanh^{-1}\frac{k_0}{\Lambda}} \end{aligned} \tag{6}$$

$$\int_0^\Lambda dp \frac{1}{k_0^2 - p^2} = \int_0^\infty dp \frac{1}{k_0^2 - p^2} \underbrace{-\frac{1}{2k_0}\int_\Lambda^\infty dp \left(\frac{-1}{p - k_0} + \frac{1}{p + k_0}\right)}_{-\frac{1}{2k_0}\log\frac{p+k_0}{p-k_0}\Big|_\Lambda^\infty = \frac{1}{2k_0}\log\frac{1+\frac{k_0}{\Lambda}}{1-\frac{k_0}{\Lambda}} = \frac{1}{2k_0}\log\frac{\Lambda + k_0}{\Lambda - k_0}}$$

(assuming $k_0 < \Lambda$)

- Now convert the integral to quadratic points $i = 1$ to N (and drop the l label):

$$R_l(k_i, k_0) = \quad V(k_i, k_0) + \frac{2}{\pi} \sum_{j=1}^{N} \frac{k_l^2 V(k_i, k_l) R(k_l, k_0) w_l}{k_0^2 - k_l^2} \tag{7}$$
$$-\frac{2}{\pi} \left(\left[\sum_{m=1}^{N} \frac{w_m}{k_0^2 - k_m^2} \right] - \frac{1}{2k_0} \log \frac{\Lambda + k_0}{\Lambda - k_0} \right) k_0^2 V(k_i, k_0) R(k_0, k_0)$$

- We now add k_0 as the $(N+1)^{th}$ mesh point and define the vectors

$$\begin{aligned} \tilde{R}_i &= R(k_i, k_0) \qquad i = 1, N+1 \text{ and } k_{N+1} \equiv k_0 \\ \tilde{V}_i &= V(k_i, k_0) \end{aligned} \tag{8}$$

  Let's write down the standard operations by Landau.

  He lets $i = N + 1$ be the k_0 point

$$\Rightarrow R_i = R(k_i, k_0) \qquad i = 1, N+1, \quad \text{also } V_i = V(k_i, k_0) \tag{9}$$

  N+1 linear equations $(2\mu = 1)$

$$R_i = \quad V_i - \frac{2}{\pi} \sum_{j=1}^{N} \frac{k_j^2 V_{ij} R_j w_j}{k_j^2 - k_0^2} \tag{10}$$
$$+\frac{2}{\pi} \left(\sum_{m=1}^{N} \frac{w_m}{k_m^2 - k_0^2} + \frac{1}{2k_0} \log \frac{\Lambda + k_0}{\Lambda - k_0} \right) k_0^2 V_{ii} R_0$$

  define

$$D_i = \begin{cases} \frac{2}{\pi} \frac{w_i k_i^2}{k_i^2 - k_0^2} & i = 1, N \\ -\frac{2}{\pi} k_0^2 \left(\sum_{j=1}^{N} \frac{w_j}{k_j^2 - k_0^2} + \frac{1}{2k_0} \log \frac{\Lambda + k_0}{\Lambda - k_0} \right) & i = N+1 \end{cases} \tag{11}$$

$$\Rightarrow R_i + \sum_{j=1}^{N+1} V_{ij} D_j R_j = V_i \tag{12}$$

  or $F_{ij} \overset{def}{=} \delta_{ij} + D_j V_{ij}$ (no sum; F is an (N+1)x(N+1) matrix)

$$\Rightarrow F\vec{R} = \vec{V} \qquad \leftarrow \text{or solve inversion problem}$$

$$\Rightarrow \vec{R} = F^{-1}\vec{V}$$

- OK, so for the starting attempt

  V_vector

  R_vector

  D_vector

  are formed. Actually, V_vector and D_vector are formed.

  Then F_matrix is formed.

Then R_vector=inv(F_matrix)*V_vector

Most everything is given.

We step through the k_0 points we want, probably by stepping through E_{lab}

$\Rightarrow E_{lab}$ in MeV

$k_0 = \sqrt{\frac{E_{lab}}{2(\hbar^2/m)}}$

Given k_0, D_vector is built. We'll use i=N+1 as the k_0 point.

$V_i = V(k_i, k_0)$ so we interpolate all of these, and its a double interpolation to get V_0

Then filling the matrix F_{ij} we have all that we need.

- Extending to coupled channels

  Once we get r_{11}, r_{12}, r_{22} $\Leftarrow$from extremes of R_matrix

  Then (using radians)

$$\begin{aligned}
\varepsilon &= \frac{1}{2}\text{atan}\left(\frac{2.0\, r_{12}}{r_{11}-r_{22}}\right) \\
r_\varepsilon &= \frac{r_{11}-r_{22}}{\cos(2.0\,\varepsilon)} \\
\delta_a &= -\text{atan}\left(\frac{1}{2}k_0(r_{11}+r_{22}+r_\varepsilon)\right) \\
\delta_b &= -\text{atan}\left(\frac{1}{2}k_0(r_{11}+r_{22}-r_\varepsilon)\right) \\
\bar{\varepsilon} &= \frac{1}{2}\text{asin}\left(\sin(2\varepsilon)\,\sin(\delta_a-\delta_b)\right) \\
\bar{\delta}_a &= \frac{1}{2}\text{atan}\left(\delta_a+\delta_b+\text{asin}\left(\frac{\tan(2\bar{\varepsilon})}{\tan(2\varepsilon)}\right)\right) \\
\bar{\delta}_b &= \frac{1}{2}\text{atan}\left(\delta_a+\delta_b-\text{asin}\left(\frac{\tan(2\bar{\varepsilon})}{\tan(2\varepsilon)}\right)\right)
\end{aligned} \tag{13}$$

- Interpolate v_{11}, v_{12}, v_{21}, v_{22} onto next higher size

  Then form big $\begin{pmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{pmatrix}$ matrix

  F is a big matrix. Is it better to recast as vector?

  What is V? No, a matrix is fine.

- Matrix form of phase shift code

  If we take the discretized form without restricting to k_0 column

$$i, j = 1, N+1 \quad \rightarrow \quad R(k_i, k_j) = V($$

$$m = max = N$$

R_{ij} corresponding to k_0 . . .

$$R_{ij} = \quad V_{ij} + \frac{2}{\pi}\sum_{l=1}^{N} \frac{k_l^2 V_{il} R_{lj} w_l}{k_0^2 - k_l^2} \qquad (14)$$
$$-\frac{2}{\pi}\left(\sum_{l=1}^{N} \frac{w_l}{k_0^2 - k_l^2} - \frac{1}{2k_0} log \frac{\Lambda + k_0}{\Lambda - k_0}\right) k_0^2 V_{i,N+1} R_{N+1,j}$$

$$R_{ij} + \frac{2}{\pi}\sum_{l=1}^{N} \frac{k_l^2 V_{il} R_{lj} w_l}{k_l^2 - k_0^2} \qquad (15)$$
$$-\frac{2}{\pi}\left(\sum_{l=1}^{N} \frac{w_l}{k_l^2 - k_0^2} + \frac{1}{2k_0} log \frac{\Lambda + k_0}{\Lambda - k_0}\right) k_0^2 V_{i,N+1} R_{N+1,j} = V_{ij}$$

$$D_i = \begin{cases} \frac{2}{\pi}\frac{w_i k_i^2}{k_i^2 - k_0^2} & i = 1, N \qquad \Rightarrow \text{same as before} \\ -\frac{2}{\pi} k_0^2 \left(\sum_{l=1}^{N} \frac{w_l}{k_l^2 - k_0^2} + \frac{1}{2k_0} log \frac{\Lambda + k_0}{\Lambda - k_0}\right) & i = N+1 \end{cases} \qquad (16)$$

$$R_{ij} + \sum_{l=1}^{N+1} V_{il} D_l R_{lj} = V_{ij} \qquad (17)$$

$$\sum_l F_{il} R_{lj} = V_{ij} \qquad (18)$$
$$\Rightarrow \vec{R} = F^{-1}\vec{V}$$

Now simply as matrices

Then still the N+1,N+1 element of R that we want

OK that works immediately

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[1] R. H. Landau, *Quantum Mechanics II* (John Wiley & Sons, Inc., New York, 1996), 2nd ed.