Scattering Theory Note: Two body

Young-Ho Song

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Contents

Chapter 1

Basic Conventions

The basic object of this note is to summarize basic relations between scattering observables(or phase shift, t-matrix) and potentials and the algorithm to solve the two-body scattering problem. We will use time-independent formalism.

엄밀하게 말하자면, scattering은 물리적으로 non-stationary and normalizable wave를 사용해야 한다. (이것은 time-dependent formalism 에 wave-packet solution을 사용하는 것을 의미). 그러나, 실제로는 stationary and non-normalizable wave를 이용하는 것이 편리하다. (즉, plane wave solution을 기본으로 사용하는 것을 의미).

wave packet $|\psi_a\rangle = \int d^3p|\psi_p\rangle\tilde{\psi}_a(\boldsymbol{p})$ 는 normalizable이 되도록 할 수 있는데, 이 때 normalizable $|\psi_a\rangle$는 free Hamiltonian H_0의 eigen-state가 아님에 유의. (즉, $H_0|\psi_a\rangle \neq E|\psi_a\rangle$ with definite energy E.) 따라서, time-evolution of the state는 $|\psi_a(t)\rangle \neq e^{-iEt/\hbar}|\psi_a\rangle$ 이다. 즉, non-stationary.

일반적으로, general initial state $\psi_a(0)\rangle$ 의 time-evolution은

$$\psi(\boldsymbol{x},t) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \int d^3x' e^{\frac{im(\boldsymbol{x}-\boldsymbol{x}')^2}{\hbar 2t}} \psi(\boldsymbol{x},0) \tag{1.1}$$

로 나타낼 수 있다. 그러면, probability density는

$$\rho(\boldsymbol{x},t) = |\psi(\boldsymbol{x},t)|^2 \leq \frac{\text{constant}}{|t|^{3/2}} \tag{1.2}$$

가 되어 시간에 따라 변하게 됨을 알 수 있다. 하지만, 이 경우에도 전체 공간에 대해 적분한 total probability는 입자의 갯수의 보존에 의해 시간에 따라 변하지 않음을 보일 수 있다.

그러나, 앞으로는 interaction이 short range 임을 가정하고 plane wave basis에서 이야기를 전개해 가도록 하자.

1.1 Box normalization

In a cube box with size L, the free solution $\psi(x) = Ae^{ikx} + Be^{ikx}$ inside box have to satisfy the periodic boundary condition $\psi(0) = \psi(L) = 0$. This gives the condition, $\psi(x) = \sqrt{\frac{2}{L}}\sin(k_n x)$ with $k_n L = \pi n \geq 0$. On the other hand, in periodic boundary condition of box, $\psi(x) = \psi(x+L)$ gives $\psi(x) = Ae^{ikx}$ with $k_n L = 2\pi n$ with integer n. (note the difference with the box).

If we normalize the wave function such that there is one particle in one periodic box, (in other words, set number density of particles of a specific momentum as $1/L^3$), the wave function becomes

$$\begin{aligned} \psi(\boldsymbol{x}) &= \frac{1}{\sqrt{L^3}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \\ k_x &= \frac{2\pi}{L}n_x, \quad k_y = \frac{2\pi}{L}n_y, \quad k_z = \frac{2\pi}{L}n_z \end{aligned} \tag{1.3}$$

and orthogonality, (Be careful that always finite volume integral is assumed for integral)

$$\int_{L^3} \psi_{\boldsymbol{k}}^\dagger(\boldsymbol{x})\psi_{\boldsymbol{l}}(\boldsymbol{x})d^3x = \int_{-L/2}^{L/2} dx \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dz \frac{1}{L^3} e^{i(\boldsymbol{l}-\boldsymbol{k})\cdot\boldsymbol{x}} = \delta_{\boldsymbol{kl}} \tag{1.4}$$

In continuum limit, we may use a representation of Dirac δ function,

$$\delta(x) = \lim_{g\to\infty} \frac{\sin gx}{\pi x} = \lim_{g\to\infty} \delta_g(x), \tag{1.5}$$

$$\begin{aligned} \int_{L^3} \psi_{\boldsymbol{k}}^\dagger(\boldsymbol{x})\psi_{\boldsymbol{l}}(\boldsymbol{x})d^3x &= \frac{2^3}{L^3} \frac{\sin((k_x-l_x)\frac{L}{2})}{(k_x-l_x)} \frac{\sin((k_y-l_y)\frac{L}{2})}{(k_y-l_y)} \frac{\sin((k_y-l_x)\frac{L}{2})}{(k_z-l_z)} \\ &= \frac{(2\pi)^3}{L^3} \delta_{L/2}^{(3)}(\boldsymbol{k}-\boldsymbol{l}) \end{aligned} \tag{1.6}$$

For the momentum space, in large box limit, we can approximate the sum over nodes as a integral over momentum(wave number)

$$\sum_{n=-\infty}^{\infty} \to \frac{L}{2\pi} \int_{-\infty}^{\infty} dk. \tag{1.7}$$

Then, we have closure relation,

$$\sum_{\boldsymbol{n}} \psi_{\boldsymbol{k}_n}^\dagger(\boldsymbol{r}')\psi_{\boldsymbol{k}_n}(\boldsymbol{r}) \to \frac{L^3}{(2\pi)^3} \int d^3k \psi_{\boldsymbol{k}}^\dagger(\boldsymbol{r}')\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{L^3}{(2\pi)^3} \int d^3k \frac{1}{L^3} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}') \tag{1.8}$$

Thus, we can get continuum limit,

$$\lim_{L\to\infty} \int_{L^3} d^3x \frac{1}{L^3} e^{i(\boldsymbol{k}-\boldsymbol{l})\cdot\boldsymbol{x}} = (2\pi)^3 \delta^{(3)}(\boldsymbol{k}-\boldsymbol{l}) \tag{1.9}$$

On the other hand, from the consistency(or completeness), we require

$$\lim_{L\to\infty} \frac{L^3}{(2\pi)^3} \int d^3k \frac{1}{L^3} e^{i(\boldsymbol{k}-\boldsymbol{l})\cdot\boldsymbol{x}} = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \tag{1.10}$$

Note that the volume part disappears in both expression.

Or, we may absorb 2π factors into the wave function,

$$\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \sqrt{\frac{1}{(2\pi)^3 L^3}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{1.11}$$

In this case the relation becomes

$$\begin{aligned} &\lim_{L\to\infty} \int_{L^3} d^3x \psi_{\boldsymbol{k}}^\dagger(\boldsymbol{x})\psi_{\boldsymbol{k}'}(\boldsymbol{x}) = \lim_{L\to\infty} \int_{L^3} d^3x \frac{1}{(2\pi)^3 L^3} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{x}} = \delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}'), \\ &\sum_{n=-\infty}^{\infty} \to L \int_{-\infty}^{\infty} dk, (?) \\ &\lim_{L\to\infty} L^3 \int d^3k \psi_{\boldsymbol{k}}^\dagger(\boldsymbol{x})\psi_{\boldsymbol{k}}(\boldsymbol{x}') = \lim_{L\to\infty} L^3 \int d^3k \frac{1}{L^3} \frac{1}{(2\pi)^3} e^{i(\boldsymbol{x}-\boldsymbol{x}')\cdot\boldsymbol{k}} = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{y}) \end{aligned} \tag{1.12}$$

1.2 Normalization convention of bra-ket

In c.m. frame $E_k = \frac{\boldsymbol{k}^2}{2\mu}$ with $\boldsymbol{k} = \mu \boldsymbol{v}_{rel}$ relative momentum between two cluster, μ reduced mass.

Usual normalization convention of states are

$$\begin{aligned}
\langle \boldsymbol{x}' | \boldsymbol{x} \rangle &= \delta^{(3)}(\boldsymbol{x} - \boldsymbol{x}'), \quad \int d^3x |\boldsymbol{x}\rangle\langle\boldsymbol{x}| = 1, \\
\langle \boldsymbol{p} | \boldsymbol{p}' \rangle &= \mathcal{N}\delta^{(3)}(\boldsymbol{p} - \boldsymbol{p}'), \quad \int \frac{d^3p}{\mathcal{N}} |\boldsymbol{p}\rangle\langle\boldsymbol{p}| = 1, \\
\langle \boldsymbol{x} | \boldsymbol{p} \rangle &= \sqrt{\frac{\mathcal{N}}{(2\pi\hbar)^3}} e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}}
\end{aligned} \tag{1.13}$$

앞으로는 natual unit을 사용하여 $\hbar = 1$ 로 두어 $\hbar$를 생략하기도 한다.

Sakurai book, Rimas 논문, Glockle 의 책은 이 $\mathcal{N} = 1$ convention을 사용한다. 이 된다. 이 노트에서는 $\langle \boldsymbol{k}' | \boldsymbol{k} \rangle = \delta^3(\boldsymbol{k} - \boldsymbol{k}')$을 사용하기로 하자.

반면, $\mathcal{N} = (2\pi)^3$ 도 많이 이용된다.[1] [2]

1.3 Note: Resolution

If the experiment have some resolution limitation, the observed signal will be different from the actual signal. This can be related with convolution integral with resolution function. Suppose, the original signal is $f(x)$ and the experimental resolution function is $g(x)$, then the detected signal $c(x)$ is related as

$$c(x) = \int dy\ g(x-y) f(y). \tag{1.17}$$

For example, if original signal is a delta function and resolution is Gaussian, the observed signal is broaden as a Gaussian.

[1] high energy 에서는 state를 4-vector로 생각하고,

$$\langle k^\mu | k'^\mu \rangle = (2\pi)^4 (2E_k) \delta^{(4)}(k - k') \tag{1.14}$$

로 정하는 것이 편리하고, 이 때는 energy conservation을 $(2\pi)\delta(k^0 - k'^0)$로 뽑아내는 것이 편리하다.

[2] Origin of normalization convention is from the definition(or representation) of Dirac delta function

$$\delta(x-a) = \frac{1}{2\pi} \int dp e^{i(x-a)p} \tag{1.15}$$

On the other hand, if we consider finite volume $\int d^3r = \Omega$, the corresponding momentum becomes a discrete values to satisfy the boundary condition. But, assuming volume is large enough and approximate sums over momentum as a integral,

$$\sum_k \to \frac{\Omega}{(2\pi)^3} \int d^3k \tag{1.16}$$

Chapter 2

Kinematics

2.1 Laboratory frame

- Let us consider reaction $a+A \to b+B$, where a is a projectile, A is a target, b is projectile-like particle, B is a target-like particle. This is usually expressed in form of $A(a,b)B$ in nuclear physics. The laboratory angle θ is an angle between a and b. The recoil angle ϕ is an angle between a and B.

- In normal kinematics, $m_a < m_A$ and $m_b < m_B$, usually b is detected but recoil B is not measured. Thus, it is convenient to remove E_B and ϕ from Kinematic relation.

- In inverse kinematics, $m_a > m_A$ and $m_b > m_B$, one can measure either both b and B or only B which is lighter.

- Non-relativistic kinematic relation is given as

$$\begin{aligned}
&m_a c^2 + E_a + m_A c^2 = m_b c^2 + E_b + m_B c^2 + E_B, \\
&\sqrt{2m_a E_a} = \sqrt{2m_B E_B}\cos\phi + \sqrt{2m_b E_b}\cos\theta, \\
&0 = \sqrt{2m_B E_B}\sin\phi - \sqrt{2m_b E_b}\sin\theta.
\end{aligned} \tag{2.1}$$

  where energy E is a kinetic energy in Laboratory frame with momentum $p = \sqrt{2mE}$. (Here ϕ is defined to be positive for forward angle scattering.)

  Square sum of two equation gives

$$2m_B E_B \quad = \quad 2m_B E_B + 2m_a E_a - 4\sqrt{m_a E_a m_b E_b}\cos\theta \tag{2.2}$$

- Q-value is defined

$$Q = (m_a + m_A - m_b - m_B)c^2 = E_B + E_b - E_a. \tag{2.3}$$

  Note here mass include excitation energy if the particle is excited.

- By eliminating E_B and ϕ, one gets

$$\begin{aligned}
Q &= E_B + E_b - E_a \\
&= E_b\left(1 + \frac{m_b}{m_B}\right) - E_a\left(1 - \frac{m_a}{m_B}\right) - \frac{2}{m_B}\sqrt{m_a m_b E_a E_b}\cos\theta.
\end{aligned} \tag{2.4}$$

  This can be used, if Q is not known, to get Q-value (or m_A) from experiment.

- By solving equation for E_b,

$$\sqrt{E_b} = r \pm \sqrt{r^2 + s}, \tag{2.5}$$

where

$$\begin{aligned} r &= \frac{\sqrt{m_a m_b E_a}}{m_b + m_B} \cos\theta, \\ s &= \frac{E_a(m_B - m_a) + m_B Q}{m_b + m_B}. \end{aligned} \tag{2.6}$$

A reverse relation is

$$\cos\theta = \frac{m_b + m_B}{\sqrt{m_a m_b E_a}} \frac{E_b - s}{2\sqrt{E_b}}. \tag{2.7}$$

- If $s > 0$, θ can be any value, and only one energy is possible for a angle. the range of energy $E_b^{min} \le E \le E_b^{max}$ ($E_b^{min,max} = (r + \sqrt{r^2+s})^2$ at $\cos\theta = \mp 1$.)

  If $s = 0$, $0 \le \theta \le 90$ degree is allowed and $0 \le E_b \le E_b^{max}$ ($E_b^{max} = (r + \sqrt{r^2+s})^2$ at $\cos\theta = 1$).

  If $s < 0$, there can be two energy $(r \pm \sqrt{r^2+s})^2$ for the same angle. The energy range $E_b^{min} \le E \le E_b^{max}$ ($E_b^{min,max} = (r \pm \sqrt{r^2+s})^2$ at $\cos\theta = 1$.) The range of angle $0 \le \theta \le \theta^{max}$ ($\cos\theta^{max}$ is determined at $E_b = -s > 0$.)

- The threshold energy (for one angle) is (from $r^2 + s \ge 0$)

$$E_t = \frac{-Q m_B (m_B + m_b)}{m_a m_b \cos^2\theta + (m_B + m_b)(m_B - m_a)} \ge \frac{-Q(m_B + m_b)}{m_B + m_b - m_a} \tag{2.8}$$

  Thus reaction can occur only when $E_a \ge E_t$. Relativistic expression of threshold energy is

$$T_t = \frac{-Q(m_a + m_A + m_b + m_B)}{2m_A} \tag{2.9}$$

- Once E_b is fixed for a θ, we get information for B as

$$\begin{aligned} E_B &= Q - E_b + E_a, \\ \sin\phi &= \sqrt{\frac{m_b E_b}{m_B E_B}} \sin\theta \end{aligned} \tag{2.10}$$

  range of E_B is obvious. However, the range of ϕ is not explicit. Instead, one can use alternative expressions (by $m_b \leftrightarrow m_B$ and $\theta \leftrightarrow \phi$),

$$Q = (\frac{m_a}{m_b} - 1)E_a + (1 + \frac{m_B}{m_b})E_B - \frac{2}{m_b}\sqrt{m_B m_a E_B E_a} \cos\phi \tag{2.11}$$

$$\begin{aligned} \sqrt{E_B} &= r_B \pm \sqrt{r_B^2 + s_B}, \\ r_B &= \frac{\sqrt{m_a m_B E_a} \cos\phi}{m_b + m_B}, s_B = \frac{Q m_b - E_a(m_a - m_b)}{m_b + m_B} \end{aligned} \tag{2.12}$$

  Thus, we can use similar criteria to determine the range of angle ϕ and E_B.

- Or, one can obtain from CM angle,

$$\begin{aligned}
\tan\theta_{lab} &= \frac{\sin\theta_{cm}}{\cos\theta_{cm}+\rho},\ \rho=\sqrt{\frac{m_a m_b}{m_A m_B}\frac{E_{a,lab}}{(1+m_a/m_A)Q+E_{a,lab}}}, \\
\tan\phi_{lab} &= \frac{\sin(\pi\pm\theta_{cm})}{\cos(\pi\pm\theta_{cm})+\rho_B},\ \rho_B=\sqrt{\frac{m_a m_B}{m_A m_b}\frac{E_{a,lab}}{(1+m_a/m_A)Q+E_{a,lab}}}
\end{aligned} \tag{2.13}$$

(The sign depends on the convention of ϕ.)

- In case of radiative capture , $a+A\to B+\gamma$, replace $m_bc^2+E_b\to E_\gamma$ and $\sqrt{2m_bE_b}\to E_\gamma/c$,

$$E_\gamma = Q+\frac{m_A}{m_B}E_a+E_\gamma\frac{v_B}{c}\cos\theta-\frac{E_\gamma^2}{2m_Bc^2}=Q+\frac{m_A}{m_B}E_a+\Delta E_{Dopp}-\Delta E_{rec} \tag{2.14}$$

Photon energy is from Q-value, CM energy, Doppler shift and recoil shift.

$$\begin{aligned}
\Delta E_{Dopp} &= 4.63367\times10^{-2}\frac{\sqrt{m_aE_a}}{m_B}E_\gamma\cos\theta, \quad (MeV) \\
\Delta E_{rec} &= 5.36772\times10^{-4}\frac{E_\gamma^2}{m_B}, \quad (MeV)
\end{aligned} \tag{2.15}$$

Exact relativistic expression

$$E_\gamma=\frac{Q(m_ac^2+m_Ac^2+m_Bc^2)/2+m_Ac^2E_a}{m_ac^2+m_Ac^2+E_a-\cos\theta\sqrt{E_a(2m_ac^2+E_a)}} \tag{2.16}$$

Recoil angle for photon emission angle θ,

$$\phi=\arctan\left(\frac{\sin\theta}{E_\gamma^{-1}\sqrt{2m_ac^2E_a}-\cos\theta}\right)\le\arctan\left(\frac{E_\gamma}{\sqrt{2m_ac^2E_a}}\right) \tag{2.17}$$

2.2 Lab frame and CM frame

- 일반적인 two-body problem can be decomposed as center of mass kinetic energy and two-body relative motion.

$$\langle \boldsymbol{r}_1\boldsymbol{r}_2|H|\boldsymbol{r}_1'\boldsymbol{r}_2'\rangle=\langle \boldsymbol{R}\boldsymbol{r}|H|\boldsymbol{R}'\boldsymbol{r}'\rangle=\delta^{(3)}(\boldsymbol{R}-\boldsymbol{R}')\left[\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')\left(-\frac{\nabla_R^2}{2M_{tot}}-\frac{\nabla_r^2}{2\mu}\right)+V(\boldsymbol{r},\boldsymbol{r}')\right] \tag{2.18}$$

C.M. frame 에서, scattering 에너지는 two-body 의 relative kinetic energy 이고, $E=\frac{\boldsymbol{k}^2}{2\mu}$ with reduced mass $\mu=\frac{m_1m_2}{m_1+m_2}$로 나타내진다. [1] [2]

- Let us consider non-relativistic kinematics of two-body reaction $A(a,b)B$.

- Non-relativistic kinematics(before collision): In lab frame, usually m_a, m_A and $E_{a,lab}$ is given,

$$\begin{aligned}
T_{lab} &= E_a^{lab}=\frac{1}{2}m_av_{a,lab}^2=\frac{p_{a,lab}^2}{2m_a}, \quad p_{a,lab}=m_av_{a,lab}, \\
\boldsymbol{v}_{rel} &= \boldsymbol{v}_{a,lab}=\boldsymbol{v}_{a,cm}-\boldsymbol{v}_{A,cm}, \\
\mu &= \frac{m_am_A}{m_a+m_A}
\end{aligned} \tag{2.19}$$

[1] 주의: $\boldsymbol{k}_{rel}\equiv\mu v_{rel}\neq\boldsymbol{p}_1-\boldsymbol{p}_2$.

[2] **주의: state나 matrix element를 나타낼 때, $|\boldsymbol{k}\rangle$, $|k,\alpha\rangle$, $|\alpha\rangle$ 는 각각 다른 의미를 가진다. $|\boldsymbol{k}\rangle$는 plane wave, $|k,\alpha\rangle$는 partial wave with radial wave function, $|\alpha\rangle$는 angular part without radial wave function.**

In CM frame, the important quantity are T_{cm} and k_{cm} which are related with relative velocity as, ($\boldsymbol{p}_{a,cm} = \boldsymbol{p}_c = -\boldsymbol{p}_{A,cm}$),(Be careful that $\boldsymbol{k}_{rel} \neq \boldsymbol{p}_{a,cm} - \boldsymbol{p}_{A,cm}$ and direction of momentum is in direction of projectile by default.)

$$\begin{aligned}
\hbar\boldsymbol{k}_{rel} &= \mu\mathbf{v}_{rel} = \mu(\frac{\boldsymbol{p}_c}{m_a} - \frac{-\boldsymbol{p}_c}{m_A}) = \boldsymbol{p}_c \\
T_{cm} &= \frac{\hbar^2\boldsymbol{k}_{rel}^2}{2\mu} = \frac{1}{2}\mu\boldsymbol{v}_{rel}^2 = E_{a,cm} + E_{A,cm} \qquad (2.20)
\end{aligned}$$

In non-relativistic approximation, speed of center of mass,

$$v_G = \dot{\boldsymbol{S}} = \frac{m_a\boldsymbol{v}_a + m_A\boldsymbol{v}_A}{m_a + m_A} = \frac{m_a\boldsymbol{v}_a}{m_a + m_A} = \frac{\mu}{m_A}\boldsymbol{v}_{rel} \qquad (2.21)$$

Let us always use only fm as a fundamental units. Other quantities are always converted by using $\hbar = c = 1$ and $\hbar c = 1 = 197$MeV.fm. Then, we don't need to distinguish momentum and wave vector.

Then, the relation between CM velocity and Lab velocity for any particle is

$$\boldsymbol{v}_{cm} = \boldsymbol{v}_{lab} - \dot{\boldsymbol{S}} \qquad (2.22)$$

Of course, the kinetic energy relation is

$$T_{a,lab} = T_{cm} + \frac{1}{2}(m_a + m_A)v_G^2 \qquad (2.23)$$

Thus, [3],

$$\begin{aligned}
&\hbar\boldsymbol{k} = \mu\boldsymbol{v}_{rel} = \boldsymbol{p}_{a,cm} = m_a\boldsymbol{v}_{a,cm} = -\boldsymbol{p}_{A,cm} = -m_A\boldsymbol{v}_{A,cm}, \\
&T_{lab} = \frac{\hbar^2}{2m_a}\boldsymbol{p}_{a,lab}^2 = \frac{1}{2}m_a v_{rel}^2 = \frac{m_a}{\mu}T_{cm} = \frac{m_a + m_A}{m_A}T_{cm}, \\
&T_{cm} = \frac{\hbar^2}{2\mu}\boldsymbol{k}^2 = \frac{1}{2}\mu v_{rel}^2 = \frac{\mu}{m_a}T_{a,lab} = \frac{m_A}{m_a + m_A}T_{a,lab} = T_{a,cm} + T_{A,cm}, \\
&\boldsymbol{p}_{a,lab} = m_a\boldsymbol{v}_{rel} = \frac{m_a}{\mu}\boldsymbol{k}_{rel}, \qquad (2.24)
\end{aligned}$$

For equivalent inverse kinematics, we have relation

$$T_{cm} = \frac{\mu}{m_A}T_{A,lab} \qquad (2.25)$$

This can be used for the case we consider equivalent target and projectile is reversed.

- E/A : If we ignore small binding energy compared to the total mass of nuclei, We may use $m_i \to A_i u$ and $\mu \to \frac{A_a A_A}{A_a + A_A}u = \mu_A u$ with u is the atomic mass unit. Then, energy per nucleon $\left(\frac{E}{A}\right)$ can be easily written in both normal and inverse kinematics,

$$\left(\frac{E}{A}\right) = \frac{T_a^L}{A_a} = \frac{T_A^L}{A_A} = \frac{T^C}{\mu_A}. \qquad (2.26)$$

In other words, it becomes easy to convert kinetic energy between equivalent reactions in different kinematics.

If the reaction have non-zero Q-value, equivalent reverse energy are given as

$$T_f^C = T_i^C + Q, \quad (E/A)_f = T_f^C/\mu_f \qquad (2.27)$$

[3]Note that thermal neutron corresponds to $v_{rel} = 2200$ m/s which is $T_L = 2.53 \times 10^{-8}$ MeV.

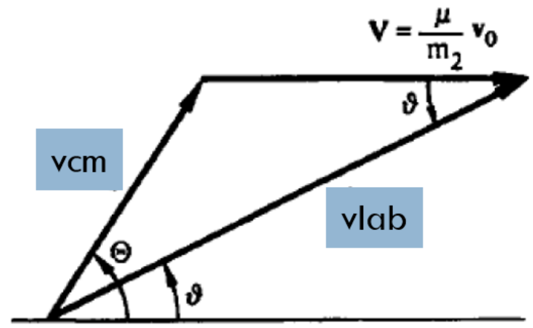

Figure 2.1

- After collision: the particles may have different masses. Then,

$$Q = (m_a + m_A - m_b - m_B)c^2 \tag{2.28}$$

where, mass includes internal binding energies. This implies energy conservation relation,

$$T_f = T_b + T_B = T_i + Q = T_a + T_A + Q \tag{2.29}$$

in both cm frame and lab frame.[4] Also the momentum conservation gives

$$\boldsymbol{p}_a + \boldsymbol{p}_A = \boldsymbol{p}_b + \boldsymbol{p}_B \tag{2.30}$$

in both lab and cm frame.

- **In non-relativistic** inelastic scattering, let us suppose the b is the **forward scattered particle**. The angle of particle b from the lab. frame($\theta_{b,lab}$) and C.M. frame($\theta_{b,cm}$) is related by

$$\boldsymbol{v}_{b,cm} = \boldsymbol{v}_{b,lab} - \dot{\boldsymbol{S}},$$

$$\begin{aligned} v_{b,cm}\sin\theta_{b,cm} &= v_{3,lab}\sin\theta_{b,lab}, \\ v_G + v_{b,cm}\cos\theta_{b,cm} &= v_{b,lab}\cos\theta_{b,lab} \end{aligned} \tag{2.31}$$

Also, from

$$\begin{aligned} 0 &= m_b v_{b,cm} + m_B v_{b,cm}, \\ Q + T_{cm} &= T_{b,cm} + T_{B,cm} = \frac{1}{2}m_b v_{b,cm}^2 + \frac{1}{2}m_B v_{B,cm}^2, \\ &= \frac{1}{2}\frac{m_b}{m_B}(m_b + m_B)v_{b,cm}^2 \end{aligned} \tag{2.32}$$

Thus, we get[5] [6]

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[4]Note that in lab frame $T_{1,lab} + Q = T_{3,lab} + T_{4,lab}$ while $T_{cm} + Q = T_{3,cm} + T_{4,cm}$ in cm frame. But, relation between cm and lab frame requires boost transformation.

[5]More exactly,

$$\rho = \left(\frac{m_1 m_3}{m_2 m_4}\frac{m_3 + m_4}{m_1 + m_2}\frac{T_{cm}}{Q + T_{cm}}\right)^{\frac{1}{2}} \tag{2.33}$$

However, $\frac{m_3+m_4}{m_1+m_2} = (1 + \frac{Q}{m_3c^2+m_4c^2})^{-1} \simeq 1$.

[6]To obtain θ_{cm} from θ_{lab}

$$\frac{\sin\theta_{lab}}{\cos\theta_{lab}} = \frac{\sin\theta_{cm}}{\rho + \cos\theta_{cm}} \to \sin\theta_{cm}\cos\theta_{lab} - \sin\theta_{lab}\cos\theta_{cm} = \sin(\theta_{cm} - \theta_{lab}) = \rho\sin\theta_{lab}$$

$$\begin{aligned}\tan\theta_{b,lab} &= \frac{\sin\theta_{b,cm}}{\rho+\cos\theta_{b,cm}}, \\ \rho &= \frac{v_G}{v_{b,cm}} = \left(\frac{m_a m_b}{m_A m_B}\frac{T_{cm}}{Q+T_{cm}}\right)^{\frac{1}{2}} = \sqrt{\frac{m_a m_b}{m_A m_B}\frac{E_{a,lab}}{(1+m_a/m_A)Q+E_{a,lab}}}\end{aligned} \tag{2.36}$$

where, $Q + T_{a,cm} + T_{A,cm} = T_{b,cm} + T_{B,cm}$ with T_{cm} is the relative energy in the incident channel.

For inverse relation, we may use

$$\sin(\theta_{cm} - \theta_{lab}) = \rho\sin\theta_{lab}. \tag{2.37}$$

Though as a function of θ_{cm} above relation gives unique θ_{lab}. However, when $\rho > 1$, the reverse can be ambiguous because there can be two θ_{cm} for one θ_{lab}. Either one can have

$$\theta_{cm} = \theta_{lab} + \sin^{-1}(\rho\sin\theta_{lab}), \quad \text{or} \quad \theta_{lab} + (\pi - \sin^{-1}(\rho\sin\theta_{lab})) \tag{2.38}$$

$v_G = |\dot{\boldsymbol{S}}|$.

Q is the internal energy released in the reaction. Q is $Q > 0$ (means final states have more kinetic energy than initial) for exothermic(발열) reaction and $Q < 0$ for endorthermic reaction.

Alternative form is, $x = \rho$,

$$\cos\theta_{lab} = \frac{1 + x^{-1}\cos\theta_{cm}}{\sqrt{1 + x^{-2} + 2x^{-1}\cos\theta_{cm}}} \tag{2.39}$$

$$\cos\theta_{cm} = \cos\theta_{lab}\left[x\cos\theta_{lab} + \sqrt{1 - x^2\sin^2\theta_{lab}}\right] - x \tag{2.40}$$

These equation works regardless whether $m_1 > m_2$ or $m_1 < m_2$.

One can obtain the c.m. angle of B as $\phi_{B,cm} = \pi \pm \theta_{b,cm}$. Then, one can obtain lab angle by change $m_b \leftrightarrow m_B$,

$$\begin{aligned}\tan\phi_{B,lab} &= \frac{\sin\phi_{B,cm}}{\rho+\cos\phi_{B,cm}}, \\ \rho &= \sqrt{\frac{m_a m_B}{m_A m_b}\frac{E_{a,lab}}{(1+m_a/m_A)Q+E_{a,lab}}},\end{aligned} \tag{2.41}$$

For two identical particles $m_1 = m_2$, $\theta_1 = \frac{1}{2}\theta_{cm}$ and $\theta_2 = \frac{1}{2}(\pi - \theta_{cm}) = \frac{\pi}{2} - \theta_1$. Thus, perpendicular relation $\theta_1 + \theta_2 = \frac{\pi}{2}$.

Thus, for the equivalent binary reaction $m_1 + m_2 + T_C \leftrightarrow m_3 + m_4 + T'_C$, $T'_C = T_C + Q$ and also $T'_C = \frac{\mu'}{m'_3}T_3^L = \frac{\mu'}{m'_4}T_4^L$.

Thus, we can use following relation to convert θ_{lab} into θ_{cm}

$$\theta^{cm} = \theta^{lab} + \sin^{-1}(\rho\sin\theta^{lab})$$

. However, there is an ambiguity and depending on ρ, one lab angle can come from two cm angles.

Another way is to solve $\chi = \cos\theta_{cm}$ from

$$\chi^2 + 2\rho\sin^2\theta_{lab}\chi + \rho^2\sin^2\theta_{lab} - \cos^2\theta_{lab} = 0 \tag{2.34}$$

Thus,

$$\cos\theta_{cm} = -\rho\sin^2\theta_{lab} \pm \sqrt{\cos^2\theta_{lab}}\sqrt{1 - \rho^2\sin^2\theta_{lab}} \tag{2.35}$$

Again, there is a problem of ambiguity. There can be two possible solutions of θ_{cm} and it is not possible to determine which one is the correct one.

- relativistic kinematics: We want a Lorentz transformation from four vector $(E_1 + m_2, k_1)$ to $(\omega, 0)$ where $E_1^2 = m_1^2 + k_1^2 = m_1 + T_{1,lab}$.

$$\begin{pmatrix} \omega \\ 0 \end{pmatrix} = \begin{pmatrix} -\gamma & -\gamma\beta \\ -\gamma\beta & \gamma \end{pmatrix} \begin{pmatrix} E_1 + m_2 \\ k_1 \end{pmatrix} \tag{2.42}$$

with

$$\begin{aligned} \beta_{cm} &= \frac{k_1}{E_1 + m_2} \quad \text{(velocity of c.m. wrt lab frame)}, \\ \gamma_{cm} &= \frac{1}{\sqrt{1-\beta^2}} = \frac{E_1 + m_2}{\sqrt{(E_1 + m_2)^2 - k_1^2}} = \frac{E_1 + m_2}{\sqrt{s}}, \\ s &= \omega^2 = (E_1 + m_2)^2 - k_1^2 = (m_1 + m_2)^2 + 2T_{1,lab} m_2 \end{aligned} \tag{2.43}$$

Also,

$$T_{cm} = \omega - (m_1 + m_2) = \sqrt{s} - (m_1 + m_2) \tag{2.44}$$

In other words,

$$\omega^2 = (m_2 + \sqrt{m_1^2 + \boldsymbol{p}_1^2})^2 - \boldsymbol{p}_1^2 = (\sqrt{m_1^2 + \boldsymbol{p}_c^2} + \sqrt{m_2^2 + \boldsymbol{p}_c^2})^2, \tag{2.45}$$

where $\boldsymbol{p}_1$ is momentum in Lab. frame, $\boldsymbol{p}_c$ is momentum in C.M. frame. Solving this equation gives a relation between, $\boldsymbol{p}_1$ and $\boldsymbol{p}_c$.

Since we found β_{cm} and γ_{cm}, we can Lorentz transform each particles energy momentum to C.M. frame,

$$\begin{pmatrix} E_1^{cm} \\ k_1^{cm} \end{pmatrix} = \begin{pmatrix} -\gamma & -\gamma\beta \\ -\gamma\beta & \gamma \end{pmatrix} \begin{pmatrix} E_1 \\ k_1 \end{pmatrix} = \frac{1}{\sqrt{s}} \begin{pmatrix} s - m_2^2 - m_2 E_1 \\ m_2 k_1 \end{pmatrix} \tag{2.46}$$

Thus, wave number in C.M. frame are

$$k_{1,cm}^2 = \frac{(m_2 k_1)^2}{s} = \frac{m_2^2}{s}(T_{1,lab}^2 + 2T_{1,lab} m_1) \tag{2.47}$$

2.2.1 Differential cross section between c.m. frame and lab. frame

Basic principle is that the number of particles into certain solid angle does not change from reference frame. Total cross sections, as ratios of fluxes, are not changed by Lorentz transformation. However, differential cross section can change by Lorentz transformation.

Thus,

$$\left(\frac{d\sigma}{d\Omega}\right)' d\Omega' = \left(\frac{d\sigma}{d\Omega}\right) d\Omega, \quad \left(\frac{d\sigma}{d\Omega}\right)' = \left(\frac{d\sigma}{d\Omega}\right)\left(\frac{d\Omega}{d\Omega'}\right) \tag{2.48}$$

In non-relativistic kinematics,

$$\left(\frac{d\sigma}{d\Omega_1}\right)_{Lab} = \left(\frac{d\sigma}{d\Omega}\right)_{cm} \frac{d\cos\theta_C}{d\cos\theta_{1L}} \simeq \left(\frac{d\sigma}{d\Omega}\right)_{cm} \frac{(1 + 2\lambda\cos\theta_{cm} + \lambda^2)^{\frac{3}{2}}}{|1 + \lambda\cos\theta_{cm}|} \tag{2.49}$$

where, $\lambda = m_1/m_2 \to \rho$.

$$\left(\frac{d\sigma}{d\Omega_2}\right)_{Lab} \simeq 4\sin(\frac{\theta_C}{2}) \left(\frac{d\sigma}{d\Omega_2}\right)_{cm} \tag{2.50}$$

For inelastic reaction, we replace λ by ρ.

relativistic expression is

$$\theta_{lab} = \arctan\left(\frac{\sin\theta_{cm}}{\gamma[\cos\theta_{cm} + xg(x, \mathcal{E}_1)]}\right) \tag{2.51}$$

More details from can be found in Goldstein book or Betulani book.

2.2.2 Inverse kinematics

Let us denote the differential cross section in c.m. frame as $\sigma(\theta_{13}^{cm})$ where θ_{13}^{cm} is an angle between particle 1 and 3 in reaction $A_2(A_1, A_3)A_4$ for given T_{cm} and Q-value of the reaction. Normally, we consider light projectile 1 and light fragment 3 is detected. In c.m. frame the angle of particle 4 can be easily obtained as $\theta_{14}^{cm} = \pi - \theta_{13}^{cm}$. (But it should understood that the angle is w.r.t. incoming particle 1.)

- (1) Normal kinematics : $A_2(A_1, A_3)A_4$, $A_1 < A_2$ and $A_3 < A_4$. The observed cross section is in terms of $\sigma_{cm}^{(1)}(\theta_{13}^{cm})$.

  We can convert between lab frame and cm frame as

$$\begin{aligned}
\tan\theta_{13}^{lab} &= \frac{\sin\theta_{13}^{cm}}{\rho_{13} + \cos\theta_{13}^{cm}}, \\
\theta_{13}^{cm} &= \theta_{13}^{lab} + \sin^{-1}(\rho_{13}\sin\theta_{13}^{lab}), \\
\rho_{13} &= \left(\frac{m_1 m_3}{m_2 m_4}\frac{T_{cm}}{Q + T_{cm}}\right)^{\frac{1}{2}}, \\
\sigma_{lab}^{(1)}(\theta_{13}^{lab}) &= \sigma_{cm}^{(1)}(\theta_{13}^{cm}) \times \frac{(1 + 2\rho_{13}\cos\theta_{13}^{cm} + \rho_{13}^2)^{\frac{3}{2}}}{|1 + \rho\cos\theta_{13}^{cm}|}
\end{aligned} \tag{2.52}$$

- (2) heavy in - light particle detected : $A_1(A_2, A_3)A_4$. The observed cross section is in terms of $\sigma(\theta_{23}^{cm} = \pi - \theta_{13}^{cm})$. Thus one can relate inverse kinematics cross section from normal kinematics cross section,

$$\sigma_{cm}^{(2)}(\theta_{23}^{cm}) = \sigma_{cm}^{(1)}(\theta_{13}^{cm} = \pi - \theta_{23}^{cm}) \tag{2.53}$$

  Conversion between lab frame and cm frame is

$$\begin{aligned}
\tan\theta_{23}^{lab} &= \frac{\sin(\pi - \theta_{13}^{cm})}{\rho_{23} + \cos(\pi - \theta_{13}^{cm})}, \\
\theta_{13}^{cm} &= \pi - (\theta_{23}^{lab} + \sin^{-1}(\rho_{23}\sin\theta_{23}^{lab})), \\
\rho_{23} &= \left(\frac{m_2 m_3}{m_1 m_4}\frac{T_{cm}}{Q + T_{cm}}\right)^{\frac{1}{2}}, \\
\sigma_{lab}^{(2)}(\theta_{23}^{lab}) &= \sigma_{cm}^{(1)}(\theta_{13}^{cm}) \times \frac{(1 - 2\rho_{23}\cos\theta_{13}^{cm} + \rho_{23}^2)^{\frac{3}{2}}}{|1 - \rho_{23}\cos\theta_{13}^{cm}|}
\end{aligned} \tag{2.54}$$

- (3) heavy in - heavy detected : $A_1(A_2, A_4)A_3$. The observed cross section is in terms of $\sigma(\theta_{24}^{cm} = \theta_{13}^{cm})$. Thus,

$$\sigma_{cm}^{(3)}(\theta_{24}^{cm}) = \sigma_{cm}^{(1)}(\theta_{13}^{cm} = \theta_{24}^{cm}) \tag{2.55}$$

  Conversion between lab and cm frame is

$$\begin{aligned}
\tan\theta_{24}^{lab} &= \frac{\sin\theta_{13}^{cm}}{\rho_{24} + \cos\theta_{13}^{cm}}, \\
\theta_{13}^{cm} &= \theta_{24}^{lab} + \sin^{-1}(\rho_{24}\sin\theta_{24}^{lab}), \\
\rho_{24} &= \left(\frac{m_2 m_4}{m_1 m_3}\frac{T_{cm}}{Q + T_{cm}}\right)^{\frac{1}{2}}, \\
\sigma_{lab}^{(3)}(\theta_{24}^{lab}) &= \sigma_{cm}^{(1)}(\theta_{13}^{cm}) \times \frac{(1 + 2\rho_{24}\cos\theta_{13}^{cm} + \rho_{24}^2)^{\frac{3}{2}}}{|1 + \rho_{24}\cos\theta_{13}^{cm}|}
\end{aligned} \tag{2.56}$$

In case of $A_1(A_2, A_4)A_3$(heavy particle in and heavy particle is detected), we want to convert between $\sigma(\theta_{24}^{cm})$ and $\sigma(\theta_{24}^{lab})$. Since $\theta_{24}^{cm} = \theta_{13}^{cm}$, we can simply get $\sigma(\theta_{24}^{cm}) = \sigma(\theta_{13}^{cm})$. And, ρ_{13} need to be changed into ρ_{24} (exchange particle and target, $1 \leftrightarrow 2$ and $3 \leftrightarrow 4$) [7]

The case of $A_1(A_2, A_3)A_4$ (the heavy particle in and light fragment is detected) is similar except that $\theta_{23}^{cm} = \pi - \theta_{13}^{cm}$. Thus,

$$\begin{aligned}
\tan\theta_{23}^{lab} &= \frac{\sin(\pi - \theta_{13}^{cm})}{\rho_{23} + \cos(\pi - \theta_{13}^{cm})}, \\
\theta_{13}^{cm} &= \pi - (\theta_{23}^{lab} + \sin^{-1}(\rho_{23}\sin\theta_{23}^{lab})), \\
\rho_{23} &= \left(\frac{m_2 m_3}{m_1 m_4}\frac{T_{cm}}{Q + T_{cm}}\right)^{\frac{1}{2}}, \\
\sigma(\theta_{23}^{lab}) &= \sigma(\theta_{13}^{cm}) \times \frac{(1 - 2\rho_{23}\cos\theta_{13}^{cm} + \rho_{23}^2)^{\frac{3}{2}}}{|1 - \rho_{23}\cos\theta_{13}^{cm}|}
\end{aligned} \tag{2.57}$$

In numerical calculation, to get the correct quadrant from the angle inversion, one have to use $atan2(Y, X)$ which solves $X + iY = Re^{i\theta}$, instead of $atan(Y/X)$ in Fortran. $atan2$ take into account the sign of both arguments.

[7] This can be understood as

$$\rho = \left(\frac{m_p m_{detected}}{m_{target} m_{residue}}\frac{T_{cm}}{Q + T_{cm}}\right)^{\frac{1}{2}}$$

Thus, different kinematics gives different mass ratio. Normally the $theta_{cm}$ is defined as an angle between light projectile and projectile like fragment. Thus, depending on the observed particle, the angle have to be changed.

Chapter 3

Formal scattering theory: In momentum space

3.1 Formal scattering theory: In-, Out- state and Moller operator

두 입자의 Scattering을 생각할 때, 보통은 과거($t = -\infty$) 에는 매우 멀리 떨어져 있다가 $t = 0$ 에서 산란하고 미래($t = \infty$) 에서는 다시 매우 멀리 떨어지는 경우를 생각하게 된다. 또한, 두 입자가 매우 멀리 떨어져 있는 경우에는 두 입자 사이에 작용하는 힘이 없다고 생각할 수 있고, 산란에 의한 전이 확률을 나타낼때도 free particle에 대한 quantum number를 이용하는 것이 편하다.

$$H|\psi_p^{(+)}\rangle = E|\psi_p^{(+)}\rangle = \frac{p^2}{2m}|\psi_p^{(+)}\rangle \tag{3.1}$$

Scattering 은 흔히 free incoming state 로부터 free outgoing state 로의 변화를 나타낸다.[1] 따라서, 이 둘을 연결시켜 주는 S operator(scattering operator)를

$$|\psi_{out}\rangle = S|\psi_{in}\rangle \tag{3.2}$$

을 생각할 수 있다.

그러나, 실제 산란을 기술하는 Hamiltonian은 interaction을 포함하고 있고 시간이 지난다고 해서 바뀌는 것도 아니다. 과거나 미래의 어느 순간부터는 H 와 그 solution $|\psi$ 을 H_0와 그 solution $|\psi_{in}\rangle$ 으로 바꿔쓸 수 있다고 생각하는 것이 좋다. We can consider $|\psi_{in}\rangle$ state such that time evolution of $|\psi\rangle$ at $t = 0$ state becomes

$$\begin{aligned} U(t)|\psi\rangle &\to_{t\to-\infty} U^0(t)|\psi_{in}\rangle, \\ U(t)|\psi\rangle &\to_{t\to+\infty} U^0(t)|\psi_{out}\rangle. \end{aligned} \tag{3.3}$$

where $U(t) = e^{-iHt}$ and $U_0(t) = e^{-iH_0t}$. 즉, 충분히 먼 시간 전 또는 후에는 $|\psi\rangle$ 대신 $\psi_{in,out}\rangle$ 을 사용해도 좋다는 것이다. 따라서, 정확하게는 $t = 0$에서의 상태 $|\psi\rangle$ 는

$$|\psi\rangle = \lim_{t\to-\infty} U^\dagger(t)U_0(t)|\psi_{in}\rangle = \lim_{t\to+\infty} U^\dagger(t)U_0(t)|\psi_{out}\rangle \tag{3.4}$$

따라서, Möller operator $\Omega_\pm$ 를 다음과 같이 정의하면,

$$\begin{aligned} \Omega_\pm &\equiv \lim_{t\to\mp\infty} U(t)^\dagger U_0(t), \\ |\psi\rangle &= \Omega_+|\psi_{in}\rangle = \Omega_-|\psi_{out}\rangle \end{aligned} \tag{3.5}$$

[1] scattering theory에서 사용하는 potential이 만족해야하는 조건은 흔히 (1) $V(r)$ 은 large r에 대해 r^{-3} 보다 빨리 떨어져야 한다. (2) $V(r)$은 small r에서 r^{-2} 보다 덜 singular 해야한다. (3) $V(r)$은 continuous 해야 한다.

따라서, Coulomb potential이나 attractive singular potential의 경우에는 다른 formalism을 사용해야 한다.

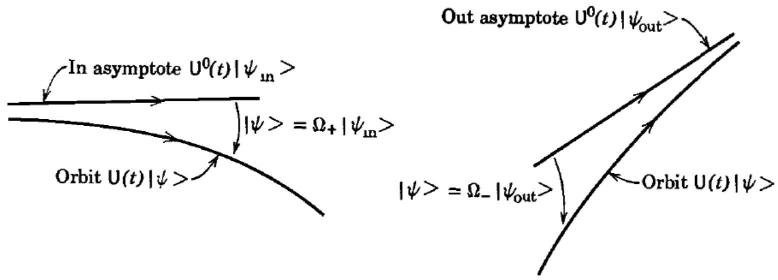

Figure 3.1: Classical Representation of the roled of the Möller operators

S-matrix는

$$
\begin{aligned}
|\psi_{out}\rangle &= \Omega_-^\dagger|\psi\rangle = \Omega_-^\dagger\Omega_+|\psi_{in}\rangle, \\
S &= \Omega_-^\dagger\Omega_+ = 1 + R \text{ or } 1 - R
\end{aligned} \tag{3.6}
$$

로 정의 될 수 있고, Unitary 임을 알 수 있다. (However, note that $\Omega_\pm$ themselves are not unitary.)

다시 정리하자면, 다음과 같다. ψ and ϕ which is in system with interaction and without interaction, their time evolution would be

$$\psi(t) = e^{-iHt}|\psi(0)\rangle, \quad \phi(t) = e^{-iH_0t}|\phi(0)\rangle \tag{3.7}$$

Since, we think the full wave function $\psi(t)$ would behave like a plane wave at very long before and after collision, we would expect,

$$
\begin{aligned}
&\psi(t \to \pm\infty) \simeq \phi(t \to \pm\infty), \\
&||e^{-iHt}|\psi(0)\rangle - e^{-iH_0t}|\phi(0)\rangle|| \xrightarrow{t\to\pm\infty} 0
\end{aligned} \tag{3.8}
$$

$$
\boxed{
\begin{array}{ccccc}
\text{in asymptote} & \to^{\Omega_+} & \text{actual state at t=0} & \leftarrow^{\Omega_-} & \text{out asymptote} \\
|\psi_{in}\rangle & \to & |\psi\rangle & \leftarrow & |\psi_{out}\rangle \\
|\phi\rangle & \to & |\phi+\rangle & & \\
 & & |\chi-\rangle & \leftarrow & |\chi\rangle
\end{array}
} \tag{3.9}
$$

일반적으로 asymptotic state는 free Hamiltonian의 eigen-state로 쓰는 것이 편하므로, scattering state 는 $|\phi\rangle^{(+)} = \Omega_+|\phi\rangle$로 scattering state를 쓰고, 이것은 t=0 에서 $|\phi\rangle^{(+)}$는 먼 과거에는 $|\phi\rangle$ 와 같은 상태였다고 생각할 수 있다는 것이다. $|\phi+\rangle$ means the actual state of the system at $t = 0$ *if the in asymptote was* $|\phi_{in}\rangle = |\phi\rangle$. (It does not mean state at $t \to +\infty$ 또는 $|\phi\rangle^{(+)}$ 가 t=0에 ϕ라는 상태에 있다는 뜻이 아님.) [2]

The actual state at time $t = 0$, which is from $|\psi_{in}\rangle = |\phi\rangle$, is $|\phi+\rangle = \Omega_+|\phi\rangle$ and actual state at time $t = 0$, which goes to $|\psi_{out}\rangle = |\chi\rangle$ is $|\chi-\rangle = \Omega_-|\chi\rangle$. Thus the probability of transition at time $t = 0$ is

$$w(\chi \leftarrow \phi) = |\langle\chi - |\phi+\rangle| = |\langle\chi|S|\phi\rangle|^2. \tag{3.10}$$

One can prove that S-matrix commutes with H_0 rather than H. In other words, S-matrix conserves the free kinetic energy between in and out states. One can use the following relation

$$H\Omega_\pm \quad = \quad \Omega_\pm H_0 \tag{3.11}$$

[2] $\Omega_+|\phi\rangle \equiv |\phi+\rangle$, $\Omega_-|\chi\rangle \equiv |\chi-\rangle$.

and because $\Omega^\dagger\Omega = 1$ (note that in general $\Omega\Omega^\dagger \neq 1$. Ω is not unitary.)

$$\Omega_\pm^\dagger H \Omega_\pm = H_0. \tag{3.12}$$

This makes to interpret $\Omega_\pm$ as operators to give free Hamiltonian H_0 from full Hamiltonian H. (If Moller operator is unitary, it implies that H and H_0 have the same spectrum, which is only true if there is no bound states for H.) And we can prove $SH_0 = H_0S$. Thus, in energy= $\langle\psi_{in}|H_0|\psi_{in}\rangle$ and out-energy= $\langle\psi_{out}|H_0|\psi_{out}\rangle$. Thus, we will have

$$\langle \boldsymbol{p}'|S|\boldsymbol{p}\rangle = \delta(E_{p'} - E_p) \times (\text{remainder}) \tag{3.13}$$

일반적으로 free state는 momentum eigen-state이므로, 앞으로 $|\boldsymbol{k}\rangle$와 $|\boldsymbol{k}\rangle^{(\pm)}$는 free LS equation과 full LS equation의 solution이다. 즉,

$$\begin{aligned} H_0|\boldsymbol{k}\rangle &= E_k|\boldsymbol{k}\rangle \\ H|\boldsymbol{k}\rangle^{(\pm)} &= (H_0 + V)|\boldsymbol{k}\rangle^{(\pm)} = E_k|\boldsymbol{k}\rangle^{(\pm)}. \end{aligned} \tag{3.14}$$

여기서, $\pm$는 서로 다른 boundary condition을 만족하는 해 임을 나타낸다.

We may introduce operator R such that $S = 1 + R$. From the energy conservation, one may write

$$\langle \boldsymbol{p}'|R|\boldsymbol{p}\rangle = -2\pi i\delta(E_{p'} - E_p)t(\boldsymbol{p}' \leftarrow \boldsymbol{p}) \tag{3.15}$$

This,

$$\boxed{\langle \boldsymbol{p}'|S|\boldsymbol{p}\rangle = \langle \boldsymbol{p}'|\boldsymbol{p}\rangle - 2\pi i\delta(E_{p'} - E_p)\langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle^{(+)}} \tag{3.16}$$

where normalization convention $\langle \boldsymbol{p}'|\boldsymbol{p}\rangle = \delta^{(3)}(\boldsymbol{p}' - \boldsymbol{p})$ is used and $t(\boldsymbol{p}' \leftarrow \boldsymbol{p}) = \langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle^{(+)}$. And this choice of convention, makes $t(\boldsymbol{p}' \leftarrow \boldsymbol{p}) \simeq \langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle$ in Born approximation. $t(\boldsymbol{p}' \leftarrow \boldsymbol{p})$ is called T matrix on the energy shell. This does not fully define operator T. ($t(\boldsymbol{p}' \leftarrow \boldsymbol{p})$ is an matrix elements of T). To fully define operator T one have to define $\langle \boldsymbol{p}'|T(E+i0)|\boldsymbol{p}\rangle$ for all $\boldsymbol{p}'$ and $\boldsymbol{p}$ (not just $|\boldsymbol{p}'| = |\boldsymbol{p}|$)

Later scattering amplitude is related to on-shell T-matrix as

$$\boxed{f(\boldsymbol{p}; \leftarrow \boldsymbol{p}) = -(2\pi)^2\mu t(\boldsymbol{p}' \leftarrow \boldsymbol{p})} \tag{3.17}$$

3.2 LS equation for scattering

- Useful relation:

$$\theta(t - t_0) = -\int \frac{dE'}{2\pi i}\frac{e^{-\frac{i}{\hbar}E'(t-t_0)}}{E' + i\epsilon}, \quad \frac{d}{dt}\theta(t - t_0) = \delta(t - t_0) \tag{3.18}$$

- Note that

$$\begin{aligned} &\int_{-\infty}^{0} dt\frac{d}{dt}\left(e^{\frac{\epsilon}{\hbar}t}X(t)\right) = e^{\frac{\epsilon}{\hbar}t}X(t)|_{-\infty}^{0} = X(0) \quad \text{if } \epsilon > 0. \\ &= \frac{\epsilon}{\hbar}\int_{-\infty}^{0} dte^{\frac{\epsilon}{\hbar}t}X(t) + \int_{-\infty}^{0} dte^{\frac{\epsilon}{\hbar}t}\frac{d}{dt}X(t) \end{aligned} \tag{3.19}$$

  Thus,

$$\begin{aligned} \lim_{\epsilon\to 0+}\frac{\epsilon}{\hbar}\int_{-\infty}^{0} dte^{\frac{\epsilon}{\hbar}t}X(t) &= X(0) - \int_{-\infty}^{0} dt\left(\lim_{\epsilon\to 0+} e^{\frac{\epsilon}{\hbar}t}\right)\frac{d}{dt}X(t) \\ &= X(0) - X(t)|_{-\infty}^{0} = \lim_{t\to-\infty} X(t) \end{aligned} \tag{3.20}$$

  In a similar way,

$$\lim_{\epsilon\to 0+} -\frac{\epsilon}{\hbar}\int_{+\infty}^{0} dte^{-\frac{\epsilon}{\hbar}t}X(t) = \lim_{t\to+\infty} X(t) \tag{3.21}$$

- For Moller operator

$$
\begin{aligned}
|\boldsymbol{k}\rangle^{(+)} &= \Omega_+|\boldsymbol{k}\rangle = \lim_{t\to-\infty} U(t)^\dagger U_0(t)|\boldsymbol{k}\rangle \\
&= \lim_{\epsilon\to 0+}\frac{\epsilon}{\hbar}\int_{-\infty}^{0} dt e^{\frac{\epsilon}{\hbar}t}U^\dagger(t)U_0(t)|\boldsymbol{k}\rangle = \lim_{\epsilon\to 0+}\frac{\epsilon}{\hbar}\int_{-\infty}^{0} dt e^{i(H-E_k-i\epsilon)t/\hbar}|\boldsymbol{k}\rangle \\
&= \lim_{\epsilon\to 0+}\frac{\epsilon}{\hbar}\frac{e^{i(H-E_k-i\epsilon)t/\hbar}}{i(H-E_k-i\epsilon)/\hbar}|_{-\infty}^{0}|\boldsymbol{k}\rangle = \lim_{\epsilon\to 0+}\frac{i\epsilon}{E_k+i\epsilon-H}|\boldsymbol{k}\rangle
\end{aligned} \tag{3.22}
$$

여기서 $t\to-\infty$ part is zero 를 이용했다.(즉, ϵ 항이 일종의 boundary condition역할 을 한다.)

- 앞의 Moller operator 결과를 이용하여, 다음과 같은 결과를 얻을 수 있다.

$$
\boxed{|\boldsymbol{k}\rangle^{(\pm)} = \lim_{\epsilon\to 0}\frac{\pm i\epsilon}{E_k\pm i\epsilon-H}|\boldsymbol{k}\rangle = \lim_{\epsilon\to 0}\pm i\epsilon G(E_k\pm i\epsilon)|\boldsymbol{k}\rangle} \tag{3.23}
$$

즉, $|\boldsymbol{k}\rangle^{(\pm)} = \lim_{\epsilon\to 0}|\boldsymbol{k}\rangle^{\pm\epsilon}$ 으로 정의하면, $|\boldsymbol{k}\rangle^{\pm\epsilon}$ 는 다음식을 만족한다. $(H_0-E_k)|\boldsymbol{k}\rangle = 0$를 만족시키는 $|\boldsymbol{k}\rangle$ 에 대해 $H|\boldsymbol{k}\rangle^{\pm} = E_k|\boldsymbol{k}\rangle^{\pm}$ 를 만족시키는 $|\boldsymbol{k}\rangle^{\pm\epsilon}$을 다음과 같이 정의할 수 있다.

$$
\begin{aligned}
&(E_k\pm i\epsilon-H)|\boldsymbol{k}\rangle^{\pm\epsilon} = \pm i\epsilon|\boldsymbol{k}\rangle \leftrightarrow |\boldsymbol{k}\rangle^{\pm\epsilon} = \frac{\pm i\epsilon}{E_k\pm i\epsilon-H}|\boldsymbol{k}\rangle, \\
&(E_k\pm i\epsilon-H_0)|\boldsymbol{k}\rangle^{\pm\epsilon} = \pm i\epsilon|\boldsymbol{k}\rangle + V|\boldsymbol{k}\rangle^{\pm\epsilon}
\end{aligned} \tag{3.24}
$$

이 경우 $|\boldsymbol{k}\rangle^{\pm\epsilon}$ 는 inhomogeneous equation 을 만족하고 unique solution을 가지며, 동시에 특정 boundary condition을 만족시킨다. 또한 inverse operator 도 잘 정의된다.

Thus, we get LS equation

$$
\boxed{|\boldsymbol{k}\rangle^{(\pm)} = |\boldsymbol{k}\rangle + \lim_{\epsilon\to 0}\frac{1}{E_k-H_0\pm i\epsilon}V|\boldsymbol{k}\rangle^{(\pm)},} \tag{3.25}
$$

이고, ±는 각각 서로 다른 boundary consition을 준다.[3] 이 식에서 $E_k = \frac{\boldsymbol{k}^2}{2\mu}$. 중간에 complete set 을 넣는다고 할 때, $|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|$, H_0 becomes $H_0 = \frac{\boldsymbol{k}'^2}{2\mu}$ for relative two-body.

Momentum component of wave function. How one define $\psi_{\boldsymbol{p}}^{(+)}(\boldsymbol{k})$? From L.S. equation, we expect,

$$
\begin{aligned}
\langle\boldsymbol{k}|\boldsymbol{p}\rangle^{(+)} &= \langle\boldsymbol{k}|\boldsymbol{p}\rangle + \int\frac{dk'}{\mathcal{N}}\langle\boldsymbol{k}|G_0(E)|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|V|\boldsymbol{p}\rangle^{(+)} \\
&= \mathcal{N}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{p}) + \frac{1}{\mathcal{N}}\frac{\mathcal{N}}{E-\frac{\boldsymbol{k}^2}{2\mu}}\langle\boldsymbol{k}|V|\boldsymbol{p}\rangle^{(+)}
\end{aligned} \tag{3.26}
$$

Thus,

$$
\frac{1}{\mathcal{N}}\langle\boldsymbol{k}|\boldsymbol{p}\rangle^{(+)} = \delta^{(3)}(\boldsymbol{k}-\boldsymbol{p}) + \frac{1}{\mathcal{N}}\frac{1}{E-\frac{\boldsymbol{k}^2}{2\mu}}\langle\boldsymbol{k}|V|\boldsymbol{p}\rangle^{(+)} \tag{3.27}
$$

Should we define

$$
\psi_{\boldsymbol{p}}^{(+)}(\boldsymbol{k}) = \langle\boldsymbol{k}|\psi_{\boldsymbol{p}}\rangle^{(+)} = \int d^3r\sqrt{\frac{\mathcal{N}}{(2\pi)^3}}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi_{\boldsymbol{p}}^{(+)}(\boldsymbol{r})? \tag{3.28}
$$

[3](1)이미 이 섹션의 첫 식에서 $\pm i\epsilon$ 과 boundary condition 의 관계를 보여준다. (2) 두 boundary condition은 Causality와 관련이 있다. Causality를 정의하는 방법은 여러가지가 있을 수 있겠지만, 일단, 반응 함수의 경우는 $f(t) = \int dt' F(t-t')g(t')$ 에서 $F(t<0) = 0$ 으로 생각할 수 있다. (3) 또는 position space 에서의 scattering solution 이 $e^{ikx} + f(k)e^{ikr}/r$ 꼴이 되는 것을 의미한다. 이것은 이후에 보여질 것이다.

Or

$$\psi_p^{(+)}(\boldsymbol{k}) = \frac{1}{\mathcal{N}}\langle \boldsymbol{k}|\psi_{\boldsymbol{p}}\rangle^{(+)} = \frac{1}{\mathcal{N}}\sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\int d^3r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi_p^{(+)}(\boldsymbol{r})? \tag{3.29}$$

- Green's function or resolvant : Green function(free resolvant or free propagator) is defined as

$$G(z) \equiv \frac{1}{z-H}, \quad G_0(z) \equiv \frac{1}{z-H_0} \tag{3.30}$$

Matrix에 대한 다음 식을 이용하면,

$$\boxed{\frac{1}{A} - \frac{1}{B} = \frac{1}{B}(B-A)\frac{1}{A} = \frac{1}{A}(B-A)\frac{1}{B}} \tag{3.31}$$

This satisfies (LS equation for Green function)

$$G(z) = G_0(z) + G_0(z)VG(z) = G_0(z) + G(z)VG_0(z) \tag{3.32}$$

for $z = E \pm i\epsilon$. Or we can define,

$$G^{\pm}(E) = G(E \pm i\epsilon) \tag{3.33}$$

이를 이용하면, (그리고 $\pm i\epsilon G_0(E \pm i\epsilon)|\boldsymbol{k}\rangle = |\boldsymbol{k}\rangle$ 를 이용)

$$|\boldsymbol{k}\rangle^{\pm\epsilon} = \pm i\epsilon G(E \pm i\epsilon)|\boldsymbol{k}\rangle = |\boldsymbol{k}\rangle + G(E \pm i\epsilon)V|\boldsymbol{k}\rangle \tag{3.34}$$

즉,

$$\boxed{|\boldsymbol{k}\rangle^{(\pm)} = |\boldsymbol{k}\rangle + \lim_{\epsilon\to 0}\frac{1}{E_k \pm i\epsilon - H}V|\boldsymbol{k}\rangle} \tag{3.35}$$

로도 쓸 수 있음을 알 수 있다. $(G_0V|\boldsymbol{k}\rangle^{(+)} = GV|\boldsymbol{k}\rangle)$

- **S-matrix:** 만약 $\boldsymbol{k}' \to \boldsymbol{k}$ 의 S-matrix를 생각하면, S-matrix의 정의로부터, $S = \Omega_-^\dagger\Omega_+$, $\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle = {}^{(-)}\langle \boldsymbol{k}|\boldsymbol{k}'\rangle^{(+)}$ 이고,

$$\begin{aligned}
\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle &= {}^{(-)}\langle \boldsymbol{k}|\boldsymbol{k}'\rangle^{(+)} = \langle \boldsymbol{k}|\boldsymbol{k}'\rangle^{(+)} + \lim_{\epsilon\to 0}\langle \boldsymbol{k}|V\frac{1}{E_k + i\epsilon - H}|\boldsymbol{k}'\rangle^{(+)} \\
&= \langle \boldsymbol{k}|\boldsymbol{k}'\rangle + \lim_{\epsilon\to 0}\langle \boldsymbol{k}|\frac{1}{E_k' + i\epsilon - H_0}V|\boldsymbol{k}'\rangle^{(+)} + \lim_{\epsilon\to 0}\langle \boldsymbol{k}|V\frac{1}{E_k + i\epsilon - H}|\boldsymbol{k}'\rangle^{(+)} \\
&= \langle \boldsymbol{k}|\boldsymbol{k}'\rangle + \lim_{\epsilon\to 0}\frac{\langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)}}{E_{k'} + i\epsilon - E_k} + \lim_{\epsilon\to 0}\frac{\langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)}}{E_k + i\epsilon - E_{k'}} \\
&= \langle \boldsymbol{k}|\boldsymbol{k}'\rangle - 2\pi i\delta(E_k - E_{k'})\langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)}
\end{aligned} \tag{3.36}$$

The final expression

$$\boxed{\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle = \langle \boldsymbol{k}|\boldsymbol{k}'\rangle - 2\pi i\delta(E_k - E_{k'})\langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)}} \tag{3.37}$$

is independent of normalization convention.

- **T-matrix:** 위 식으로 부터 ($E_k = E_{k'}$이어야 하므로) on-shell T-matrix 를

$$t(\boldsymbol{k} \leftarrow \boldsymbol{k}') \equiv \langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)} \tag{3.38}$$

으로 정의 할 수 있다. 반면, off-shell T-matrix는 $T(\boldsymbol{k}, \boldsymbol{k}'; E \neq E_{\boldsymbol{k},\boldsymbol{k}'})$ 로써, additional energy index가 필요하다.

보통은 S-matrix 식에서 에너지 보존 delta function을 빼내고,

$$\hat{S} = I - i(factor)\hat{T} \tag{3.39}$$

와 같은 식으로 나타낼 수도 있다. 그러나, 이경우 convention에 따라서 T-matrix의 정의가 달라짐에 주의. 또한, partial wave decompose하기 전에는 첫번째 항이 숫자 1이 아니라 operator임. 예를 들어,

$$\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle = \delta(E_k - E_{k'})s_{\boldsymbol{k},\boldsymbol{k}'}, \quad \langle \boldsymbol{k}|\hat{T}|\boldsymbol{k}'\rangle = \delta(E_k - E_{k'})t_{\boldsymbol{k},\boldsymbol{k}'} = \frac{\mu}{k}\delta(k - k')t_{\boldsymbol{k},\boldsymbol{k}'} \tag{3.40}$$

와 같이 정의하는 것이 하나의 convention 이다.

만약, T-matrix를 위와 같이 정의하면,

$$\boxed{\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)} \equiv \langle \boldsymbol{k}'|T|\boldsymbol{k}\rangle, \text{ or } V|\boldsymbol{k}\rangle^{(+)} = T|\boldsymbol{k}\rangle} \tag{3.41}$$

이고 LS equation을 이용하면[4]

$$\begin{aligned} T|\boldsymbol{p}\rangle &= V|\psi_p\rangle^{(+)} = V|\boldsymbol{p}\rangle + VG_0^{+}V|\psi_p\rangle^{(+)} \\ &= V|\boldsymbol{p}\rangle + VG_0^{(+)}T|\boldsymbol{p}\rangle \end{aligned} \tag{3.42}$$

이므로, formal하게 T-matrix의 LS eq.이 얻어진다.

$$\begin{aligned} T(E) &= V + VG_0(E)T(E) \\ &= V + VG_0V + VG_0VG_0V + \ldots \end{aligned} \tag{3.43}$$

Convention과 상관 없이 momentum space에서 다음과 같이 쓸 수 있다.

$$\boxed{\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)} = \langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle + \int \frac{d\tilde{\boldsymbol{k}}}{\mathcal{N}}\langle \boldsymbol{k}'|V|\tilde{\boldsymbol{k}}\rangle \frac{1}{E_{\boldsymbol{k}} - E_{\tilde{\boldsymbol{k}}} + i\epsilon}\langle \tilde{\boldsymbol{k}}|V|\boldsymbol{k}\rangle^{(+)}} \tag{3.44}$$

여기서, $\mathcal{N}$은 state vector 의 normalization에 관계 된다. 한편, 왼쪽의 T -matrix는 on-shell 이지만, 오른쪽의 T-matrix는 half-onshell 임에 유의. 즉, LS equation 의 해는 half-on-shell T-matrix 가 된다. 만약, T-matrix element를 아래와 같이 정의하면,

$$T(\boldsymbol{k}', \boldsymbol{k}; E_{\boldsymbol{k}}) = \frac{1}{\mathcal{C}}\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)}, \tag{3.45}$$

LS equation for T-matrix becomes

$$\boxed{T(\boldsymbol{k}', \boldsymbol{k}) = \frac{1}{\mathcal{C}}\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle + \int \frac{d\tilde{\boldsymbol{k}}}{\mathcal{N}}\langle \boldsymbol{k}'|V|\tilde{\boldsymbol{k}}\rangle \frac{1}{E_{\boldsymbol{k}} - E_{\tilde{\boldsymbol{k}}} + i\epsilon}T(\tilde{\boldsymbol{k}}, \boldsymbol{k})} \tag{3.46}$$

[4]**주의** 할 것은 $T = V + VG_0^{+}T$ 나 $V|\boldsymbol{k}\rangle^{+} = T|\boldsymbol{k}\rangle$ 와 같이 쓸 때의 T는 사실 $\hat{T}$가 아니라, 위 식에서의 $t_{\boldsymbol{k},\boldsymbol{k}'} = \langle \boldsymbol{k}|t|\boldsymbol{k}'\rangle$와 같이 쓸 때의 t-matrix에 해당한다는 것이다.

- **LS equation in different normalization**: Though we can formally write LS equation as $\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{T}$, the exact number depends on the representation basis.

  If we use normalization $\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}')$, LS equation for T-matrix becomes

$$\langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle^{(+)} = \langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle + \int d\tilde{\boldsymbol{p}} \langle \boldsymbol{p}'|V|\tilde{\boldsymbol{p}}\rangle \frac{1}{E_{\boldsymbol{p}} - E_{\tilde{\boldsymbol{p}}} + i\epsilon} \langle \tilde{\boldsymbol{p}}|V|\boldsymbol{p}\rangle^{(+)} \tag{3.47}$$

  If we use normalization $\langle \boldsymbol{k}|\boldsymbol{k}'\rangle = (2\pi)^3\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}')$,

$$\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)} = \langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle + \int \frac{d\tilde{\boldsymbol{k}}}{(2\pi)^3} \langle \boldsymbol{k}'|V|\tilde{\boldsymbol{k}}\rangle \frac{1}{E_{\boldsymbol{k}} - E_{\tilde{\boldsymbol{k}}} + i\epsilon} \langle \tilde{\boldsymbol{k}}|V|\boldsymbol{k}\rangle^{(+)} \tag{3.48}$$

  Then, there will be relation between different representation,

$$\langle \boldsymbol{p}'|\text{V or T}|\boldsymbol{p}\rangle = \frac{1}{(2\pi)^3} \langle \boldsymbol{k}'|\text{V or T}|\boldsymbol{k}\rangle \tag{3.49}$$

  Thus, we have to use consistent definition for LS equation and potential representation. 만약, $T(\boldsymbol{k}', \boldsymbol{k}) = \frac{1}{(2\pi)^3}\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)}$ 로 정의할 경우,

$$T(\boldsymbol{k}', \boldsymbol{k}) = \frac{V(\boldsymbol{k}', \boldsymbol{k})}{(2\pi)^3} + \int d^3\tilde{\boldsymbol{k}} \frac{V(\boldsymbol{k}', \tilde{\boldsymbol{k}})}{(2\pi)^3} \frac{2\mu}{k^2 - \tilde{k}^2 + i\epsilon} T(\boldsymbol{k}', \boldsymbol{k}) \tag{3.50}$$

  가 된다.

- **Free Green's function:** in configuration space, $r = |\boldsymbol{x} - \boldsymbol{x}'|$

$$\begin{aligned}
&\langle \boldsymbol{x}|G_0(E \pm i\epsilon)|\boldsymbol{x}'\rangle = \langle \boldsymbol{x}|\frac{1}{E \pm i\epsilon - H_0}|\boldsymbol{x}'\rangle \\
= &\int \frac{d^3p}{\mathcal{N}} \langle \boldsymbol{x}|\boldsymbol{p}\rangle \frac{1}{E \pm i\epsilon - p^2/2\mu} \langle \boldsymbol{p}|\boldsymbol{x}'\rangle = \frac{1}{(2\pi)^3} \int d^3p e^{i\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}')} \frac{1}{E \pm i\epsilon - p^2/2\mu} \\
= &\frac{2\pi}{(2\pi)^3} \int dp p^2 \int_{-1}^{+1} dz e^{ip|\boldsymbol{x}-\boldsymbol{x}'|z} \frac{1}{E \pm i\epsilon - p^2/2\mu} \\
= &\frac{2\pi}{(2\pi)^3} \int dp p^2 \frac{e^{ipr} - e^{-ipr}}{ipr} \frac{1}{E \pm i\epsilon - p^2/2\mu} = \frac{1}{(2\pi)^3}(4\pi) \int_0^\infty dp p^2 j_0(pr) \frac{1}{E \pm i\epsilon - p^2/2\mu} \\
= &\frac{2\pi}{(2\pi)^3} \int_{-\infty}^{\infty} dz \frac{e^{izr}}{ir} \frac{2\mu z}{k^2 \pm i2\mu\epsilon - z^2}
\end{aligned} \tag{3.51}$$

  where, $k = \sqrt{2\mu E}$ and $\mu = \frac{m}{2}$로 two nucleon reduced mass. . This can be converted into contour integral if the surface integral vanishes. There are two poles,

$$\frac{1}{k^2 \pm i2\mu\epsilon - z^2} \simeq \frac{-1}{(z - k \mp i\frac{\mu\epsilon}{k})(z + k \pm i\frac{\mu\epsilon}{k})} \tag{3.52}$$

  To make the surface integral vanish at large $|z|$, we have to choose upper half plane. Then, in case of $+i\epsilon$, we have to choose $z = k + i\epsilon$ pole, and in case of $-i\epsilon$, we have to choose $z = -k + i\epsilon$ pole. Thus, we get

$$\boxed{\langle \boldsymbol{x}|\frac{1}{E \pm i\epsilon - H_0}|\boldsymbol{x}'\rangle = -\frac{\mu}{2\pi\hbar^2} \frac{e^{\pm ik|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|} e^{-\frac{\epsilon k}{2E}|x-x'|}} \tag{3.53}$$

  Final expression is independent of normalization convention and the last exponential term disappears when $\epsilon \to 0$.

  This result shows that the ϵ prescription choose a specific boundary condition. This can be explicitly shown in the configuration space expression of LS equation at large distance as following.

- **scattering amplitude:** In configuration space, LS equation implies

$$\begin{aligned}\langle \boldsymbol{r}|\boldsymbol{k}\rangle^{(+)} &= \langle \boldsymbol{r}|\boldsymbol{k}\rangle + \int d^3\boldsymbol{r}' \langle \boldsymbol{r}|G_0(E+i\epsilon)|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|V|\boldsymbol{k}\rangle^{(+)} \\ &= \langle \boldsymbol{r}|\boldsymbol{k}\rangle - \int d^3\boldsymbol{r}' \frac{\mu}{2\pi\hbar^2}\frac{e^{ik|\boldsymbol{r}'-\boldsymbol{r}|}}{|\boldsymbol{r}'-\boldsymbol{r}|}\langle \boldsymbol{r}'|V|\boldsymbol{k}\rangle^{(+)} \end{aligned} \tag{3.54}$$

By using

$$\begin{aligned}|\boldsymbol{r}-\boldsymbol{r}'| &= r - r'\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}' + \ldots, \\ \lim_{\boldsymbol{r}\to\infty}\langle \boldsymbol{r}'|G_0(E\pm i\epsilon)|\boldsymbol{r}\rangle &\to -\frac{\mu}{2\pi\hbar^2}\frac{e^{ikr-ikr'\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}}'}}{r} = -\frac{e^{ikr}}{r}\frac{\mu}{2\pi\hbar^2}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \end{aligned} \tag{3.55}$$

where $\boldsymbol{k}' = k\hat{\boldsymbol{r}}$. 따라서, we can define scattering amplitude asymptotically[5]

$$\psi_{out}(\boldsymbol{r}) \to_{\boldsymbol{r}\to\infty} \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\boldsymbol{k}',\boldsymbol{k})\frac{e^{ikr}}{r}\right). \tag{3.56}$$

where

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\sqrt{\frac{(2\pi)^3}{\mathcal{N}}}\frac{\mu}{2\pi\hbar^2}\int d^3\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}\langle \boldsymbol{r}'|V|\boldsymbol{k}\rangle^{(+)} \tag{3.57}$$

scattering matrix $\hat{f}$를 scattering amplitude로 부터 정의하면,

$$\boxed{\langle \boldsymbol{k}'|\hat{f}|\boldsymbol{k}\rangle \equiv f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{(2\pi)^3}{\mathcal{N}}\frac{\mu}{2\pi\hbar^2}\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)}} \tag{3.58}$$

으로 formal 하게 쓸 수 있다.(엄밀하게는 $\boldsymbol{k}' = k\hat{\boldsymbol{r}}$인 관계가 있음에 주의해야한다.)

From the definition T-matrix, $\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)} = \langle \boldsymbol{k}'|T|\boldsymbol{k}\rangle$, 즉 $V|\boldsymbol{k}\rangle^{(+)} = T|\boldsymbol{k}\rangle$, then we get

$$f(\boldsymbol{k}',\boldsymbol{k}) = -\frac{(2\pi)^3}{\mathcal{N}}\frac{\mu}{2\pi\hbar^2}\langle \boldsymbol{k}'|T|\boldsymbol{k}\rangle \tag{3.59}$$

만약, Coulomb interaction과 같은 long range interaction이 있는 경우에는 asymptotic wave 로 plane wave 를 사용할 수 없기 때문에, scattering amplitude를 다르게 정의 해야한다. 단, 이 때, differential cross section은 잘 정의되더라도, total cross ssection은 diverge 할 수 있다.

- relation between S-, T-, R- matrix and scattering amplitude and potential.

$$\begin{aligned}\langle \boldsymbol{k}|\hat{T}|\boldsymbol{k}'\rangle &\equiv \langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)} \\ \langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle &= \langle \boldsymbol{k}|\boldsymbol{k}'\rangle - 2\pi i\delta(E_k - E_{k'})\langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)} \\ &= \langle \boldsymbol{k}|\boldsymbol{k}'\rangle - 2\pi i\delta(E_k - E_{k'})\langle \boldsymbol{k}|T|\boldsymbol{k}'\rangle \\ &= \langle \boldsymbol{k}|\boldsymbol{k}'\rangle + i\delta(E_k - E_{k'})\frac{\mathcal{N}}{(2\pi)^3}\frac{(2\pi)^2\hbar^2}{\mu}f(\boldsymbol{k}',\boldsymbol{k}) \end{aligned} \tag{3.60}$$

- factoring Energy conservation : In case of elastic scattering, we can factor out energy conservation part and only consider matrix elements for angles,

$$\begin{aligned}&\langle \boldsymbol{k}|\boldsymbol{k}'\rangle = \mathcal{N}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}') = \mathcal{N}\frac{\delta(k-k')}{kk'}\delta^{(2)}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}') \\ &\delta(E_k - E_{k'}) = \frac{\mu}{k}\delta(k-k'),\ \text{in case } E_k = \tfrac{k^2}{2\mu}. \end{aligned} \tag{3.61}$$

[5]여기서 우리는 potential과 scattering amplitude 사이의 관계를 보였다. 보통의 경우 asymptotic boundary condition(**Sommerfeld Radiation Condition**) 을 가정하는 것으로 시작하기도 한다.

따라서 angle에 대한 정보만 생각하면,

$$
\begin{aligned}
\langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle &\equiv \mathcal{N}\frac{\delta(k-k')}{kk'}\langle\hat{\boldsymbol{k}}|\hat{S}(k)|\hat{\boldsymbol{k}}'\rangle = \mathcal{N}\frac{\delta(k-k')}{kk'}S(k,\theta) \\
&= \mathcal{N}\frac{\delta(k-k')}{kk'}\left(\delta^{(2)}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}') - \frac{2\pi i\mu k}{\mathcal{N}}\langle\boldsymbol{k}|T|\boldsymbol{k}'\rangle\right) \\
&= \mathcal{N}\frac{\delta(k-k')}{kk'}\left(\delta^{(2)}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}') + \frac{ik}{2\pi}f(\boldsymbol{k}',\boldsymbol{k})\right) \qquad (3.62)
\end{aligned}
$$

따라서,

$$
\boxed{\hat{S}(k,\theta) = \hat{\delta} - \frac{1}{\mathcal{N}}2\pi i\mu k\hat{T}(k,\theta) = \hat{\delta} + \frac{ik}{2\pi}f(k,\theta)} \qquad (3.63)
$$

와 같이 나타낼 수 있다. 단, 이 경우, $k = k'$ is already implied and only consider angles for S-matrix 그리고 delta는 angle에 대한 operator.

- K-matrix: Since $S = I + icT$ is unitary, (where c is a constant factor depending on the convention),

$$
\begin{aligned}
&S^\dagger S = SS^\dagger = I, \\
\rightarrow\ & T - T^\dagger = ciTT^\dagger = ciT^\dagger T, \\
\rightarrow\ & (T^\dagger)^{-1} - T^{-1} = ciI \rightarrow (T^{-1}/(c/2) + iI)^\dagger = (T^{-1}/(c/2) + iI) \qquad (3.64)
\end{aligned}
$$

Thus, $K \equiv (T^{-1}/(c/2) + iI)^{-1}$ is a Hermitian. (Note that we may multiply constant factors in the definition of K)

$$
\begin{aligned}
&K \equiv \left[\frac{2}{c}T^{-1} + iI\right]^{-1}, \\
\rightarrow\ & \frac{c}{2}T = K(I - iK)^{-1}, \\
\rightarrow\ & S = \frac{I + iK}{I - iK}, \quad K = i\frac{I - S}{I + S}. \qquad (3.65)
\end{aligned}
$$

commonly used factors are $c = \pm 1, \pm 2, \pm 2\pi\mu k$,

3.2.1 Examples

Example: Born approximation

Let us consider the case of scattering by weak local potential $V(\boldsymbol{x})$. If the potential is weak enough we may approximate $|\psi\rangle^{(+)} \simeq |\phi\rangle + \ldots$. Then, by the first-order Born approximation,

$$
\begin{aligned}
f^{(1)}(\boldsymbol{k}',\boldsymbol{k}) &= -\sqrt{\frac{(2\pi)^3}{\mathcal{N}}}\frac{\mu}{2\pi\hbar^2}\int d^3\boldsymbol{r}' e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}\langle\boldsymbol{r}'|V|\boldsymbol{k}\rangle \\
&= -\frac{2\mu}{4\pi\hbar^2}\int d^3x' e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{x}'}V(\boldsymbol{x}') \qquad (3.66)
\end{aligned}
$$

For the case of Yukawa potential,

$$
\begin{aligned}
V(r) &= V_0\frac{e^{-mr}}{mr}, \\
f^{(1)}(\theta) &= -\frac{2\mu V_0}{m\hbar^2}\frac{1}{q^2+m^2}, \quad q = |\boldsymbol{k}-\boldsymbol{k}'| = 4k^2\sin^2\frac{\theta}{2}, \\
|f^{(1)}(\theta)|^2 &= \left(\frac{2\mu V_0}{m\hbar^2}\right)^2\frac{1}{(q^2+m^2)^2} \qquad (3.67)
\end{aligned}
$$

$m \rightarrow 0$ limit gives Rutherford scattering amplitude(replace q into θ's).

Example: Eikonal approximation

If potential $V(\boldsymbol{x})$ varies very slowly compared to the wave length λ(which is small), we may approximate the wave function as semi-classical wave function, $E = \frac{\hbar^2 k^2}{2\mu}$

$$\begin{aligned}\psi^{(+)} &\sim e^{iS(\boldsymbol{x})/\hbar}, \\ \frac{\hbar^2 k^2}{2\mu} &= \frac{(\nabla S)^2}{2\mu} + V, \quad \text{Hamilton-Jacobi equation.}\end{aligned} \tag{3.68}$$

With further assumption that the classical trajectory is just a straight line path with impact parameter b, we have

$$\begin{aligned}\frac{S(\boldsymbol{x} = \boldsymbol{b} + z\hat{z})}{\hbar} &= kz + \int_{-\infty}^{z} dz' \left[\sqrt{k^2 - \frac{2\mu}{\hbar^2} V(\sqrt{b^2 + z'^2})} - k\right] \\ &\simeq kz - \frac{\mu}{\hbar^2 k} \int_{-\infty}^{z} dz' V(\sqrt{b^2 + z'^2})\end{aligned} \tag{3.69}$$

This means that the particle wave function only changes the phase during inside the scattering region. Then, We may obtain scattering amplitude by putting $\psi^{(+)} \sim e^{iS(\boldsymbol{x})/\hbar}$ to $\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)} \simeq \langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle_{eik}$. Then, scattering amplitude

$$\begin{aligned}f(\boldsymbol{k}', \boldsymbol{k}) &\simeq -\sqrt{\frac{(2\pi)^3}{\mathcal{N}}} \frac{\mu}{2\pi\hbar^2} \langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle_{eik} \\ &= -\sqrt{\frac{(2\pi)^3}{\mathcal{N}}} \frac{\mu}{2\pi\hbar^2} \frac{\mathcal{N}}{(2\pi)^3} \int d^3\boldsymbol{x} e^{-i\boldsymbol{k}'\cdot\boldsymbol{x}} V(\boldsymbol{x}) e^{iS(\boldsymbol{x})/\hbar} \\ &= \ldots\end{aligned} \tag{3.70}$$

By using

$$\int_0^{2\pi} d\phi_b e^{-ikb\theta\cos\phi_b} = 2\pi J_0(kb\theta), \tag{3.71}$$

the final result

$$\begin{aligned}f(\boldsymbol{k}', \boldsymbol{k}) &= -ik \int_0^{\infty} db b J_0(kb\theta)[e^{2i\Delta(b)} - 1], \\ \Delta(b) &= -\frac{\mu}{2k\hbar^2} \int_{-\infty}^{\infty} V(\sqrt{b^2 + z^2}) dz.\end{aligned} \tag{3.72}$$

3.2.2 Differential cross section, total cross section and Optical theorem

- current density can be defined from the continuity equation.

$$\frac{\partial \rho(\boldsymbol{x}, t)}{\partial t} + \nabla \cdot \boldsymbol{j}(\boldsymbol{x}, t) = 0 \tag{3.73}$$

With $\rho(\boldsymbol{x}, t) = |\psi(\boldsymbol{x}, t)|^2$ and Schrodinger equation for both ψ,

$$i\hbar \frac{\partial \psi}{\partial t} = [\hat{T} + \hat{V}]\psi \tag{3.74}$$

we get

$$\frac{\partial \psi^* \psi}{\partial t} = \frac{\hbar}{2i\mu} \nabla \cdot [(\nabla\psi)^* \psi - \psi^* \nabla\psi] + \frac{1}{i\hbar}[\psi^* \hat{V}\psi - (\hat{V}\psi)^* \psi] \tag{3.75}$$

Thus,

$$\frac{\partial \rho(\boldsymbol{x},t)}{\partial t} = -\nabla \cdot \boldsymbol{j}_{free} - \frac{i}{\hbar}\langle\psi|\left[\delta(\boldsymbol{r}-\boldsymbol{r}_i)\hat{V} - \hat{V}^\dagger\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right]|\psi\rangle \tag{3.76}$$

with

$$\boldsymbol{j}_{free} = \frac{\hbar}{2i\mu}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \langle\psi|\frac{\hbar}{2i\mu}\left[\delta(\boldsymbol{r}-\boldsymbol{r}_i)\nabla_i - \nabla_i\delta(\boldsymbol{r}-\boldsymbol{r}_i)\right]|\psi\rangle, \tag{3.77}$$

This simply corresponds to $j = v|\psi|^2$ with $v = \hbar k/\mu$ for plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{x}}$

- current와 flux의 차이: current는 vector quantity이고 flux(current density)는 scalar quantity 이다. If electric current I_A (ampere=(charge)/(time)) flowing through A at point x, electric current density is $j = \lim_{A\to 0}\frac{I_A}{A}$. The current density vector is the vector whose magnitude is the electric current density, $\boldsymbol{j} = \rho\boldsymbol{v}$. flux of $\boldsymbol{j}$ for area dA is $\boldsymbol{j}\cdot\hat{n}dA$. (다른 말로 flux는 단위 시간당 단위 면적당 통과하는 입자의 수.) density라는 말을 사용할 때 probability density, charge density 인지 number density 인지 구분할 것.

- α 가 작은 angle 범위에서 detect 될때, the count rate $N_\alpha(\Omega,\Delta\Omega)$ 는 $\Delta\Omega$에 비례 해야 하고, multiple scattering을 무시한다면, 빔이 있는 곳의 number of target particle n에 비례할 것이고, beam 사이의 interaction을 무시한다면, beam flux에 비례할 것이다.

$$\begin{aligned} N_\alpha(\Omega,\Delta\Omega) &\propto nJ\Delta\Omega \\ &= (\Delta\Omega nJ)\frac{d\sigma}{d\Omega} \end{aligned} \tag{3.78}$$

여기서 비례상수를 differential cross section으로 정의할 수 있다. 거꾸로

$$\frac{d\sigma}{d\Omega} = \frac{N_\alpha(\Omega,\Delta\Omega)}{(\Delta\Omega nJ)} \tag{3.79}$$

- In a classical mechanics, number of scattered particles in a specific solid angle $\Delta\Omega$ is the same as number of incident particles in a specific area.

$$N_{sc}(\Delta\Omega) = n_{inc}\sigma(\Delta\Omega), \tag{3.80}$$

where n_{inc} is number of projectiles incident per unit area. One define differential cross section as

$$\sigma(d\Omega) = \frac{d\sigma}{d\Omega}d\Omega \tag{3.81}$$

- In quantum mechanics, a probability of finding a scattered particle in solid angle is

$$w(d\Omega \leftarrow \psi_{in}) = d\Omega\int_0^\infty p^2dp|\psi_{out}(\boldsymbol{p})|^2 \tag{3.82}$$

By considering variation of impact parameter ρ, one may consider

$$N_{sc}(d\Omega) = \int d^2\rho n_{inc}w(d\Omega \leftarrow \phi_\rho) = n_{inc}\int d^2\rho w(d\Omega \leftarrow \phi_\rho), \tag{3.83}$$

where ϕ_ρ is a wave packet peaked around impact parameter ρ. We assumed ρ is random and so n_{inc} is practically constant. Then, comparison with classical expression,

$$\sigma(d\Omega \leftarrow \phi) = \int d^2\rho\ w(d\Omega \leftarrow \phi_\rho) \tag{3.84}$$

we can view $\sigma(d\Omega \leftarrow \phi)$ is an effective cross sectional area of the target potential for scattering ϕ_ρ into $d\Omega$. If the beam is sufficiently peaked over momentum $\boldsymbol{p}_0$, one may consider $\sigma(d\Omega \leftarrow \boldsymbol{p}_0)$. Note that this requires that each incident particle scatter separately off one scattering center at most. Thus, beam should be weak enough and target should be thin and so on.

- From the S-matrix,

$$\begin{aligned}\psi_{out}(\boldsymbol{p}) &= \int d^3p' \langle \boldsymbol{p}|S|\boldsymbol{p}'\rangle \psi_{in}(\boldsymbol{p}'), \\ &= \psi_{in}(\boldsymbol{p}) + \frac{i}{2\pi m}\int d^3p' \delta(E_p - E_{p'}) f(\boldsymbol{p} \leftarrow \boldsymbol{p}')\psi_{in}(\boldsymbol{p}') \end{aligned} \tag{3.85}$$

If we do not consider forward angle, $\boldsymbol{p}$ is not near $\boldsymbol{p}_0$, we can ignore the first term and $\psi_{in}(\boldsymbol{p}) = e^{-i\boldsymbol{\rho}\cdot\boldsymbol{p}}\phi(\boldsymbol{p})$. To be continued.

- Asymptotic wave [6]

$$\psi \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \tag{3.86}$$

Then incident flux and scattered flux into area $\Delta A = r^2 d\Omega$

$$\begin{aligned}|\vec{j}_{inc}|d\sigma &= \frac{k}{\mu}d\sigma = \text{(number of incident particles per unit time for effective area per one target)}, \\ \vec{j}_{scatt}\cdot\hat{r}r^2 d\Omega &= \frac{k}{\mu}\frac{|f(\theta)|^2}{r^2}r^2 d\Omega = \text{(number of scattered particles per unit time for solid area)}\end{aligned} \tag{3.87}$$

We can consider that the total number of scattered particles to solid angle $d\Omega$ per unit time is related to the number of incident particles to effective area of target,

$$\vec{j}_{scatt}\cdot\hat{r}r^2 d\Omega = |\vec{j}_{inc}|d\sigma \tag{3.88}$$

In other words, effective target area for the solid angle is

$$\sigma(\Delta\Omega) = \frac{d\sigma}{d\Omega}d\Omega = \frac{|j_{scatt}|r^2}{|j_{inc}|}d\Omega. \tag{3.89}$$

즉,

$$d\sigma(\Omega) = \frac{\text{probability current into } d\Omega \text{ in the direction } d\Omega}{\text{probability current density of the incident wave}}, \tag{3.90}$$

단, 위의 경우 cross section은 하나의 projectile과 하나의 target인 경우를 말한다. 따라서, 실험의 경우에는 target/projectile의 갯수를 고려해야한다.

$$d\sigma^{exp}(\Omega) = \frac{\text{particle current into } d\Omega \text{ in the direction } d\Omega}{\text{particle current density of the incident particles}} \tag{3.91}$$

When computing the actual number of particles scattered, one have to consider how many targets presents in a beam area and their effective area for scattering. One can consider a density of particles as number of particles for unit area. (this is not usual volume density defined as number of particles for unit volume.) This makes some confusion when making a relation with actual observed scattered particle number and density of incident particles and target particles.

[6] For long range scattering case, the asymptotic wave should be distorted. Thus, we need to include logarithmic phase factor in asymptotic form. In case of long range force, total cross section becomes infinite, because total number of particle incident are infinite for plane waves and they all have to scatter.

- Confusing !!: Differential cross section $\frac{d\sigma}{d\Omega}$ is defined as **the flux of scattered particles through the area $dA = r^2 d\Omega$ in the direction θ, per unit incident flux.**

$$
\begin{aligned}
d\sigma = \frac{d\sigma}{d\Omega} d\Omega &= \frac{\text{flux of scattered particles through } r^2 d\Omega}{\text{incident flux}} \\
&= \frac{(\text{\# of particles scattered})/\text{sec}}{(\text{\# of particles incident})/\text{area}/\text{sec}} = \frac{|j_{scatt}| r^2 d\Omega}{|j_{inc}|}
\end{aligned}
\tag{3.92}
$$

This corresponds to an effective surface area of a target for one incident particle and also proportional to the probability of one incident particle to be scattered by a target nuclei. 여기서, 입자의 갯수로 생각하면 ,

$$
\frac{(\text{\# of scattered particle per time})}{(\text{\# of incident particle per time})} = \frac{(\text{effective area by target})}{(\text{incident beam area})},
$$

$$
(\text{effective area by target }) = (\text{\# of target nuclei in beam area }) \times \frac{d\sigma}{d\Omega} \tag{3.93}
$$

$$
\frac{dN}{dt} = j_i n_t \Delta\Omega \sigma(\theta, \phi) \tag{3.94}
$$

with $\sigma(\theta, \phi)$ is the number of particles scattered per unit time per unit scattering center and per unit incident flux into a unit solid angle. units are usually, mb/sr. $10\ mb = 1\ fm^2$

The same expression can be written as

$$
\Delta I = I_0 n_t \frac{d\sigma}{d\Omega} \Delta\Omega \tag{3.95}
$$

where I_0 is the number of incident particles per unit time, $\Delta\Omega$ is the solid angle subtended by the detector, ΔI is the number of detected particles per unit time in $\Delta\Omega$, and n_t is the number of target nuclei per unit surface area. ($I_0 = \rho_b * A * v = n_b v$, where n_b is a number of beam particles in unit length,A is the beam surface area, $n_t = \rho_t d$ with ρ is the target volume density, d is the target thickness) Actual number of particles detected depends on the experimental conditions(beam intensity and target thickness), but the differential cross section is independent of such conditions.

- differential cross section and scattering amplitude: Thus, differential cross section becomes [7]

$$
\frac{d\sigma}{d\Omega_k} = |f(\boldsymbol{k}, \boldsymbol{k}')|^2 \tag{3.96}
$$

In case of inelastic scattering, $v_i \neq v_f$, asymptotic wave

$$
\psi^{asym} = A[e^{ikz} + f(\theta, \phi) \frac{e^{ik_f r}}{r}], \tag{3.97}
$$

implies

$$
\sigma(\theta, \phi) = \frac{v_f}{v_i} |f(\theta, \phi)|^2. \tag{3.98}
$$

Sometimes the flux factor v_f/v_i can be absorbed to the definition of scattering amplitudes, $\tilde{f} = \sqrt{v_f/v_i} f$.

[7] 이 관계는 normalization convention 과 무관.

- Optical throem: Let us derive optical theorem, from the definition, $V|\psi\rangle^{(+)} = T|\boldsymbol{k}\rangle$,

$$\mathrm{Im}\langle\boldsymbol{k}|V|\psi\rangle^{+} = \mathrm{Im}\left[\left({}^{+}\langle\psi| - {}^{+}\langle\psi|V\frac{1}{E-H_0-i\epsilon}\right)V|\psi\rangle\right] \tag{3.99}$$

에서 imaginary part는 $i\epsilon$ 으로 부터 온다. 따라서,

$$\frac{1}{E-H_0-i\epsilon} = \frac{P}{E-H_0} + i\pi\delta(E-H_0) \tag{3.100}$$

를 이용하면,

$$\begin{aligned}\mathrm{Im}\langle\boldsymbol{k}|V|\psi\rangle^{+} &= -\pi\langle\psi^{(+)}|V\delta(E-H_0)V|\psi\rangle^{(+)}, \\ \mathrm{Im}\langle\boldsymbol{k}|T|\boldsymbol{k}\rangle &= -\pi\langle\psi|V\delta(E-H_0)V|\psi\rangle = -\pi\langle\boldsymbol{k}|T^{\dagger}\delta(E-H_0)T|\boldsymbol{k}\rangle\end{aligned} \tag{3.101}$$

plane wave의 complete set을 넣으면,

$$\begin{aligned}\mathrm{Im}\langle\boldsymbol{k}|T|\boldsymbol{k}\rangle &= -\pi\langle\boldsymbol{k}|T^{\dagger}\delta(E-H_0)T|\boldsymbol{k}\rangle \\ &= -\pi\int\frac{d^3k'}{\mathcal{N}}\langle\boldsymbol{k}|T^{\dagger}|\boldsymbol{k}'\rangle\langle\boldsymbol{k}'|T|\boldsymbol{k}\rangle\delta(E-\frac{\hbar^2k'^2}{2\mu}) \\ &= -\pi\int d\Omega'\frac{1}{\mathcal{N}}\frac{\mu k}{\hbar^2}|\langle\boldsymbol{k}'|T|\boldsymbol{k}\rangle|^2\end{aligned} \tag{3.102}$$

이 되고, 이것을 scattering amplitude의 식으로 바꾸면, $f = -\frac{(2\pi)^3}{\mathcal{N}}\frac{\mu}{2\pi\hbar^2}t$,

$$\mathrm{Im}\langle\boldsymbol{k}|f|\boldsymbol{k}\rangle = \frac{k}{4\pi\hbar^2}\int d\Omega'|\langle\boldsymbol{k}'|f|\boldsymbol{k}\rangle|^2 = \frac{k}{4\pi\hbar^2}\sigma_{tot} \tag{3.103}$$

따라서, 잘 알려진 optical theorem 이 만족된다.

$$\boxed{\mathrm{Im}f(\theta=0) = \frac{k}{4\pi}\sigma_{tot}} \tag{3.104}$$

optical relation 식은 convention independent이다.

3.2.3 cross section again: relativistic

REF: arXiv:1605.005692

- Reaction $1+2\to f$, final state f can be with two or more particles.
- reaction rate $\mathcal{R}_f$

$$\mathcal{R}_f = \frac{dN_f}{dV\,dt} = \frac{dN_f}{d^4x} \tag{3.105}$$

Because N_f and d^4x is independent of reference frame, reaction rate is invariant under Lorentz transformation.

- reaction rate is proportional to number density of particles n_1,n_2 and relative velocity. This is initial flux F.
- cross section σ is defined so that it contain intrinsic property of the system independent of details of initial state.

$$\sigma = \frac{\mathcal{R}_f}{F} \tag{3.106}$$

To $\mathcal{R}_f$ is invariant under L.T., cross section and initial flux should be invariant. However, non-relativistic flux is not invariant under L.T.

- non-relativistic flux is

$$F_{nr} = n_1 n_2 v_r, \quad v_r = |\boldsymbol{v}_1 - \boldsymbol{v}_2|. \tag{3.107}$$

- Theoretical calculation of reaction rate (unpolarized) in normalization $\langle p|p'\rangle = (2\pi)^3 2E\delta^3(\boldsymbol{p}-\boldsymbol{p}')$(thus, $n = 2E$ in number density.)

$$R^{th}_{fi} = \frac{dP_{fi}}{dVdt} = \int \overline{|\mathcal{M}_{fi}|^2}(2\pi)^4\delta^4(P_i - P_f)\prod_{j=3}^{n}\frac{d^3p_j}{(2\pi)^3 2E_j} \tag{3.108}$$

- non-relativistic flux can be written as

$$\begin{aligned} F_{nr} &= n_1 n_2 |\boldsymbol{v}_1 - \boldsymbol{v}_2| = \frac{n_1 n_2}{E_1 E_2}\mathcal{F} = 4\mathcal{F}, \\ \mathcal{F} &= \sqrt{(p_1 \cdot p_2) - m_1^2 m_2^2} \end{aligned} \tag{3.109}$$

  for collinear velocity(in other words, direction of two velocity is in the same or opposite direction.) However, non-relativistic flux is not L.T. invariant. On the other hand, $\mathcal{F}$ is L.T. invariant, we get

$$\frac{\mathcal{F}}{E_1 E_2} = \sqrt{(\boldsymbol{v}_1 - \boldsymbol{v}_2)^2 - (\boldsymbol{v}_1 \times \boldsymbol{v}_2)^2} = \bar{v} \tag{3.110}$$

  In other words, we can write

$$F = n_1 n_2 \sqrt{(\boldsymbol{v}_1 - \boldsymbol{v}_2)^2 - (\boldsymbol{v}_1 \times \boldsymbol{v}_2)^2}. \tag{3.111}$$

  Thus, F_{nr} is only a special case. The flux may be generalized as Moller flux

$$F = \frac{n_1 n_2}{E_1 E_2}\sqrt{-\frac{1}{2}A^{\mu\nu}A_{\mu\nu}}, \quad A^{\mu\nu} = p_1^\mu p_2^\mu - p_1^\nu p_2^\mu. \tag{3.112}$$

- However, does $\bar{v}$ correspond to relative velocity in relativity? Densities are also not invariant under L.T.

- we may define $\mathcal{R} = An_1 n_2$ where A reduces to σv_{rel} in the rest frame of collinear velocities.

$$A = \frac{p_1 \cdot p_2}{E_1 E_2}\sigma v_{rel} \tag{3.113}$$

$$v_{rel} = \frac{\sqrt{(\boldsymbol{v}_1 - \boldsymbol{v}_2)^2 - (\boldsymbol{v}_1 \times \boldsymbol{v}_2)^2}}{1 - \boldsymbol{v}_1 \cdot \boldsymbol{v}_2} \tag{3.114}$$

3.2.4 LS equation for bound state

Bound state 의 경우는

$$\begin{aligned} (H_0 + V)|\psi_b\rangle &= E_b|\psi_b\rangle, \quad E = E_b < 0, \\ (H_0 - E_b)|\psi_b\rangle &= -V|\psi_b\rangle \end{aligned} \tag{3.115}$$

여기서, $H_0 > 0$이고, $E_b < 0$ 이므로, homogeneous LS equation

$$|\psi_b\rangle = \frac{1}{E_b - H_0}V|\psi_b\rangle \tag{3.116}$$

가 얻어진다. boundstate 의 경우는 $E_b - H_0$ cannot give pole 이므로 $i\epsilon$ 을 Green function에 포함하지 않아도 되고, free solution $|\psi\rangle$,(such that $(H_0 - E_b)|\phi\rangle = 0$), 를 포함하지 않아도 된다는 점에 주의.

위 식을 configuration space 에서 쓰면, $|E_b| = \frac{\kappa^2}{2\mu}$ or $k = i\kappa$ 일 때,

$$\langle \boldsymbol{x}|\psi_b\rangle = \psi_b(\boldsymbol{x}) = -\frac{\mu}{2\pi\hbar^2}\int d^3x' \frac{e^{-\kappa|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|}V(\boldsymbol{x}')\psi_b(\boldsymbol{x}') \tag{3.117}$$

이 되어 large r 에서 exponential fall-off 형태가 됨을 알 수 있다.

3.2.5 Bound-state 와 scattering state 의 관계.

이미 보았듯이 bound state 와 scattering state가 만족하는 식은 약간 다르다.

$$\begin{aligned} |\Psi_b\rangle &= G_0(E_b)V|\Psi_b\rangle, \quad E = E_b < 0, \\ t(E) &= V + VG_0(E+i\epsilon)t(E), \quad E > 0 \end{aligned} \tag{3.118}$$

여기서, transition operator 의 E를 E_b로 continuation 시키면 어떻게 될까? Formally, we can express t-matrix as sum of series

$$t(E) = (1 - VG_0(E))^{-1}V \tag{3.119}$$

Expanding in $VG_0(E)$

$$t(E) = (1 + VG_0 + VG_0VG_0 + \dots)V = V(1 + G_0V + G_0VG_0V + \dots) \tag{3.120}$$

then,

$$t(E_b)|\Psi_b\rangle = V(1 + 1 + 1 + \dots)|\Psi_b\rangle \tag{3.121}$$

bound state 에 대한 관계식으로부터 $t(E_b < 0)$는 diverging 하는 것을 알 수 있다. 즉 bound state에 대해 $T(E = -E_b)$ 는 pole을 가진다.

또는 약간 다르게,

$$\begin{aligned} t(E) &= [(G_0^{-1} - V)G_0]^{-1}V = G_0^{-1}\frac{1}{E - H_0 - V}V \\ &= G_0^{-1}\frac{1}{E - H}V = G_0^{-1}GV \end{aligned} \tag{3.122}$$

로 바꿔 쓴다음 complete set을 넣으면,

$$|\Psi_b\rangle\langle\Psi_b| + \int d^3p|\Psi_p^+\rangle\langle\Psi_p^+| = 1 \tag{3.123}$$

$$\begin{aligned} t(E) &= (E - H_0)|\Psi_b\rangle\frac{1}{E - E_b}\langle\Psi_b|V + \int d^3p(E - H_0)|\boldsymbol{p}\rangle^+\frac{1}{E - \boldsymbol{p}^2/m}\langle\boldsymbol{p}^+|V \\ &= V|\Psi_b\rangle\frac{1}{E - E_b}\langle\Psi_b|V + \int d^3pV|\boldsymbol{p}\rangle^+\frac{1}{E - \boldsymbol{p}^2/m}\langle\boldsymbol{p}^+|V \end{aligned} \tag{3.124}$$

가 되고, $E \to E_b$ 일 때, pole을 가지는 것을 볼 수 있다.

$$t(E) \to V|\Psi_b\rangle\frac{1}{E - E_b}\langle\Psi_b|V, \quad E \to E_b \tag{3.125}$$

또는 , scattering wave의 asymptotic form으로 부터 $E_b = -\kappa^2/(2\mu)$,

$$\bar{u}(r,k) \simeq [s(k)e^{ikr} - e^{-ikr}] \to [s(\pm i\kappa)e^{\mp\kappa r} - e^{\pm\kappa r}] \tag{3.126}$$

인데, 여기서 물리적으로 중요한 것은 ratio between incoming and outgoing wave, 즉 S 이다. Bound state는 outgoing wave without incoming wave라고 생각할 수 있고, 따라서 ratio가 infinite여야한다. 이경우, $k = i\kappa$ 에서 $S(k = i\kappa)$ 가 pole을 가지는 것이 correct bound state solution을 줌을 알 수 있다. 단지, $S(E)$ 의 negative energy axis 에서의 pole은 $\pm i\kappa$ 를 모두 의미하므로, 적합하지 않고, $S(k)$ 가 positive imaginary axis 에서 pole을 가져야 함을 알 수 있다.

3.2.6 $\chi^{(-)}(R)$?

$\pm i\epsilon$ prescription corresponds to two different boundary condition in the wave function.

$$(T_R + V(R))\chi^{(+)}_{\boldsymbol{k}}(\boldsymbol{R}) = E\chi^{(+)}_{\boldsymbol{k}}(\boldsymbol{R}) \tag{3.127}$$

$$\chi^{(+)}_{\boldsymbol{k}}(\boldsymbol{R}) \to e^{i\boldsymbol{k}\cdot\boldsymbol{R}} + f^{(+)}(\hat{R})\frac{e^{ikR}}{R}, \tag{3.128}$$

$$\chi_{\boldsymbol{k}}(\boldsymbol{R}) = 4\pi \sum_{LM} i^L Y^*_{LM}(\hat{k})Y_{LM}(\hat{R})e^{i\delta_L}\chi^{(+)}_L(R), \tag{3.129}$$

$$\chi^{(+)}_L(R) \to (\cos\delta_L j_L(kR) + \sin\delta_L n_L(kR)) \tag{3.130}$$

$$f^{(+)}(\theta,\phi) = 4\pi \sum_{LM} Y^*_{LM}(\hat{k})Y_{LM}(\theta,\phi)e^{i\delta_L}\frac{\sin\delta_L}{k} \tag{3.131}$$

we can consider $\chi^{(-)}_{\boldsymbol{k}}(\boldsymbol{R})$ as a solution of

$$(T_R + V^*(R))\chi^{(-)}_{\boldsymbol{k}}(\boldsymbol{R}) = E\chi^{(-)}_{\boldsymbol{k}}(\boldsymbol{R}) \tag{3.132}$$

$$\chi^{(-)}_{\boldsymbol{k}}(\boldsymbol{R}) \to e^{i\boldsymbol{k}\cdot\boldsymbol{R}} + f^{(-)}(\hat{R})\frac{e^{-ikR}}{R}, \tag{3.133}$$

$$\chi^{(-)}_{\boldsymbol{k}}(\boldsymbol{R}) = 4\pi \sum_{LM} i^L Y^*_{LM}(\hat{k})Y_{LM}(\hat{R})e^{-i\delta^*_L}(\chi^{(+)}_L(R))^*, \tag{3.134}$$

$$f^{(-)}(\theta,\phi) = 4\pi \sum_{LM} (-1)^L Y^*_{LM}(\hat{k})Y_{LM}(\theta,\phi)e^{-i\delta^*_L}\frac{\sin\delta^*_L}{k} \tag{3.135}$$

Thus,

$$(\chi^{(-)}_{\boldsymbol{k}}(\boldsymbol{R}))^* = \chi^{(+)}_{-\boldsymbol{k}}(\boldsymbol{R}) \tag{3.136}$$

Chapter 4

Partial wave decomposition

4.1 Basic relations

In general, any function of angle between two vector $\cos\theta = \hat{\boldsymbol{r}}_1 \cdot \hat{\boldsymbol{r}}_2$ can be expanded in terms of Legendre Polynomial and more generally by spherical harmonics.

- delta function expansion is

$$\boxed{\delta^{(3)}(\boldsymbol{r}_1 - \boldsymbol{r}_2) = \frac{\delta(r_1 - r_2)}{r_1 r_2}\delta^{(2)}(\hat{r}_1 - \hat{r}_2) = \frac{\delta(r_1 - r_2)}{r_1 r_2}\sum_{lm} Y_{lm}(\hat{r}_1)Y^*_{lm}(\hat{r}_2)} \tag{4.1}$$

  Or,

$$\langle\hat{r}_1|\hat{r}_2\rangle = \delta^{(2)}(\hat{r}_1 - \hat{r}_2) = \delta(\phi_1 - \phi_2)\delta(\cos\theta_1 - \cos\theta_2) = \sum_{lm} Y_{lm}(\hat{r}_1)Y^*_{lm}(\hat{r}_2) \tag{4.2}$$

- Useful relation for spherical harmonics:

$$\boxed{\sum_m Y^*_{lm}(\hat{r}_1)Y_{lm}(\hat{r}_2) = \frac{(2l+1)}{4\pi}P_l(\hat{r}_1 \cdot \hat{r}_2), \qquad \text{addition theorem}} \tag{4.3}$$

$$\begin{aligned}
Y_{lm}(\hat{z}) &= \sqrt{\frac{2l+1}{4\pi}}\delta_{m0} \quad \text{if } \hat{p} = \hat{z}, \\
Y_{l0}(\hat{r}) &= \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta) \quad \text{if } m = 0, \\
Y_{lm}(-\hat{r}) &= (-1)^l Y_{lm}(\hat{r}), \\
Y^*_{lm}(\hat{r}) &= (-1)^m Y_{l-m}(\hat{r}).
\end{aligned} \tag{4.4}$$

  Orthogonality of Legendre Polynomial:

$$\int_{-1}^{1} dx P_n(x)P_m(x) = \frac{2}{2n+1}\delta_{mn} \tag{4.5}$$

  Orthogonality of Spherical Harmonics:

$$\int d\Omega Y^*_{lm}(\Omega)Y^*_{l'm'}(\Omega) = \delta_{ll'}\delta_{mm'} \tag{4.6}$$

- Completeness relation from spherical bessel functions,

$$\boxed{\int_0^\infty x^2 j_n(ax) j_n(bx) dx = \frac{\pi}{2}\frac{\delta(a-b)}{ab}} \tag{4.7}$$

$$j_l(kr) = \frac{1}{2i^l}\int_{-1}^{+1} e^{ikr\cos\theta} P_l(\cos\theta) d\cos\theta \tag{4.8}$$

Let us consider some general matrix A in basis χ_α. If the basis is complete, we may express any matrix as

$$\begin{aligned} \hat{A} &= \sum_{\alpha\alpha'} A_{\alpha\alpha'} \chi_\alpha \chi^\dagger_{\alpha'}, \\ A_{\alpha\alpha'} &\equiv \mathcal{Z}_{\alpha\alpha'} \chi^\dagger_\alpha \hat{A} \chi_{\alpha'} \end{aligned} \tag{4.9}$$

here the index α can be any discrete or continuous quantity. If index is a continuous quantity, the sum have to be replaced to integral. $\mathcal{Z}_{\alpha\alpha'}$ can be any number and one can re-define the matrix elements We can think the partial wave expansion in this way.

If we think there are some complete set describing spatial space which both acts on radial and angular quantity such that

$$\begin{aligned} &\sum_\alpha |\alpha\rangle\langle\alpha| = \hat{I}, \\ &\langle \boldsymbol{k}|\alpha\rangle \equiv \langle k\alpha| \otimes \langle\hat{k}|\alpha\rangle, \\ &|\boldsymbol{k}\rangle = \left(\sum_\alpha |\alpha\rangle\langle\alpha|\right)|\boldsymbol{k}\rangle = \sum_\alpha |k\alpha\rangle\langle\alpha|\hat{k}\rangle, \\ &|\boldsymbol{r}\rangle = \sum_\alpha |r\alpha\rangle\langle\alpha|\hat{r}\rangle \end{aligned} \tag{4.10}$$

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \langle \boldsymbol{r}|\left(\sum_\alpha |\alpha\rangle\langle\alpha|\right)|\boldsymbol{k}\rangle = \sum_\alpha \langle\hat{r}|\alpha\rangle\langle r\alpha|k\alpha\rangle\langle\alpha|\hat{k}\rangle \tag{4.11}$$

If we introduce explicit forms by spherical harmonics and so on,

$$\begin{aligned} &\langle\hat{r}|\alpha\rangle \to Y_\alpha(\hat{r}), \quad \langle\alpha|\hat{k}\rangle \to Y^*_\alpha(\hat{k}), \\ &\langle r\alpha|k\alpha\rangle \to Z_\alpha \psi_\alpha(r;k) \end{aligned} \tag{4.12}$$

we can write

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \sum_\alpha Z_\alpha \psi_\alpha(r;k) Y_\alpha(\hat{r}) Y^*_\alpha(\hat{k}) \tag{4.13}$$

With an appropriate choice of $Z_\alpha\psi_\alpha(r;k)$, we can express $\langle \boldsymbol{r}|\boldsymbol{k}\rangle$ in terms of partial wave components. We can generalize the expression by extending α to include other quantum numbers acting on spin, isospin. In a similar way, a matrix function may be written such that We may also consider the matrix element as

$$\begin{aligned} A_{mm'}(\boldsymbol{k},\boldsymbol{k}') &= \left(\langle\boldsymbol{k}| \otimes \langle m|\right) \hat{A} \left(|\boldsymbol{k}'\rangle \otimes |m'\rangle\right) \\ &= \sum_{\alpha\beta} \left(\langle\hat{k}|\alpha\rangle\langle k\alpha| \otimes \langle m|\right) \hat{A} \left(|k',\beta\rangle\langle\beta|\hat{k}'\rangle \otimes |m'\rangle\right) \end{aligned} \tag{4.14}$$

If we can combine spatial and spin quantum numbers into f and i such that

$$|k\alpha\rangle \otimes |m\rangle = \left(\sum_i |i\rangle\langle i|\right)|k\alpha\rangle \otimes |m\rangle = \sum_i |ki\rangle\langle i|k\alpha, m\rangle \tag{4.15}$$

where $\langle i|k\alpha, m\rangle$ is a kind of Clebsch-Gordon coefficients and $|k, i\rangle$ contains information of radial, angular and spins. This will allow one to convert any matrix in space, spins into some combination of matrix elements defined in combined states,

$$\begin{aligned} A_{mm'}(\boldsymbol{k}, \boldsymbol{k}') &= \sum_{fi} \langle \hat{k}|f\rangle\langle k, f|\hat{A}|k', i\rangle\langle i|\hat{k}'\rangle \\ &= \sum_{fi} A_{fi}(k, k')\langle \hat{k}|f\rangle\langle i|\hat{k}'\rangle \end{aligned} \tag{4.16}$$

Here $A_{fi}(k, k')$ includes the factors like $\langle i|k\alpha, m\rangle$. We have freedom to choose the definition of each parts in the equation.

4.2 Partial wave expansion of plane wave

- Plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ in partial waves as [1]

$$\boxed{e^{i\boldsymbol{p}\cdot\boldsymbol{r}} = 4\pi \sum_{lm} j_l(pr) i^l Y_{lm}(\hat{r}) Y^*_{lm}(\hat{p}) = \sum_l j_l(pr) i^l (2l+1) P_l(\cos\theta) \text{ if } \hat{p} = \hat{z}} \tag{4.17}$$

(Note that because one can change index $m' = -m$, $\sum_m Y^*_{lm}(\hat{p})Y_{lm}(\hat{r}) = \sum_m Y_{lm}(\hat{p})Y^*_{lm}(\hat{r})$) (Thus, expansion of $e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$ is the same as $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ except $i^L \to i^{-L}$.) Here the radial wave function is spherical Bessel function. But, later it would be more convenient to represent radial wave in Coulomb function

$$j_L(kR) = \frac{1}{kR} F_L(\eta = 0, \rho = kR) \tag{4.18}$$

Thus, we may write

$$\begin{aligned} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} &= 4\pi \sum_{lm} \frac{F_L(0, kR)}{kR} i^l Y_{lm}(\hat{r}) Y^*_{lm}(\hat{p}), \\ &= \sum_L (2L+1) i^L P_L(\cos\theta) \frac{F_L(0, kR)}{kR}, \text{ if } \hat{k} = \hat{z} \end{aligned} \tag{4.19}$$

Note that there is $1/k$ in the expression.

Convention of definition of radial partial wave function $\chi_L(R)$ and it's normalization is arbitrary. There may be two different convention on the defining radial wave function.

$$\chi^{(+)}_{\boldsymbol{k}}(\boldsymbol{R}) = 4\pi \sum_{LM} i^L Y^*_{LM}(\hat{k}) Y_{LM}(\hat{R}) \exp(i\delta_L) \chi^{(+)}_L(R) \tag{4.20}$$

or

$$\chi^{(+)}_{\boldsymbol{k}}(\boldsymbol{R}) = 4\pi \sum_{LM} i^L Y^*_{LM}(\hat{k}) Y_{LM}(\hat{R}) \chi^{(+)}_L(R) \tag{4.21}$$

Note that depending on the convention the relation between S-matrix,T-matrix, scattering amplitude and wave function may change.

[1] Simple explanation of the origin of $(2l+1)$ factor: Consider a plane perpendicular to the flow and a slap of circles at impact parameter b. Then angular momentum $L = b*k$. Thus, we can set $b_l = l/k$. Then, the probability of particle have angular momentum l is proportional to the area of circles, $A = \pi(b^2_{l+1} - b^2_l) = \pi((l+1)^2 - l^2)/k^2 = \pi(2l+1)/k^2$.

- In normalization $\langle \boldsymbol{k}|\boldsymbol{k}'\rangle = \mathcal{N}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}')$, free particle wave function becomes

$$\begin{aligned}
\langle \boldsymbol{r}|\boldsymbol{p}\rangle &= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}e^{i\boldsymbol{p}\cdot\boldsymbol{r}} \\
&= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}} \times 4\pi \sum_{lm} j_l(pr) i^l Y_{lm}(\hat{r}) Y^*_{lm}(\hat{p}) \\
&= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}} \sum_l j_l(pr) i^l (2l+1) P_l(\cos\theta) \text{ if } \hat{p}=\hat{z}, \\
&= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}} \sum_l \frac{F_L(0,\rho)}{kR} i^l (2l+1) P_l(\cos\theta) \text{ if } \hat{p}=\hat{z} \qquad (4.22)
\end{aligned}$$

Since we will consider Coulomb wave function later, we may express free radial wave as

$$\begin{aligned}
j_L(\rho) &= \frac{F_L(0,\rho)}{\rho} \\
&= \frac{1}{\rho}\frac{i}{2}[H_L^{(-)}(0,\rho) - H_L^{(+)}(0,\rho)], \\
&\to \frac{1}{\rho}\frac{i}{2}[e^{-i(\rho - l\pi/2)} - e^{i(\rho-l\pi/2)}], \quad \rho \gg 1 \\
&= \frac{\sin(\rho - l\pi/2)}{\rho} \qquad (4.23)
\end{aligned}$$

즉, 다음과 같은 wave function form을 생각할 수 있다.

- incident wave: e^{ikz}
- Spherical ingoing/outgoing waves: $e^{\pm ikr}$
- angular advancing(?) waves: $e^{\pm ik\theta}$ The usual expansion is incident wave expanded in terms of spherical partial waves, with l, and each radial waves are decomposed into ingoing/outgoing or incident/scattered waves. Now this case is to decompose angular waves into clock wise or anti-clock wise angular advancing waves. This involves 2nd kind Legendre polynomial $Q_{lm}(\theta)$,

$$\begin{aligned}
Q^{\pm}_{lm}(\cos\theta) &\equiv \frac{1}{2}[P_{lm}(\cos\theta) \pm \frac{2}{i\pi}Q_{lm}(\cos\theta) \\
&\sim_{l\gg m} \frac{1}{\sqrt{2\pi\sin\theta}}\frac{(l+m)!}{\Gamma(l+3/2)} \exp\left(\pm i[(l+\frac{1}{2})\theta + m\frac{\pi}{2} - \frac{\pi}{4}]\right) + \mathcal{O}(l^{-1}) \qquad (4.24)
\end{aligned}$$

Inverse relation is

$$P_{lm}(\cos\theta) = \frac{1}{2}[Q^{(+)}_{lm}(\cos\theta) + Q^{(-)}_{lm}(\cos\theta)] \qquad (4.25)$$

This implies that usual Spherical Harmonics(or Legendre polynomial) contains both counter-clock wise part and clock-wise part. Thus, P_l is a kind of standing angular wave and $Q_l^{(\pm)}$ are traveling angular waves. In this decomposition, $Q_l^{(-)}$ is near-side(In the sense thet detector is in the $\theta > 0$ side) and $Q_l^{(+)}$ is called far-side, making the scattering amplitude decomposed into near-side amplitude and far-side amplitude. This concept may be useful for semi-classical description(?).

4.3 Scattering wave for short range interaction

- Note that there are always a convention dependence in the partial wave expansion and normalization of radial wave function. They have to go together.

$$\psi_k(\boldsymbol{r}) = \sum_L (factor)(2L+1) i^L \psi_L(r) P_L(\cos\theta) \tag{4.26}$$

Let us assume that the effect of interaction is to introduce phase shift δ_l in asymptotic wave function. We may use the following asymptotic form,

$$\begin{aligned}
& e^{i\delta_l}\frac{\sin(\rho - \frac{l}{2}\pi + \delta_l)}{\rho}, \quad \text{phase shift in sin function,} \\
= & \; e^{i\delta_l}\frac{i}{2}\left(\frac{e^{-i(\rho - l\pi/2+\delta_l)}}{\rho} - \frac{e^{i(\rho - l\pi/2+\delta_l)}}{\rho}\right) \\
= & \; \frac{i}{2}\left(\frac{e^{-i(\rho - l\pi/2)}}{\rho} - e^{2i\delta_l}\frac{e^{i(\rho - l\pi/2)}}{\rho}\right), \quad \text{incoming and outgoing wave} \\
= & \; \frac{i}{2}\left(\frac{e^{-i(\rho - l\pi/2)}}{\rho} - \frac{e^{+i(\rho - l\pi/2)}}{\rho} + (1-e^{2i\delta_l})\frac{e^{i(\rho - l\pi/2)}}{\rho}\right) \\
= & \; \frac{\sin(\rho - \frac{l}{2}\pi)}{\rho} + i^{-l}\frac{e^{2i\delta_l}-1}{2i}\frac{e^{i\rho}}{\rho}, \quad \text{incident and scattered wave}
\end{aligned} \tag{4.27}$$

where $e^{i\delta_l}$ factor in the first line makes that the incoming wave have no phase shift and only outgoing wave have a phase shift factor.

If I set $(factor) = 1$ and inserting this into partial wave expansion $\psi_L(r)$,

$$\begin{aligned}
\psi_k(\boldsymbol{r}) &= \sum_l (2l+1) i^l \psi_l(r) P_l(\cos\theta), \\
&\to \sum_l (2l+1) i^l \left(\frac{\sin(\rho - \frac{l}{2}\pi)}{\rho} + i^{-l}\frac{e^{2i\delta_l}-1}{2i}\frac{e^{i\rho}}{\rho}\right) P_L(\cos\theta) \\
&\simeq e^{ikz} + \left(\sum_l (2l+1)\frac{e^{2i\delta_l}-1}{2ik} P_l(\cos\theta)\right)\frac{e^{ikr}}{r}, \quad \rho \gg 1
\end{aligned} \tag{4.28}$$

Thus, we find the relation between the scattering amplitude and phase shifts,

$$f(\theta) = \sum_l (2l+1)\frac{e^{2i\delta_l}-1}{2ik} P_l(\cos\theta) \tag{4.29}$$

where note that there is no i^l factor here.

In fact, we can define S-matrix and asymptotic normalization of wave as

$$\begin{aligned}
u_l(kr) &\sim A_L \exp(-i(kr - \frac{l\pi}{2})) - B_L \exp(i(kr - \frac{l\pi}{2})), \\
B_L &\equiv \sum_{L'} S_{LL'} A_{L'}
\end{aligned} \tag{4.30}$$

with any factor of A_L. ($A_L = \frac{i}{2}$ in above equation. We may use $\frac{i}{2}\cos\delta_l$) However, note that we would have additional expansion coefficients in other normalization convention.

Magnitude of S_L are sometimes called as a **reflection coefficient** in 1-D scattering. This implies that $1-|S_L|^2$ can be interpreted as a probability of absorption and $|S_L|^2$ as a probability of survival(?).

In the same normalization, we will write the full scattering wave function as in form of

$$
\begin{aligned}
\psi_k^{(+)}(\boldsymbol{R}) &= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\sum_l i^l(2l+1)P_l(\cos\theta)\psi_L^{(+)}(R), \quad \psi_L^{(+)}(R) = \frac{u_L^{(+)}(R)}{R}, \\
&\xrightarrow{r\to\infty} \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\sum_l i^l(2l+1)P_l(\cos\theta)\frac{1}{kR}\frac{i}{2}[H_L^{(-)}(\eta,\rho) - S_L H_L^{(+)}(\eta,\rho)], \\
&= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\sum_l i^l(2l+1)P_l(\cos\theta)\frac{1}{kR}[F_L(\eta,\rho) + T_L H_L^{(+)}(\eta,\rho)], \quad T_L \equiv \frac{S_L - 1}{2i} \\
&\xrightarrow[\eta\to 0]{r\to\infty} \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\sum_l i^l(2l+1)P_l(\cos\theta)\frac{e^{i\delta_L}\cos\delta_L}{kR}[F_L(0,\rho) + K_L G_L(0,\rho)], \quad K_L = \tan\delta_L,
\end{aligned}
\tag{4.31}
$$

$$
S_L = 1 + 2iT_L = \frac{1+iK_L}{1-iK_L} \tag{4.32}
$$

where $H_L^{(\pm)} = G_L \pm iF_L$. $H_L^{(-)} = H_L^{(+)} - 2iF_L$ 임을 이용. And the phase shift, scattering amplitude and cross section are related

$$
f(\theta) = \sum_l (2l+1)\frac{S_l - 1}{2ik}P_l(\cos\theta), \quad \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \tag{4.33}
$$

interpretation of coefficient: In case of S-matrix, in analogy of 1-dimensional scattering, S-matrix can be considered as reflection coefficient (ratio between ingoing and outgoing wave) or survival coefficient.(if $S = 1$, all ingoing wave survives.) This way of thinking is useful for eikonal approximation.

However, in case of long range Coulomb interaction, the normalization and expansion may have additional phase factor related with Coulomb phase shift.

Also, if the expansion is done with Spherical Harmonics, there will be another factor 4π will appear from the addition theorem eq. (..).

Convention의 차이?

However, in case of multi-channel, it is not clear how the final wave function form should be written for $\alpha' \neq \alpha$,

$$
\begin{aligned}
\psi_k^{(+)}(R) &\to 4\pi\sum_L i^L e^{i\sigma_L}Y_L^*(\hat{k})\sum_{L'}\frac{u_{L'L}^{(+)}(R)}{kR}Y_{L'}(\hat{R})(?), \\
&\to 4\pi\sum_L e^{i\sigma_L}Y_L^*(\hat{k})\sum_{L'}\frac{u_{L'L}^{(+)}(R)}{kR}i^{L'}Y_{L'}(\hat{R})(?)
\end{aligned}
\tag{4.34}
$$

From the asymptotic form,

$$
\begin{aligned}
\frac{u_{\alpha'\alpha}}{kR} &\to \frac{1}{kR}\frac{i}{2}\left(H_{L'}^{(-)}\delta_{\alpha'\alpha} - S_{\alpha'\alpha}H_{L'}^{(+)}\right) \\
&\to \frac{1}{kR}\frac{i}{2}\left(e^{-i\Theta_{L'}}\delta_{\alpha'\alpha} - e^{+i\Theta_L}S_{\alpha'\alpha}\right) \\
&\to \frac{1}{kR}\frac{i}{2}\left[(e^{-i\Theta_{L'}} - e^{+i\Theta_{L'}})\delta_{\alpha'\alpha} - e^{+i\Theta_{L'}}(S_{\alpha'\alpha} - \delta_{\alpha'\alpha})\right] \\
&\to \frac{1}{kR}\sin\Theta_{L'}\delta_{\alpha'\alpha} + \frac{e^{i\Theta_{L'}}}{R}\frac{(S_{\alpha'\alpha} - \delta_{\alpha'\alpha})}{2ik},
\end{aligned}
\tag{4.35}
$$

where

$$\Theta_L = kR - \frac{L\pi}{2} + \sigma_L - \eta \ln 2kR. \tag{4.36}$$

The first term becomes original Coulomb function which gives Coulomb scattering amplitude $f_C(\theta)$. the second term becomes

$$\frac{e^{i(\rho-\eta\ln 2\rho)}}{R} e^{i\sigma_{L'}} i^{-L'} \frac{(S_{\alpha'\alpha} - \delta_{\alpha'\alpha})}{2ik} \tag{4.37}$$

This implies the scattering amplitude $f(\theta)$ becomes in the first convention,

$$f(\theta) = 4\pi \sum_{L,L'} e^{i\sigma_L + i\sigma_{L'}} i^{L-L'} \frac{(S_{\alpha'\alpha} - \delta_{\alpha'\alpha})}{2ik} Y_{L'}(\hat{R}) Y_L^*(\hat{p}) \tag{4.38}$$

while in the second convention,

$$f(\theta) = 4\pi \sum_{L,L'} e^{i\sigma_L + i\sigma_{L'}} \frac{(S_{\alpha'\alpha} - \delta_{\alpha'\alpha})}{2ik} Y_{L'}(\hat{R}) Y_L^*(\hat{p}) \tag{4.39}$$

Since the scattering amplitude itself should be the same in both case, it implies the S-matrix in two convention have different phase factor.

These two convention corresponds to usual spherical Harmonics convention and modified spherical harmonics convention.

On the other hand, for in-elastic scattering, $k' \neq k$, the outgoing flux and incident flux are

$$j_{out} = v_f |f(\theta)|^2, \quad j_{inc} = v_i \tag{4.40}$$

Thus, differential cross section becomes

$$\frac{d\sigma}{d\Omega} = \frac{v_f}{v_i} |f(\theta)|^2 \tag{4.41}$$

This factor can be absorbed into the definition of S-matrix, which corresponds to change the normalization of asymptotic wave function,

4.3.1 How to get the phase shift from the Schrödinger equation

For a partial wave expansion of wave function

$$\psi_k(\boldsymbol{r}) = \sum_L i^L (2L+1) P_L(\cos\theta) \frac{\chi_L(r;k)}{kr} \tag{4.42}$$

We can get the radial wave function $\chi_L(r;k)$ by solving the Schrödinger equation with $\chi_L(0) = 0$ and $\chi'_L(0)$ which is not known a priori.

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} \right) + V(R) - E \right] \chi_L(R) = 0. \tag{4.43}$$

Let us consider the case $V(R) = V_C(R) + V_S(R)$, $V_C(R) = \frac{Z_1 Z_2 e^2}{R}$ (in Gaussian unit)

$$\begin{aligned}
&\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} \right) + \frac{Z_1 Z_2 e^2}{R} + V_S(R) - E \right] \chi_L(R) = 0, \\
&\left[\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} \right) - \frac{2\mu}{\hbar^2} \frac{Z_1 Z_2 e^2}{R} - \frac{2\mu}{\hbar^2} V_S(R) + k^2 \right] \chi_L(R) = 0, \\
&\left[\left(\frac{d^2}{d\rho^2} - \frac{L(L+1)}{\rho^2} \right) - \frac{\eta}{\rho} - \frac{2\mu}{\hbar^2 k^2} V_S(R) + 1 \right] \chi_L(R) = 0, \quad \rho = kR
\end{aligned} \tag{4.44}$$

where $\eta = \frac{2\mu Z_1 Z_2 e^2}{\hbar^2 k}$.

Then, we can obtain numerical solution $u_L(R)$ with initial condition, $u_L(0) = 0$ and $u'_L(0) \neq 0$ with arbitrary value. Then, the true solution will be $\chi_L(R) = B_L u_L(R)$ with unknown constant B_L. We want to obtain $S-$matrix or equivalently phase shift by using matching condition with asymptotic boundary condition.

$$B_L u_L(R) = \chi_L(R) \xrightarrow{R>R_n} \chi_L^{ext}(R) = \frac{i}{2}\left[H_L^{(-)}(0,kR) - S_L H_L^{(+)}(0,kR)\right] \tag{4.45}$$

We require the χ_L and χ'_L to be continuous at matching radius $R = a$. It is convenient to define R-matrix,

$$R_L = \frac{1}{a}\frac{\chi_L(a)}{\chi'_L(a)} = \frac{1}{a}\frac{u_L(a)}{u'_L(a)} \tag{4.46}$$

This gives

$$\begin{aligned} R_L &= \frac{1}{a}\frac{H_L^{(-)}(a) - S_L H_L^{(+)}(a)}{H_L^{'(-)}(a) - S_L H_L^{'(+)}(a)}, \\ S_L &= \left(\frac{H_L^{(-)} - aR_L H_L^{'(-)}}{H_L^{(+)} - aR_L H_L^{'(+)}}\right)_{R=a} \end{aligned} \tag{4.47}$$

As an example, hard sphere scattering implies that $R_L = 0$. Thus, we get the $S-$matrix for hard sphere scattering.

In a similar way, we can relate the R-matrix with other matrix forms,

$$\begin{aligned} R_L &= \frac{1}{a}\frac{F_L(a) + T_L H_L^{(+)}(a)}{F'_L(a) + T_L H_L^{'(+)}(a)}, \quad T_L = -\left(\frac{F_L - aR_L F'_L}{H_L^{(+)} - aR_L H_L^{'(+)}}\right)_{R=a}, \\ R_L &= \frac{1}{a}\frac{F_L(a) + K_L G_L(a)}{F'_L(a) + K_L G'_L(a)}, \quad K_L = -\left(\frac{F_L - aR_L F'_L}{G_L - aR_L G'_L}\right)_{R=a} \end{aligned} \tag{4.48}$$

4.3.2 Phase shift and potential

Let us consider two equations,

$$\begin{aligned} &\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2}\right) - E\right] u_L(R) = 0, \\ &\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2}\right) + V(R) - E\right] \chi_L(R) = 0. \end{aligned} \tag{4.49}$$

We already know one solution $u_L(\rho) = \rho j_L(\rho) = F_L(0,\rho)$. Then, take difference of two equation after multiplying each other's wave function,

$$-\frac{\hbar^2}{2\mu}\left(\chi_L \frac{d^2}{dR^2} u_L - u_L \frac{d^2}{dR^2}\chi_L\right) - V(R) u_L \chi_L = 0. \tag{4.50}$$

Integration over R and do integration by parts to remove surface term

$$\begin{aligned} &\int_0^\infty dR \frac{d}{dR}\left(\chi_L \frac{d}{dR} u_L - u_L \frac{d}{dR}\chi_L\right) = -\frac{2\mu}{\hbar^2}\int_0^\infty dR u_L V \chi_L, \\ &\left(\chi_L \frac{d}{dR} u_L - u_L \frac{d}{dR}\chi_L\right)\Big|_0^\infty = -\frac{2\mu}{\hbar^2}\int_0^\infty dR u_L V \chi_L \end{aligned} \tag{4.51}$$

where we used the regular property of $\chi_L(0) = u_L(0) = 0$. Use the asymptotic form of χ_L, and $u_L = F_L$ and Wronskian property $G_L(\rho)\frac{d}{dR}F_L(\rho) - F_L(\rho)\frac{d}{dR}G_L(\rho) = k$, we get

$$e^{i\delta_L}\sin\delta_L = -\frac{2\mu}{\hbar^2}\int dRRj_L(\rho)V\chi_L(\rho) \tag{4.52}$$

Note that this relation depends on the choice of asymptotic form of wave function. [2]

Roughly speaking, the effective potential which is a sum of nuclear interaction and centrifugal interaction implies that the phase shifts should be diminish as increasing partial wave. (Because centrifugal barrier increase as increasing partial wave l, eventually particle cannot reach the nuclear interaction above some l. Thus, phase shift becomes zero at high partial waves.)

4.3.3 Resonance

From the total cross section expression in partial wave decomposition, which is proportional to $\sin^2\delta_L$, we can see that if phase shift rapidly grows from 0 to $\pi/2$ and further to π as energy changes, the cross section will also change rapidly showing resonance peak. Let us look more details.

Let us define $\gamma(E;R)$ which is a logarithmic derivative of radial wave function, $\psi_L(r) = \frac{u_L(r)}{r} = \frac{\chi_L(r)}{kr}$, (this choice is not unique)

$$\gamma_L(E;R) = \frac{1}{\psi_L}\frac{d\psi_L}{dr}|_{r=R} \tag{4.53}$$

When the energy is very low, $E \ll |V|$, the wave function inside the potential would not so sensitive to the E, since kinetic would be $E + |V| \sim |V|$. Thus, we may think as a first approximation, $\gamma_L(E)$ is almost constant at very low energy.

From the boundary condition,

$$\psi_L \to e^{i\delta_L}\cos\delta_L[j_L - K_L n_L], \tag{4.54}$$

$$\tan\delta_L = \frac{kj'_L(\rho) - \gamma_L j_L(\rho)}{kn'_L(\rho) - \gamma_L n_L(\rho)}, \quad j'_L(\rho) = \frac{dj_L(\rho)}{d\rho} \tag{4.55}$$

In low energy limit,$\rho \to 0$, we get

$$j_L(\rho) \to \frac{\rho^L}{(2L-1)!!}, \quad n_L(\rho) \to -(2L+1)!!\rho^{-L-1} \tag{4.56}$$

$$\begin{aligned} \tan\delta_L \quad &\xrightarrow{k\to 0} \quad \frac{(l+1) - R\gamma_0}{l + R\gamma_0}\frac{(kR)^{2l+1}}{[(2l-1)!!]^2(2l+1)} \\ &\simeq \quad a_l p^{2l+1} \end{aligned} \tag{4.57}$$

where γ_0 is the zero energy logarithmic derivative, [3] Let us consider the limit that the denominator $l + R\gamma_0(E) \to 0$. At a specific energy, $E = E_r$, $\tan\delta$ diverges and $\delta = \frac{\pi}{2} + n\pi$. Divergence of $\tan\delta_L$

---

[2] In terms of $\tilde{\chi}_L$ convention($\chi_L = e^{i\delta_L}\tilde{\chi}_L$), we gets

$$\sin\delta_L = -\frac{2\mu}{\hbar^2}\int dRRj_L(\rho)V\tilde{\chi}_L(\rho)$$

If we had used other convention, $\chi_L = e^{i\delta_L}\cos\delta_L\tilde{\chi}_L$, we gets

$$\tan\delta_L = -\frac{2\mu}{\hbar^2}\int dRRj_L(\rho)V\tilde{\chi}_L(\rho)$$

[3] In case of S-wave, we get

$$\tan\delta_{L=0} \xrightarrow{k\to 0} \frac{1 - R\gamma_0}{\gamma_0}p = -pa_0 \tag{4.58}$$

here we defined zero energy scattering length a_0 in terms of γ_0.

implies a relatively long life time [**This requires additional explanation**]. Near such resonance energy, we may express $\gamma_L(E)$ as,

$$R\gamma_L(E) \simeq -l + (E - E_r)\frac{d(R\gamma_L)}{dE}|_{E=E_r} + \dots \tag{4.59}$$

Then,

4.3.4 Bra-Ket representation in partial wave expansion

First note that bra- and ket- are rather abstract in itself. Let us consider, position and momentum bra and ket such that,

$$\begin{aligned}
&\langle \boldsymbol{x}|\boldsymbol{x}'\rangle = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}'), \quad \int d^3x|\boldsymbol{x}\rangle\langle\boldsymbol{x}| = 1. \\
&\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \mathcal{N}\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}'), \quad \int \frac{d^3p}{\mathcal{N}}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| = 1. \\
&\langle \boldsymbol{x}|\boldsymbol{p}\rangle = \sqrt{\frac{\mathcal{N}}{(2\pi\hbar)^3}}e^{i\frac{\boldsymbol{p}\cdot\boldsymbol{x}}{\hbar}}, \\
&\langle \boldsymbol{p}|\boldsymbol{x}\rangle = (\langle\boldsymbol{x}|\boldsymbol{p}\rangle)^\dagger
\end{aligned} \tag{4.60}$$

Then We may think the local and non-local function in position space as

$$\begin{aligned}
\langle \boldsymbol{r}|\psi\rangle &= \psi(\boldsymbol{r}), \\
\langle \boldsymbol{r}|\hat{V}|\boldsymbol{r}'\rangle &= V(\boldsymbol{r},\boldsymbol{r}') \to V(\boldsymbol{r})\delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}') \quad \text{local limit}
\end{aligned} \tag{4.61}$$

Then, we may think its momentum space expression as

$$\begin{aligned}
\langle \boldsymbol{k}|\psi\rangle &= \psi(\boldsymbol{k}) = \sqrt{\frac{\mathcal{N}}{(2\pi\hbar)^3}}\int d^3r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi(\boldsymbol{r}), \\
\langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle &= V(\boldsymbol{k},\boldsymbol{k}') \\
&= \int d^3r\int d^3r'\langle\boldsymbol{k}|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\hat{V}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\boldsymbol{k}'\rangle \\
&= \frac{\mathcal{N}}{(2\pi\hbar)^3}\int d^3r\int d^3r' e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}V(\boldsymbol{r},\boldsymbol{r}')e^{i\boldsymbol{k}'\cdot\boldsymbol{r}'}
\end{aligned} \tag{4.62}$$

From the partial wave expansion of plane wave

- Position state expansion: $\langle\boldsymbol{x}|\boldsymbol{x}'\rangle = \delta^{(3)}(\boldsymbol{x}-\boldsymbol{x}')$ can be rewritten as partial expansion of $|\boldsymbol{x}\rangle$, by introducing $|xlm\rangle$ and $\langle\hat{x}|xlm\rangle$

  $$\boxed{|\boldsymbol{x}\rangle = \sum_{lm}|xlm\rangle\langle xlm|\hat{x}\rangle} \tag{4.63}$$

  such that

  $$\langle xlm|x'l'm'\rangle = \frac{\delta(x-x')}{xx'}\delta_{ll'}\delta_{mm'}, \quad \sum_{lm}\int dx x^2|xlm\rangle\langle xlm| = 1. \tag{4.64}$$

  We have two choices for the definition of $\langle\hat{x}|xlm\rangle$:

  $$\begin{aligned}
  \langle\hat{x}|xlm\rangle &\equiv Y_{lm}(\hat{x}), \quad \textbf{spherical harmonics convention}, \\
  \langle\hat{x}|xlm\rangle &\equiv i^l Y_{lm}(\hat{x}), \quad \textbf{modified spherical harmonics convention}.
  \end{aligned} \tag{4.65}$$

- Momentum state expansion: Though angular part $\langle\hat{p}|plm\rangle = Y_{lm}(\hat{p})$ is almost universal, definition of radial component varies according to convention. Let us define expansion as

$$\boxed{|\boldsymbol{p}\rangle = \sum_{lm} C_{pl}|plm\rangle\langle plm|\hat{p}\rangle} \tag{4.66}$$

such that,

$$|C_{pl}|^2\langle plm|p'lm\rangle = \mathcal{N}\frac{\delta(p-p')}{pp'}\delta_{ll'}\delta_{mm'}, \quad \sum_{lm}\int \frac{dpp^2}{\mathcal{N}}|C_{pl}|^2|plm\rangle\langle p'lm| = 1. \tag{4.67}$$

By using the partial wave expansion of plane wave,

$$\begin{aligned}\langle\boldsymbol{x}|\boldsymbol{p}\rangle &= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}e^{i\boldsymbol{p}\cdot\boldsymbol{x}} \\ &= \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}4\pi\sum_{lm} j_l(pr)i^l Y_{lm}(\hat{r})Y^*_{lm}(\hat{p}) \\ &= \sum_{lm,l'm'} C_{pl}\langle xlm|pl'm'\rangle\langle\hat{x}|xlm\rangle\langle pl'm'|\hat{p}\rangle\end{aligned} \tag{4.68}$$

If we use spherical harmonics convention, $\langle\hat{x}|xlm\rangle = Y_{lm}(\hat{x})$, We have relation

$$C_{pl}\langle xlm|pl'm'\rangle = \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}4\pi j_l(pr)i^l\delta_{ll'}\delta_{mm'} \tag{4.69}$$

On the other hand, if we use modified spherical harmonics convention, $\langle\hat{x}|xlm\rangle = i^l Y_{lm}(\hat{x})$,

$$C_{pl}\langle xlm|pl'm'\rangle = \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}4\pi j_l(pr)\delta_{ll'}\delta_{mm'} \tag{4.70}$$

We have many choices: $C_{pl} = 1$, $C_{pl} = i^l$, $C_{pl} = 4\pi$ and so on. This fixes the normalization of $\langle xlm|pl'm'\rangle$ too. Be careful for where i^l factor is absorbed. This can change the relations among wave functions and S-matrix.

- Whether to include i^l factor to the definition of $\langle\hat{x}|xlm\rangle$ or $\langle xlm|plm\rangle$ or treat them explicitly for the expansion are convention dependent. Personally I prefer to use modified spherical harmonics convention with $\langle\hat{x}|xlm\rangle = i^l Y_{lm}(\hat{x})$, $C_{pl} = 1$, $\mathcal{N} = 1$, $\langle xlm|plm\rangle = \sqrt{\frac{2}{\pi}}j_l(px)$.

- If we fix the normalization of $|plm\rangle$ as $\langle xlm|pj_{lm}\rangle = j_l(px)$, then, up to i^l factors,

$$C_{pl} = \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}4\pi \quad\to\quad \sqrt{\frac{2}{\pi}} \text{ or } 4\pi \tag{4.71}$$

But, be careful that

$$\langle pj_{lm}|p'j_{lm}\rangle = \frac{\pi}{2}\frac{\delta(p-p')}{pp'} = \int dxx^2 j_l(px)j_l(p'x) \tag{4.72}$$

- 때로는 $|p,lm\rangle$ 이외에 $|E,lm\rangle$ state를 정의하여 사용하기도 한다. $E = p^2/(2\mu)$ 인 경우에는

$$\begin{aligned}|E,lm\rangle &= \sqrt{\mu p}|plm\rangle, \quad \langle E'l'm'|Elm\rangle = \delta(E-E')\delta_{l'l}\delta_{m'm} \\ \langle\boldsymbol{x}|Elm\rangle &= i^l\sqrt{\frac{2}{\pi}}\sqrt{\mu p}j_l(pr)Y_{lm}(\hat{x}), \quad \langle\boldsymbol{p}|Elm\rangle = \frac{1}{\sqrt{\mu p}}\delta(E_p-E)Y_{lm}(\hat{p})\end{aligned} \tag{4.73}$$

- Configuration space In spherical harmonics convention,

$$\langle \boldsymbol{x}|rlm\rangle_{sp} \equiv \frac{\delta(x-r)}{xr} Y_{lm}(\hat{x}) \tag{4.74}$$

In modified spherical harmonics convention,

$$\langle \boldsymbol{x}|rlm\rangle_{ms} \equiv \frac{\delta(x-r)}{xr} i^l Y_{lm}(\hat{x}) \tag{4.75}$$

$$\sum_{lm}\int dx x^2 |xlm\rangle\langle xlm| = 1, \quad \langle x'l'm'|xlm\rangle = \frac{\delta(x'-x)}{xx'}\delta_{ll'}\delta_{mm'} \tag{4.76}$$

In both spherical harmonics convention and modified spherical harmonics convention

$$|\boldsymbol{x}\rangle = \sum_{lm} |xlm\rangle_{sp}\langle xlm|\hat{x}\rangle_{sp} = \sum_{lm} |xlm\rangle_{ms}\langle xlm|\hat{x}\rangle_{ms} \tag{4.77}$$

- Momentum space expansion:

$$\langle \boldsymbol{p}'|plm\rangle \equiv \frac{\delta(p'-p)}{pp'} Y_{lm}(\hat{\boldsymbol{p}}'), \quad \langle plm|p'l'm'\rangle = \frac{\delta(p'-p)}{pp'}\delta_{ll'}\delta_{mm'} \tag{4.78}$$

Thus, in spherical Harmonics convention, we can write

$$|\boldsymbol{p}\rangle = \sum_{lm} |plm\rangle_{sp} i^l \langle plm|\hat{p}\rangle_{sp} \tag{4.79}$$

and in modified spherical harmonics convention

$$|\boldsymbol{p}\rangle = \sum_{lm} |plm\rangle_{ms}\langle plm|\hat{p}\rangle_{ms} \tag{4.80}$$

We have completeness relation in (ms) convention

$$\sum_{lm}\int dp p^2 |plm\rangle\langle plm| = 1 \tag{4.81}$$

- $\langle xlm|plm\rangle = j_l(px)$ 가 되도록 정의하면, completeness relation은

$$\begin{aligned}&\sum_{lm}\int \frac{dpp^2}{(2\pi)^3}|plm\rangle\langle plm| = 1, \quad \langle plm|p'l'm'\rangle = \frac{\pi}{2}\frac{\delta(p-p')}{pp'}\delta_{ll'}\delta_{mm'},\\ &\langle p'lm|\boldsymbol{p}\rangle = i^l(2\pi^2)\frac{\delta(p-p')}{pp'}Y^*_{lm}(\hat{p})\end{aligned} \tag{4.82}$$

이 된다.

- Note that from the relation for spherical bessel functions,

$$\boxed{\int_0^\infty x^2 j_n(ax) j_n(bx) dx = \frac{\pi}{2}\frac{\delta(a-b)}{ab}} \tag{4.83}$$

여기서, $\langle plm|p'l'm'\rangle \neq \delta(p-p')\delta_{ll'}\delta_{mm'}$ 임에 주의하자. 또한 이 때 $\langle rl|pl\rangle = \sqrt{\frac{2}{\pi}} j_l(pr)$ 이라는 것에 주의할 것.

- $\langle \hat{x}|lm\rangle = Y_{lm}(\hat{x})$ 인 경우

$$\begin{aligned}\langle rlm|plm\rangle &= \int d\boldsymbol{x}\int d\boldsymbol{p}\langle plm|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\boldsymbol{x}\rangle\langle\boldsymbol{x}|rlm\rangle \\ &= \int d^3p'\int d^3x\frac{\delta(p'-p)}{p'p}Y^*_{lm}(\hat{p}')\frac{1}{(2\pi)^{3/2}}e^{-i\boldsymbol{p}'\cdot\boldsymbol{x}}\frac{\delta(x-r)}{xr}Y_{lm}(\hat{x}) \\ &= \sqrt{\frac{2}{\pi}}j_l(pr)i^l \end{aligned} \quad (4.84)$$

또는 $\langle \hat{x}|lm\rangle = i^l Y_{lm}(\hat{x})$ 인 경우

$$\langle rlm|plm\rangle = \sqrt{\frac{2}{\pi}}j_l(pr) \quad (4.85)$$

이 된다.

- 여기서 $|xlm\rangle$ 이나 $|plm\rangle$ 를 $|x\rangle_l|lm\rangle$과 $|p\rangle_l|lm\rangle$ 로 쓰는 convention을 사용할 경우,

$$\begin{aligned}&\int d\hat{x}|\hat{x}\rangle\langle\hat{x}| = 1, \quad \int dx^2x^2|x\rangle_l\langle x|_l = 1, \\ &\sum_{lm}|lm\rangle\langle lm| = 1\end{aligned} \quad (4.86)$$

으로 vector 의 radial part 와 angular part를 분리할 수 있게 된다. 즉, $|\boldsymbol{x}\rangle = |x\rangle|\hat{x}\rangle$ 로써,

$$\begin{aligned}&\langle p'|p\rangle_l = \int drr^2\langle p'|r\rangle_l\langle r|p\rangle_l = \frac{1}{p^2}\delta(p'-p) \\ &\langle\boldsymbol{p}'|\boldsymbol{p}\rangle = \langle p'|p\rangle\langle\hat{p}'|\hat{p}\rangle = \delta(\boldsymbol{p}'-\boldsymbol{p}) = \frac{1}{p^2}\delta(p'-p)\delta(\hat{p}'-\hat{p})\end{aligned} \quad (4.87)$$

로 정의할 수 있다.[4]

4.4 Time reversal invariance and the choice of convention

- Under time reversal Θ,

$$\Theta\boldsymbol{x}\Theta^{-1} = \boldsymbol{x}, \quad \Theta\boldsymbol{p}\Theta^{-1} = -\boldsymbol{p}, \quad \Theta\boldsymbol{\sigma}\Theta^{-1} = -\boldsymbol{\sigma}. \quad (4.88)$$

From the fundamental commutation relation, $[x_i,p_j] = i\hbar\delta_{ij}$,

$$\Theta[x_i,p_j]\Theta^{-1} = [x_i,(-)p_j] = \Theta i\hbar\delta_{ij}\Theta^{-1} = -i\hbar\delta_{ij} \quad (4.89)$$

We can know that Θ is an anti-unitary operator. And,

$$\Theta\boldsymbol{J}\Theta^{-1} = -\boldsymbol{J}, \quad \text{from } [J_i,J_j] = i\hbar\epsilon_{ijk}J_k \quad (4.90)$$

For spatial wave,

$$\begin{aligned}\Theta Y_{lm}(\theta,\phi)\Theta^{-1} &= Y^*_{lm}(\theta,\phi) = (-1)^mY_{l-m}(\theta,\phi), \\ \Theta|l,m\rangle &= (-1)^m|l,-m\rangle\end{aligned} \quad (4.91)$$

For spinor, $\Theta = \eta UK$, with η is an intrinsic phase factor, U is unitary, K is complex conjugation operator,

$$\Theta = \eta e^{-i\frac{\pi}{\hbar}J_y}K \quad (4.92)$$

We may choose convention of η such that

$$\Theta|S,m\rangle = (-1)^{S-m}|j,-m\rangle \quad (4.93)$$

[4] 이 식들은 spherical harmonics의 convention에 무관하다. 왜냐면, 왼쪽과 오른쪽이 같은 l을 가지므로, convention의 차이는 $(-i)^li^l = i^{-l}i^l = 1$ 을 주기 때문이다.

- time-reversal 을 생각할 때는 $\langle \hat{x}|lm\rangle = i^l Y_{lm}(\hat{x})$, modified spherical harmonics convention 로 정의하는 것이 편리하다. Then, 모든 $|jm\rangle$ 상태에 대해

$$\begin{aligned}\mathcal{T}|jm\rangle^{\pm} &= (-1)^{j-m}|j-m\rangle^{(\mp)}, \\ \mathcal{T}|(j_1j_2)jm\rangle^{\pm} &= (-1)^{j-m}|(j_1j_2)j-m\rangle^{(\mp)}\end{aligned} \tag{4.94}$$

가 성립한다. i^l factor가 없으면,

$$\mathcal{T}|(ls)jm\rangle^{\pm} = (-1)^{l+j-m}|(ls)j-m\rangle^{\mp} \tag{4.95}$$

가 되어, orbital angular momentum 에 대해서는 특별히 다르게 취급해야한다. 하지만, 어느 경우에나,

$$\begin{aligned}|\boldsymbol{x}\rangle &= \sum_{lm}|xlm\rangle\langle xlm|\hat{x}\rangle \\ |\boldsymbol{p}\rangle &= \sum_{lm}|plm\rangle\langle plm|\hat{p}\rangle\end{aligned} \tag{4.96}$$

로 나타내어 지는 것은 같다. [5]

4.4.1 Relation between incoming and outgoing boundary condition wave function.

Let us consider spin-less particle state. Because $T|\boldsymbol{p}\rangle = |-\boldsymbol{p}\rangle$,

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = \langle \boldsymbol{x}|T^{\dagger}T|\boldsymbol{p}\rangle = \langle \boldsymbol{x}|T^{\dagger}|-\boldsymbol{p}\rangle = \langle -\boldsymbol{p}|\boldsymbol{x}\rangle \tag{4.98}$$

it implies $\langle x|\boldsymbol{p}\rangle = \langle \boldsymbol{x}|-\boldsymbol{p}\rangle^*$ which is trivial for plane wave. However, let us consider the scattering wave. Because Time reversal changes $\Omega_{\pm} \to \Omega_{\mp}$, We would have $T|\boldsymbol{p}\rangle^{(+)} = |-\boldsymbol{p}\rangle^{(-)}$. Then, it implies

$$\langle x|\boldsymbol{p}\rangle^{(-)} = \langle \boldsymbol{x}|-\boldsymbol{p}\rangle^{(+)*} \to \left[\psi^{(\pm)}_{\boldsymbol{k}}(\boldsymbol{R})\right]^* = \psi^{(\mp)}_{-\boldsymbol{k}}(\boldsymbol{R}) \tag{4.99}$$

Asymptotic form is

$$\begin{aligned}\psi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}) &\to A\left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta)\frac{e^{ikr}}{r}\right), \\ \psi^{(-)}_{\boldsymbol{k}}(\boldsymbol{r}) &\to A\left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f^*(\pi-\theta)\frac{e^{-ikr}}{r}\right).\end{aligned} \tag{4.100}$$

If the orbital angular momentum is conserved, partial wave expansion becomes

$$\langle x|\boldsymbol{p}\rangle^{(\pm)} = \sum_{LL_z} i^L R^{(\pm)}_L(px)Y_{LL_z}(\hat{x})Y^*_{LL_z}(\hat{p}). \tag{4.101}$$

By using the property of spherical harmonics,

$$Y^*_{lm}(x) = (-1)^m Y_{l-m}(x), \quad Y_{lm}(-x) = (-1)^l Y_{lm}(x), \tag{4.102}$$

we can get the relation

$$\begin{aligned}\langle x|\boldsymbol{p}\rangle^{(-)} &= \langle \boldsymbol{x}|-\boldsymbol{p}\rangle^{(+)*} = \sum_{LL_z}(-i)^L R^{(+),*}_L(px)Y^*_{LL_z}(\hat{x})Y_{LL_z}(-\hat{p}) \\ &= \sum_{LL_z} i^L R^{(+),*}_L(px)Y_{L-L_z}(\hat{x})Y^*_{L-L_z}(\hat{p})\end{aligned} \tag{4.103}$$

[5] 특별히, $\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = (2\pi)^3\delta^3(\boldsymbol{p}-\boldsymbol{p}')$ and $\langle xl|pl\rangle = j_l(px)$ 의 convention을 사용할 경우는 expansion을

$$|\boldsymbol{x}\rangle = \sum_{lm}|xlm\rangle\langle xlm|\hat{x}\rangle, \quad |\boldsymbol{p}\rangle = \sum_{lm}(4\pi)i^l|plm\rangle\langle plm|\hat{p}\rangle \tag{4.97}$$

임에 유의.

And thus,

$$R_L^{(-)}(px) = \left(R_L^{(+)}(px)\right)^* \tag{4.104}$$

Or, we may consider $\psi_{\boldsymbol{k}}^{(-)}(\boldsymbol{R})$ as a solution of equation,

$$(T_R + V^*(R))\psi_{\boldsymbol{k}}^{(-)}(\boldsymbol{R}) = E\psi_{\boldsymbol{k}}^{(-)}(\boldsymbol{R}). \tag{4.105}$$

When orbital angular momentum is not conserved, we may write partial wave expansion as either

$$\begin{aligned}
\langle x|\boldsymbol{p}, SM_S\rangle^{(\pm)} &= \sum_{\alpha',\alpha} i^{L'} R_{\alpha',\alpha}^{(\pm),ms} \mathcal{Y}_{\alpha'}(x) Y_{LM_L}^*(p)\langle LM_L, SM_S|JM_J\rangle \\
&= \sum_{\alpha}\left(\sum_{\alpha'} i^{L'} R_{\alpha',\alpha}^{(\pm),ms}\mathcal{Y}_{\alpha'}(x)\right) Y_{LM_L}^*(p)\langle LM_L, SM_S|JM_J\rangle \\
&= \sum_{\alpha}\langle x|p,\alpha\rangle_{ms}^{(\pm)} Y_{LM_L}^*(p)\langle LM_L, SM_S|JM_J\rangle
\end{aligned} \tag{4.106}$$

or

$$\begin{aligned}
\langle x|\boldsymbol{p}, SM_S\rangle^{(\pm)} &= \sum_{\alpha',\alpha} i^{L} R_{\alpha',\alpha}^{(\pm),sp} \mathcal{Y}_{\alpha'}(x) Y_{LM_L}^*(p)\langle LM_L, SM_S|JM_J\rangle \\
&= \sum_{\alpha} i^L \left(\sum_{\alpha'} R_{\alpha',\alpha}^{(\pm),sp}\mathcal{Y}_{\alpha'}(x)\right) Y_{LM_L}^*(p)\langle LM_L, SM_S|JM_J\rangle \\
&= \sum_{\alpha} i^L \langle x|p,\alpha\rangle_{sp}^{(\pm)} Y_{LM_L}^*(p)\langle LM_L, SM_S|JM_J\rangle
\end{aligned} \tag{4.107}$$

where, radial wave function are normalized as $R_{\alpha'\alpha} \propto \delta_{\alpha'\alpha} h_{\alpha'}^{(-)} + S_{\alpha'\alpha} h_{\alpha'}^{(+)}$ in both case. But resulting S-matrix definition becomes different by phase factor. Though the choice is a matter of convention, one have to use one convention consistently because different convention would leads to different phase factors and relations between outgoing wave function and incoming wave function.

First convention corresponds to modified spherical harmonics convention and second one corresponds to spherical harmonics convention.

From T-reversal,

$$T|\boldsymbol{p}, SM_S\rangle^{(+)} = (-1)^{S-M_S}|-\boldsymbol{p}, S-M_S\rangle^{(-)} \tag{4.108}$$

Thus,

$$\langle x|\boldsymbol{p}, SM_S\rangle^{(-)} = \left((-1)^{S-M_S}\langle x|-\boldsymbol{p}, S-M_S\rangle^{(+)}\right)^* \tag{4.109}$$

Then in modified spherical harmonics convention,

$$\begin{aligned}
& \left((-1)^{S-M_S}\langle x|-\boldsymbol{p}, S-M_S\rangle^{(+)}\right)^* \\
= \;& (-1)^{S-M_S}\Big(\sum_{L,M_L}\sum_{J,M_J}\sum_{L'S'} i^{L'} R_{L'S',LS}^{(+),ms}\mathcal{Y}_{L'S'}^{J-M_J}(\hat{x}) \\
& \times Y_{L-M_L}^*(-\hat{p}) C_{L-M_L,S-M_S}^{J-M_J}\Big)^* \\
= \;& (-1)^{S-M_S}\sum_{L,M_L}\sum_{J,M_J}\sum_{L'S'}(-i)^{L'} R_{L'S',LS}^{(+)*,ms}(-1)^{J+M_J+L'}\mathcal{Y}_{L'S'}^{JM_J}(\hat{x}) Y_{L-M_L}(-\hat{p})(-1)^{L+S-J} C_{LM_L,SM_S}^{JM_J} \\
= \;& \sum_{L,M_L}\sum_{J,M_J}\sum_{L'S'} i^{L'} R_{L'S',LS}^{(+)*,ms}\mathcal{Y}_{L'S'}^{JM_J}(\hat{x}) Y_{LM_L}^*(\hat{p}) C_{LM_L,SM_S}^{JM_J} \\
& \times(-1)^{S-M_S}(-1)^{L'}(-1)^{J+M_J+L'}(-1)^{L-M_L}(-1)^{L+S-J} \\
= \;& \sum_{L,M_L}\sum_{J,M_J}\sum_{L'S'} i^{L'} R_{L'S',LS}^{(+)*,ms}\mathcal{Y}_{L'S'}^{JM_J}(\hat{x}) Y_{LM_L}^*(\hat{p}) C_{LM_L,SM_S}^{JM_J}.
\end{aligned} \tag{4.110}$$

Thus, it implies that

$$R^{(+)*}_{L'S',LS} = R^{(-)}_{L'S',LS}, \quad \text{m.s. convention.} \tag{4.111}$$

In similar way, spherical harmonics convention,

$$R^{(+)*}_{L'S',LS}(-1)^{L'+L} = R^{(-)}_{L'S',LS}, \quad \text{sp. convention.} \tag{4.112}$$

In fact from the convention, we have relations [6]

$$R^{ms}_{\alpha',\alpha} = i^{-L'+L} R^{sp}_{\alpha',\alpha} \tag{4.115}$$

Also at the same time, if S-matrix is defined from the boundary condition of $R_{\alpha'\alpha}$, we will have

$$S^{ms}_{\alpha',\alpha} = i^{-L'+L} S^{sp}_{\alpha'\alpha} \tag{4.116}$$

4.5 Partial wave Decomposition

4.5.1 Partial wave decomposition convention

- $|\boldsymbol{p}\rangle$ 의 normalization을 정하더라도, partial wave로 decompose 시킬 때 새로운 convention dependence 가 생긴다. 어떠한 convention을 사용하거나, $\langle \boldsymbol{p}'|\boldsymbol{p}\rangle = \delta^{(3)}(\boldsymbol{p}'-\boldsymbol{p})$ 인 것은 같다. 하지만,

  $$\langle xlm|plm\rangle = \sqrt{\frac{2}{\pi}} j_l(px) \text{ 또는 } \sqrt{\frac{2}{\pi}} j_l(px) i^l \tag{4.117}$$

  의 convention을 사용하면,

  $$\langle p'l'm'|plm\rangle = \frac{\delta(p'-p)}{pp'}\delta_{l'l}\delta_{m'm}, \quad \sum_{lm}\int dpp^2|plm\rangle\langle plm| = 1 \tag{4.118}$$

  이 된다.

- general partial wave expansion: For general case of many body scattering and non-conservation of angular momentum, let us denote α as general 'angular-spin' quantum numbers. Let us distinguish $|k,\alpha\rangle$ with $|\alpha\rangle$, where the first includes radial wave function while the second only contains 'angular' quantum numbers, thus is dimensionless.

  Define

  $$\begin{aligned} Y_\alpha(\hat{k}) &\equiv \langle \hat{k}|k\alpha\rangle, \\ \langle \hat{k}|\hat{k}'\rangle &= \delta^{(2)}(\hat{k}-\hat{k}') = \sum_{\alpha\beta}\delta_{\alpha\beta}Y_\alpha(\hat{k})Y^*_\beta(\hat{k}') \end{aligned} \tag{4.119}$$

  For each convention

  $$|\boldsymbol{k}\rangle = \sum_\alpha |k,\alpha\rangle_{sp} i^\alpha \langle\alpha|\hat{k}\rangle_{sp} = \sum_\alpha |k,\alpha\rangle_{ms}\langle\alpha|\hat{k}\rangle_{ms}. \tag{4.120}$$

---

[6] Or, we may define radial function such that

$$\langle x|\boldsymbol{p}, SM_S\rangle^{(\pm)} = \sum_{\alpha',\alpha} R^{(\pm)}_{\alpha',\alpha}\mathcal{Y}_{\alpha'}(x)Y^*_{LM_L}(p)\langle LM_L, SM_S|JM_J\rangle \tag{4.113}$$

In this case, $R_{\alpha'\alpha} = i^{L'}R^{ms}_{\alpha'\alpha} = i^L R^{sp}_{\alpha'\alpha}$. And,

$$(-1)^{L'}R^{(+),*}_{\alpha'\alpha} = R^{(-)}_{\alpha'\alpha} \tag{4.114}$$

However, this is not desirable.

$$|\boldsymbol{x}\rangle = \sum_{\alpha} |x,\alpha\rangle_{sp}\langle x,\alpha|\hat{x}\rangle_{sp} = \sum_{\alpha} |x,\alpha\rangle_{ms}\langle x,\alpha|\hat{x}\rangle_{ms} \tag{4.121}$$

with $\langle\hat{x}|x,\alpha\rangle_{sp} = Y_\alpha(\hat{x})$ and $\langle\hat{x}|x,\alpha\rangle_{ms} = i^\alpha Y_\alpha(\hat{x})$

- partial wave expansion of scattering amplitude

$$\begin{aligned} f(\boldsymbol{k},\boldsymbol{k}') &= -\frac{(2\pi)^2\mu}{\mathcal{N}}\langle\boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)} \\ &= -\frac{(2\pi)^2\mu}{\mathcal{N}}\sum_{\alpha\beta}\langle k,\alpha|V|k,\beta\rangle_{sp}^{(+)} i^{-\alpha+\beta} Y_\alpha(\hat{k})Y^*_\beta(\hat{k}') \\ &= -\frac{(2\pi)^2\mu}{\mathcal{N}}\sum_{\alpha\beta}\langle k,\alpha|V|k,\beta\rangle_{ms}^{(+)} Y_\alpha(\hat{k})Y^*_\beta(\hat{k}') \end{aligned} \tag{4.122}$$

How can we define $S_{\alpha,\beta}(k)$($f_{\alpha\beta}(k)$ and $T_{\alpha,\beta}(k)$) from $\langle\boldsymbol{k}|S|\boldsymbol{k}'\rangle$?

Thus, if we define $S_{\alpha\beta}$, $f_{\alpha\beta}$ and $T_{\alpha\beta}$ as, we have [7]

$$\begin{aligned} \langle\hat{k}|\hat{S}(k)|\hat{k}'\rangle &\equiv \sum_{\alpha\beta} i^{-\alpha+\beta} Y_\alpha(\hat{k})Y^*_\beta(\hat{k}')S_{\alpha\beta}(k) \text{ in sp convention,} \\ &\equiv \sum_{\alpha\beta} Y_\alpha(\hat{k})Y^*_\beta(\hat{k}')S_{\alpha\beta}(k) \text{ in ms convention} \end{aligned} \tag{4.123}$$

Similar relation holds for T and f.

Regardless of convention, we can write

$$\boxed{\begin{aligned} S_{\alpha\beta}(k) &= \delta_{\alpha\beta} - (2\pi)i\mu k\langle k,\alpha|V|k,\beta\rangle^{(+)}, \\ &= \delta_{\alpha\beta} - (2\pi)i\mu k T_{\alpha\beta}(k), \\ &= \delta_{\alpha\beta} + i\tfrac{k}{2\pi} f_{\alpha\beta}(k) \end{aligned}} \tag{4.124}$$

However, $S^{(ms)}_{\alpha\beta}$ and $S^{(sp)}_{\alpha\beta}$ is different. And the definition of T-matrix can be different by factor $(2\pi)^3$.

the relation between potential matrix element with $f_{\alpha\beta}$ depends on the convention,

$$\boxed{\begin{aligned} f^{(ms)}_{\alpha\beta}(k) &= -(2\pi)^2\mu\langle k,\alpha|V|k,\beta\rangle^{(+)}_{ms} \\ f^{(sp)}_{\alpha\beta}(k) &= -(2\pi)^2\mu\langle k,\alpha|V|k,\beta\rangle^{(+)}_{sp} \end{aligned}} \tag{4.125}$$

Thus,

$$\begin{aligned} S^{(ms)}_{\alpha\beta}(k) &= \delta_{\alpha\beta} - i2\pi\mu k\langle k,\alpha|V|k,\beta\rangle^{(+)}_{ms} \\ &= \delta_{\alpha\beta} - i4\mu k\langle k,\alpha|V|k,\beta\rangle^{(+)}_{ms'} \\ S^{(sp)}_{\alpha\beta}(k) &= \delta_{\alpha\beta} - 4i\mu k\langle k,\alpha|V|k,\beta\rangle^{(+)}_{sp'} \end{aligned} \tag{4.126}$$

- In general scattered state does not have the same quantum numbers with asymptotic state. Thus, let us further expands scattered state as

$$\begin{aligned} \langle\boldsymbol{x}|\Psi_\alpha(k)\rangle^{(+)}_{sp} &= \sum_{\alpha'}\langle x,\alpha'|\Psi^{(+)}_{\alpha',\alpha}(k)\rangle_{sp} Y_{\alpha'}(\hat{x}), \\ \langle\boldsymbol{x}|\Psi_\alpha(k)\rangle^{(+)}_{ms} &= \sum_{\alpha'}\langle x,\alpha'|\Psi^{(+)}_{\alpha',\alpha}(k)\rangle_{ms} i^{\alpha'} Y_{\alpha'}(\hat{x}) \end{aligned} \tag{4.127}$$

[7] My mistake? Because the S-matrix here only involves direction of momentums ??? Not quite clear. $i^{-\alpha+\beta}$ factor might be wrong.... Though those factor should appear when we write potential matrix element which involves integration with radial wave function.

where,

$$\langle x, \alpha' | \Psi^{(+)}_{\alpha',\alpha}(k) \rangle_{sp} \equiv \Psi^{(+)}_{\alpha',\alpha}(k, x) \tag{4.128}$$

is radial wave function solution of the scattering with boundary condition,

$$\langle x\alpha' | \Psi_{\alpha',\alpha}(k) \rangle^{(+)}_{sp} = \sqrt{\frac{2}{\pi}} \frac{i}{2} [h^{(2)}_{l'}(pr)\delta_{\alpha'\alpha} - S^{J,(sp)}_{\alpha'\alpha} h^{(1)}_{l'}(pr)] \text{ at large r} \tag{4.129}$$

In modified spherical harmonics convention,

$$\begin{aligned}
\langle x\alpha' | \Psi_{\alpha'\alpha} \rangle^{(+)}_{ms} &= \sqrt{\frac{2}{\pi}} \frac{i}{2} [h^{(2)}_{l'}(pr)\delta_{\alpha'\alpha} - S^{J,(ms)}_{\alpha'\alpha} h^{(1)}_{l'}(pr)] \text{ at large r} \\
&= \sqrt{\frac{2}{\pi}} i^{-\alpha'+\alpha} \frac{i}{2} [h^{(2)}_{l'}(pr)\delta_{\alpha'\alpha} - S^{J,(sp)}_{\alpha'\alpha} h^{(1)}_{l'}(pr)] \text{ at large r} \\
&= i^{-\alpha'+\alpha} \langle x\alpha' | \Psi_{\alpha'\alpha} \rangle^{(+)}_{sp}
\end{aligned} \tag{4.130}$$

Thus, we can write, in both primed conventions,

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} - 4i\mu k \sum_{\beta'} \langle k, \alpha | V | \Psi^{(+)}_{\beta',\beta}(k), \beta' \rangle \tag{4.131}$$

We may consider it as, because wave function $\langle \boldsymbol{x} | \boldsymbol{p} \rangle^{(+)}$ is written before any convention,

$$\begin{aligned}
\langle \boldsymbol{x} | \boldsymbol{p} \rangle^{(+)} &= \sum_l \langle \hat{x} | x, \alpha \rangle_{sp} \langle x, \alpha | p, \alpha' \rangle^{(+)}_{sp} \langle p, \alpha' | \hat{p} \rangle_{sp} i^{\alpha'} \\
&= \sum_l \langle \hat{x} | x, \alpha \rangle_{ms} \langle x, \alpha | p, \alpha' \rangle^{(+)}_{ms} \langle p, \alpha' | \hat{p} \rangle_{ms}
\end{aligned} \tag{4.132}$$

Thus, we should have a relation,

$$\langle x, \alpha | p, \alpha' \rangle^{(+)}_{sp} i^{\alpha'} = i^{\alpha} \langle x, \alpha | p, \alpha' \rangle^{(+)}_{ms}. \tag{4.133}$$

- expansion of momentum function: Any function depends on momentum chould be partial wave expanded. Common definition of partial wave component $f_l(p)$ and $f_{\alpha\beta}(p, p')$ are

$$\begin{aligned}
f(\boldsymbol{p}) &= \sum_{\alpha} f_{\alpha}(p)(2l+1)P_l(\cos\theta), \\
f(\boldsymbol{p}, \boldsymbol{p'}) &= \sum_{\alpha,\beta} f_{\alpha,\beta}(p, p') Y_{\alpha}(\hat{p}) Y^*_{\beta}(\hat{p}')
\end{aligned} \tag{4.134}$$

However, if we represent them as matrix elements of operators $\hat{f}$, the relation between f_{α}, $f_{\alpha,\beta}$ and $\langle p, \alpha | \hat{f} | p, \beta \rangle$ depends on conventions.

$$\begin{aligned}
\langle \boldsymbol{p'} | \hat{f} | \boldsymbol{p} \rangle &= \sum_{\alpha,\beta} C^*_{p'\alpha} C_{p\beta} \langle \hat{p}' | p', \alpha \rangle \langle p', \alpha | \hat{f} | p, \beta \rangle \langle p, \beta | \hat{p} \rangle \\
&= \sum_{\alpha,\beta} \langle p', \alpha | \hat{f} | p, \beta \rangle C^*_{p'\alpha} C_{p\beta} Y_{\alpha}(\hat{p}') Y^*_{\beta}(\hat{p}) \\
&= \sum_{\alpha,\beta} \langle p', \alpha | \hat{f} | p, \beta \rangle C^*_{p'\alpha} C_{p\beta} \sqrt{\frac{(2l_{\alpha}+1)(2l_{\beta}+1)}{(4\pi)^2}} P_{\alpha}(\cos\theta), \quad \text{if } \hat{p} = \hat{z}
\end{aligned} \tag{4.135}$$

Uncoupled case can be considered for the case $\boldsymbol{p} = \boldsymbol{p'}$, $\alpha = \beta$. Thus, if we had $|C_{pl}|^2 = 1$, $\frac{f_{\alpha\alpha}(p,p)}{4\pi} \leftrightarrow f_{\alpha}(p)$.

- For S-matrix and scattering amplitudes, usual convention is to relate them by

$$f_{\alpha,\beta}(p) = \left(\frac{S-1}{2ip}\right)_{\alpha\beta} \tag{4.136}$$

To be consistent with the normalization of S-matrix $S_{\alpha\beta} = \delta_{\alpha\beta} + \dots$,

$$\boxed{f(\boldsymbol{p},\boldsymbol{p}') = \sum_{\alpha\beta} 4\pi \left(\frac{S-1}{2ip}\right)_{\alpha\beta} i^{-\alpha+\beta} Y_\alpha(\hat{p}) Y^*_\beta(\hat{p}')} \tag{4.137}$$

(However, $i^{-\alpha+\beta}$ factor can be absorbed to the definition of S-matrix depending on the convention.)

we get,

$$\frac{\mathcal{N}}{(2\pi)^3} 4\pi \langle p\alpha|\hat{f}|p\beta\rangle = f_{\alpha,\beta}(p) = \left(\frac{S-1}{2ip}\right)_{\alpha\beta} \tag{4.138}$$

and treating

$$\hat{f} = -\frac{(2\pi)^3}{\mathcal{N}}\frac{\mu}{2\pi\hbar}\hat{V} \quad \rightarrow \quad \left(\frac{S-1}{2ip}\right)_{\alpha\beta} = -2\mu\langle j_\alpha|\hat{V}|j_\beta\rangle^{(+)} \tag{4.139}$$

Thus, to have a normalization convention independent expression can be obtained by

$$\boxed{\left(\frac{S-1}{2ip}\right)_{\alpha\beta} = -2\mu\sum_{\beta'}\langle \mathcal{Y}_\alpha j_\alpha|\hat{V}|\mathcal{Y}_{\beta'}\psi_{\beta'\beta}\rangle^{(+)}} \tag{4.140}$$

with radial partial wave function is normalized as $\psi_{\beta'\beta}(x) \to \delta_{\beta'\beta} j_{\beta'}(px)$.

4.5.2 Partial wave expressions

We can define partial wave matrix elements of potential such that

$$V_{\alpha\beta}(x', x) = \langle x', \alpha|\hat{V}|x, \beta\rangle = \int d\Omega' \int d\Omega \mathcal{Y}^*_\alpha(\hat{x}') V(\boldsymbol{x}', \boldsymbol{x}) \mathcal{Y}_\beta(\hat{x}) \tag{4.141}$$

In momentum space,

$$V_{\alpha\beta}(p', p) = \langle p', \alpha|\hat{V}|p, \beta\rangle = \frac{2}{\pi}\int dx' dx x'^2 \int dx x^2 j_{l'}(p'x') V_{\alpha,\beta}(x', x) j_l(px) \tag{4.142}$$

t-matrix 에 대한 LS equation을 partial wave basis 에서 나타내면,

$$t_{\alpha',\alpha}(E, p'p) \quad = \quad V_{\alpha',\alpha}(p'p) + \sum_{\tilde{\alpha}}\int d\tilde{p}\tilde{p}^2 V_{\alpha',\tilde{\alpha}}(p'\tilde{p}) \frac{1}{E - \tilde{p}^2/(2\mu) + i\epsilon} t_{\tilde{\alpha},\alpha}(\tilde{p}, p) \tag{4.143}$$

where,

$$[t \text{ or } V]_{\alpha',\alpha}(E, p'p) \equiv \langle p', \alpha'|(T \text{ or } V)|p, \alpha\rangle \tag{4.144}$$

여기서 V가 rotationally invariant 라면, partial wave component $t_l(p'p)$와 $V_l(p'p)$를 다음과 같이 정의할 수 있다.,

$$\langle p'l'm'|t(E), \text{ or } V|plm\rangle \quad = \quad [t_l(p'p), \text{ or } V_l(p'p)]\delta_{l'l}\delta_{m'm} \tag{4.145}$$

$$t_l(p'p) = V_l(p'p) + \int_0^\infty dp'' p''^2 V_l(p'p'') \frac{1}{E + i\epsilon - p''^2/2\mu} t_l(p''p) \quad (4.146)$$

따라서 , local potential 의 partial wave representation 은

$$\begin{aligned} V_l(p'p) &= \langle p'lm|V|plm\rangle = \int d\hat{p}' Y^*_{lm}(\hat{p}') \int d\hat{p} Y_{lm}(\hat{p}) \langle p'\hat{p}'|V|p\hat{p}\rangle \\ &= \frac{2}{\pi} \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 j_l(p'r') \frac{\delta(r-r')}{rr'} V(r) j_l(pr) \\ &= \frac{2}{\pi} \int_0^\infty dr r^2 j_l(p'r) V(r) j_l(pr) \end{aligned} \quad (4.147)$$

이 된다. 또는 local potential 의 경우

$$\begin{aligned} \langle \boldsymbol{q}|V|\boldsymbol{q}'\rangle &= \tilde{V}(|\boldsymbol{q} - \boldsymbol{q}'|) = \frac{4\pi}{(2\pi)^3} \int dr r^2 j_0(|\boldsymbol{q} - \boldsymbol{q}'|r) V(r) \\ V_l(p'p) &= 2\pi \int_{-1}^1 dx P_l(x) \tilde{V}(\sqrt{p^2 + p'^2 - 2pp'x}) \end{aligned} \quad (4.148)$$

주의할 것은 $\langle plm|V|plm\rangle$ 이 radial function $\sqrt{\frac{2}{\pi}} j_l(pr)$을 포함한다는 것이다. 만약 partial wave representation을 정의할 때, $\langle j_l lm|V|j_l lm\rangle$ 과 같이 정의하면, 이 둘 사이엔

$$\begin{aligned} \langle p'lm|V|plm\rangle &= \frac{2}{\pi} \langle j_l(p'r) lm|V|j_l(pr) lm\rangle, \text{ OR} \\ \langle p'lm|V|plm\rangle^{(+)} &= \frac{2}{\pi} \langle j_l(p'r) lm|V|\psi_l(pr) lm\rangle \end{aligned} \quad (4.149)$$

인 관계가 있게 된다.[8]

어느 operator 의 partial wave matrix element를 나타 낼 때, position space에서의 representation 이 필요한 경우에는 언제나 i^l factor에 유의해야하지만, momentum space나 spin, isospin space 에 작용하는 operator의 경우에는 어느 경우나 같다.

S-matrix, T-matrix의 on-energy-shell element 는

$$\begin{aligned} \langle \boldsymbol{k}|S|\boldsymbol{k}'\rangle &\equiv \frac{\delta(k-k')}{kk'} \langle k, \hat{k}|S|k, \hat{k}'\rangle = \frac{\delta(k-k')}{kk'} \hat{S}_{\hat{k}\hat{k}'}(k)\rangle, \\ \hat{S}_{\hat{k}\hat{k}'}(k) &= \delta_{\hat{k}\hat{k}'} - 2\pi i \mu k \hat{t}_{\hat{k}\hat{k}'}(k) \\ &= \delta_{\hat{k}\hat{k}'} + i \frac{k}{2\pi} \hat{f}_{\hat{k}\hat{k}'}(k) \end{aligned} \quad (4.151)$$

마찬가지로

$$\hat{S}^J_{\alpha\beta}(p) = \delta_{\alpha\beta} - 2\pi i \mu k t^J_{\alpha\beta}(p) = \delta_{\alpha\beta} + i \frac{p}{2\pi} f^J_{\alpha\beta}(p) \quad (4.152)$$

로 나타낼 수 있다. [9] 여기서, $S_{\alpha\beta}$ 와 $f_{\alpha\beta}$는 radial wave function의 normalization까지 모두 포함한 것이다.

$$S^J_{\alpha\beta} = \delta_{\alpha\beta} - 4i\mu q \sum_\gamma \langle \mathcal{Y}_\alpha, j_\alpha|V|\mathcal{Y}_\gamma, \Psi_{\gamma\beta}\rangle = \delta_{\alpha\beta} - 4i\mu q t^J_{\alpha\beta} \quad (4.155)$$

[8] 따라서, 다음과 같이 쓸 수도 있다.

$$\langle j_{l'}(p')l'|T|j_l(p)l\rangle = \langle j_{l'}(p')l'|V|j_l(p)l\rangle + \frac{2}{\pi} \sum_{\tilde{l}} \int d\tilde{p}\tilde{p}^2 \langle j_{l'}(p')l'|V|j_{\tilde{l}}(\tilde{p})\tilde{l}\rangle \frac{1}{E - \tilde{p}^2/(2\mu) + i\epsilon} \langle j_{\tilde{l}}(\tilde{p})\tilde{l}|T|j_l(p)l\rangle \quad (4.150)$$

[9] R-matrix is defined as $\hat{R} = \hat{1} - \hat{S}$.

와 같이 정의 할 수도 있다. 이 때, $t^J_{\alpha\beta} \equiv \sum_\gamma \langle \mathcal{Y}_\alpha, j_\alpha | V | \mathcal{Y}_\gamma, \Psi_{\gamma\beta}\rangle$ 이고, $t^J_{\alpha\beta} = \langle p, \alpha | V | p, \beta \rangle^{(+)}$ 는 다르다.

- partial wave expansion: denoting α as 'angular-spin' quantum numbers and let us separate pure angular part and radial part for convenience,

$$\begin{aligned} |\boldsymbol{k}\rangle &= \sum_\alpha |k,\alpha\rangle\langle\alpha|\hat{k}\rangle, \quad |\hat{k}\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|\hat{k}\rangle, \\ \langle\hat{k}|\hat{k}'\rangle &= \delta^{(2)}(\hat{k}-\hat{k}') = \sum_{\alpha\beta}\delta_{\alpha\beta}Y_\alpha(\hat{k})Y^*_\beta(\hat{k}') \end{aligned} \tag{4.156}$$

where $|k,\alpha\rangle$ contains 'radial' wave function and spherical harmonics thus have dimension, while $|\alpha\rangle$ only contains 'angular' part and dimensionless. Note that the $|k,\alpha\rangle$ in this definition have to include i^α factor from $\langle \boldsymbol{x}|k,\alpha\rangle = i^\alpha f_\alpha(k,x)Y_\alpha(\hat{x})$.

- partial wave expansion of scattering amplitude

$$\begin{aligned} f(\boldsymbol{k},\boldsymbol{k}') &= -(2\pi)^2\mu\langle\boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)} \\ &= -(2\pi)^2\mu\sum_{\alpha\beta}\langle k,\alpha|V|k,\beta\rangle^{(+)}Y_\alpha(\hat{k})Y^*_\beta(\hat{k}') \end{aligned} \tag{4.157}$$

Thus, if we define $S_{\alpha\beta}$, $f_{\alpha\beta}$ and $T_{\alpha\beta}$ as

$$\begin{aligned} \langle\hat{k}|[\hat{S}\text{ or }\hat{T}]|\hat{k}'\rangle &\equiv \sum_{\alpha\beta}Y_\alpha(\hat{k})Y^*_\beta(\hat{k}')[S\text{ or }T]_{\alpha\beta}(k), \\ f(\boldsymbol{k},\boldsymbol{k}') &\equiv \sum_{\alpha\beta}Y_\alpha(\hat{k})Y^*_\beta(\hat{k}')f_{\alpha\beta}(k), \\ S_{\alpha\beta}(k) &= \delta_{\alpha\beta} - (2\pi)i\mu k\langle k,\alpha|V|k,\beta\rangle^{(+)}, \\ &= \delta_{\alpha\beta} - (2\pi)i\mu kT_{\alpha\beta}(k), \\ &= \delta_{\alpha\beta} + i\frac{k}{2\pi}f_{\alpha\beta}(k) \end{aligned} \tag{4.158}$$

- Special case : angular momentum conserved case. $\langle pl|V|pl'\rangle^{(+)} = t(p)\delta_{ll'}$

Usual definition of $f_l(E)$ is

$$f(E,\theta) \equiv \sum_l (2l+1)f_l(E)P_l(\cos\theta) \tag{4.159}$$

Comparing this with previous expansion,

$$\begin{aligned} f(\boldsymbol{k},\boldsymbol{k}'=k\hat{z}) &= \sum_{lm,l'm'}Y_{lm}(\hat{k})Y^*_{l'm'}(\hat{k}')f_{ll'}(k) \\ &= \sum_{ll'}\delta_{ll'}f_{ll}(k)\frac{2l+1}{4\pi}P_l(\cos\theta) \end{aligned} \tag{4.160}$$

In different normalization convention, we have

$$\langle\boldsymbol{k}|S|\boldsymbol{k}'\rangle = (2\pi)^3\frac{\delta(k-k')}{kk'}\delta_{\hat{k}\hat{k}'} - 2\pi i\frac{\mu}{k}\delta(k-k')t_{\hat{k}\hat{k}'}(k) \tag{4.153}$$

and factoring $(2\pi)^3\frac{\delta(k-k')}{k^2}$, and replacing $f = -\frac{\mu}{2\pi}t$, then

$$\hat{S}_{\hat{k}\hat{k}'} = \delta_{\hat{k}\hat{k}'} + i\frac{k}{2\pi}f_{\hat{k}\hat{k}'}(k) \tag{4.154}$$

Thus, $f_l(E) = \frac{f_{l,l}(k)}{4\pi}$ and $S_{ll'}(k) = \delta_{ll'} s_l(k)$,

$$s_l(k) = 1 + 2ikf_l(k), \quad f_l(k) = \frac{s_l(k) - 1}{2ik} \tag{4.161}$$

By using

$$\int d\Omega P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{4\pi}{2l+1}\delta_{ll'} \tag{4.162}$$

We get

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l \tag{4.163}$$

4.5.3 Partial wave decomposition of LS equation and convention dependence

Let us consider some convention dependence. In momentum vector form, the S-matrix can be related to the potential by,

$$\boxed{\begin{gathered}\langle \boldsymbol{k}|\boldsymbol{k}'\rangle = \mathcal{N}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}'), \quad \int \frac{d^3k}{\mathcal{N}}|\boldsymbol{k}\rangle\langle\boldsymbol{k}| = 1, \\ \langle \boldsymbol{k}|\hat{S}|\boldsymbol{k}'\rangle = \langle \boldsymbol{k}|\boldsymbol{k}'\rangle - 2\pi i\delta(E_k - E_k')\langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle^{(+)}, \\ \langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle^{(+)} = \langle \boldsymbol{k}|\hat{V}|\boldsymbol{k}'\rangle + \int \frac{d^3q}{\mathcal{N}}\langle \boldsymbol{k}|\hat{V}|\boldsymbol{q}\rangle\frac{1}{E_k - E_q + i\epsilon}\langle \boldsymbol{q}|\hat{V}|\boldsymbol{k}'\rangle^{(+)}\end{gathered}}$$

For the partial wave expansion of potential, let us use plane wave expansion,

$$\langle \boldsymbol{k}|\boldsymbol{k}'\rangle = \mathcal{N}\delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}') = \mathcal{N}\frac{\delta(k-k')}{kk'}\sum_{\alpha\beta}\delta_{\alpha\beta}Y_\alpha(\hat{k})Y^*_\beta(\hat{k}') \tag{4.164}$$

Usually, the $V(\boldsymbol{x},\boldsymbol{x}') \equiv \langle \boldsymbol{x}'|\hat{V}|\boldsymbol{x}\rangle$ and its partial wave expression has fixed convention.

$$V_{l'l}(x',x) \equiv \int d\Omega_{x'}\int d\Omega_x Y^*_{l'm'}(\hat{x}')V(\boldsymbol{x}',\boldsymbol{x})Y_{lm}(\hat{x}) \tag{4.165}$$

However, the momentum space matrix elements and it's partial wave components are convention dependent.

$$\begin{aligned}\langle \boldsymbol{k}'|\hat{V}|\boldsymbol{k}\rangle &= \int d^3x'\int d^3x \langle \boldsymbol{k}'|\boldsymbol{x}'\rangle\langle \boldsymbol{x}'|\hat{V}|\boldsymbol{x}\rangle\langle \boldsymbol{x}|\boldsymbol{k}\rangle \\ &= \left(\sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\right)^2\int d^3x'\int d^3x\left(4\pi\sum_\alpha i^{-\alpha}j_\alpha(k'x')Y^*_\alpha(\hat{x}')Y_\alpha(\hat{k}')\right)\times\langle \boldsymbol{x}'|\hat{V}|\boldsymbol{x}\rangle \\ &\quad\times\left(4\pi\sum_\beta i^\beta j_\beta(kx)Y_\beta(\hat{x})Y^*_\beta(\hat{k})\right) \\ &= \left(\sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\right)^2(4\pi)^2\sum_{\alpha\beta}i^{-\alpha+\beta}Y_\alpha(\hat{k}')Y^*_\beta(\hat{k})\langle j_\alpha Y_\alpha|\hat{V}|j_\beta Y_\beta\rangle, \\ &= \mathcal{N}\frac{2}{\pi}\sum_{\alpha\beta}i^{-\alpha+\beta}Y_\alpha(\hat{k}')Y^*_\beta(\hat{k})\langle j_\alpha Y_\alpha, k'|\hat{V}|j_\beta Y_\beta, k\rangle. \end{aligned} \tag{4.166}$$

where,

$$\begin{aligned}\langle j_\alpha Y_\alpha, k'|\hat{V}|j_\beta Y_\beta, k\rangle &\equiv \int d^3x' \int d^3x j_\alpha(k'x') Y^*_\alpha(\hat{x}') V(\boldsymbol{x}', \boldsymbol{x}) j_\alpha(kx) Y_\alpha(\hat{x}) \\ &= \int dx' x'^2 \int dx x^2 j_\alpha(k'x') V_{\alpha\beta}(x', x) j_\beta(kx) \end{aligned} \tag{4.167}$$

Now we may have various different ways to define partial wave component $V_{\alpha\beta}(k', k)$. (For example, If we absorb $i^{-\alpha+\beta}$ into the definition of $Y(\hat{x})$, we get modified spherical harmonics convention. or also we can absorb $\frac{2}{\pi}$ factor or $\mathcal{N}$ into radial wave function definition.)

It is beneficial to define partial wave on-shell S-matrix such that

$$\boxed{\frac{S_{\alpha\beta}(q) - \delta_{\alpha\beta}}{2iq} = -2\mu\langle j_\alpha Y_\alpha|\hat{V}|j_\beta Y_\beta\rangle^{(+)}(q, q).}$$

so that it can be related to the convention independent scattering amplitudes.

This definition of on-shell $S_{\alpha\beta}$ leads to the relation,

$$\begin{aligned}\langle \boldsymbol{k}'|S|\boldsymbol{k}\rangle &\equiv \langle \boldsymbol{k}'|\boldsymbol{k}\rangle - 2\pi i\delta(E_k - E_{k'})\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle^{(+)} \\ &= \mathcal{N}\frac{\delta(k-k')}{kk'}\sum_{\alpha\beta} i^{-\alpha+\beta} Y_\alpha(\hat{k}') Y^*_\beta(\hat{k}) \left(\delta_{\alpha\beta} - 4i\mu k\langle j_\alpha Y_\alpha|V|j_\beta Y_\beta\rangle^{(+)}\right) \\ &= \mathcal{N}\frac{\delta(k-k')}{kk'}\sum_{\alpha\beta} i^{-\alpha+\beta} Y_\alpha(\hat{k}') Y^*_\beta(\hat{k}) S_{\alpha\beta}(k) \end{aligned} \tag{4.168}$$

Rewriting the LS-equation as normalization independent way,

$$\boxed{\begin{aligned}\langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle^{(+)} &= \langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle \\ &+ \frac{2}{\pi}\sum_\gamma \int dq q^2 \langle j_\alpha Y_\alpha, k'|V|j_\gamma Y_\gamma, q\rangle \frac{1}{E_k - E_q + i\epsilon}\langle j_\gamma Y_\gamma, q|V|j_\beta Y_\beta, k\rangle^{(+)}\end{aligned}}$$

Now the definition of $T-$ matrix and $V_{\alpha\beta}$ depends on the convention. And further we may solve $K-$matrix equation, replacing $T_{\alpha\beta} \to K_{\alpha\beta}$.

- (a) If we define, on-shell T-matrix relation as

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} - 4i\mu q T_{\alpha\beta}(k, k), \quad T_{\alpha\beta}(k', k) \equiv \langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle^{(+)}, \tag{4.169}$$

LS-equation becomes

$$T_{\alpha\beta}(k', k) = V_{\alpha\beta}(k', k) + \frac{2}{\pi}\sum_\gamma \int dq q^2 V_{\alpha\gamma}(k', q)\frac{1}{E_k - E_q + i\epsilon} T_{\gamma\beta}(q, k) \tag{4.170}$$

where we define

$$\begin{aligned}V_{\alpha\beta}(k', k) &\equiv \langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle \\ &= \int d\Omega_{k'} \int d\Omega_k i^{\alpha-\beta} Y^*_\alpha(\hat{k}')\left(\frac{\pi}{2}\frac{\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle}{\mathcal{N}}\right) Y_\beta(\hat{k}) \end{aligned} \tag{4.171}$$

Also the K-matrix can be related with

$$T = K(1 - i2\mu p T) \tag{4.172}$$

- (b) If we define, on-shell T-matrix relation as

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} - 2\pi i\mu q T_{\alpha\beta}(k,k), \quad T_{\alpha\beta}(k',k) \equiv \langle\sqrt{\frac{2}{\pi}}j_\alpha Y_\alpha, k'|V|\sqrt{\frac{2}{\pi}}j_\beta Y_\beta, k\rangle^{(+)}, \tag{4.173}$$

LS-equation becomes

$$T_{\alpha\beta}(k',k) = V_{\alpha\beta}(k',k) + \sum_\gamma \int dq q^2 V_{\alpha\gamma}(k',q)\frac{1}{E_k - E_q + i\epsilon}T_{\gamma\beta}(q,k) \tag{4.174}$$

where we define

$$\begin{aligned} V_{\alpha\beta}(k',k) &\equiv \langle\sqrt{\frac{2}{\pi}}j_\alpha Y_\alpha, k'|V|\sqrt{\frac{2}{\pi}}j_\beta Y_\beta, k\rangle \\ &= \int d\Omega_{k'} \int d\Omega_k i^{\alpha-\beta} Y^*_\alpha(\hat{k}')\left(\frac{\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle}{\mathcal{N}}\right)Y_\beta(\hat{k}) \end{aligned} \tag{4.175}$$

and K-matrix is

$$T = K(1 - i\pi\mu p T) \tag{4.176}$$

- Machleidt's CD-Bonn potential paper follows convention (b) with $\mathcal{N} = 1$ but replacing $T_{\alpha\beta} \to R_{\alpha\beta}$. This $R_{\alpha\beta}$ is related with K-matrix in (a) convention as $R^{(b)}_{\alpha\beta} = \frac{2}{\pi}K^{(a)}_{\alpha\beta}$

- (c) In the paper of Haftel-Tabakin, they defined partial wave components as

$$\begin{aligned} V_{\alpha\beta}(k',k) &\equiv m_N\langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle \\ &= m_N \int d\Omega_{k'} \int d\Omega_k i^{\alpha-\beta} Y^*_\alpha(\hat{k}')\left(\frac{\pi}{2}\frac{\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle}{\mathcal{N}}\right)Y_\beta(\hat{k}), \quad \text{with } \mathcal{N} = 1 \end{aligned} \tag{4.177}$$

This leads to the LS equation such that

$$T_{\alpha\beta}(k',k) = V_{\alpha\beta}(k',k) + \frac{2}{\pi}\sum_\gamma \int dq q^2 V_{\alpha\gamma}(k',q)\frac{1}{k^2 - q^2 + i\epsilon}T_{\gamma\beta}(q,k) \tag{4.178}$$

with $E_k = \frac{k^2}{2\mu}$, $m_N = 2\mu$,

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} - 2iqT_{\alpha\beta}(k,k), \quad T_{\alpha\beta}(k',k) \equiv m_N\langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle^{(+)}, \tag{4.179}$$

- (d) In Epelbaum's paper, the $T_{\alpha\beta}$ is defined such as

$$S_{\alpha\beta} = \delta_{\alpha\beta} - \frac{i}{8\pi^2}pmT_{\alpha\beta}, \quad T_{\alpha\beta} = (2\pi)^3\langle\sqrt{\frac{2}{\pi}}j_\alpha Y_\alpha, k'|V|\sqrt{\frac{2}{\pi}}j_\beta Y_\beta, k\rangle^{(+)}, \tag{4.180}$$

and LS equation

$$T_{\alpha\beta}(k',k) = V_{\alpha\beta}(k',k) + \sum_\gamma \int \frac{dq q^2}{(2\pi)^3} V_{\alpha\gamma}(k',q)\frac{m}{k^2 - q^2 + i\epsilon}T_{\gamma\beta}(q,k) \tag{4.181}$$

This corresponds to

$$\begin{aligned} V_{\alpha\beta}(k',k) &\equiv (2\pi)^3\langle\sqrt{\frac{2}{\pi}}j_\alpha Y_\alpha, k'|V|\sqrt{\frac{2}{\pi}}j_\beta Y_\beta, k\rangle \\ &= (2\pi)^3 \int d\Omega_{k'} \int d\Omega_k i^{\alpha-\beta} Y^*_\alpha(\hat{k}')\left(\frac{\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle}{\mathcal{N}}\right)Y_\beta(\hat{k}). \end{aligned} \tag{4.182}$$

- Thus, the usual convention of one-pion exchange potential and contact potentials are defined in the $\mathcal{N} = (2\pi)^3$ convention.

$$\begin{aligned} V_{1\pi}(\boldsymbol{p}', \boldsymbol{p}) &= -\frac{g_A^2}{4f_\pi^2}\tau_1 \cdot \tau_2 \frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{q}\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}}{q^2 + m_\pi^2}, \\ V_{ct}^{(0)}(\boldsymbol{p}', \boldsymbol{p}) &= C_S + C_T \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2. \end{aligned} \tag{4.183}$$

Thus, the partial wave expression becomes

$$V_{ct}^{(0)}({}^1S_0) = 4\pi(C_S - 3C_T) \quad \text{in convention (d)} \tag{4.184}$$

- (e) We may define

$$S_{\alpha\beta} = \delta_{\alpha\beta} - iT_{\alpha\beta}, \quad T_{\alpha\beta}(k', k) = 4\mu k \langle j_\alpha Y_\alpha, k'|V|j_\beta Y_\beta, k\rangle^{(+)} \tag{4.185}$$

- Note that the 1-pion exchange potential is defined as

$$\langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle = -\frac{g_A^2}{4f_\pi^2}\tau_1 \cdot \tau_1 \frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{q}\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}}{q^2 + m_\pi^2}, \quad \langle \boldsymbol{p}'|\boldsymbol{p}\rangle = (2\pi)^3 \delta^{(3)}(\boldsymbol{p}' vp). \tag{4.186}$$

The code chiral_pion_p is written in this normalization. However, at the end of the chiral_pot_p ,it is divided by $(2\pi)^3$ so that the final return results is

$$\langle \boldsymbol{p}'|V|\boldsymbol{p}\rangle = -\frac{1}{(2\pi)^3}\frac{g_A^2}{4f_\pi^2}\tau_1 \cdot \tau_1 \frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{q}\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}}{q^2 + m_\pi^2}, \quad \langle \boldsymbol{p}'|\boldsymbol{p}\rangle = \delta^{(3)}(\boldsymbol{p}' vp). \tag{4.187}$$

Thus, we solve LS equation in the form of (b) in the 'phase' code.

Note that parity conserving strong interaction case, we can always set $i^{\alpha-\beta} \to 1$. Because there is no unique definition of $T_{\alpha\beta}$ or $V_{\alpha\beta}$, it is better to explicitly write equation as above.

4.5.4 Relation between T-matrix and K-matrix

Let us consider a relation between T-matrix and K-matrix. For orbital angular momentum conservation, let us consider

$$\begin{aligned} T_l(p', p) &= V_l(p', p) + \mathcal{C}\int dq \frac{q^2}{q^2 - p^2 - i\epsilon} V_l(p', q) T_l(q, p), \\ &= V_l(p', p) + \mathcal{C}\int dq P\frac{q^2}{q^2 - p^2} V_l(p', q) T_l(q, p) + \mathcal{C}\frac{i\pi}{2} p V_l(p', p) T_l(p, p), \\ &\to \int dq \left(\delta(q - p) - \mathcal{C}P\frac{q^2}{q^2 - p^2} V_l(p', q)\right) T(q, p) = V_l(p', p)(1 + \mathcal{C}\frac{i\pi}{2} p T_l(p, p)) \end{aligned}$$

and from K-matrix equation

$$\int dq \left(\delta(q - p) - \mathcal{C}P\frac{q^2}{q^2 - p^2} V_l(p', q)\right) K(q, p) = V_l(p', p) \tag{4.188}$$

$$\begin{aligned} &\int dq \left(\delta(q - p) - \mathcal{C}P\frac{q^2}{q^2 - p^2} V_l(p', q)\right) T(q, p) \\ = &\int dq \left(\delta(q - p) - \mathcal{C}P\frac{q^2}{q^2 - p^2} V_l(p', q)\right) K(q, p) \left(1 + \mathcal{C}\frac{i\pi}{2} p T(p, p)\right) \end{aligned} \tag{4.189}$$

Thus, removing integral in both sides, we get half-on-shell relations, [10]

$$T(q,p) = K(q,p)\left(1 + \mathcal{C}\frac{i\pi}{2}pT(p,p)\right). \tag{4.191}$$

4.5.5 Integral representation of scattering amplitudes

When angular momentum is conserved, we can write

$$\begin{aligned}\langle \boldsymbol{x}|\boldsymbol{p}\rangle^{(+)} &= \sum_{l'm'}\langle xl'm'|pl'm'\rangle^{(+)}\langle\hat{x}|xl'm'\rangle\langle pl'm'|\hat{p}\rangle \\ &= \sum_{l'm'}\langle xl'm'|pl'm'\rangle^{(+)} i^l Y_{l'm'}(\hat{x})Y^*_{l'm'}(\hat{p})\end{aligned} \tag{4.192}$$

With

$$\langle xl'm'|pl'm'\rangle^{(+)} \to \sqrt{\frac{2}{\pi}}j_l(pr) \text{ free limit} \tag{4.193}$$

But, if angular momentum is not conserved, then we have to consider something like

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle^{(+)} = \sum_{l'm',lm}\langle xl'm'|plm\rangle^{(+)}\langle\hat{x}|xl'm'\rangle\langle plm|\hat{p}\rangle \tag{4.194}$$

where

$$\begin{aligned}\langle xl'm'|plm\rangle^{(+)} &= \sqrt{\frac{2}{\pi}}\psi_{l'l}(x,p) \\ &\to \sqrt{\frac{2}{\pi}}j_l(pr)\delta_{l'l} \text{ without interaction} \\ &\to \sqrt{\frac{2}{\pi}}\frac{1}{2}[\delta_{l'l}h^{(-)}_{l'}(px) + S_{l'l}h^{(+)}_{l'}(px)] \text{ asymptotically}\end{aligned} \tag{4.195}$$

where, $h^{(\pm)}_l(px) \equiv j_l(px) \pm iy_l(px)$ and

$$S_{l'l}(q) = \delta_{l'l} - 4i\mu q\sum_{l''}\langle j_{l'}, l'|V|l'', \psi_{l'',l}\rangle \tag{4.196}$$

OR we can write,

$$\begin{aligned}S_{\alpha\beta}(k) &= \delta_{\alpha\beta} - (2\pi)i\mu k\langle k,\alpha|V|k,\beta\rangle^{(+)}, \\ &= \delta_{\alpha,\beta} - 4i\mu k\sum_{\beta'}\langle j_\alpha(k),\alpha|V|\psi^{(+)}_{\beta'\beta},\beta'\rangle\end{aligned} \tag{4.197}$$

such that,

$$\begin{aligned}|k,\alpha\rangle &= \sqrt{\frac{2}{\pi}}|j_\alpha(k),\alpha\rangle \\ |k,\beta\rangle^{(+)} &= \sqrt{\frac{2}{\pi}}\sum_{\beta'}|\psi_{\beta'\beta},\beta'\rangle\end{aligned} \tag{4.198}$$

[10] I confirmed the half-on-shell relation with explicit numerical calculation. I tried to check whether the relation can be extended to full off-shell relation,

$$T(q',q;E) = K(q',q;E)\left(1 + \mathcal{C}\frac{i\pi}{2}T(q,q;E)\right) \quad ? \tag{4.190}$$

It looks like it is not satisfied!

We may define partial-wave projected T-matrix element by

$$
\begin{aligned}
T^J_{\alpha',\alpha} &\equiv \sum_\beta \langle j_{\alpha'},\alpha'|V|\beta,\Psi^{(+)}_{\beta\alpha}\rangle \\
S_{\alpha\beta}(k) &= \delta_{\alpha\beta} - 4i\mu k T^J_{\alpha\beta}
\end{aligned} \tag{4.199}
$$

- total cross section in partial wave: Total cross section can be written in terms of S-matrix as [11]

$$
\sigma_{tot} = \frac{4\pi}{k}\mathrm{Im}\sum_{\alpha\beta} i^{-l_\alpha+l_\beta}\sqrt{(2l_\alpha+1)(2l_\beta+1)}\left(\frac{S_{\alpha\beta}-\delta_{\alpha\beta}}{2ik}\right) \tag{4.200}
$$

Note when we use above equation, we have to be careful because α,β represent all possible quantum numbers including polarizations. Thus, unpolarized total cross section requires average over polarization. For example, $\frac{1}{(2j_1+1)(2j_2+1)}\sum_{m_1m_2} M_{m_1m_2,m_1m_2}$. If two particle were spin $\frac{1}{2}$, it will be $\frac{1}{4}[M^{J=0}+3M^{J=1}]$ and if two particle were spin 1 and $\frac{1}{2}$, $\frac{1}{6}[2M^{J=\frac{1}{2}}+4M^{J=\frac{3}{2}}]$. Thus, n-d scattering case,

$$
\sigma_{tot} = \frac{2\pi}{k^2}\mathcal{I}m(\frac{1}{3}[S^{J=1/2}_{00}-1]+\frac{2}{3}[S^{J=3/2}_{00}-1]). \tag{4.201}
$$

4.6 Optical potential case:

This part is from "Nuclear Optical Model Calculations: by M.A. Melkanoff et.al.

When optical potential including spin-orbit interaction is considered, the asymptotic radial solution at the matching radius can be written as

$$
\psi^j_l(r_m) = F_l(\eta,kr_m) + C^j_l[G_l(\eta,kr_m)+iF_l(\eta,kr_m)] \tag{4.202}
$$

where C^j_l corresponds to partial T-matrix which is related with phase shift

$$
C^j_l = -\frac{i}{2}[\exp(2i\delta^j_l)-1] = -\frac{i}{2}[\eta^j_l-1] \tag{4.203}
$$

where absorption coefficient(?) $|\eta^j_l|^2$. The total reaction cross section is written as

$$
\sigma_R = \frac{4\pi}{k^2}\frac{1}{2s+1}\sum_{l=0}^{\infty}\sum_{j=|l-s|}^{l+s}(2j+1)(\mathrm{Im C^j_l}-|\mathrm{C^j_l}|^2). \tag{4.204}
$$

4.6.1 $s=0$ case

scattering amplitude is given by

$$
\begin{aligned}
A(\theta) &= f_c(\theta) + \frac{1}{k}\sum_{l=0}^{\infty}\exp(2i\sigma_l)(2l+1)C^l_l P_l(\cos\theta), \\
\sigma(\theta) &= |A(\theta)|^2
\end{aligned} \tag{4.205}
$$

where σ_l is a Coulomb phase shift.

[11] I am not sure about $i^{-l_\alpha+l_\beta}$ factor. Is it correct? It seems to be....

4.6.2 $s = \frac{1}{2}$ case

two independent scattering amplitudes are

$$\begin{aligned}
A(\theta) &= f_c(\theta) + \frac{1}{k}\sum_{l=0}^{\infty} \exp(2i\sigma_l)[(l+1)C_l^{l+1/2} + lC_l^{l-1/2}]P_l(\cos\theta), \\
B(\theta) &= \frac{i}{k}\sum_{l=0}^{\infty} \exp(2i\sigma_l)[C_l^{l+1/2} - C_l^{l-1/2}]P_l^1(\cos\theta)
\end{aligned} \tag{4.206}$$

Then differential cross section and polarization for unpolarized incident beam are

$$\begin{aligned}
\sigma(\theta) &= |A(\theta)|^2 + |B(\theta)|^2, \\
P(\theta) &= [A^*(\theta)B(\theta) + A(\theta)B^*(\theta)]/\sigma(\theta).
\end{aligned} \tag{4.207}$$

4.6.3 $s = 1$ case

(There are four independent scattering amplitudes. There are different sets of them) In helicity formalism,

$$\begin{aligned}
A(\theta) &= f_c(\theta)\frac{(1+\cos\theta)}{2} + \frac{1}{2k}\sum_{J=1}^{\infty}\big((J+1)\exp(2i\sigma_{J-1})C_{J-1}^J + J\exp(2i\sigma_{J+1})C_{J+1}^J + (2J+1)\exp(2i\sigma_J)C_J^J\big) \\
&\quad \times\left(\frac{(1-\cos\theta)}{J(J+1)\sin\theta}P_j^1(\cos\theta) + P_J(\cos\theta)\right), \\
B(\theta) &= -f_c(\theta)\frac{\sin\theta}{\sqrt{2}} + \frac{1}{\sqrt{2}k}\sum_{J=1}^{\infty}\Big\{\exp(2i\sigma_{J-1})C_{J-1}^J - \exp(2i\sigma_{J+1})C_{J+1}^J\Big\}P_J^1(\cos\theta), \\
C(\theta) &= f_c(\theta)\frac{1-\cos\theta}{2} + \frac{1}{2k}\sum_{J=1}^{\infty}\Big\{(J+1)\exp(2i\sigma_{J-1})C_{J-1}^J + J\exp(2i\sigma_{J+1})C_{J+1}^J - (2J+1)\exp(2i\sigma_J)C_J^J\Big\} \\
&\quad \times\Big\{\frac{1+\cos\theta}{J(J+1)\sin\theta}P_J^1(\cos\theta) - P_J(\cos\theta)\Big\} \\
D(\theta) &= f_c(\theta)\cos\theta + \frac{1}{k}\sum_{J=1}^{\infty}\Big\{J\exp(2i\sigma_{J-1})C_{J-1}^J + (J+1)\exp(2i\sigma_{J+1})C_{J+1}^J\Big\}P_J(\cos\theta)
\end{aligned} \tag{4.208}$$

and

$$\begin{aligned}
\sigma(\theta) &= \frac{1}{3}\left\{2|A(\theta)|^2 + 4|B(\theta)|^2 + 2|C(\theta)|^2 + |D(\theta)|^2\right\}, \\
i\langle T_{11}\rangle &= \sqrt{\frac{2}{3}}\frac{1}{\sigma(\theta)}\mathrm{Im}[B^*(\theta)(C(\theta) - A(\theta) - D(\theta))] \\
\langle T_{20}\rangle &= \frac{\sqrt{2}}{3}\frac{1}{\sigma(\theta)}[|A(\theta)|^2 + |C(\theta)|^2 - |B(\theta)|^2 - |D(\theta)|^2] \\
\langle T_{21}\rangle &= \sqrt{\frac{2}{3}}\frac{1}{\sigma(\theta)}\mathrm{Re}[B^*(\theta)(A(\theta) - C(\theta) - D(\theta))] \\
\langle T_{22}\rangle &= \frac{1}{\sqrt{3}}\frac{1}{\sigma(\theta)}[A(\theta)C^*(\theta) + C(\theta)A^*(\theta) - |B(\theta)|^2]
\end{aligned} \tag{4.209}$$

Chapter 5

Distorted Wave Born Approximation

Until now, we only considered a single channel scatterings or partial waves within the same partitions(number of particles). In other words, it was mainly for elastic or inelastic channels in reaction theory. Let us extend its concepts for general multi-channel scatterings. In many cases, the DWBA is a practical approximation of the full theory. Let us derive here DWBA

5.1 Derivation of DWBA

5.1.1 Green's function method in DWBA

Let us consider the case with both Coulomb V_c and nuclear interaction V_s. Because the Coulomb force is long range, there is a distortion in asymptotic wave and it is not appropriate to use free plane wave as basis.

$$\begin{aligned}
&[T + V_c - E]\psi_\alpha + \sum_{\alpha'} \langle \alpha | V | \alpha' \rangle \psi_{\alpha'} = 0, \\
&[E - T - V_c]\psi_\alpha = \Omega_\alpha, \quad \Omega_\alpha \equiv \sum_{\alpha'} \langle \alpha | V | \alpha' \rangle \psi_{\alpha'}, \\
&[\frac{d^2}{dR^2} - \frac{2\eta k_\alpha}{R} - \frac{L_\alpha(L_\alpha + 1)}{R^2} + k_\alpha^2]\psi_\alpha(R) = \frac{2\mu}{\hbar^2}\Omega_\alpha(R). \qquad (5.1)
\end{aligned}$$

Let us denote the homogeneous solution of equation as regular solution F_α and outgoing solution H_α^+, so that boundary condition becomes

$$\psi_{\alpha\alpha_i} = F_\alpha \delta_{\alpha\alpha_i} + H_\alpha^+ T_{\alpha\alpha_i}. \qquad (5.2)$$

If we define Green's function such that

$$\begin{aligned}
&[\frac{d^2}{dR^2} - U(R) + k_\alpha^2]G^+(R, R') = \delta(R - R'), \\
&U(R) = 2\frac{\eta k_\alpha}{R} + \frac{L_\alpha(L_\alpha + 1)}{R^2}, \quad k_\alpha^2 = \frac{1}{\hbar^2}2\mu E \qquad (5.3)
\end{aligned}$$

Formal solution becomes

$$\psi_\alpha(R) = \delta_{\alpha\alpha_i}(R) + \frac{2\mu}{\hbar^2}\int dR' G^+(R, R')\Omega_\alpha(R') \qquad (5.4)$$

Or in short,

$$\psi_\alpha = F_\alpha + [E - T - U_c]^{-1}\Omega_\alpha \qquad (5.5)$$

Because we already know the homogeneous solution form at $R < R'$ and $R > R'$, if we require the continuity of Green function and discontinuity of derivative of Green function, we can get,

$$
\begin{aligned}
G^{+}(R,R') &= \frac{1}{W(F,H^{+})(R')}\begin{cases} H^{+}(R')F(R) & \text{for } R < R' \\ F(R')H^{+}(R) & \text{for } R > R' \end{cases} \\
&= -\frac{1}{k}F(R_{<})H^{+}(R_{>}), \qquad (5.6)
\end{aligned}
$$

where Wronskian $W(F,H^{+})(R') = -k$.

By comparing this with asymptotic form,

$$
\psi_{\alpha}(R) = \delta_{\alpha\alpha_i}F_{\alpha}(R) - \frac{2\mu}{\hbar^2 k_{\alpha}}\int dR' F_{\alpha}(R_{<})H_{\alpha}^{+}(R_{>})\Omega_{\alpha}(R'), \qquad (5.7)
$$

we get

$$
\begin{aligned}
T_{\alpha\alpha_i} &= -\frac{2\mu}{\hbar^2 k_{\alpha}}\int dR' F_{\alpha}(R')\Omega_{\alpha}(R'), \\
&= -\frac{2\mu}{\hbar^2 k_{\alpha}}\langle F_{\alpha}^{*}|\Omega_{\alpha}\rangle = -\frac{2\mu}{\hbar^2 k_{\alpha}}\langle F^{(-)}|\Omega_{\alpha}\rangle \\
T &= -\frac{2\mu}{\hbar^2 k_{\alpha}}\langle F^{(-)}|V|\psi\rangle \qquad (5.8)
\end{aligned}
$$

In DWBA, we approximate $|\psi\rangle \simeq |F^{(+)}\rangle$.

5.2 Two potential formula and DWBA

Here we try to verify how to obtain three-body scattering amplitude by using distorted wave born approximation or perturbation method.

The two-body scattering case, the scattering amplitude or T-matrix can be obtained by,

$$
\begin{aligned}
\langle \boldsymbol{k}|S|\boldsymbol{k}'\rangle &\equiv {}^{(-)}\langle \boldsymbol{k}|\boldsymbol{k}'\rangle^{(+)} = \langle \boldsymbol{k}|\boldsymbol{k}'\rangle - 2\pi i\delta(E_k - E_{k'})\langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)}, \\
\langle \boldsymbol{k}|T|\boldsymbol{k}'\rangle &\equiv \langle \boldsymbol{k}|V|\boldsymbol{k}'\rangle^{(+)} \qquad (5.9)
\end{aligned}
$$

We want an approximated expression of T-matrix when the potential can be written as a sum of $V_s + V_w$, strong and weak potential writing T-matrix in terms of only states of eigen states of V_s.

DWBA can be written as

$$
\begin{aligned}
f(\theta) &= f_0(\theta) - 2\pi^2\frac{2\mu}{\hbar^2}\int d^3r\chi_{\boldsymbol{k}'}^{(-)*}(\boldsymbol{r})V_w\psi_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}) \\
f_{DWBA}(\theta) &= f_0(\theta) - 2\pi^2\frac{2\mu}{\hbar^2}\int d^3r\chi_{\boldsymbol{k}'}^{(-)*}(\boldsymbol{r})V_w\chi_{\boldsymbol{k}}^{(+)}(\boldsymbol{r}) \qquad (5.10)
\end{aligned}
$$

For inelastic scattering reaction $A(a,b)B$,

$$
f_{DWBA}^{inel}(\theta) = -2\pi^2\frac{2\mu}{\hbar^2}\int d^3r_{\alpha}d^3r_{\beta}\chi_{\beta}^{(-)*}(\boldsymbol{k}_{\beta},\boldsymbol{r}_{\beta})\langle b,B|V_w|a,A\rangle\chi_{\alpha}^{(+)}(\boldsymbol{k}_{\alpha},\boldsymbol{r}_{\alpha}) \qquad (5.11)
$$

5.2.1 derivation of DWBA for 2-body scattering: method 1

Suppose there are two potential $U_1 + U_2$ with U_1 is strong and U_2 is weak. For each partial wave let us define three wave functions,

Free:	$[E-T]\phi = 0$	$\hat{G}_0^{(+)} = [E-T]^{-1}$	$\phi = F,$
Distorted:	$[E-T-U_1]\chi = 0$	$\chi = \phi + \hat{G}_0^{+}U_1\chi$	$\chi \to \phi + \boldsymbol{T}^{(1)}H^{(+)},$
Full:	$[E-T-U_1-U_2]\psi = 0$	$\psi = \phi + \hat{G}_0^{+}(U_1+U_2)\psi$	$\psi \to \phi + \boldsymbol{T}^{(1+2)}H^{(+)}$

Let us denote $|\phi_{\boldsymbol{k}}\rangle$ as a free plane wave, which is a solution for

$$H_0|\phi_{\boldsymbol{k}}\rangle = E_k|\phi_{\boldsymbol{k}}\rangle. \tag{5.12}$$

Let us first define modified "free" states, or "distorted" waves,

$$(H_0 + V_s)|\chi_{\boldsymbol{k}}\rangle = E_k|\chi_{\boldsymbol{k}}\rangle, \tag{5.13}$$

which leads LS-equation of form,

$$|\chi_{\boldsymbol{k}}\rangle^{(\pm)} = |\phi_{\boldsymbol{k}}\rangle + G_0(E_k \pm i\epsilon)V_s|\chi_{\boldsymbol{k}}\rangle^{(\pm)} \tag{5.14}$$

also imply

$$\langle\phi_{\boldsymbol{k}}| = {}^{(-)}\langle\chi_{\boldsymbol{k}}| - {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_s G_0(E_k + i\epsilon) \tag{5.15}$$

On the other hand, full solution satisfies

$$\begin{aligned} (H_0 + V_s + V_w)|\psi_{\boldsymbol{k}}\rangle &= E_k|\psi_{\boldsymbol{k}}\rangle, \\ |\psi_{\boldsymbol{k}}\rangle^{(\pm)} &= |\phi_{\boldsymbol{k}}\rangle + G_0^{(\pm)}(V_s + V_w)|\psi_{\boldsymbol{k}}\rangle^{(\pm)} \end{aligned} \tag{5.16}$$

Then, full scattering amplitude become

$$\begin{aligned} t(\boldsymbol{k}, \boldsymbol{k}') &= \langle\phi_{\boldsymbol{k}}|(V_s + V_w)|\psi_{\boldsymbol{k}'}\rangle^{(+)} \\ &= {}^{(-)}\langle\chi_{\boldsymbol{k}}|(V_s + V_w)|\psi_{\boldsymbol{k}'}\rangle^{(+)} - {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_s G_0^{(+)}(V_s + V_w)|\psi_{\boldsymbol{k}'}\rangle^{(+)} \\ &= {}^{(-)}\langle\chi_{\boldsymbol{k}}|(V_s + V_w)|\phi_{\boldsymbol{k}'}\rangle + {}^{(-)}\langle\chi_{\boldsymbol{k}}|(V_s + V_w)G_0^{(\pm)}(V_s + V_w)|\psi_{\boldsymbol{k}'}\rangle^{(\pm)} \\ &\quad - {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_s G_0^{(+)}(V_s + V_w)|\psi_{\boldsymbol{k}'}\rangle^{(+)} \\ &= {}^{(-)}\langle\chi_{\boldsymbol{k}}|(V_s + V_w)|\phi_{\boldsymbol{k}'}\rangle + {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w G_0^{(\pm)}(V_s + V_w)|\psi_{\boldsymbol{k}'}\rangle^{(+)} \\ &= {}^{(-)}\langle\chi_{\boldsymbol{k}}|(V_s + V_w)|\phi_{\boldsymbol{k}'}\rangle + {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w|\psi_{\boldsymbol{k}'}\rangle^{(+)} - {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w|\phi_{\boldsymbol{k}'}\rangle \\ &= {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_s|\phi_{\boldsymbol{k}'}\rangle + {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w|\psi_{\boldsymbol{k}'}\rangle^{(+)} \\ &= t(\boldsymbol{k}, \boldsymbol{k}')_s + {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w|\psi_{\boldsymbol{k}'}\rangle^{(+)} \end{aligned} \tag{5.17}$$

where,

$$t(\boldsymbol{k}, \boldsymbol{k}')_s = \langle\phi_{\boldsymbol{k}}|V_s|\chi_{\boldsymbol{k}'}\rangle^{(+)} = {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_s|\phi_{\boldsymbol{k}'}\rangle \tag{5.18}$$

This result is known as two-potential formula, Watson's theorem or Gell-Mann-Goldberger result. In other words, the full solution can be written as

$$|\boldsymbol{k}\rangle^{(+)} = |\phi_k\rangle^{(+)} + G_s^{(+)}V_w|\boldsymbol{k}\rangle^{(+)}, \quad G_s^{(+)} = [E - H_0 - V_s]^{-1} \tag{5.19}$$

Explicit form of $G_s^+(R, R')$ can be written in terms of regular and irregular solutions $F(R)$, $H(R)$ such that $[E - H_0 - V_s]\{F, H\}(R) = 0$,

$$G_s^{(+)}(R, R') = -\frac{1}{k}F(R_<)H(R_>) \tag{5.20}$$

In DWBA, we approximate $|\boldsymbol{k}\rangle^{(+)} \sim |\phi_{\boldsymbol{k}}\rangle^{(+)}$ and

$$t(\boldsymbol{k}, \boldsymbol{k}') \simeq t(\boldsymbol{k}, \boldsymbol{k}')_s + {}^{(-)}\langle\phi_{\boldsymbol{k}}|V_w|\phi_{\boldsymbol{k}'}\rangle^{(+)} \tag{5.21}$$

On the other hand, if we express above equation in terms of T-matrix instead of wave function, we use formal relation

$$\begin{aligned} T|\boldsymbol{k}\rangle &= V|\boldsymbol{k}\rangle^{(+)}, \\ |\phi_k\rangle^{(+)} &= |\boldsymbol{k}\rangle + G_0 V_s|\phi_k\rangle^{(+)} = |\boldsymbol{k}\rangle + G_0 T_s|\boldsymbol{k}\rangle = (1 + G_0 T_s)|\boldsymbol{k}\rangle, \end{aligned} \tag{5.22}$$

Thus, DWBA expression becomes

$$t(\boldsymbol{k}, \boldsymbol{k}') \simeq t(\boldsymbol{k}, \boldsymbol{k}')_s + \langle\boldsymbol{k}|(1 + T_s G_0)V_w(G_0 T_s + 1)|\boldsymbol{k}\rangle. \tag{5.23}$$

5.2.2 derivation of DWBA for 2-body scattering: method 2

Previous derivation is only true for 2-body scattering. This equation seems to work for other processes.

Let us denote $V = V_s + V_w$ and

$$G^{(\pm)} = \frac{1}{E \pm i\epsilon - H}, \quad G_0^{(\pm)} = \frac{1}{E \pm i\epsilon - H_0}, \tag{5.24}$$

Let us consider T-operator ,

$$T = V_s + V_w + (V_s + V_w)G_0^{(+)}T \to (1 - V_sG_0^{(+)})T = V_s + V_w + V_wG_0^{(+)}T \tag{5.25}$$

Mulyiply both sides with $(1 - V_sG_0^{(+)})^{-1}$,

$$\begin{aligned} T &= (1 - V_sG_0^{(+)})^{-1}V_s + (1 - V_sG_0^{(+)})^{-1}V_w + (1 - V_sG_0^{(+)})^{-1}V_wG_0^{(+)}T \\ &= (1 - V_sG_0^{(+)})^{-1}V_s + (1 - V_sG_0^{(+)})^{-1}V_w(1 + G_0^{(+)}T) \end{aligned} \tag{5.26}$$

On the other hand, from the relation,

$$\begin{aligned} & T = V + G_0^{(+)}VT \to (1 - VG_0^{(+)})T = V \\ \to \quad & G^{(+)}(1 - VG_0^{(+)})T = (G^{(+)} - G^{(+)}VG_0^{(+)})T = G_0^{(+)}T = G^{(+)}V \end{aligned} \tag{5.27}$$

Thus, $G_0T = GV$. And from the LS-equation, Low equation and from Moller operator,

$$\begin{aligned} |\psi\rangle^{(\pm)} &= |\phi\rangle + G_0^{(\pm)}V|\psi\rangle^{(\pm)} \to |\psi\rangle^{(\pm)} = (1 - G_0^{(\pm)}V)^{-1}|\phi\rangle, \\ |\psi\rangle^{(\pm)} &= |\phi\rangle + G^{(\pm)}V|\phi\rangle, \\ |\psi\rangle^{(\pm)} &= \Omega_\pm|\phi\rangle \end{aligned} \tag{5.28}$$

We can rewrite Moller operator as

$$\Omega_\pm = (1 - G_0^{(\pm)}V)^{-1} = 1 + G^{(\pm)}V = 1 + G_0^{(\pm)}T \tag{5.29}$$

In a similar way, we get

$$\begin{aligned} & \langle\psi^\pm| = \langle\psi^\pm|(\Omega_\pm)^\dagger = \langle\phi| + \langle\psi^\pm|VG_0^{(\mp)}, \to \langle\psi^\pm| = \langle\phi|(1 - VG_0^\mp)^{-1}, \\ \to \quad & (\Omega_\pm)^\dagger = (1 - VG_0^\mp)^{-1} \end{aligned} \tag{5.30}$$

Also, if we define T_s such that

$$T_s = V_s + V_sG_0^{(+)}T_s \to T_s = (1 - V_sG_0^{(+)})^{-1}V_s. \tag{5.31}$$

The original T-matrix equation becomes

$$T = T_s + \Omega_s^{(-)^\dagger}V_w\Omega^{(+)} \tag{5.32}$$

This implies the matrix element,

$$\begin{aligned} T(\boldsymbol{k}, \boldsymbol{k}') &= T_s(\boldsymbol{k}, \boldsymbol{k}') + {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w|\psi_{\boldsymbol{k}'}\rangle^{(+)}, \\ &\simeq T_s(\boldsymbol{k}, \boldsymbol{k}') + {}^{(-)}\langle\chi_{\boldsymbol{k}}|V_w|\chi_{\boldsymbol{k}'}\rangle^{(+)} \quad \text{(DWBA)} \end{aligned} \tag{5.33}$$

Note that

$$\psi_{\boldsymbol{k}}^{(-)}(\boldsymbol{r}) = \left(\psi_{-\boldsymbol{k}}^{(+)}(\boldsymbol{r})\right)^* \tag{5.34}$$

Other derivation: In finite ϵ case, let us

$$
\begin{aligned}
&(E+i\epsilon-H_0)|\phi\rangle = i\epsilon|\phi\rangle \\
&(E+i\epsilon-H_1)|\chi^{(+)}\rangle = i\epsilon|\phi\rangle, \quad H_1 = H_0+V_1 \\
&(E+i\epsilon-H)|\psi^{(+)}\rangle = i\epsilon|\phi\rangle, \quad H = H_0+V_1+V_2
\end{aligned}
\tag{5.35}
$$

Then

$$
\begin{aligned}
|\chi^{(\pm)}\rangle &= \Omega_1^{(\pm)}|\phi\rangle = \frac{\pm i\epsilon}{E\pm i\epsilon-H_1}|\phi\rangle \\
|\psi^{(\pm)}\rangle &= \Omega^{(\pm)}|\phi\rangle = \frac{\pm i\epsilon}{E\pm i\epsilon-H}|\phi\rangle
\end{aligned}
\tag{5.36}
$$

T-matrix are defined

$$
T_1 = \langle\phi|V_1|\chi^{(+)}\rangle \tag{5.37}
$$

$$
T = \langle\phi|V_1+V_2|\psi^{(+)}\rangle = \langle\phi|V_1\Omega^{(+)}|\phi\rangle + \langle\phi|V_2|\psi^{(+)}\rangle \tag{5.38}
$$

from $\frac{1}{B}-\frac{1}{A} = \frac{1}{B}(A-B)\frac{1}{A} = \frac{1}{A}(A-B)\frac{1}{B}$,

$$
\begin{aligned}
\Omega_1^{(-)\dagger} &= \left(\frac{-i\epsilon}{E-i\epsilon-H_1}\right)^\dagger = \left[\left(1+\frac{1}{E-i\epsilon-H_1}V_1\right)\frac{-i\epsilon}{E-i\epsilon-H_0}\right]^\dagger \\
&= \frac{i\epsilon}{E+i\epsilon-H_0}\left(1+V_1\frac{1}{E+i\epsilon-H_1}\right)
\end{aligned}
\tag{5.39}
$$

$$
\begin{aligned}
V_1\frac{i\epsilon}{E+i\epsilon-H} &= V_1\left[\frac{i\epsilon}{E+i\epsilon-H_1} + \frac{1}{E+i\epsilon-H_1}V_2\frac{i\epsilon}{E+i\epsilon-H}\right] \\
&= V_1\frac{i\epsilon}{E+i\epsilon-H_1} + V_1\frac{1}{E+i\epsilon-H_1}V_2\frac{i\epsilon}{E+i\epsilon-H}
\end{aligned}
\tag{5.40}
$$

Then,

$$
\langle\phi|V_1\Omega^{(+)}|\phi\rangle = \langle\phi|V_1|\chi^{(+)}\rangle + \langle\phi|V_1\frac{1}{E+i\epsilon-H_1}V_2|\psi^{(+)}\rangle \tag{5.41}
$$

Thus,

$$
T = \langle\phi|V_1|\chi^{(+)}\rangle + \langle\phi|\left(1+V_1\frac{1}{E+i\epsilon-H_1}\right)V_2|\psi^{(+)}\rangle \tag{5.42}
$$

$$
T = T_1 + \langle\chi^{(-)}|V_2|\psi^{(+)}\rangle \tag{5.43}
$$

5.3 Watson's series

Let us consider a scattering T-matrix in channel $\alpha = (A+a)$,

$$
T_\alpha = V_\alpha + V_\alpha\frac{1}{E-H_A-H_a-T_\alpha+i\epsilon}T_\alpha \tag{5.44}
$$

for the case of no rearrangement of particles. Let us introduce a notation for a potential between projectile and one nucleon in bound state A as

$$
V_j = \sum_{i\in a} V_{ij}, \quad V = \sum_{j=1}^{A} V_j \tag{5.45}
$$

In channel α, we may define $G_0^{(+)} = \frac{1}{E-H_A-H_a-T_\alpha+i\epsilon}$. where H_A and H_a are target and projectile internal Hamiltonian and T_α is a relative kinetic energy. From now on, the index α in T or V may be omitted because we do not consider re-arrangement. Then, the equation can be re-written as

$$T = V(1 + G^{(+)}T) = \sum_j V_j(1 + G^{(+)}T) \tag{5.46}$$

However, note that the all operators acts on $A + a$ space. If we consider the case of scattering of two-nucleon i and j, we may write

$$t_{ij} = V_{ij} + V_{ij}\frac{1}{E - T_{ij} + e\epsilon}t_{ij}. \tag{5.47}$$

Because we consider a projectile-nucleon scattering in a bound state,

$$\tau_{ij} = V_{ij} + V_{ij}\frac{1}{E - H_A - H_a - T_\alpha + i\epsilon}\tau_{ij}. \tag{5.48}$$

Note that $t_{ij} \neq \tau_{ij}$. In a similar notation for V_j, we have

$$\begin{aligned} \tau_j &= V_j + V_jG^{(+)}\tau_j = V_j(1 + G^{(+)}\tau_j) \\ &= V_j + V_jG^{(+)}V_j + V_jG^{(+)}V_jG^{(+)}V_j + \cdots \end{aligned} \tag{5.49}$$

Let us define two-body operator ω_j such that

$$V_j(1 + G^{(+)}T) = \tau_j\omega_j \tag{5.50}$$

In other words,

$$T = \sum_{j=1}^{A} \tau_j\omega_j \tag{5.51}$$

This implies that

$$\begin{aligned} \omega_j &= 1 + G^{(+)}T - G^{(+)}\tau_j\omega_j \\ &= 1 + G^{(+)}\sum_{k\neq j}\tau_k\omega_k \\ &= 1 + G^{(+)}\sum_{k\neq j}\tau_k + G^{(+)}\sum_{k\neq j}\tau_kG^{(+)}\sum_{l\neq j}\tau_l + \cdots \end{aligned} \tag{5.52}$$

Thus,

$$T = \sum_{j=1}^{A}\tau_j + \sum_{j,k\neq j}^{A}\tau_jG^{(+)}\tau_k + \sum_{j,k\neq j,l\neq k}\tau_jG^{(+)}\tau_kG^{(+)}\tau_l + \cdots \tag{5.53}$$

This is called Watson's multiple scattering series. This is the same as formal solution and its re-arrangement,

$$T = \sum_{j=1}^{A}V_j + \sum_{j,k}V_jG^{(+)}V_k + \sum_{jkl}V_jG^{(+)}V_kG^{(+)}V_l + \cdots . \tag{5.54}$$

However, instead of possibly singular V_j, the series involves τ_j which can be well-defined.

Chapter 6

NN potential

6.1 NN potential

There are several realistic modern potentials.

-

6.1.1 spin and isospin

두 개의 nucleon system 을 생각하자. 이 경우 spin과 isospin을 고려해야 한다. full state will be represented as

$$|p(ls)jm(\frac{1}{2}\frac{1}{2})_t tm_t\rangle \tag{6.1}$$

여기서 $s = 0, 1$, $t = 0, 1$ 이 가능하며, antisymmetry of fermions leads

$$(-)^{l+s+t} = -1, \quad \text{or} \quad l + s + t = odd \tag{6.2}$$

만약 parity is conserved 이고 tensor force를 가정하면 , $l = l'$, or $l = l' \pm 2$ 의 mixing 이 가능하다. For example tensor potential cause coupled case ${}^3S_1 - {}^3D_1$ in deuteron. ${}^3P_0$를 제외하면, $S = 1$이고, $L \neq J$ 인 상태들은 모두 coupled 된다.

Thus, for $t = 1$ case,

$${}^1S_0,\ {}^3P_0,\ {}^3P_1,\ {}^1D_2,\ {}^3P_2 - {}^3F_2, \ldots \tag{6.3}$$

and for $t = 0$ case,

$${}^1P_1,\ {}^3S_1 - {}^3D_1,\ {}^3D_2, \ldots \tag{6.4}$$

are possible states. (이것은 parity나 t-reversal symmetry가 깨지더라도 옳다.)

spin 과 parity가 보존되는 경우

$$\langle p'(l's')j'm'|V|p(ls)jm\rangle \equiv \delta_{jj'}\delta_{mm'}\delta_{ss'}V^{sj}_{ll'}(pp'), \tag{6.5}$$

을 정의할 수 있다.

이 경우,

$$t^{sj}_{l'l}(p', p) = V^{sj}_{l'l}(p'p) + \sum_{l''}\int_0^\infty dp'' p''^2 V^{sj}_{l'l''}(pp'')\frac{1}{E + i\epsilon - p''^2/2\mu}t^{sj}_{l''l}(p''p) \tag{6.6}$$

6.1.2 Isospin structures

일반적으로 Isospin structure of 2N force 는 approximate isospin symmetric(invariant under rotation in iso-spin space). Charge symmetry는 reflection in iso-spin space로 $n \leftrightarrow p$. Charge independence 는 $(np = nn = pp)$를 의미 한다. 예를 들어 $\tau_1^z \tau_2^z$ 는 $pp = nn$ 으로 charge symmetry는 갖지만, $np \neq pp = nn$ 으로 charge independence breaking(CIB).

- Class I (isospin invariant forces $nn = pp = np$) : $V_I = \alpha + \beta(\tau_1 \cdot \tau_2)$
- Class II (CIB $np \neq pp = nn$) : $V_{II} = \alpha \tau_1^3 \tau_2^3$
- Class III (CSB, no isospin mixing, $nn \neq pp$): $V_{III} = \alpha(\tau_1^3 + \tau_2^3)$
- Class IV (CSB and isospin mixing): $V_{IV} = \alpha(\tau_1^3 - \tau_2^3) + \beta(\tau_1 \times \tau_2)^3$

Note that, Class III force does not mix isospin triplet and isospin singlet in 2-body, it will mix isospin triplet and isospin singlet $A \geq 3$ case.

6.1.3 Operators

General symmetry argument constraints the strong nuclear potential. Assume, (1)Heritianity of potential (real), (2) time-translation invariance(no t-dependence) (3)Rotation invariance (scalar both in orbital-spin space and isospin space), (4) Invariance of space translation and Galilean (no R-dependence, no P-dependence), (5) parity conservation,($\boldsymbol{r} \to -\boldsymbol{r}$, $\boldsymbol{p} \to -\boldsymbol{p}$),(6) invariance under particle permutation, (7) Time reversal invariance($\boldsymbol{p} \to -\boldsymbol{p}$, $\boldsymbol{\sigma}_i \to -\boldsymbol{\sigma}_i$).

Usual One boson exchange potential can be obtained by non-relativistic reduction of one-boson exchange diagrams with approximations, (1) on-shell approximation $E_{q'} = E_q$, (2) Expansion of E in powers of q.

In configuration space,

$$\left\{1, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, S_{12}(\boldsymbol{r}), S_{12}(\boldsymbol{p}), \boldsymbol{L} \cdot \boldsymbol{S}, (\boldsymbol{L} \cdot \boldsymbol{S})^2\right\} \otimes \{1, \tau_1 \cdot \tau_2\} \tag{6.7}$$

where, $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$.

In momentum space,

$$\{1, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, S_{12}(\boldsymbol{q}), S_{12}(\boldsymbol{k}), i\boldsymbol{S} \cdot \boldsymbol{q} \times \boldsymbol{k}, \boldsymbol{\sigma}_1 \cdot (\boldsymbol{q} \times \boldsymbol{k})\boldsymbol{\sigma}_2 \cdot (\boldsymbol{q} \times \boldsymbol{k})\} \otimes \{1, \tau_1 \cdot \tau_2\} \tag{6.8}$$

where $\boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p}$, $\boldsymbol{k} = (\boldsymbol{p}' + \boldsymbol{p})/2$.

total spin S는 위의 operator들과 commute 하므로, total spin does not change. However, general isospin-breaking operators can break total spin conservation.

6.1.4 Partial wave decomposition of two-body potential in momentum space

Let us summarize the results from E.Epelbaum et.al., NPA747(2005)362 about the partial wave decomposition of two body potential.

First, write the potential in the form, $\boldsymbol{k} = \frac{\boldsymbol{p}' + \boldsymbol{p}}{2}$, $\boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p}$,

$$\begin{aligned} V \;=\;& V_C + V_\sigma \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + V_{SL} i \frac{1}{2} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\boldsymbol{k} \times \boldsymbol{q}) \\ & + V_{\sigma L} \boldsymbol{\sigma}_1 \cdot (\boldsymbol{q} \times \boldsymbol{k}) \boldsymbol{\sigma}_2 \cdot (\boldsymbol{q} \times \boldsymbol{k}) + V_{\sigma q} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) + V_{\sigma k} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{k})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{k}) \end{aligned} \tag{6.9}$$

where, $V_C(p', p, z) \ldots$ are functions of $p = |\boldsymbol{p}|$, $p' = |\boldsymbol{p}'|$ and the $z = \hat{p} \cdot \hat{p}'$. Isospin dependence are treated separately. Note that these operators conserves total spin.

Then, for $j > 0$, partial wave matrix elements are

$$\begin{aligned}
\langle (j0)j|V|(j0)j\rangle &= 2\pi\int_{-1}^{1} dz\left\{V_C - 3V_\sigma + p^{'2}p^2(z^2-1)V_{\sigma L} - q^2V_{\sigma q} - k^2V_{\sigma k}\right\}P_j(z),\\
\langle (j1)j|V|(j1)j\rangle &= 2\pi\int_{-1}^{1} dz\Big\{\Big[V_C + V_\sigma + 2p'pzV_{SL} - p^{'2}p^2(1+3z^2)V_{\sigma L} + 4k^2V_{\sigma q} + \frac{1}{4}q^2V_{\sigma k}\Big]P_j(z)\\
&\quad + \Big[-p'pV_{SL} + 2p^{'2}p^2zV_{\sigma L} - 2p'p(V_{\sigma q} - \frac{1}{4}V_{\sigma k})\Big](P_{j-1}(z) + P_{j+1}(z))\Big\}, \qquad (6.10)
\end{aligned}$$

$$\begin{aligned}
\langle (j\pm1,1)j|V|(j\pm1,1)j\rangle &= 2\pi\int_{-1}^{1} dz\Big\{p'p\Big[-V_{SL} \pm \frac{2}{2j+1}\left(-p'pzV_{\sigma L} + V_{\sigma q} - \frac{1}{4}V_{\sigma k}\right)\Big]P_j(z)\\
&\quad + \Big[V_C + V_\sigma + p'pzV_{SL} + p^{'2}p^2(1-z^2)V_{\sigma L}\\
&\quad \pm \frac{1}{2j+1}\left(2p^{'2}p^2V_{\sigma L} - (p^{'2}+p^2)\left(V_{\sigma q} + \frac{1}{4}V_{\sigma k}\right)\right)\Big]P_{j\pm1}(z)\Big\},\\
\langle (j\pm1,1)j|V|(j\mp1,1)j\rangle &= \frac{\sqrt{j(j+1)}}{2j+1}2\pi\int_{-1}^{1} dz\Big\{-p'p(4V_{\sigma q} - V_{\sigma k})P_j(z)\\
&\quad + \Big[\mp\frac{2p^{'2}p^2}{2j+1}V_{\sigma L} + p^{'2}\left(2V_{\sigma q} + \frac{1}{2}V_{\sigma k}\right)\Big]P_{j\mp1}(z)\\
&\quad + \Big[\pm\frac{2p^{'2}p^2}{2j+1}V_{\sigma L} + p^{2}\left(2V_{\sigma q} + \frac{1}{2}V_{\sigma k}\right)\Big]P_{j\pm1}(z)\Big\}. \qquad (6.11)
\end{aligned}$$

where, $P_j(z)$ are the Legendre Polynomials.

For $j = 0$,

$$\begin{aligned}
\langle (00)0|V|(00)0\rangle &= 2\pi\int_{-1}^{1} dz\left\{V_C - 3V_\sigma + p^{'2}p^2(z^2-1)V_{\sigma L} - q^2V_{\sigma q} - k^2V_{\sigma k}\right\},\\
\langle (11)0|V|(11)0\rangle &= 2\pi\int_{-1}^{1} dz\Big\{zV_C + zV_\sigma + p'p(z^2-1)V_{SL} + p^{'2}p^2z(1-z^2)V_{\sigma L}\\
&\quad -((p^{'2}+p^2)z - 2p'p)V_{\sigma q} - \frac{1}{4}((p^{'2}+p^2)z + 2p'p)V_{\sigma k}\Big\}. \qquad (6.12)
\end{aligned}$$

For example, in case, single contact term, $V(\boldsymbol{p'},\boldsymbol{p}) = C$ gives $\langle (ls)j|V|(ls)j\rangle = 4\pi C\delta_{l0}$.

6.1.5 Partial wave matrix elements in coordinate space

In general, we can obtain the partial wave expression for non-local potential $V_{\alpha\beta}(r,r')$ by Fourier transform(or Bessel function integration). In case of local potential, we may represent the local potential in coordinate space as follows,

$$\begin{aligned}
U(\boldsymbol{q}) &= U_c(q) + U_S(q)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + U_T(q)\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q} + U_{SO}(q)\boldsymbol{S}\cdot(\boldsymbol{k}\times\boldsymbol{q})\\
U(\boldsymbol{r}) &= U_C(r) + U_S(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + U_T(r)S_{12}(\hat{r}) + U_{SO}(r)\boldsymbol{S}\cdot\boldsymbol{L}, \qquad (6.13)
\end{aligned}$$

where, $S_{12}(\hat{r}) = (3\boldsymbol{\sigma}_1\cdot\hat{r}\boldsymbol{\sigma}_2\cdot\hat{r} - \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)$, $\boldsymbol{S}\cdot\boldsymbol{L} = \frac{(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)}{2}\cdot(-i\boldsymbol{r}\times\nabla_r)$ However, note that $U_X(r) \neq [U_X(q)]_{FT}$ in general. And V_X contains iso-spin independent potential and iso-spin dependent potential, $U_X(r) = V_X(r) + \tau_1 \cdot \tau_2 W_X(r)$. [1]

$$\begin{aligned}
U_C(r) &= [U_C(q)]_{FT}(r), \\
U_S(r) &= [U_S(q)]_{FT}(r) - \frac{1}{3}\nabla^2 [U_T(q)]_{FT}(r), \\
U_T(r) &= -\frac{1}{3} r \frac{d}{dr}\frac{1}{r}\frac{d}{dr}[U_T(q)]_{FT}(r), \\
U_{SO}(r) &= (sign?)\frac{1}{r}\frac{d}{dr}[U_{SO}(q)]_{FT}(r)
\end{aligned} \tag{6.18}$$

Once $U_X(r)$ are obtained, we get the partial wave matrix elements by using,

$$\begin{aligned}
\langle (ls)j|\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2|(l's')j'\rangle &= \delta_{jj'}\delta_{ss'}\delta_{ll'}[2s(s+1) - 3], \\
\langle (ls)j|S_{12}|(l's')j'\rangle &= \delta_{jj'}\delta_{s1}\delta_{s'1}[\delta_{l,j}\delta_{l',j}(2) + \delta_{l',j-1}\delta_{l,j-1}(-2\frac{j-1}{2j+1}) \\
&\quad + \delta_{l',j\pm1}\delta_{l,j\mp1}(6\frac{\sqrt{j(j+1)}}{2j+1}) + \delta_{l,j+1}\delta_{l',j+1}(-2\frac{j+2}{2j+1})] \\
\langle (ls)j|\boldsymbol{L}\cdot\boldsymbol{S}|(l's')j'\rangle &= \delta_{jj'}\delta_{ss'}\delta_{ll'}\frac{1}{2}[j(j+1) - l(l+1) - s(s+1)]
\end{aligned} \tag{6.19}$$

6.1.6 Separable potential solution

In case of the separable potential, $V(p, p')$, (or $V(r, r,)$ in configuration space.) the two-body scattering problem can be solved analytically. Let us represent the separable potential in matrix notation,

$$V(\boldsymbol{p}, \boldsymbol{p}') = \sum_\mu F_\mu(p)\omega_\mu F_\mu(p') = \langle \boldsymbol{p}|\boldsymbol{F}_\mu\rangle \hat{\Omega}_{\mu\nu}\langle \boldsymbol{F}_\nu|\boldsymbol{p}'\rangle, \quad \Omega_{\mu\nu} = \omega_\mu\delta_{\mu\nu}. \tag{6.20}$$

Then the T-matrix have to be in a form of

$$T(\boldsymbol{p}, \boldsymbol{p}'; \boldsymbol{k}) = \sum_\mu F_\mu(\boldsymbol{p})\hat{t}_{\mu\nu}(k)F_\nu(\boldsymbol{p}'). \tag{6.21}$$

If we define, the matrix $\hat{G}(\boldsymbol{l}; k)$ as

$$\hat{G}(k)_{\mu\nu} \equiv \int_{\boldsymbol{l}} F_\mu(\boldsymbol{l})\frac{1}{E_k - E_l + i\epsilon}F_\nu(\boldsymbol{l}) \tag{6.22}$$

the LS equation becomes

$$\begin{aligned}
T(\boldsymbol{p}, \boldsymbol{p}'; \boldsymbol{k}) &= V(\boldsymbol{p}, \boldsymbol{p}') + \int_l V(\boldsymbol{p}, \boldsymbol{l})G_0(\boldsymbol{l}; \boldsymbol{k})T(\boldsymbol{l}, \boldsymbol{p}') \\
\hat{t}_{\mu\nu}(k) &= \hat{\Omega}_{\mu\nu} + \sum \hat{\Omega}_{\mu\alpha}\hat{G}_{\alpha\beta}(k)\hat{t}_{\beta\nu}(k)
\end{aligned} \tag{6.23}$$

[1] Because,

$$\nabla^2 \frac{e^{-\mu r}}{r} = \mu^2 \frac{e^{-\mu r}}{r} - 4\pi\delta^{(3)}(r) \tag{6.14}$$

$$\boldsymbol{\sigma}_1 \cdot \nabla \boldsymbol{\sigma}_2 \cdot \nabla f(r) = \boldsymbol{\sigma}_1 \cdot \hat{r}\boldsymbol{\sigma}_2 \cdot \hat{r}(r\frac{d}{dr}\frac{1}{r}\frac{d}{dr})f(r) + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \frac{1}{r}\frac{d}{dr}f(r) \tag{6.15}$$

$$\nabla^2 f(r) = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} \tag{6.16}$$

$$(\boldsymbol{\sigma}_1 \cdot \nabla\boldsymbol{\sigma}_2 \cdot \nabla - \frac{1}{3}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \nabla^2)f(r) = (\frac{1}{3})S_{12}(r\frac{d}{dr}\frac{1}{r}\frac{d}{dr})f(r) \tag{6.17}$$

Thus, the T-matrix can be solved as

$$\begin{aligned}\hat{t}(k) &= [\hat{\Omega}^{-1} - \hat{G}(k)]^{-1}, \\ T(\boldsymbol{p}, \boldsymbol{p}') &= \sum_{\mu\nu} F_\mu(\boldsymbol{p}) \left[\hat{\Omega}^{-1} - \hat{G}(k)\right]^{-1}_{\mu\nu} F_\nu(k)\end{aligned} \tag{6.24}$$

In a similar way, the Schrodinger equation for separable potential can be solved as

$$\begin{aligned}V(\boldsymbol{r}, \boldsymbol{r}') &= \sum_\mu v_\mu(\boldsymbol{r})\omega_\mu v_\nu^*(\boldsymbol{r}'), \\ \psi_k(\boldsymbol{r}) &= \phi_k(\boldsymbol{r}) - \sum_\mu \omega_\mu \int_{\boldsymbol{r}'} \int \boldsymbol{r}'' G(\boldsymbol{r}, \boldsymbol{r}'; k) v_\mu(\boldsymbol{r}') v_\mu^*(\boldsymbol{r}'') \psi_k(\boldsymbol{r}'')\end{aligned} \tag{6.25}$$

Scattering amplitude can be written as

$$\begin{aligned}A(k_f \leftarrow k_i) &= -\frac{m}{2\pi\hbar^2} \int d^3\boldsymbol{r}' \int d^3\boldsymbol{r}'' e^{-i\boldsymbol{k}_f\cdot\boldsymbol{r}'} V(\boldsymbol{r}', \boldsymbol{r}'')\psi_k(\boldsymbol{r}'') \\ &= -\frac{m}{2\pi\hbar^2} \langle \boldsymbol{k}_f | v_\mu \rangle \left[\hat{\Omega}^{-1} + \hat{G}\right]^{-1}_{\mu\nu} \langle v_\nu | \boldsymbol{k}_i \rangle\end{aligned} \tag{6.26}$$

where,

$$\begin{aligned}G(\boldsymbol{r}, \boldsymbol{r}'; E) &= \frac{m}{2\pi\hbar^2} \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}, \\ G_{\nu\mu} &= \int d^3r \int d^3r' v_\nu^*(\boldsymbol{r}) G(\boldsymbol{r}, \boldsymbol{r}'; E) v_\mu(\boldsymbol{r}'), \\ \langle v_\mu | \boldsymbol{k} \rangle &= \int d^3r v_\mu^*(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\end{aligned} \tag{6.27}$$

Let us consider more simple case. Suppose a separable potential

$$V(\boldsymbol{k}', \boldsymbol{k}) = \lambda g(k') g(k). \tag{6.28}$$

- Since the potential has no angular dependence, it only have $l = 0$ component, $V_{l=0}(k', k)$.
- LS equation(constant factors depends on normalization) for S-wave,

  $$T_0(p', p; E) = V_0(p', p) + \int_0^\infty d\tilde{p} \frac{\tilde{p}^2 V_0(p', \tilde{p}) T_0(\tilde{p}, p; E)}{E + i\epsilon - \tilde{p}^2/2\mu} \tag{6.29}$$

  gives solution

  $$T_0(k', k; E) = \frac{\lambda g(k') g(k)}{1 - \lambda J(E)}, \quad J(E) = \int_0^\infty d\tilde{p} \frac{\tilde{p}^2 g^2(\tilde{p})}{E + i\epsilon - \tilde{p}^2/2\mu} \tag{6.30}$$

- The scattering length can be related to $g(k = 0)$. On-shell t-matrix can be related to S-matrix as

  $$t(k) = -\frac{e^{2i\delta} - 1}{2i\pi\mu k} = \frac{-1}{\pi\mu} \frac{1}{k\cot\delta - ik}. \tag{6.31}$$

  Thus, in $k \to 0$ limit,

  $$t(0) = \frac{\lambda g(0)^2}{1 - \lambda J(0)} \simeq \frac{-1}{\pi\mu} \frac{1}{-1/a} \Rightarrow a = \frac{\lambda\pi\mu g^2(0)}{1 - \lambda J(0)} \tag{6.32}$$

- bound state condition, S-matrix have a pole at positive imaginary $k = i\kappa$ implies

$$1 + \lambda \int_0^\infty d\tilde{p} \frac{2\mu\tilde{p}^2 g^2(\tilde{p})}{\kappa^2 + \tilde{p}^2} = 0. \tag{6.33}$$

Thus, $\lambda > 0$ does not have bound state. $\lambda < 0$ support only one bound state.

- For a resonance, S-matrix have pole at $E_r = \frac{k_r^2}{2\mu}$ (More correctly pole at $E = E_r - i\Gamma/2$.) . Then, near $E = E_r$,

$$\begin{aligned}
J(E = \frac{k^2}{2\mu}) &= \int_0^\infty d\tilde{p} \frac{\tilde{p}^2 g^2(\tilde{p})}{E + i\epsilon - \tilde{p}^2/2\mu} = \mathcal{P}\int_0^\infty d\tilde{p}\left(\frac{\tilde{p}^2 g^2(\tilde{p})}{E - \tilde{p}^2/2\mu}\right) - i\pi\mu k g^2(k) \\
J(E) &\simeq J(E_r) + (E - E_r)\frac{dJ(E)}{dE}|_{E_r} + \cdots \\
&\simeq \mathcal{P}\int_0^\infty d\tilde{p}\left(\frac{\tilde{p}^2 g^2(\tilde{p})}{E_r - \tilde{p}^2/2\mu}\right) - i\pi\mu k_r g^2(k_r) + (E - E_r)\int_0^\infty d\tilde{p}\frac{-\tilde{p}^2 g^2(\tilde{p})}{(E_r + i\epsilon - \tilde{p}^2/2\mu)^2} + \cdots \\
\frac{1}{1 - \lambda J(E)} &\simeq \frac{1}{(-\lambda\frac{dJ(E)}{dE})\left(E - E_r - \frac{1}{\lambda dJ/dE}(1 - \lambda J(E_r))\right)}
\end{aligned} \tag{6.34}$$

Denominator will have a form of $E - E_r + i\Gamma/2$ for BW resonance. Thus, at resonance

$$1 - \lambda\mathcal{P}\int_0^\infty d\tilde{p}\left(\frac{\tilde{p}^2 g^2(\tilde{p})}{E_r - \tilde{p}^2/2\mu}\right) = 0. \tag{6.35}$$

and width of resonance is

$$\Gamma = B g^2(k_r), \quad B = -\frac{2\pi\mu k_r}{dJ(E)/dE|_{E_r}}(?) \tag{6.36}$$

I am not sure about factors.

6.2 Bethe-Salpeter equation: Relativistic scattering amplitude

Bethe-Salpeter equation in relativistic scattering amplitude corresponding to LS equation for non-relativistic scattering amplitude.

$$M = K + KGM = K + KGK + KGKGK + \cdots \tag{6.37}$$

where, M is relativistic T-amplitudes and G is relativistic two nucleon propagator. Relativistic kernel K is the sum of all irreducible diagrams.

If we approximate $K = K_0$ of the first tree diagram and approximating $M = K_0 + K_0 G K_0 + \cdots$ is called "ladder approximation". However, "ladder approximation" is not good because in the kernel K exchanged diagram is equally important as the tree diagram.

Usually two nucleon propagator G can be written as

$$G = \left[\frac{\gamma^\mu q_{1\mu} + m\mathbf{1}}{q_1^2 - m^2 + i\epsilon}\right]^{(1)} \left[\frac{\gamma^\mu q_{2\mu} + m\mathbf{1}}{q_2^2 - m^2 + i\epsilon}\right]^{(1)} \tag{6.38}$$

If we use center of mass momentum and relative momentum, and using projection for particle and anti-particle, we get

$$G(k, p^0) \quad = \tag{6.39}$$

6.3 Meson exchange potential

Because the meson exchange model gives some microscopic understanding on the origin of NN interaction, it could be useful to discuss here.

Chapter 7

NN phase shift

7.1 NN phase shift

7.1.1 Effective Range Theory

In zero energy limit, only S-wave scattering is important and we can write

$$\sigma = 4\pi \lim_{k\to 0}(-\frac{\delta_l}{k})^2 \tag{7.1}$$

Thus, we can define scattering length a as

$$\lim_{k\to 0}(-\frac{\delta_l}{k}) = a$$

.

from the S-wave wave function, $\psi_L = \frac{u_L}{r}$

$$u_{L=0}(r) \to e^{i\delta_0}\sin(kr+\delta_0) \to k(r-a_0) \tag{7.2}$$

Thus, the scattering length represents the position at the external wave function, or its extrapolation towards origin vanishes.

As increasing energy, we need energy dependence and higher partial wave. However, at low enough energy (less than 10 MeV), we can still have good approximation with only S-waves. The energy dependence of phase shifts can be obtained from Bethe's effective range theory.

Let us suppose two S-wave solutions u_1 and u_2 corresponding to energy E_1 and E_2 respectively. They satisfy equations,

$$\begin{aligned} \frac{d^2u_1}{dr^2} + k_1^2u_1 - \frac{2m}{\hbar^2}V(r)u_1 = 0, \\ \frac{d^2u_2}{dr^2} + k_2^2u_2 - \frac{2m}{\hbar^2}V(r)u_2 = 0. \end{aligned} \tag{7.3}$$

By multiplying u_2, u_1 and subtracting them gives

$$u_2\frac{d^2u_1}{dr^2} - u_1\frac{d^2u_2}{dr^2} + (k_1^2-k_2^2)u_1u_2 = 0. \tag{7.4}$$

If we integrate the equation up to arbitary R,

$$\int_0^R dr\frac{d}{dr}[u_1'u_2 - u_1u_2'] = [u_1'u_2 - u_1u_2']_0^R = (k_2^2-k_1^2)\int_0^R dr u_1u_2 \tag{7.5}$$

Let us consider asymptotic wave function for each energy,

$$\psi_{1,2} = \frac{\sin(k_{1,2}r + \delta_{1,2})}{\sin(\delta_{1,2})}, \quad \psi'(r) = \frac{k\cos(kr+\delta)}{\sin\delta}. \tag{7.6}$$

where normalization is chosen as $\psi(r=0)=1$. In a similar way, asymptotic wave function ψ satisfies

$$[\psi_1'\psi_2 - \psi_1\psi_2']_0^R = (k_2^2 - k_1^2)\int_0^R dr\psi_1\psi_2. \tag{7.7}$$

If R is large enough, $\psi(R) = u(R)$ and $u(0) = 0$. Thus, subtraction of two equation becomes,

$$\psi_1'(0)\psi_2(0) - \psi_1(0)\psi_2'(0) = (k_2^2 - k_1^2)\int_0^R (\psi_1\psi_2 - u_1u_2) \tag{7.8}$$

Then (1) change the range of integration to infinite, (2)use the exact form of wave function, (3)choose $k_1 = 0.$,

$$[\lim_{k\to 0} k\cot\delta(k)] - k\cot\delta(k) = k^2\int_0^\infty (\psi_1\psi_2 - u_1u_2) \tag{7.9}$$

Thus, if we replace, $[\lim_{k\to 0} k\cot\delta(k)] = -\frac{1}{a}$, we get

$$\boxed{k\cot\delta(k) = -\frac{1}{a} + k^2\int_0^\infty (\psi_{k=0}\psi_k - u_{k=0}u_k)} \tag{7.10}$$

Upto now, the equation is exact. If we approximate, $\{\psi, u\}_k \simeq \{\psi, u\}_{k=0}$, we get effective range

$$k\cot\delta(k) = -\frac{1}{a} + \frac{1}{2}k^2 r_{eff}, \quad r_{eff} \equiv 2\int_0^\infty (\psi_{k=0}^2 - u_{k=0}^2) \tag{7.11}$$

Generalized effective range expansion becomes

$$\lim_{p\to 0} f_l(p) = O(p^{2l}) \tag{7.12}$$

$$f_l(p) = \frac{p^{2l}}{p^{2l+1}\cos\delta_l(p) - ip^{2l+1}}. \tag{7.13}$$

$$p^{2l+1}\cot\delta_l(p) = -\frac{1}{a_l} + \frac{1}{2}r_l p^2 + P_l p^4 + Q_l p^6 + \mathcal{O}(p^8) \tag{7.14}$$

Scattering amplitude of S-wave in terms of phase shift is

$$\begin{aligned} f_{l=0} &= \frac{S_l - 1}{2ik} = \frac{1}{k}e^{i\delta_0}\sin\delta_0 = \frac{1}{k}\frac{1}{\cot\delta_0 - i} = \frac{1}{k\cot\delta_0 - ik}, \\ &\to \frac{1}{-\frac{1}{a_0} + \frac{1}{2}r_0k^2 - ik} = \frac{-a_0}{1 - \frac{1}{2}a_0r_0k^2 + ia_0k} \end{aligned} \tag{7.15}$$

From S-wave scattering cross section relation,

$$\sigma(k) = 4\pi|f_0|^2 = \frac{4\pi a_0^2}{(1-\frac{1}{2}a_0r_0k^2)^2 + a_0^2k^2}. \tag{7.16}$$

This form is usually good up to tens of MeV. Also, this means that any theory which can give good scattering length and effective range will give the same results at low energy. Thus, low energy physics is insensitive to the short range details of the potential.

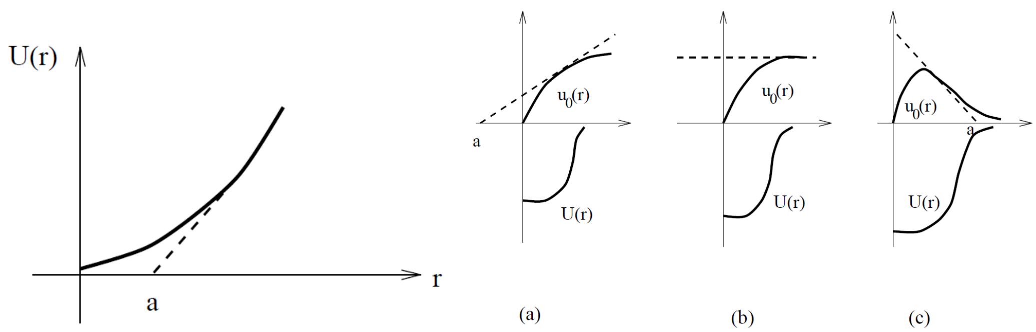

Figure 7.1: Scattering length is positive for repulsive potential. Scattering length can be (a) negative (b) infinite (c) positive depending on the strength of attaction.

We can also apply the effective range theory to bound state. We can obtain the relation between effective range and binding energy by introducing $k = i\kappa_B = i\sqrt{2mE_B}$, because positive imaginary k implies bound state wave function $e^{-\kappa_B r}$, from (1) the pole position of scattering amplitude or scattering cross section. or (2) Integration of asymptotic wave function $\psi_B = e^{-\kappa r}$, $\psi_1 = \psi_{k=0}$, $\psi_2 = \psi_B$,

$$\begin{aligned} \text{Pole of scattering cross section:} \quad & -a_t^2\kappa_B^2 + (1 + \frac{1}{2}a_t r_t \kappa_B^2)^2 = 0, \\ \text{Effective range integration:} \quad & -\kappa_B + \frac{1}{a_t} = -k_B^2 \frac{1}{2} a_t r_t \end{aligned} \tag{7.17}$$

Scattering length have a geometric interpretation. S-wave at large r in low energy,

$$u_0(r) \to_{r\to\infty} e^{i\delta_0} \sin(pr + \delta_0) \to_{p\to 0} p(r - a_0). \tag{7.18}$$

Thus, a_0 is a point nearest to the origin at which the external wave function or its extrapolation vanishes. This leads, for weak potential,

$$\begin{aligned} V > 0 \quad &\leftrightarrow \quad a_0 > 0, \quad \text{repulsive}, \\ V < 0 \quad &\leftrightarrow \quad a_0 < 0, \quad \text{attractive but no bound state}, \\ &\leftrightarrow \quad a_0 = \infty, \quad \text{attractive producing s-wave virtual state (zero energy resonance)}, \\ &\leftrightarrow \quad a_0 > 0, \quad \text{attractive producing s-wave bound state}, \end{aligned} \tag{7.19}$$

Note that single real number a_0 completely parametrize **all** low energy scattering.

Also, for the attractive potential, the knowledge of bound state corresponds to the knowledge of scattering length because of the pole relation of scattering amplitude equation ($k \simeq -1/a$ at pole). This allows (1) if one know there is a bound state, one can estimate the cross section,

$$\sigma \simeq |f_0|^2 \simeq \frac{1}{2m(E + E_B)} \tag{7.20}$$

(2) Or, if one know the scattering length, one can also estimate the bound state energy $E_B = \frac{1}{2ma_0^2}$.

The s-wave neuteal scattering can generate very large negative scattering length state, which corresponds to a Unitary limit or virtual state. In this case, wave function is very long ranged. This corresponds to negative imaginary pole of S-matrix at $k = \frac{i}{a}, a < 0$. In other words, the unitary limit corresponds to $a_0 \to \infty$, $r_0 \to 0$,and $\delta_0 \to \frac{\pi}{2}$. This can occur at a certain interaction among particles.

7.1.2 Levinson's theorem

When the attractive potential is strong enough to have several bound state, the change from negative scattering length to positive scattering length can happen several times. $\tan \delta_0 = pa_0$ where tan is a multi-valued function. (In other words, scattering length changes from negative$\rightarrow$infinite$\rightarrow$positive as attraction allows more bound states. Thus, number of positive scattering length corresponds to number of supported bound states.) This is also affects the phase shifts.

Because we may expect that for very large energy $k \gg 1$, phase shift would be very small, $\delta_l \rightarrow 0$. On the other hand, at zero energy, we will also have zero phase shift. Then, we can plot the energy dependence of phase shift so that it to be continuous. (i.e. add $\pm n\pi$ as necessary). Then, starting from large energy and reducing energy, whenever the phase shift pass $\pm\pi/2$, one have to add/subtract π.

The general result is Levinson's theorem:

$$\delta(k=0) - \delta(k \rightarrow \infty) = n_B \pi, \tag{7.21}$$

where n_B is the number of bound states supported by the specific potential $U(r)$. It implies that the energy dependence of phase shift at zero energy and large energy is related with number of bound state.(예를 들어 만약 bound state가 하나라면, phase shift는 zero energy에서 π 로 시작해 infinite energy에서는 zero.) Proof for simple square well can be found in Bertulani's book. More general proof can be found at Taylor's book

7.1.3 Unitarity and parametrization of S-matrix

t-matrix notation

$$t \equiv t^{sj}_{l'l}(p'p) \tag{7.22}$$

Then, since $V^\dagger = V$,

$$\begin{aligned} t &= V + VG_0 t = V + tG_0 V \\ t^\dagger &= V + VG_0^* t^\dagger \end{aligned} \tag{7.23}$$

and

$$\begin{aligned} t - t^\dagger &= VG_0 t - VG_0^* t^\dagger = V(G_0 - G_0^*)t^\dagger \\ &= VG_0(t - t^\dagger) + V(G_0 - G_0^*)t^\dagger(1 - VG_0)(t - t^\dagger) \\ &= (1 - VG_0)^{-1} V(G_0 - G_0^*)t^\dagger = t(G_0 - G_0^*)t^\dagger \end{aligned} \tag{7.24}$$

Because $G_0 = \frac{1}{E + i\epsilon - H_0}$,

$$G_0 - G_0^* = -2\pi i \delta(E - H_0) \tag{7.25}$$

and,$p_0 = \sqrt{2\mu E}$,

$$\begin{aligned} t_{l'l}(p'p) - t^*_{ll'}(pp') &= \int_0^\infty dp'' p''^2 \sum_{l''} t_{l'l''}(p'p'')(-2\pi i)\delta(E - \frac{p''^2}{2\mu}) t^*_{ll''}(pp'') \\ &= -2\pi i \mu p_0 \sum_{l''} t_{l'l''}(p'p_0) t^*_{ll''}(pp_0) \end{aligned} \tag{7.26}$$

여기서 on-energy shell value를 취하여, $p = p' = \sqrt{2\mu E}$ 인 경우,

$$t_{l'l}(pp) - t^*_{ll'}(pp) = -2\pi i \mu p \sum_{l''} t_{l'l''}(pp) t^*_{ll''}(pp), \quad \text{or} \quad t - t^\dagger = -2i\pi\mu p t t^\dagger \tag{7.27}$$

여기서 , S-matrix를 [1]

$$S = 1 - i2\pi\mu p t \tag{7.29}$$

로 쓰면, 위 식은

$$SS^\dagger = (1 - 2i\pi\mu p t)(1 + 2i\pi\mu p t^\dagger) = 1 \tag{7.30}$$

이 되어, S-matrix가 Unitary 임을 나타낸다.

S-matrix를 partial wave decompose 시키면, 일반적으로 couple 이 되어 $J \neq 0$ 일 때 다음과 같은 형태를 갖는다.

$$S^{J\neq 0}_{l'S',lS} = \delta_{S'S} \begin{pmatrix} S^J_{J-1,1,J-1,1} & S^J_{J-1,1,J+1,1} & 0 & 0 \\ S^J_{J+1,1,J-1,1} & S^J_{J+1,1,J+1,1} & 0 & 0 \\ 0 & 0 & S^J_{J0J0} & 0 \\ 0 & 0 & 0 & S^J_{J1J1} \end{pmatrix} \tag{7.31}$$

$J = 0$인 경우 $^1S_0$와 $^3P_0$ 만 특별히 따로 계산한다.

$$S^{J=0}_{l'S',lS} = \delta_{l'l}\delta_{SS}(S^0_{00,00} \text{ or } S^0_{11,11}) \tag{7.32}$$

7.1.4 Uncoupled channel

Uncoupled 인 경우에는 , 하나의 parameter δ로 나타낼 수 있다.

$$S = e^{2i\delta_l}, \quad K = \tan\delta_l, \quad \delta_l \sim k^{2l+1} \tag{7.33}$$

$$S = \frac{1 + iK}{1 - iK} \tag{7.34}$$

Note that the phase shift can be determined from S-matrix,

$$\delta_L(E) = \frac{1}{2i}\ln \boldsymbol{S}_L + n(E)\pi, \tag{7.35}$$

where integer $n(E)$ is chosen suitably for E. However, this does not affect the cross section because, $e^{2i\pi n} = 1$.

This also implies that scattering amplitude can be written as

$$f_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k} = \frac{1}{k\cot\delta_l - ik} \tag{7.36}$$

The threshold behavior of phase shift can be obtained from

$$f_l = \frac{e^{i\delta_l}\sin\delta_l}{k} = -\frac{2\mu}{\hbar^2}\int_0^\infty j_l(kr)V(r)\psi_l(r)r^2 dr \tag{7.37}$$

If $1/k$ is much larger than the range of potential, and $\psi_l(r)$ is not much different from $j_l(kr)$, (i.e. at very low energy and small phase shift) the right hand side vary as k^{2l} and left hand side as δ_l/k. Thus, $\delta_l \sim k^{2l+1}$.

[1] $\langle \boldsymbol{k}|\boldsymbol{k}'\rangle = (2\pi)^3\delta^{(3)}(\boldsymbol{k} - \boldsymbol{k}')$ 인 convention을 사용하는 SChiavilla의 경우 $p = p'$인 on-shell S-matrix 와 T-matrix의 partial wave amplitude를

$$S^J_{\alpha\alpha'}(p) = \delta_{\alpha\alpha'} - 4i\mu p T^J_{\alpha\alpha'}(p) \tag{7.28}$$

로 나타내었다. 확인이 필요하다.

Also, we may consider the S-matrix pole or scattering amplitude at low energy as

$$S(k) = \frac{k\cot\delta(k) + ik}{k\cot\delta(k) - ik}, \quad f(k) = \frac{1}{k\cot\delta(k) - ik}. \tag{7.38}$$

This implies that the scattering wave function as

$$\frac{e^{-ikr}}{r} + f(k)\frac{e^{ikr}}{r}. \tag{7.39}$$

To have a bound state, which is on decaying wave function in a specific negative energy without incoming wave, the scattering amplitude and S-matrix have to diverge at $k = ik_B$. Thus, we have a relation that the pole of S-matrix in positive imaginary k axis corresponds to bound state.

If there is a pole on negative imaginary k axis, this state cannot make bound state because the wave function does not decay. But, still this state would exists even without incoming waves and wave function will be extended because of $e^{k_s r}$. This is called "virtual states".

7.1.5 Stapp parametrization or bar parametrization

In "Stapp-" or "bar"- parametrization, Coupled S-matrix between $l = j-1$ and $l = j+1$ states is written as

$$\begin{aligned} S &= \begin{pmatrix} e^{i\bar{\delta}_{J-1}} & 0 \\ 0 & e^{i\bar{\delta}_{J+1}} \end{pmatrix} \begin{pmatrix} \cos 2\bar{\epsilon} & i\sin 2\bar{\epsilon} \\ i\sin 2\bar{\epsilon} & \cos 2\bar{\epsilon} \end{pmatrix} \begin{pmatrix} e^{i\bar{\delta}_{J-1}} & 0 \\ 0 & e^{i\bar{\delta}_{J+1}} \end{pmatrix} \\ &= \begin{pmatrix} \cos 2\bar{\epsilon} e^{2i\bar{\delta}_1} & i\sin 2\bar{\epsilon} e^{i(\bar{\delta}_1+\bar{\delta}_2)} \\ i\sin 2\bar{\epsilon} e^{i(\bar{\delta}_1+\bar{\delta}_2)} & \cos 2\bar{\epsilon} e^{2i\bar{\delta}_2} \end{pmatrix} \end{aligned} \tag{7.40}$$

S-matrix scales like

$$(S-1)_{l'l} \sim -2i\alpha_{l'l} k^{l'+l+1} + \cdots \tag{7.41}$$

and each phase shift parameters scales like [2]

$$\bar{\delta}_{J-1} \sim k^{2J-1}, \quad \bar{\delta}_{J+1} \sim k^{2J+3}, \quad \bar{\epsilon}_J \sim k^{2J+1} \tag{7.43}$$

Nijmegen phase shift analysis use "bar" representation.

In case, matrix is larger than 2×2, we can generalize the representation such that

$$\begin{aligned} S &= e^{i\Delta} e^{2iE} e^{i\Delta}, \\ \Delta &= \begin{pmatrix} \delta_1 & & & \\ & \delta_2 & & \\ & & \delta_3 & \\ & & & ... \end{pmatrix}, \quad E = \begin{pmatrix} 0 & \alpha & \beta & ... \\ \alpha & 0 & \gamma & ... \\ \beta & \gamma & 0 & ... \\ ... & & & \end{pmatrix} \end{aligned} \tag{7.44}$$

where E is a symmetric non-diagonal matrix

[2]Hermitian matrix $\alpha_{l'l}$ is called a scattering length matrix, though it's dimension is not length. Once the scaling of S matrix is given as $k^{l'+l+1}$, it is easy to see the scaling of each phase shift parameters by comparing S-matrix form.

$$S \sim \begin{pmatrix} 1 - 2i\alpha_{11}k^{2j-1} & -2i\alpha_{12}k^{2j+1} \\ -2i\alpha_{21}k^{2j+1} & 1 - 2i\alpha_{22}k^{2j+3} \end{pmatrix} \tag{7.42}$$

7.1.6 Blatt parametrization

In "Blatt and Bierdenharn" parametrization,

$$\begin{aligned}
S &= U^{-1}\begin{pmatrix} e^{2i\delta_-} & 0 \\ 0 & e^{2i\delta_+} \end{pmatrix} U, \text{ with } U = \begin{pmatrix} \cos\epsilon & \sin\epsilon \\ -\sin\epsilon & \cos\epsilon \end{pmatrix}, \\
&= \begin{pmatrix} \cos^2\epsilon e^{2i\delta_-} + \sin^2\epsilon e^{2i\delta_+} & \frac{1}{2}\sin 2\epsilon(e^{2i\delta_-} - e^{2i\delta_+}) \\ \frac{1}{2}\sin 2\epsilon(e^{2i\delta_-} - e^{2i\delta_+}) & \cos^2\epsilon e^{2i\delta_+} + \sin^2\epsilon e^{2i\delta_-} \end{pmatrix}
\end{aligned} \tag{7.45}$$

$K = U^{-1}K_{diag}U$ Here, each scales like

$$\delta_{J-1} \sim k^{2J-1}, \quad \delta_{J+1} \sim k^{2J+3}, \quad \epsilon_J \sim k^{2J} \tag{7.46}$$

We can generalize representation for larger matrix,

$$\begin{aligned}
S &= U^T S_d U, \quad U = \prod_{i<j} U^{(ij)}, \\
S_d &= \begin{pmatrix} e^{2i\delta_1} & & & \\ & e^{2i\delta_2} & & \\ & & e^{2i\delta_3} & \\ & & & ... \end{pmatrix}, \\
U^{(13)} &= \begin{pmatrix} \cos\epsilon_{13} & 0 & \sin\epsilon_{13} & ... \\ 0 & 0 & 0 & ... \\ -\sin\epsilon_{13} & 0 & \cos\epsilon_{13} & ... \\ ... & & & ... \end{pmatrix}
\end{aligned} \tag{7.47}$$

In particular, Kievsky et.al., Nucl. Phys. A 607(1996) 402-424, used notation, given in Blatt representation convention which is defined in D. Hüber et.al, Phys. Rev. C 51(1995)51. n-d S-matrix for parity $\Pi = (-1)^{J\pm\frac{1}{2}}$ is given as

$$[S]^J_{L'S',LS} = \begin{pmatrix} S^J_{J\mp\frac{3}{2}\frac{3}{2},J\mp\frac{3}{2}\frac{3}{2}} & S^J_{J\mp\frac{3}{2}\frac{3}{2},J\pm\frac{1}{2}\frac{1}{2}} & S^J_{J\mp\frac{3}{2}\frac{3}{2},J\pm\frac{1}{2}\frac{3}{2}} \\ S^J_{J\pm\frac{1}{2}\frac{1}{2},J\mp\frac{3}{2}\frac{3}{2}} & S^J_{J\pm\frac{1}{2}\frac{1}{2},J\pm\frac{1}{2}\frac{1}{2}} & S^J_{J\pm\frac{1}{2}\frac{1}{2},J\pm\frac{1}{2}\frac{3}{2}} \\ S^J_{J\pm\frac{1}{2}\frac{3}{2},J\mp\frac{3}{2}\frac{3}{2}} & S^J_{J\pm\frac{1}{2}\frac{3}{2},J\pm\frac{1}{2}\frac{1}{2}} & S^J_{J\pm\frac{1}{2}\frac{3}{2},J\pm\frac{1}{2}\frac{3}{2}} \end{pmatrix} \tag{7.48}$$

$$\begin{aligned}
\boldsymbol{S} &= \boldsymbol{U}^T e^{2i\Delta}\boldsymbol{U}, \quad \boldsymbol{U} = \boldsymbol{vwx}, \\
\boldsymbol{v} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\epsilon & \sin\epsilon \\ 0 & -\sin\epsilon & \cos\epsilon \end{pmatrix}, \boldsymbol{w} = \begin{pmatrix} \cos\xi & 0 & \sin\xi \\ 0 & 1 & 0 \\ -\sin\xi & 0 & \cos\xi \end{pmatrix}, \boldsymbol{x} = \begin{pmatrix} \cos\eta & \sin\eta & 0 \\ -\sin\eta & \cos\eta & 0 \\ 0 & 0 & 1 \end{pmatrix}
\end{aligned} \tag{7.49}$$

Transform between LS basis and JJ basis

Note that transform matrix between LS basis and $l_y j_y$ basis was given in Huber paper as as

$$S^J_{L'S',LS} = \sum_{j'_y,j_y} \sqrt{\hat{j}'_y\hat{S}'}(-1)^{J-j'_y}\begin{Bmatrix} L' & \frac{1}{2} & j'_y \\ j_x & J & S' \end{Bmatrix}\sqrt{\hat{j}_y\hat{S}}(-1)^{J-j_y}\begin{Bmatrix} L & \frac{1}{2} & j_y \\ j_x & J & S \end{Bmatrix} S^J_{L'j'_y,Lj_y} \tag{7.50}$$

which has different sign factor from what I used. Possible resolution is that they are using different basis with mine. For the definition of $l_y - S$ basis. I am using $|l_y(j_x s)\Sigma, J\rangle$ basis, but they might be using $|(j_x s)\Sigma l_y, J\rangle$ basis which would give $(-1)^{(l_y+\Sigma-J)}$ sign difference. For example,

$$\begin{aligned}
|l_y(j_x s)\Sigma, J\rangle &= \sum_{j_y} |j_x(l_y s)j_y, J\rangle\langle j_x(l_y s)j_y|l_y(j_x s)\Sigma\rangle, \\
\langle j_x(l_y s)j_y|l_y(j_x s)\Sigma\rangle &= \langle l_y(j_x s)\Sigma|j_x(l_y s)j_y\rangle = (-1)^{s+j_x-\Sigma}(-1)^{j_x+j_y-J}\langle l_y,(sj_x)\Sigma|(l_y s)j_y, j_x\rangle \\
&= (-1)^{s+j_x-\Sigma}(-1)^{j_x+j_y-J}(-1)^{l_y+s+j_x+J}\sqrt{\hat{j}_y\hat{\Sigma}}\left\{\begin{array}{ccc} l_y & s & j_y \\ j_x & J & \Sigma \end{array}\right\} \\
&= (-1)^{l_y+\Sigma-J}(-1)^{J-j_y}\sqrt{\hat{j}_y\hat{\Sigma}}\left\{\begin{array}{ccc} l_y & s & j_y \\ j_x & J & \Sigma \end{array}\right\} \qquad (7.51)
\end{aligned}$$

where, I used $(-1)^{integer} = (-1)^{-integer}$ and (half integer)$\pm$(half integer)=(integer)

Example of scattering phase shift in Nd scattering

Let us try a numerical example. The paper by Kievsky et.al., Nuclear Physics A 607 (1996) 402-424, gives tables of phase shifts for N-D scattering. One calculation results is that the p-D scattering phase shifts using AV18(AV18+U9 potential) at $T_L = 1.5$ MeV (or $T_C = 1.0$ MeV) are

$$\delta(^2S_{1/2}) = -19.2(-15.5),\ \delta(^4D_{1/2}) = -1.50(-1.50),\ \eta_{1/2} = 1.07(1.56) \qquad (7.52)$$

in degree. From the parametrization, ignoring other mixing angles, we get for AV18+U9,

$$\begin{aligned}
S^{1/2}_{2\,\frac{3}{2},2\,\frac{3}{2}} &= \cos^2\eta e^{2i\delta_{3/2}} + \sin^2\eta e^{2i\delta_{1/2}} \simeq 0.9985 - i0.0527, \\
S^{1/2}_{2\,\frac{3}{2},0\,\frac{1}{2}} &= \frac{1}{2}\sin 2\eta(e^{2i\delta_{3/2}} - e^{2i\delta_{1/2}}) \simeq 0.003849 + i0.01259, \\
S^{1/2}_{0\,\frac{1}{2},0\,\frac{1}{2}} &= \sin^2\eta e^{2i\delta_{3/2}} + \cos^2\eta e^{2i\delta_{1/2}} \simeq 0.857 - i0.515, \qquad (7.53)
\end{aligned}$$

Comparison with Rimas code results, $1-S$, is in agreement.

7.1.7 Analytic property

- From the relation

$$f_l(k) = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k\cot\delta_l - ik} \qquad (7.54)$$

  Unitarity $|s_l(k)| = 1$ gives restriction on the f_l.

$$[kf_l] = \frac{i}{2} + \frac{1}{2}e^{-i\pi/2+2i\delta_l} \qquad (7.55)$$

  Argand diagram is a plot of $kf_l(k)$ in complex plane (x-axis is Re(kf_l) and y-axis is Im(kf_l)). In this diagram, kf_l position is on the **unitary circle** which center is at $\frac{1}{2}i$ and radius $\frac{1}{2}$. The angle between kf_l and y-axis becomes $2\delta_l$. Thus, when δ_l is small, f_l is almost purely real. $f_l \sim \delta_l/k$. When δ_l is near $\pi/2$, kf_l have maximum value. This can correspond to the resonance(quasi-bound state) at $E > 0$. When there is a resonance, as energy increases, phase shift pass through $\pi/2$(it should be increase) and the scattering amplitude and cross section have maximum value.

- One way to understand the relation between resonance and phase shift increase is using **time-delay**. Let us consider outgoing wave packet which have phase shift from scattering,

$$\psi_{out}(r,t) = \frac{1}{r}\int dkA(k)e^{+ikr-i\omega(k)t+2i\delta(k)}. \qquad (7.56)$$

Suppose the $A(k)$ is centered around k_0, we can approximate $k = k_0 + (k - k_0)$, $\omega_k \simeq \omega(k_0) + \omega'(k_0)(k - k_0)$, $\delta_k \simeq \delta(k_0) + \delta'(k_0)(k - k_0)$. Then we can approximate

$$|\psi_{out}(r,t)| = |\frac{1}{r} \int dk A(k) e^{+ik(r-\omega' t+2\delta')}|. \tag{7.57}$$

Thus, we can consider

$$|\psi_{out}(r,t)| = |\psi_{out}(r - \omega' t + 2\delta', 0)| \tag{7.58}$$

Thus wave front moves in relation, $r - \omega' t + 2\delta' = 0$. If there was no phase shift, wave front moves in velocity $v_g = \frac{d\omega}{dk}$ and take time to the detector, $\tau = \frac{L}{v_g}$ where L is the distance to the detector. Because of phase shift, time is delayed by $\tau = \frac{2\delta'}{v_g} = 2\frac{d\delta}{d\omega}$. Thus we can say the time-delay as $\tau = 2\frac{d\delta}{d\omega}$. Note that the factor 2 in front is not the same in the book of Ian Tompson. Thus, only increase of phase shift in energy corresponds to time-delay and rapid change could be interpreted as resonance.

- For S-matrix, $S(k)$: The pole of $S(k)$ at positive imaginary axis $k = i\kappa$ corresponds to the bound state $E < 0$. The pole at $k = -i\kappa$ is called "virtual" state. The pole of S-matrix at fourth quadrant (positive real and negative imaginary) in k-space corresponds to resonance. Note that the δ_l must goes through $\pi/2$ from below as increasing energy and $\cot\delta_l$ must goes through zero from above to have resonance.

- There is $n\pi$ ambiguity in the definition of phase shift because $\delta_l + n\pi$ gives the same S-matrix, $e^{2i\delta_l}$. This ambiguity can be removed if we require δ_l goes to zero at high energy. In this convention, δ_l is not zero at zero energy in general. **Levinson's theorem** determines $\delta_l(0) = n_l\pi$ with n_l is the number of bound states in the channel.

- Near resonance energy E_r, we may expand as

$$\cot\delta_l \simeq \cot\delta_l(E = E_R) - c(E - E_r) \simeq -c(E - E_r), \tag{7.59}$$

or

$$\begin{aligned} \delta(E) &= \delta_{bg}(E) + \delta_{res}(E), \\ \delta_{res}(E) &= \arctan(\frac{\Gamma/2}{E_r - E}) + n(E)\pi, \end{aligned} \tag{7.60}$$

then

$$\begin{aligned} f_l(k) &= \frac{1}{k\cot\delta_l - ik} = -\frac{\Gamma/2}{k\left[(E - E_r) + i\frac{\Gamma}{2}\right]}, \quad \frac{d(\cot\delta_l)}{dE}|_{E=E_r} = -c = -\frac{2}{\Gamma}, \\ s_l(k) &= e^{2i\delta_{bg}} \frac{k\cot\delta_l + ik}{k\cot\delta_l - ik} = e^{2i\delta_{bg}} \frac{E - E_r - i\Gamma/2}{E - E_r + i\Gamma/2}, \\ \sigma_l &= \frac{4\pi}{k^2} \frac{(2l+1)(\Gamma/2)^2}{(E - E_r)^2 + \Gamma^2/4} \end{aligned} \tag{7.61}$$

- How we can obtain resonance energy, width? If we simply solve the LS- or Sch- equation with proper potential to obtain phase shift for varying energy, we would get the resonance behavior naturally. What about the pionless EFT? One have to solve the scattering amplitude with diagrams and find a pole position of scattering amplitude. Or one may try to find a case $\cot\delta_l \simeq -c(E - E_r)$.

7.1.8 Jost function

When wave function is normalized at the origin as

$$\bar{u}_l(k, r \to 0) = \hat{j}_l(kr) \tag{7.62}$$

where $\hat{j}$ is Ricatti-Bessel function, its asymptotic form can be written as

$$\bar{u}_l(k, r > R) = \frac{i}{2}[\mathcal{J}_l(k)\hat{h}_l^{(-)}(kr) - \mathcal{J}_l^*(k)\hat{h}_l^{(+)}(kr)] \tag{7.63}$$

where $\mathcal{J}_l(k)$ is called **Jost function**.

$\bar{u}_l$ satisfies following equation,

$$\bar{u}_l(kr) = \hat{j}_l(kr) + \int_0^r dr' \bar{g}_l(r, r')V(r')\bar{u}_l(k, r') \tag{7.64}$$

$$\begin{aligned} \bar{g}_l(r, r') &= (\frac{2\mu}{\hbar^2})\frac{1}{k}[\hat{j}_l(kr)\hat{n}_l(kr') - \hat{j}_l(kr')\hat{n}_l(kr)] \\ &= (\frac{2\mu}{\hbar^2})\frac{i}{2k}[\hat{h}_l^{(-)}(kr)\hat{h}_l^{(+)}(kr') - \hat{h}_l^{(+)}(kr)\hat{h}_l^{(-)}(kr')] \end{aligned} \tag{7.65}$$

we get

$$\mathcal{J}_l(k) = 1 + \int_0^\infty dr \hat{h}_l^{(+)}(kr)V(r)\bar{u}_l(k, r) \tag{7.66}$$

and this integral converges.

7.1.9 In K-matrix

The K-matrix can be written in terms of phase shift parameters in Blatt parametrization as [3]

$$K = -i\frac{S-1}{S+1} = U^T(\tan\Delta)U = \begin{pmatrix} \cos^2\epsilon\tan\delta_- + \sin^2\epsilon\tan\delta_+ & \cos\epsilon\sin\epsilon(\tan\delta_- - \tan\delta_+) \\ \cos\epsilon\sin\epsilon(\tan\delta_- - \tan\delta_+) & \sin^2\epsilon\tan\delta_- + \cos^2\epsilon\tan\delta_+ \end{pmatrix} \tag{7.67}$$

We can obtain phase shifts in Blatt parametrization as

$$\begin{aligned} \tan 2\epsilon &= \frac{2K_{-+}}{K_{--} - K_{++}} = \frac{2\mathrm{Re}T_{-+}}{\mathrm{Re}[T_{--} - T_{++}]}, \\ \tan\delta_- &= \frac{1}{2}\left(K_{--} + K_{++} + \frac{K_{--} - K_{++}}{\cos 2\epsilon}\right), \\ \tan\delta_+ &= \frac{1}{2}\left(K_{--} + K_{++} - \frac{K_{--} - K_{++}}{\cos 2\epsilon}\right). \end{aligned} \tag{7.68}$$

These are related with Stapp- parametrization,

$$\begin{aligned} &\sin(\delta_- - \delta_+) = \sin 2\bar{\epsilon}/\sin 2\epsilon, \\ &\bar{\delta}_1 + \bar{\delta}_2 = \delta_- + \delta_+, \\ &\sin(\bar{\delta}_1 - \bar{\delta}_2) = \tan 2\bar{\epsilon}/\tan 2\epsilon, \end{aligned} \tag{7.69}$$

[3] The definition of K-matrix is different from Glockle's. Here $\hat{S} = (1 - i\hat{K})^{-1}(1 + i\hat{K})$, but in Glockle's book, $\hat{S} = (1 + 2i\mu qK)^{-1}(1 - 2i\mu qK)$. Thus, $K = -2\mu qK_{Glockle}$.

- However, note that some case, $K_{--} >> K_{++}$ case like ${}^3S_1 - {}^3D_1$ near $E_{lab} = 16..18$ MeV, $\delta_- \simeq 90$ degree, $\epsilon << 1$ require special attention because there will be numerical uncertainty δ_+ which requires subtle cancellation of $K_{--} + K_{++} - (K_{--} - K_{++})(1 + 2\epsilon^2 + \dots) = 2K_{++} - (K_{--} - K_{++}) * (2\epsilon^2 + \dots)$. Thus, it is better to expand $\cos(2\epsilon)$ first.

  Because basic equation to determine K-matrix is inhomogeneous, the sign and normalization of K-matrix is determined by the potential. On the other hand, the phase shifts can have ambiguity.

- In Blatt-Biedernhann parameters from above equation can have phase ambiguity up to π for $\delta_\mp$ and $\frac{\pi}{2}$ for ϵ.

- If we convert these phase to Stapp parametrization by above relation, $\sin(2\bar{\epsilon}) = (number) * \sin(2\epsilon + n\pi)$, sign of $\bar{\epsilon}$ can be ambiguous. Also, $\bar{\delta}_\mp$ can be ambiguous up to $n\pi$.

Note that according to the definition of T matrix or K matrix, there could be some factor $(factor)K = i\frac{1-S}{1+S}$.

In S-matrix

In a similar way, we can obtain phase shifts from S-matrix (or T-matrix.) In Blatt parametrization, we have

$$S = \begin{pmatrix} \cos^2\epsilon e^{2i\delta_-} + \sin^2\epsilon e^{2i\delta_+} & \frac{1}{2}\sin 2\epsilon(e^{2i\delta_-} - e^{2i\delta_+}) \\ \frac{1}{2}\sin 2\epsilon(e^{2i\delta_-} - e^{2i\delta_+}) & \cos^2\epsilon e^{2i\delta_+} + \sin^2\epsilon e^{2i\delta_-} \end{pmatrix}, \tag{7.70}$$

In Stapp(or bar) parametrization,

$$S = \begin{pmatrix} \cos 2\bar{\epsilon} e^{2i\bar{\delta}_1} & i\sin 2\bar{\epsilon} e^{i(\bar{\delta}_1+\bar{\delta}_2)} \\ i\sin 2\bar{\epsilon} e^{i(\bar{\delta}_1+\bar{\delta}_2)} & \cos 2\bar{\epsilon} e^{2i\bar{\delta}_2} \end{pmatrix} \tag{7.71}$$

Let us first consider Blatt parametrization, by using, [4]

$$\begin{aligned} \frac{S_{-+}}{S_{--} - S_{++}} &= \frac{1}{2}\tan 2\epsilon, \\ S_{--} + S_{++} + \frac{S_{--} - S_{++}}{\cos 2\epsilon} &= 2e^{2i\delta_-}, \\ S_{--} + S_{++} - \frac{S_{--} - S_{++}}{\cos 2\epsilon} &= 2e^{2i\delta_+}. \end{aligned} \tag{7.73}$$

Once Blatt phase shifts are obtained we can change them into Stapp phase shifts by using relations.

Or we may try directly relate Stapp phase shifts with S-matrix by

$$\begin{aligned} \frac{S_{12}S_{21}}{S_{11}S_{22}} &= -\tan^2(2\bar{\epsilon}), \\ \frac{S_{11}}{\cos 2\bar{\epsilon}} &= e^{2i\bar{\delta}_1}, \quad \frac{S_{22}}{\cos 2\bar{\epsilon}} = e^{2i\bar{\delta}_2}. \end{aligned} \tag{7.74}$$

[4]

$$\begin{aligned} S_{--} - S_{++} &= \cos 2\epsilon(e^{2i\delta_-} - e^{2i\delta_+}), \\ S_{--} + S_{++} &= e^{2i\delta_-} + e^{2i\delta_+}. \end{aligned} \tag{7.72}$$

7.1.10 Effective range function

Define effective range function,

$$\begin{aligned} \boldsymbol{M}(k^2) &= k^{l+1}\boldsymbol{K}^{-1}k^l \\ &= M_0 + M_1 k^2 + M_2 k^4 + \cdots, \quad \text{effective range expansion} \end{aligned} \tag{7.75}$$

Thus, we define general scattering length and effective range as,

$$\frac{k^{2l+1}}{\boldsymbol{K}} = -\frac{1}{a_l} + \frac{1}{2} r_l k^2 + \cdots \tag{7.76}$$

where, note that $\frac{k^{2l+1}}{\boldsymbol{K}} \to k\cot\delta_0$ for $l = 0$ [5] At low energy, effective range parameters can be written as

$$\begin{aligned} &k\cot\delta \to -\frac{1}{a} + \frac{1}{2} r k^2 + \mathcal{O}(k^4), \\ &\frac{\tan\delta}{k} = \frac{K_{11}}{k} = -a_0 - \frac{1}{2} a_0^2 r_0 k^2 + \mathcal{O}(k^4) \end{aligned} \tag{7.77}$$

In case of multi-channel scattering,

$$\sum_{m',n'} \boldsymbol{p}_{mm'} [\boldsymbol{K}^{-1}]_{m'n'} \boldsymbol{p}_{n'n} = -\frac{1}{\boldsymbol{a}_{mn}} + \frac{1}{2}\boldsymbol{r}_{mn} p^2 + \boldsymbol{P}_{mn} p^4 + \dots \tag{7.78}$$

where, $\boldsymbol{p}$ is a diagonal momentum matrix

$$\boldsymbol{p} = \begin{pmatrix} p^{j-s+\frac{1}{2}} & & \\ & \ddots & \\ & & p^{j+s+\frac{1}{2}} \end{pmatrix} \tag{7.79}$$

6

If phase shifts at two different energies, k_i (which can be related to energies as $T_{i,c} = \frac{1}{2\mu} k_i^2$, $T_{i,L} = \frac{m_1}{\mu} T_{i,C} \simeq \frac{k_i^2}{\mu}$) are known, we can obtain effective range parameters as

$$\begin{aligned} r &= \frac{k_1\cot\delta_1 - k_2\cot\delta_2}{(k_1^2 - k_2^2)/2}, \\ \frac{1}{a} &= \frac{1}{2} r k_i^2 - k_i\cot\delta_i, \quad i = 1, 2 \end{aligned} \tag{7.81}$$

effective range를 파동함수를 통해서 구할 수도 있다. S-wave의 경우

$$\begin{aligned} \bar{u}_0(r) &\equiv \lim_{k\to 0} \bar{u}(r) = r - a_0, \quad \bar{u}(r) = u(r > R), \\ r_0 &= \frac{2}{a_0^2}\int_0^\infty dr[\bar{u}_0^2 - u_0^2]. \end{aligned} \tag{7.82}$$

[5]Scattering length can be alternatively defined as the point at $u(r = a_0) = 0$ when $kR << 1$.

In case of multi-channel, $M_{l_1,l_2} = k_1^{l_1+\frac{1}{2}} k_2^{l_1+\frac{1}{2}} [K^{-1}]_{l_1,l_2}$.

[6]For example, two nucleon scattering in elastic singlet or uncoupled channel $j = l$, $[p] = p^{l+\frac{1}{2}}$, so, $M(k) = k^{2l+1}[K^{-1}]_{ll}$. On the other hand, triplet coupled channel, $l_1 = j - 1$ and $l_2 = j + 1$,

$$[M](k) = \frac{1}{K_{11}K_{22} - K_{12}K_{21}} \begin{pmatrix} p^{2l_1+1}K_{22} & -p^{l_1+l_2+1}K_{12} \\ -p^{l_1+l_2+1}K_{21} & p^{2l_2+1}K_{11} \end{pmatrix} \tag{7.80}$$

zero mixing case, $K_{12} = 0$ restores uncoupled case.

For the weak potential, we may have relation between scattering length and effective range. For very weak potential, scattering length approaches zero, while effective range diverges. But, their product,

$$ar_{eff} = \pm 2R^2/3, \quad V \to 0_\pm, \tag{7.83}$$

where $\pm$ means repulsive/attractive weak potential.

7.1.11 partial wave decompose for s-matrix, scattering amplitude

- **Spinless particle scattering**: Because usual potential are rotational invariant, it is convenient to introduce partial wave decomposition.

$$\langle k'l'm'|S|klm\rangle = \delta(k'-k)\delta_{l'l}\delta_{m'm}s_l(k) \tag{7.84}$$

where overall energy conservation factor is factored out. Because S-matrix have to be unitary, $s_l(k)$ can be written as

$$s_l(k) = e^{2i\delta_l(k)} \tag{7.85}$$

this defines phase shift $\delta_l(k)$. Scattering amplitude can be expanded as

$$f(\boldsymbol{k}', \boldsymbol{k}) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\hat{\boldsymbol{k}}' \cdot \hat{\boldsymbol{k}}) \tag{7.86}$$

$$f_l(k) = \frac{s_l(k)-1}{2ik} = \frac{e^{i\delta_l(k)}\sin\delta_l(k)}{k} \tag{7.87}$$

This gives

$$\sigma(k) = \sum_{l=0}^{\infty}\sigma_l(k) = 4\pi\sum_{l=0}^{\infty}(2l+1)|f_l(k)|^2 = 4\pi\sum_{l=0}^{\infty}(2l+1)\frac{\sin^2\delta_l(k)}{k^2} \tag{7.88}$$

- **Coupled channels:** Once the S-matrix or phase shifts are calculated, we can compute differential cross section.

For the case of two particle scattering,

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{1}{(2s_1+1)(2s_2+1)}\sum_{m_1,m_2,m_1',m_2'}|\langle s_1m_1', s_2m_2'|f|s_1m_1, s_2m_2\rangle|^2 \\ &= \frac{1}{(2s_1+1)(2s_2+1)}\sum_{SM,S'M'}|\langle S'M'|f|SM\rangle|^2\end{aligned} \tag{7.89}$$

$$\begin{aligned}\langle S'M'|f|SM\rangle &= \sum(4\pi)i^{-L'+L}Y_{L'L_z'}(\hat{k})Y^*_{LL_z}(\hat{k})f^J_{L'S',LS} \\ &\quad \times\langle L'L_z', S'M'|JJ_z\rangle\langle LL_z, SM|JJ_z\rangle, \\ f^J_{L'S',LS} &= \left(\frac{S^J_{L'S',LS} - \delta_{L'L}\delta_{S'S}}{2ik}\right).\end{aligned} \tag{7.90}$$

Be careful about the factor $i^{-L'+L}$. We may absorb this factor to S matrix definition or, Spherical harmonics definition or radial wave function, however, it is important to keep this factor in the formula. In above case, we use conventional spherical harmonics definition or radial wave function is defined such that $\langle xl|pl\rangle_0 = \mathcal{N} j_l(px)$.

It might be useful to use T-reversal symmetry,

$$\langle S' - M'|f|SM\rangle = (-1)^{S+M+S'+M'}\langle S'M'|f|SM\rangle \tag{7.91}$$

In special case of ignoring orbital angular momentum mixing ,total angular momentum dependence and Coulomb interaction, we can simplify the differential cross section as

$$\begin{aligned}
f^J_{L'S',LS} &= f_{LS}\delta_{LL'}\delta_{SS'}, \quad f_{LS} = \left(\frac{e^{2i\delta_{LS}} - 1}{2ik}\right), \\
g_S\delta_{SS'}\delta_{MM'} &\equiv \left(\sum_{LL_zL'_z}(4\pi)Y_{LL'_z}(\hat{k})Y^*_{LL_z}(\hat{k})f_{LS}\delta_{L_zL'_z}\right)\delta_{SS'}\delta_{MM'}, \\
\frac{d\sigma}{d\Omega} &= \frac{1}{(2s_1+1)(2s_2+1)}\sum_S (2S+1)|g_S|^2
\end{aligned} \tag{7.92}$$

7.1.12 Differential equation

Schrodinger equation for two-body scattering in C.M. can be written as

$$\begin{aligned}
&[\hat{T} + V - E]\psi(\boldsymbol{r}) = 0, \\
&\hat{T} = -\frac{\nabla^2}{2\mu} = \frac{1}{2\mu}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{\hat{L}^2}{r^2}\right], \\
&\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right], \\
&\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}.
\end{aligned} \tag{7.93}$$

Scattering wave 를 spherical wave 로 나타내면,

$$\frac{u_{l,k}(r)}{r} = \sqrt{\frac{\pi}{2}}\langle rlm|klm+\rangle, \tag{7.94}$$

이렇게 $\psi_{l,k}(r)$ 을 정의하면, asymptotically, Gives radial Schrodinger equation

$$\left[\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} - V(r) + E\right]u_{l,k}(r) = 0. \tag{7.95}$$

We seek solution with boundary condition,

$$u_{l,k}(r) \to_{r\to 0} cr^{l+1}, \tag{7.96}$$

$$u_{l,k}(r) \quad \to_{r\to\infty} \quad N[\hat{j}_l(kr) - \tan\delta_l(k)\hat{n}_l(kr)], \tag{7.97}$$

If we choose the normalization $N = -2i\cos\delta_l e^{i\delta_l}$, we may rewrite

$$\begin{aligned}
u_l(r) &\to \exp(-i\theta_l) - \exp(i\theta_l)S_l(k), \quad \theta_l = kr - \frac{l\pi}{2}, \\
S_l(k) &= \exp[2i\delta_l(k)] = \frac{1+iK_l(k)}{1-iK_l(k)}, \quad K_l(k) = \tan\delta_l(k)
\end{aligned} \tag{7.98}$$

$$
\begin{aligned}
u_{l,k}(r) &\to_{r\to\infty} \hat{j}_l(kr) + kf_l(k)e^{i(kr-l\pi/2)}, \\
&\to_{r\to\infty} e^{i\delta_l(k)}\sin[kr - l\frac{\pi}{2} + \delta_l(k)], \\
&\to_{r\to\infty} \frac{i}{2}[\hat{h}_l^-(kr) - s_l(k)\hat{h}_l^+(kr)],
\end{aligned} \tag{7.99}
$$

단, 이 식에서 $\hat{j}_l(z) = zj_l(z)$ 로써, Ricatti-Bessel function, $\hat{h}_l^{(\pm)}(z)$ are Ricatti-Hankel function 으로써, $\hat{h}_l^{(\pm)}(z) = z(-y_l \pm ij_l)$ or $z(n_l \pm ij_l)$ if use convention $n_l(z) = -y_l(z)$.

• potential 과 phase shift 의 관계: We may obtain the direct relation between phase shift and integral of a potential by computing difference from the free Schrodinger equation.

$$
\frac{d}{dr}[(rj_l(kr))'u_l(r) - (rj_l(kr))u_l'(r)] = -(rj_l(pr))\frac{2\mu V(r)}{\hbar^2}u_l(r) \tag{7.100}
$$

Then, integration over r with asymptotic form of $u_l(r)$ gives

$$
\sin\delta_l(k) = -\frac{2\mu}{\hbar^2 k}\int_0^\infty j_l(kr)V(r)\psi_{l,k}(r)dr \tag{7.101}
$$

(if $u_l(r) \to \frac{1}{k}\sin(kr - l\pi/2 + \delta_l)$). If we use different normalization, $u_l(r) \to j_l(kr + \tan\delta_l n_l(kr)$, we get,

$$
\tan\delta_l(k) = -\frac{2\mu}{\hbar^2 k}\int_0^\infty j_l(kr)V(r)\psi_{l,k}(r)dr \tag{7.102}
$$

만약 두 포텐셜이 거의 비슷하여 wave function 의 차이가 거의 없는 경우는, infinitesima phase shift difference 를,

$$
\Delta\delta_l(k) = -\frac{2\mu}{\hbar^2 k}\int_0^\infty \Delta V(r)\psi_{l,k}^2(r)dr \tag{7.103}
$$

로 구할 수 있다.

이것은, phase shift의 부호와 potential 사이에, bron approximation에서

$$
\begin{aligned}
\delta_l < 0 \leftrightarrow V(r) > 0, &\quad \text{repulsive}, \\
\delta_l > 0 \leftrightarrow V(r) < 0, &\quad \text{attractive}.
\end{aligned} \tag{7.104}
$$

그러나, 이것은 potential이 매우 약한 경우에만 성립한다.

• phase shift 와 effective range parameter는 관계가 있다. 정확한 관계식, 그리고, 주어진 phase shift 로 부터 또는 주어진 potential 로부터 scattering length 와 effective range를 구하는 식을 추가할 필요가 있다.

7.1.13 K-matrix equation

In literature, there are several different conventions to define K-matrix or R-matrix.

- I (and Rimas) use the K-matrix definition such that $K_0 = \tan\delta_0$ for S-waves.
- Glockle uses $K_{Rimas} = -2\mu q K_{Glockle}$ but also use partial wave notation of $V_{l'l}^{(Glockle)}(p'p) = \int_0^\infty dxx^2 j_{l'}(p'x)V_{l'l}(x)j_l(px)$ with $V_{l'l}(x) = \langle Y_{l'}(\hat{x})|V(\boldsymbol{x})|Y_l(\hat{x})\rangle$. In Glockle's notation, the equation for K-matrix is

$$
K_{\alpha\beta}^{(Glockle)}(q'q) = V_{\alpha\beta}^{(Glockle)}(q'q) + \frac{2}{\pi}\sum_\gamma \int dkk^2 V_{\alpha\gamma}^{(Glockle)}(q'k)\mathcal{P}\left(\frac{1}{q^2/(2\mu) - k^2/(2\mu)}\right)K_{\gamma\beta}^{(Glockle)}(kq) \tag{7.105}
$$

- On the other hand, Machleidt(Bonn potential) uses, partial wave potential as $V_{l'l}(p'p) = \frac{2}{\pi} V^{(Glockle)}_{l'l}(p'p) = \langle Y_{l'}(\hat{p'})|V|Y_l(\hat{p})\rangle$ and R-matrix so that, $R = \frac{\pi}{2} K^{(Glockle)}$

$$R_{\alpha\beta}(q'q) = V_{\alpha\beta}(q'q) + \sum_{\gamma} \int dk k^2 V_{\alpha\gamma}(q'k)\mathcal{P}\left(\frac{1}{q^2/(2\mu) - k^2/(2\mu)}\right) R_{\gamma\beta}(kq) \tag{7.106}$$

7.2 Asymptotic form of scattering wave

먼저, Schrodinger equation 에서, $u(r)$ 의 equation은

$$\frac{d^2 u_l}{dr^2} + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right] u_l = 0. \tag{7.107}$$

여기서, $u_l(r) = v(r)e^{\pm ikr}$ 로 가정하면, $v(r)$은

$$v'' \pm ikv' = \left[U(r) + \frac{l(l+1)}{r^2}\right] v \tag{7.108}$$

식을 만족시킨다. 만약, $v(r)$ 이 slowly varying function으로 가정하여, v''을 무시하면,

$$\pm 2ik \ln v(r) = \int^r \left[U(r) + \frac{l(l+1)}{r^2}\right] + (constant) \tag{7.109}$$

이 된다. 만약, $U(r)$이 $1/r$보다 빠르게 떨어진다면, 오른쪽 항은 r이 커짐에 따라, $\int^r \left[U(r) + \frac{l(l+1)}{r^2}\right] \to \frac{1}{r}$로 상수로 접근하게된다. 따라서, $u(r) \sim e^{\pm ikr + \delta}$ 와 같이 phase shift를 얻게 된다. 하지만, $U(r) \sim C/r$ 인 경우에는 $v(r) \simeq e^{\pm \frac{C}{2ik}\ln r} + \dots$ 가 되어, $u(r) \sim e^{\pm i(kr - \frac{C}{2k}\ln r) + \delta} + \dots$ 와 같이 long range force 에 의한 phase shift가 더 생기게 된다.

따라서, total wave 의 radial wave function은 asymptotically

$$\begin{aligned}
R_l(r) &\simeq j_l(kr) + \frac{s_l - 1}{2i}\frac{e^{i(kr - l\pi/2)}}{kr} \\
&\simeq e^{i\delta_l(k)}\frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} \\
&\simeq j_l(kr) + \frac{s_l - 1}{2i}(-n_l(kr) + ij_l(kr)) \\
&\simeq e^{i\delta_l(k)}[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)] \\
&\simeq \frac{1}{2}[h_l^{(-)}(kr) + s_l h_l^{(+)}(kr)]
\end{aligned} \tag{7.110}$$

where, spherical hanke functions are $h_l^{(\pm)}(kr) = j_l(kr) \pm in_l(kr)$. [7]

여기서 real numerical solution 을 $\hat{R}_l(r)$ 이라고 쓰면,

$$\begin{aligned}
R_l(r) &= e^{i\delta_l(k)}\cos\delta_l \hat{R}_l(r), \\
\hat{R}_l(r) &\simeq [j_l(kr) - \tan\delta_l n_l(kr)]
\end{aligned} \tag{7.113}$$

[7]

$$h^{(+)}(\rho) \to \frac{e^{i(\rho - l\pi/2)}}{i\rho}, \quad h^{(-)}(\rho) \to -\frac{e^{-i(\rho - l\pi/2)}}{i\rho}, \quad , \rho \to \infty \tag{7.111}$$

여기서 $n_l(kr)$은 second kind modified spherical bessel function으로 $y_l(kr)$ 로 쓰기도하고, Nueman function과는 부호가 반대이다.

$$j_l(z \to \infty) = -\frac{1}{z}\sin(z - \frac{l\pi}{2}), \quad n_l(z \to \infty) = -\frac{1}{z}\cos(z - \frac{l\pi}{2}). \tag{7.112}$$

In the zero energy limit, we can use the boundary condition,

$$j_l(\rho \to 0) \simeq \frac{\rho^l}{(2l+1)!!}, \quad n_l(\rho \to 0) \simeq -\frac{(2l-1)!!}{\rho^{l+1}} \tag{7.114}$$

$$\begin{aligned}
\hat{R}_l(k \to 0) &\simeq [\frac{(kr)^l}{(2l+1)!!} + \tan\delta_l \frac{(2l-1)!!}{(kr)^{l+1}}] \\
&\simeq k^l \left[\frac{r^l}{(2l-1)!!} + \left(\frac{\tan\delta_l}{k^{2l+1}}\right)\frac{(2l-1)!!}{r^{l+1}}\right] \\
&\simeq k^l \left[\frac{r^l}{(2l-1)!!} - a_l \frac{(2l-1)!!}{r^{l+1}}\right]
\end{aligned} \tag{7.115}$$

7.2.1 cross section

The full wave function which is solution of scattering Schrodinger equation includes both incident wave function and scattered wave function. The same wave function can also be separated into incoming wave function and outgoing wave function. 여기서 incident wave 는 incoming wave 와 outgoing wave 를 모두 가짐에 주의.

$$\begin{aligned}
\psi(\boldsymbol{r}) &\sim \underbrace{e^{ikz}}_{\text{incident wave}} + \underbrace{\left[\sum_l (2l+1)\frac{(s_l-1)}{2ik}P_l(\cos\theta)\right]\frac{e^{ikr}}{r}}_{\text{scattered wave}}, \\
&= \sum_l i^l(2l+1)P_l(\cos\theta)\frac{1}{2}[\underbrace{h_l^{(-)}}_{\text{incoming wave}} + \underbrace{s_l h_l^{(+)}}_{\text{outgoing wave}}]
\end{aligned} \tag{7.116}$$

flux(or current density) of incident wave of particle 1 of mass m_1.

$$J_{in} = \frac{\hbar k_{in}}{m_1} \tag{7.117}$$

current density of scattered wave of particle mass m into $r^2 d\Omega$ becomes

$$J^r_{scatt} = \frac{k}{m}|f(\theta)|^2\frac{1}{r^2} \tag{7.118}$$

On the other hand, total flux in sphere r is given by integrating the current density computed from full wave function including both incoming wave and outgoing wave.

위에서 scattering amplitude를

$$f(\theta) = \frac{1}{2ik}\sum_l (2l+1)(s_l-1)P_l(\cos\theta) \tag{7.119}$$

로 쓸 수 있음을 알 수 있었는데, 지금까지 $s_l = e^{2i\delta_l}$ 에 대해서는 어떠한 가정도 하지 않았다. Elastic Differntial cross section은 section (2.1)에 정의된 것처럼 scattered particle flux를 incident flux로 나눈것이다.

$$\frac{d\sigma_{el}}{d\Omega} \equiv |f(\theta)|^2 = \frac{1}{4k^2}\sum_{l=0}^{\infty}(2l+1)(s_l-1)\sum_{l'=0}^{\infty}(2l'+1)(s^*_{l'}-1)P_l(\cos\theta)P_{l'}(\cos\theta) \tag{7.120}$$

만약, δ_l 이 real number 라면, angle integrated cross section becomes

$$\sigma_{el} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)|1-s_l|^2 = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l, \tag{7.121}$$

while using

$$\int_0^\pi d\theta \sin\theta P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1}\delta_{ll'}. \tag{7.122}$$

으로 쓸 수 있고 $|s_l| = 1$. 따라서, Real phase shift means total cross section is the same with the elastic scattering cross section

만약, δ_l 이 complex number 일 경우, $|s_l|^2 = \exp(-4\mathrm{Im}\delta_l) < 1$ 이 된다. 이 경우에는 전체 l-th partial wave flux중 $|s_l|^2$ fraction 만큼만 elastic scattering을 하고, $1-|s_l|^2$ 는 다른 reaction을 겪게 되어 total cross section과 elastic cross section이 달라지게 된다.

Reaction cross section: 만약 일정 입자의 total current density 를 large sphere surface($r = R_0$)에 대해서 적분 할 경우, total flux(number of particles per unit time)는 입자의 개수가 보존되는 한 산란이 되건 안되건 언제나 0 이 되어야한다. 하지만, reaction 이 있을 경우 total flux into the sphere

$$J_r = -\int df v_r = -\int d\Omega R_0^2 \frac{1}{2m_1}\frac{\hbar}{i}\left(\phi^*\frac{\partial\phi}{\partial r} - \frac{\partial\phi^*}{\partial r}\phi\right)_{r=R_0} = \frac{\hbar R_0^2}{m_1}\mathrm{Re}i\int d\omega\left(\phi^*\frac{\partial\phi}{\partial r}\right)_{r=R_0} \tag{7.123}$$

이고, asymptotic form of full (elastic channel) wave function

$$\phi_l(x) = \frac{2l+1}{2ikr}[s_l e^{ikr} - (-1)^l e^{-ikr}] \tag{7.124}$$

으로 부터,(주의: elastic cross section 계산의 경우에는 scattered flux를 scattered part of wave function $f(\theta)\frac{e^{ikr}}{r}$ 로 부터 계산한다. 하지만, total flux into the sphere의 경우에는 intital incoming wave를 포함한 전체 wave function으로 flux를 계산한다. 따라서, $J_r \neq J_{sc}$.)

$$\left(\frac{\partial\phi}{\partial r}\right)_{r=R_0} \simeq \sum_{l=0}^{\infty}\frac{2l+1}{2R_0}[s_l e^{ikR_0} + (-1)^l e^{-ikR_0}]P_l(\cos\theta), \tag{7.125}$$

$$\begin{aligned} J_r &= \frac{\hbar R_0^2}{m_1}\mathrm{Re}i\sum_{l=0}^{\infty}\frac{2l+1}{-2ikR_0}\sum_{l'=0}^{\infty}\frac{2l'+1}{2R_0}\int d\Omega[s_l^* e^{-ikR_0} - (-1)^l e^{ikR_0}][s_{l'}e^{ikR_0} + (-1)^{l'}e^{-ikR_0}]P_l(\cos\theta)P_{l'}(\cos\theta) \\ &= \frac{\pi\hbar}{m_1 k}\sum_{l=0}^{\infty}(2l+1)(1-|s_l|^2) \end{aligned} \tag{7.126}$$

Density of incoming stream of particles 는

$$I = \mathrm{Re}\left(\phi_{in}^*\frac{1}{m_1}\frac{\hbar}{i}\frac{\partial\phi_{in}}{\partial x_3}\right) = \frac{\hbar k}{m_1} \tag{7.127}$$

따라서, reaction cross section는 incident flux와 사라진 총량(flux into the sphere)의 비율로 정의할 수 있다. 당연히, 사라지는 것에 대해서 angle을 정할 수 없으므로, reaction cross section 은 angular dependence가 없이 정의되었다.(하지만, 만약, 구체적인 reaction의 final product를 고려하면, angle dependence도 정의할 수 있을 것이다.) 또한, 여기서, reaction cross section이 elastic scattering amplitude 만으로 완전히 정해짐에 유의!

$$\sigma_r \equiv \frac{J_r}{I} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-|s_l|^2) \tag{7.128}$$

And

$$\sigma_{tot} = \sigma_{el} + \sigma_r \tag{7.129}$$

다르게 표현하면,

$$\sigma_t = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(|1-s_l|^2+1-|s_l|^2) = \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-\text{Re } s_l) \tag{7.130}$$

$$f(\theta=0) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(s_l-1) \tag{7.131}$$

따라서,

$$\sigma_t = \frac{4\pi}{k}\text{Im}f(0) \tag{7.132}$$

위 계산은 elastic channel에서 들어가는 flux와 나가는 flux만 계산했을 뿐이므로 optical theorem은 completely general 하다. 하지만, 실제로는 in-elastic channel을 생각할 때, complex phase shift를 얻을 수 있어야하므로, potential 자체가 complex (또는 relativistic filed theory 계산처럼 scattering amplitude 계산에 in-elastic channel이 포함되거나) 이어야만 optical theorem이 만족된다. 다만, 낮은 에너지 에서는 $\sigma_r = 0$, $\sigma_{tot} = \sigma_{el}$ 이고, δ_l 이 real number 이므로, forward elastic scattering amplitude 만으로 optical theorem이 만족되어 total cross section을 계산 할 수 있다.

한편, 특별히 elastic channel에서 absorption이 일어나는 경우 absorption cross section은 total cross section에서 non-elastic channel 과 elastic cross section을 제외한 양으로 정의할 수 있는데, complex potential,$V \to V + iW$, 을 도입하면, 직접 계산할 수 있다.

$$\begin{aligned}
[\hat{T} + V + iW]\psi &= i\hbar\frac{\partial}{\partial t}\psi, \\
\frac{\partial\rho}{\partial t} &= -\nabla\cdot j + \frac{2}{\hbar}W\rho,
\end{aligned} \tag{7.133}$$

where, $\rho(x,t) = \psi^*(x,t)\psi(x,t)$ 이고, $\rho(t) \propto e^{2Wt/\hbar}$ 로써, $W < 0$이면, sink 가 있음을 의미하게 된다. (If density does not change in time,

$$\nabla\cdot\boldsymbol{j}(\boldsymbol{r}) = \frac{2}{\hbar}\rho(\boldsymbol{r})W(r) \tag{7.134}$$

thus loss of flux, $\nabla\cdot\boldsymbol{j}(\boldsymbol{r}) < 0$, requires negative imaginary part $W(r) < 0$.)

Absorptive cross section을 정의하면,

$$\begin{aligned}
\sigma_A &= \frac{2}{\hbar v}\int[-W(R)]|\psi(\boldsymbol{R})|^2 d^3\boldsymbol{R} \\
&= \frac{2}{\hbar v}\frac{4\pi}{k^2}\sum_L(2L+1)\int[-W(R)]|\chi_L(R)|^2 dR
\end{aligned} \tag{7.135}$$

On the other hand, reaction cross section은 각 partial wave에서 사라지는 flux를 모두 더하면,

$$\sigma_R = \frac{\pi}{k^2}\sum_L(2L+1)(1-|S_L|^2) \tag{7.136}$$

In spherical case, $\sigma_A = \sigma_R$. If we introduce additional coupling to non-elastic channel. The reaction cross section becomes $\sigma_R \geq \sigma_A$,

$$\sigma_R = \sigma_A + \sum_{\alpha\neq el}\sigma_\alpha \tag{7.137}$$

Reaction cross section은 elastic scttering 이 아닌 모든 반응을 포함한다.

$$\begin{aligned}\sigma_{tot} &= \sigma_{el} + \sigma_R, \\ &= \frac{2\pi}{k^2}\sum_L (2L+1)(1 - \mathrm{Re}S_L) \\ &= \end{aligned} \tag{7.138}$$

가능한 모든 channel들은

- elastic scattering channel: $A(B,B)A$
- inelastic scattering channel : $A(B,B)A^*$ or $A(B,B^*)A$. target이나 projectile 이 excite 되고, $k_i \neq k_f$ 가 된다. 이러한, 반응은 optical potential에 의해 기술 가능하며, absorption cross section 이라 불리기도 한다.
- non-elastic channels: transfer, fusion, capture, fission and so on.

따라서,

$$\sigma_{tot} = \sigma_{el} + \sigma_R, \quad \sigma_R = \sigma_A + \sigma_{non-el} \tag{7.139}$$

여기서, imaginary potential을 도입하지 않는 microscopic theory에서는 σ_A 는 σ_R 중에서 σ_{non-el}을 뺀 것으로 정의된다. 따라서 σ_{non-el} 에 포함되는 channel의 수에 따라 그 값이 달라진다.

Hard sphere scattering Example

hard sphere scattering 의 경우 wave function의 phase shift는 boundary condition에 의해, $\tan\delta_L = j_L(kR)/n_L(kR)$ 로 결정된다.

낮은 에너지($kR \ll 1$)에서는 S-wave만이 중요하고, $\delta_0 \sim -kR$.

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2\delta_0}{k^2} \simeq R^2 \tag{7.140}$$

이므로, cross section becomes $4\pi R^2$.

반면, high energy($kR \gg 1$) 의 경우에는 L 에 대한 sum을 $l_{max} = kR$ 까지 하는 것으로 생각할 수 있고, $\delta_L \to L * \pi/2 - kR$ 로 approximate 할 수 있다.

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_L^{kR}(2L+1)\sin^2\delta_L \tag{7.141}$$

여기서, many L summation에 대한 approximation으로, average avg$(\sin^2\delta_L) \simeq \frac{1}{2}$, avg$(2L+1) \simeq kR$ 을 취하면,

$$\sigma_{tot} \simeq \frac{4\pi}{k^2}(kR)^2\frac{1}{2} = 2\pi R^2 \tag{7.142}$$

이 얻어진다. high energy에서도 classical limit을 얻지 못함에 유의.

이것은 (total cross section)=(reflection cross section)+(shadow cross section) 으로 이해할 수 있다 여기서, "shadow" is not "absorption". scattering amplitude를 scattering(reflection) amplitude와 shadow amplitude로 나누어 보자.

$$\begin{aligned}f(\theta) &= \sum_l (2l+1)\frac{s_l - 1}{2ik}P_l(\cos\theta) = \sum_{l=0}^{kR}(2l+1)\frac{e^{2i\delta_l}}{2ik}P_l(\cos\theta) + \sum_{l=0}^{kR}(2l+1)\frac{-1}{2ik}P_l(\cos\theta) \\ &= f_{ref}(\theta) + f_{shad}(\theta)\end{aligned} \tag{7.143}$$

By computing $\int |f_{ref}|^2 d\Omega \simeq \pi R^2$, $\int |f_{shad}|^2 d\Omega \simeq \pi R^2$ and $\mathrm{Re}(f^*_{ref} f_{shad}) \simeq 0$, we get $2\pi R^2$. scattering cross section은 incident flux와 outgoing spherical flux의 ratio만을 의미한다. 따라서, 오직 scattering amplitude의 square로 주어진다. 그러나, high energy에서는 물체 뒤에 shadow가 생기고, 이 것은 shadow는 incident wave와 scattering wave의 destructive interference로 이해해야한다. incoming wave는 scattering 에 의해 영향을 받지 않고, full amplitude의 outgoing wave는 $\psi \to \sum_l (2l+1) P_l(\cos\theta)[1 + 2ikf_l = 1 + (s_l - 1)]\frac{e^{ikr}}{r}$ 이므로, no outgoing wave at forward 가 되기 위해서는, pure imaginary f_l 이 필요하다. (-1) term 이 shadow를 만드는 역할을 함을 알수 있다. Thus, we need a scattering to create shadow! 또한, Note that $\mathrm{Im}[f(0)] \simeq \mathrm{Im}[f_{shad}(0)]$.

Mean free path

Imaginary part of optical potential $W < 0$, describes the absorption. By using this, let us consider the mean free path of a particle within optical potential. From the plane wave, e^{iKz} we can roughly write (like WKB approximation), while assume W is smaller than $E + V$

$$\frac{\hbar^2 K^2}{2\mu} + U = E, \quad U = -(V + iW),$$

$$K \simeq \left(\frac{2\mu}{\hbar^2}(E - U)\right)^{\frac{1}{2}} \simeq \left(\frac{2\mu}{\hbar^2}(E + V)\right)^{\frac{1}{2}} \left(1 + \frac{i}{2}\frac{W}{E + V}\right) \tag{7.144}$$

Let us define mean free path length l by $|\psi|^2 \sim e^{-z/l}$. Then, we can approximately get

$$l \simeq \left(\frac{\hbar^2}{2\mu}\right)^{\frac{1}{2}} \frac{(E + V)^{\frac{1}{2}}}{W} \tag{7.145}$$

This mean free path length can be considered as a penetration length for collision.

7.2.2 Coupled equations

In general, potential can change quantum numbers and connect different partial waves. Thus, we have to solve coupled equations. For example, nuclear interaction can connect S-wave and D-wave. Also, nuclear interaction can change spins. Thus, though final scattering wave can have different quantum numbers from initial incoming waves. Let us consider, at infinite past, wave function was $|\phi_\alpha\rangle$. After scattering, we will have $|\psi_\alpha\rangle^{(+)}$. But this scattering wave can be decomposed by

$$|\psi_\alpha\rangle^{(+)} = \sum_{\alpha'} \psi_{\alpha'\alpha} |\alpha'\rangle. \tag{7.146}$$

Thus, partial wave function $\psi_{\alpha'\alpha}$ is a final scattering wave with $|\alpha'\rangle$ which originally came from $|\alpha\rangle$ in the past. [8]

Thus, we can write the asymptotic form as

$$\begin{aligned}
R_{\alpha',\alpha} &\simeq \frac{1}{2}[\delta_{\alpha'\alpha} h^{(-)}_{l'}(kr) + S^J_{\alpha'\alpha} h^{(+)}_{l'}(kr)] \\
&= \left[(j_{L'}(kr) + \frac{1}{i}\frac{(1 - \hat{S})}{1 + \hat{S}} n_{L'}(kr))\left(\frac{1 + \hat{S}}{2}\right)\right]_{\alpha'\alpha} \\
&\equiv \left[(j_{L'}(kr) - \hat{K} n_{L'}(kr))\left(\frac{1 + \hat{S}}{2}\right)\right]_{\alpha'\alpha} \\
&\equiv \left[(j_{L'}(kr) - \hat{K} n_{L'}(kr))(1 - i\hat{K})^{-1}\right]_{\alpha'\alpha}
\end{aligned} \tag{7.147}$$

[8] In physical scattering, if initial beam was a linear combination $|\phi\rangle = \sum_\alpha c_\alpha |\alpha\rangle$, we will also have total scattering wave

$$|\psi\rangle^{(+)} = \sum_\alpha c_\alpha \sum_{\alpha'} \psi_{\alpha'\alpha} |\alpha'\rangle$$

above definition gives [9]

$$
\begin{aligned}
\hat{K} &\equiv i(1-\hat{S})(1+\hat{S})^{-1} \\
\hat{S} &= (1-i\hat{K})^{-1}(1+i\hat{K})
\end{aligned} \tag{7.149}
$$

Thus real valued solution can be written as

$$
\begin{aligned}
\hat{R}_{\alpha'\alpha}(p,r) &\equiv \Big[R(1-i\hat{K})\Big]_{\alpha'\alpha} \\
&\simeq \Big(\delta_{\alpha'\alpha} j_{L'}(kr) - \hat{K}_{\alpha'\alpha} n_{L'}(kr)\Big)
\end{aligned} \tag{7.150}
$$

For zero energy limit, in terms of phase shift or scattering length, in Blatt representation for $l_{\mp} = j \mp 1$,

$$
\begin{aligned}
\hat{R}_{--} &\to k^{j-1}[\frac{r^{j-1}}{(2j-1)!!} + \frac{K_{--}}{k^{2j-1}}\frac{(2j-3)!!}{r^j}], \\
\hat{R}_{-+} &\to k^{j+1}\frac{K_{-+}}{k^{2j+1}}\frac{(2j-3)!!}{r^j} \\
\hat{R}_{+-} &\to k^{j-1}\frac{K_{+-}}{k^{2j+1}}\frac{(2j+1)!!}{r^{j+2}}, \\
\hat{R}_{++} &\to k^{j+1}[\frac{r^{j+1}}{(2j+3)!!} + \frac{K_{++}}{k^{2j+3}}\frac{(2j+1)!!}{r^{j+2}}],
\end{aligned} \tag{7.151}
$$

3-Body or 2-cluster scattering case, we may write pure real solution as

$$
\hat{R}_{\alpha'\alpha}(p,x,y) \simeq \phi_B^{\alpha'}(x)\Big(\delta_{\alpha'\alpha} j_{L'}(kr) - \hat{K}_{\alpha'\alpha} n_{L'}(kr)\Big) \tag{7.152}
$$

7.2.3 Deuteron 의 경우

$l = 0, 2$, $s = j = 1$, $t = 0$인 two nucleon의 bound state(Deuteron)에 대한 homogeneous LS equation 은 다음과 같다.

$$
\begin{aligned}
\Psi_l(p) &= \langle p(ls)jt|\Psi_b\rangle, \\
\Psi_l(p) &= \frac{1}{E_b - \frac{p^2}{m}} \sum_{l'=0,2} \int_0^\infty dp' p'^2 V_{ll'}(pp')\Psi_{l'}(p')
\end{aligned} \tag{7.153}
$$

위 식을 풀면, deuteron의 binding energy $E_b = -2.2246$ MeV와 wave function이 얻어진다. wave function 을 얻었다고 하면, deuteron의 몇가지 성질을 wave function으로부터 구할 수 있다.

- deuteron D-state probability[10]

$$
p_D \equiv \frac{\int_0^\infty \Psi_2^2(p)p^2dp}{\int_0^\infty dpp^2(\Psi_0^2(p) + \Psi_2^2(p))} \tag{7.154}
$$

- single nucleon momentum distribution

$$
\begin{aligned}
n(k) &\equiv \frac{1}{2}\frac{1}{3}\sum_m \langle\Psi_b, 1m| \sum_{i=1}^{2} \delta(\boldsymbol{k} - \boldsymbol{k}_i^{cm})|\Psi_b, 1m\rangle \\
&= \frac{1}{4\pi}\sum_{l=0,2}\Psi_l^2(k)
\end{aligned} \tag{7.155}
$$

[9] Convention에 따라서,

$$
\begin{aligned}
S^J_{\alpha',\alpha}(p) &= \delta_{\alpha'\alpha} - 4i\mu p T^J_{\alpha'\alpha}(p,p) \\
S^J(p) &= [1 + 2i\mu p K^J(p;p)]^{-1}[1 - 2i\mu p K^J(p;p)]
\end{aligned} \tag{7.148}
$$

matrix K is real symmetric and S is unitary. 로 쓰기도 한다. 이 경우의 K^J는 위의 $\hat{K}$와 부호가 반대이다.

[10] Smaller p_d goes larger 3-body,4-body binding energy.

• NN correlation function, the probability to find 2 nucleons at distance r,

$$C(r) \equiv \frac{1}{3}\sum_m \langle \Psi_b, 1m|\delta(\boldsymbol{r}-\boldsymbol{x})|\Psi_b, 1m\rangle = \frac{1}{4\pi}\sum_{l=0,2}\Psi_l(r)^2 \tag{7.156}$$

여기서, Partial wave 의 Fourier transformation은

$$\Psi_l(r) = \sqrt{\frac{2}{\pi}}\int_0^\infty dpp^2 j_l(pr)\Psi_l(p) \tag{7.157}$$

로 얻어진다.

• deuteron magnetic moment from one-nucleon operator:

$$\mu_d = \mu_p + \mu_n + \frac{3}{2}\left(\frac{m_n}{m_p+m_n}\mu_N - \mu_p - \mu_n\right)p_D = (0.879805 - 0.569191 * p_D) \tag{7.158}$$

• Quadropole moment from one-nucleon operator: $\frac{m_n}{m_n+m_p} \simeq 0.50344$,

$$Q = \frac{1}{5}\left(\frac{m_n}{m_n+m_p}\right)^2 \int_0^\infty drr^2 u_D(\sqrt{8}u_S - u_D) \tag{7.159}$$

• radius r_D

$$r_D = \left(\frac{1}{4}\int_0^\infty drr^2(|u_S|^2 + |u_D|^2)\right)^{\frac{1}{2}} \tag{7.160}$$

• D/S ratio $\eta = \frac{A_D}{A_S}$: $\kappa = \sqrt{-ME_b}$ for large r,

$$\frac{u_S(r)}{r} = A_S\frac{e^{-\kappa r}}{r}, \quad \frac{u_D(r)}{r} = A_D\frac{e^{-\kappa r}}{r}\left(1 + \frac{3}{(\kappa r)} + \frac{3}{(\kappa r)^2}\right) \tag{7.161}$$

7.3 Electromagnetic Interaction between nucleon

up to $O(\alpha^2)$ and $O(1/m^2)$, EM potential have Coulomb+Vacuum polarization+ Magnetic interaction,

$$V_{EM}(pp) = V_C^{improved} + V_{VP} + V_{MM}(pp), \quad V_{EM}(np) = V_{MM}(np), \quad V_{EM}(nn) = V_{MM}(nn) \tag{7.162}$$

• Improved Coulomb potential (leading $1/m^2$ correction to $1\gamma + 2\gamma$ exchange): Austin, de Swart '83

$$V_C^{improved} = \frac{\alpha'}{r}\left(1 - \frac{\alpha}{m_p r}\right), \quad \text{with } \alpha' \equiv \alpha\frac{m_p^2 + 2k^2}{m_p\sqrt{m_p^2+k^2}}, \text{ k is sc. on-shell mom.} \tag{7.163}$$

• Vacuum polarization: Ueling'35, Durand III '57

$$V_{VP} = \frac{2\alpha}{3\pi}\frac{\alpha'}{r}\int_1^\infty dxe^{-2m_e rx}\left(1 + \frac{1}{2x^2}\right)\frac{(x^2-1)^{\frac{1}{2}}}{x^2}, \tag{7.164}$$

• Magnetic moment interaction: Schwinger'48; Breit'55,'62; Stoks, de Swart, PRC 42 (1990) 1235

$$\begin{aligned} V_{MM}(pp) &= -\frac{\alpha}{4m_p^2 r^3}\left[\mu_p^2 S_{12} + (6+8\kappa_p)\vec{L}\cdot\vec{S}\right], \\ V_{MM}(np) &= -\frac{\alpha\kappa_n}{2m_n r^3}\left[\frac{\mu_p}{2m_p}S_{12} + \frac{1}{m}\left(\vec{L}\cdot\vec{S} + \frac{1}{2}\vec{L}\cdot(\vec{\sigma}_1 - \vec{\sigma}_2)\right)\right], \\ V_{MM}(nn) &= -\frac{\alpha\mu_n^2}{4m_n^2 r^3}S_{12} \end{aligned} \tag{7.165}$$

7.4 Coulomb scattering

The previous asymptotic form of wave function or boundary condition is based on the assumption that they are free solutions at large separation. However, in case of Coulomb scattering, the wave function have to be distorted even at large separation.

Let us introduce notations:

$$\begin{aligned}
&\rho = kr, \quad k = \sqrt{2\mu E}, \quad U(r) = 2\mu V(r) \\
&a = \frac{q_1 q_2}{2E}, \quad \text{half distance of closest approach} \\
&\eta = \frac{\mu e_1 e_2}{k} = \frac{Z_1 Z_2 \mu \alpha}{k} = \frac{q_1 q_2}{\hbar v} = ka, \quad \text{Sommerfeld parameter.}
\end{aligned} \tag{7.166}$$

NUMERICAL NOTE: the unit of charge is usually chosen in cgs. So that the Coulomb interaction is $\frac{Z_1 Z_2 e^2}{r}$. Then, $e_{cgs}^2 = \alpha_{em} \hbar c = 1.44$ MeV fm.

Shrodinger equation for simple Coulomb scattering is (in CGS unit)

$$\begin{aligned}
& -\frac{\nabla^2}{2\mu}\psi + \frac{Z_1 Z_2 e^2}{r}\psi = E\psi \\
\rightarrow \quad & \left[-\nabla^2 + \frac{2\eta k}{r} - k^2\right]\psi = 0.
\end{aligned} \tag{7.167}$$

We can see the asymptotic solution is, with some constant δ,

$$\psi \rightarrow e^{\pm i(kr - \eta \ln r) + \delta} \tag{7.168}$$

7.4.1 Classical Mechanics

The equation of motion under Coulomb force is

$$m\frac{d^2 \boldsymbol{r}}{dt^2} = \frac{C}{r^3}\boldsymbol{r}, \quad C = \frac{Zze^2}{4\pi\epsilon_0} \tag{7.169}$$

There are three conserved quantities,

$$\begin{aligned}
\text{Energy:} \quad & \frac{dE}{dt} = 0, \quad E = \frac{mv^2}{2} + \frac{C}{r} \\
\text{angular momentum:} \quad & \frac{d}{dt}\boldsymbol{L} = 0, \quad \boldsymbol{L} = m\boldsymbol{r} \times \boldsymbol{v}, \\
\text{...vector} \quad & \frac{d}{dt}\boldsymbol{\epsilon} = 0, \quad \boldsymbol{\epsilon} = \frac{\boldsymbol{v} \times \boldsymbol{L}}{C} + \frac{\boldsymbol{r}}{r}
\end{aligned} \tag{7.170}$$

Note that

$$\epsilon^2 = 1 + 2\frac{EL^2}{mC^2} \tag{7.171}$$

and, trajectory is

$$r(t) = \frac{l}{\epsilon \cos\theta - 1}, \quad l = \frac{L^2}{mC} \tag{7.172}$$

We can define parameter a, which is $\frac{1}{2}$ of the distance of closest approach in a **head-on** collision($\theta = \pi$),

$$a = \frac{Z_P Z_T e^2}{\mu v_0^2} \tag{7.173}$$

and Sommerfeld parameter η as ($\hbar k = \mu v_0$)

$$\eta = ka = \frac{Z_P Z_T e^2}{\hbar v_0} \tag{7.174}$$

For impact parameter b, which would be the closest approach without Coulomb force for given l,

$$L = mbv_0 = \sqrt{2\mu E}b, \quad \rightarrow \quad b = \frac{\eta}{k}\cot\frac{\theta}{2} \tag{7.175}$$

Cross section

$$\begin{aligned} -bdbd\Phi &= \frac{d\sigma}{d\Omega}d\Omega = \frac{\cos\Theta/2}{2\sin^3\Theta/2}(\frac{C}{2E})^2 d\Theta d\Phi \\ \sigma(\theta) &= \frac{b}{\sin\theta}|\frac{db}{d\theta}| = \frac{1}{4}(\frac{Z_P Z_T e^2}{2E})^2\csc^4(\frac{\theta}{2}) \end{aligned} \tag{7.176}$$

The **distance of closest approach** d is

$$d = a(1+\epsilon), \rightarrow \quad kd = \eta + \sqrt{\eta^2 + L^2} \tag{7.177}$$

If there is a nuclear force in addition to Coulomb, the distance of closest approach is called "**grazing**" value, R_{gr} which gives "grazing" orbital angular momentum, $L_{gr}^2 = kR_{gr}(kR_{gr} - 2\eta)$. For varying orbital angular momentum , the grazing distance(or scattering angle) suddenly changes near some orbital angular momentum, L_c ('critical angular momentum')($L > L_c$, scattering is dominated by Coulomb and $L < L_c$ short range nuclear force is active)

cut-off angular momentum l_c: the value of l above which the partial-wave solution is prevented by the centrifugal-plus-Coulomb barrier from penetrating into the regrion $r < a$ where the nuclear potential acts. From the condition,

$$\frac{l_c^2}{a^2} + \frac{2k\eta}{a} = k^2 \tag{7.178}$$

cutoff anguar momentum is

$$l_c = ka\sqrt{1 - \frac{2\eta}{ka}}. \tag{7.179}$$

cutoff value for charged particle scattering is smaller than neutral case(ka). (In other words, because of coulomb repulsion, nuclear interaction acts to less number of orbital angular momentum).

As increasing energy, at low energy the scattering is dominated by Coulomb. (매우 낮은 에너지, 즉 large wave length의 경우는 point particle scattering 으로 볼 수 있다.) For large grazing angular momentum, $l_g \gg 1$, For $\eta \gg 1$(low energy), the short range absorption of nucleus takes effects and reduces the flux in large angle.(Fresnel-like). (에너지가 약간 높아져서 핵의 내부를 들여다보기 시작하되, wave length에 비해 screen의 거리를 finite로 볼 수 있는 경우, screen에 핵의 그림자 같은 윤곽이 나올것이다. 사실은 large scattering쪽은 strongly apsrob되고, impact parameter가 작은 쪽은 투과할 수 있으므로, 벽에 구멍이 뚫려 있고, 반투명한 유리가 끼워져 있는 경우와 비슷하게 생각할 수 있다. 이 경우, 구멍의 크기와 비슷한 밝은 영역이 스크린에 나올 것이다.) As the wave length becomes shorter, $\eta \leq 1$, the distance of upper path and lower path becomes evident and makes a interference.(Fraunhoffer-like) (screen과의 거리가 wave length와 비교해서 무한대라고 생각할 정도가 되면, screen에는 interference pattern이 나오게 된다. 가장 밝은 영역의 크기는 구멍의 크기보다 작아진다.)

7.4.2 Full Solution: Parabolic Coordinate

When there is a strong interaction potential, $U(r) = 2\mu V(r)$,

$$\left[\nabla^2 - \frac{2\eta k}{r} + k^2 - U(r)\right]\psi(r) = 0. \tag{7.180}$$

먼저 pure Coulomb interaction만 있는 경우($U(r) = 0$) 의 해를 구해보자.

Parabolic coordinate 로 변환하여, [11]

$$\begin{aligned} x_1 &= \sqrt{\xi\zeta}\cos\phi, & \xi &= r + x_3, \\ x_2 &= \sqrt{\xi\zeta}\sin\phi, & \zeta &= r - x_3, \\ x_3 &= (\xi - \zeta)/2, & \phi &= \arctan(x_2/x_2), \end{aligned} \tag{7.181}$$

식을 바꾸어 쓰면,

$$\begin{aligned} d^3x = \frac{1}{4}(\xi+\zeta)d\xi d\zeta d\phi, \quad \nabla^2 = \frac{4}{\xi+\zeta}\left[\frac{\partial}{\partial\xi}(\xi\frac{\partial}{\partial\xi}) + \frac{\partial}{\partial\zeta}(\zeta\frac{\partial}{\partial\zeta})\right] + \frac{1}{\xi\zeta}\frac{\partial^2}{\partial\phi^2}, \\ \left[\frac{\partial}{\partial\xi}(\xi\frac{\partial}{\partial\xi}) + \frac{\partial}{\partial\zeta}(\zeta\frac{\partial}{\partial\zeta}) + \frac{\xi+\zeta}{4\xi\zeta}\frac{\partial^2}{\partial\phi^2} - \eta k + \frac{k^2}{4}(\xi+\zeta)\right]\psi(\xi,\zeta,\phi) = 0. \end{aligned} \tag{7.182}$$

From the axial symmetry, the solution will be independent of ϕ and we can expect it as

$$\psi = e^{ikz} f \tag{7.183}$$

with no ξ dependence in f. Since the wave function have to have asymptotically, $r^{-1}e^{ikr}$ but no $r^{-1}e^{+ikr}$, we can expect $e^{ikz}f(r-z) = e^{ik(\xi-\zeta)/2}f(\zeta)$ not $e^{ikz}f(r+z)$. Then,

$$\zeta\frac{d^2}{d\zeta^2}f + (1 - ik\zeta)\frac{d}{d\zeta}f - \eta k f = 0 \leftrightarrow z\frac{d^2F}{dz^2} + (b - z)\frac{dF}{dz} - aF = 0 \tag{7.184}$$

이 식의 regular 해($r = 0$에서 regular이면서, outgoing spherical wave) [12] 는, confluent fypergeometric function을 이용하여

$$\psi_k(\xi,\zeta) = C\exp(ik\frac{\xi-\zeta}{2})F(-i\eta, 1, ik\zeta). \tag{7.185}$$

[11] Arfken 참조. $g_{ij} = \sum_l \frac{\partial x_l}{\partial q_i}\frac{\partial x_l}{\partial q_j}$, $g_{ii} = h_i^2$, $ds_i = h_i dq_i$, $d\sigma_{ij} = h_i h_j dq_i dq_j$, $dv = h_1 h_2 h_3 dq_1 dq_2 dq_3$. 이경우, $h_1^2 = (\xi+\zeta)/(4\xi)$,$h_2^2 = (\xi+\zeta)/(4\zeta)$, $h_3^2 = \xi\zeta$.

[12] Pure Coulomb case, the exact solution have to be regular at $r = 0$. In this case, the solution is correct in all range. However, in case there is other short range force, asymptotic form does not need to be regular. In that case, the asymptotic solution will be a combination of regular and irregular Coulomb functions.

으로 쓸 수 있고, 일반적인 momentum $\boldsymbol{k}$에 대해서, C를 정하여 다음과 같이 쓸 수 있다. [13]

$$
\begin{aligned}
\phi_c(r,\boldsymbol{k}) &= \exp(i\boldsymbol{k}\cdot\boldsymbol{r})_1F_1(-i\eta,1,i(kr-\boldsymbol{k}\cdot\boldsymbol{r})),\\
\psi_k(\boldsymbol{r}) &= C\phi_c(r,\boldsymbol{k}) = \underbrace{\sqrt{\frac{\mathcal{N}}{(2\pi)^3}}e^{-\frac{\pi}{2}\eta}\Gamma(1+i\eta)}_{normalization}\phi_c(r,\boldsymbol{k}).
\end{aligned}
\tag{7.190}
$$

asymptotic form (Confluent Hypergeometric function 항목 참조)

$$
\begin{aligned}
&F(-i\eta,1,ik\zeta) = W_1(-i\eta,1,ik\zeta)+W_2(-i\eta,1,ik\zeta),\\
&W_1(-i\eta,1,ik\zeta) \to \frac{1}{\Gamma(1+i\eta)}e^{\pi\eta/2+i\eta\ln(k\zeta)}\left\{1-\frac{i\eta^2}{k\zeta}+\mathcal{O}(\zeta^{-2})\right\},\\
&W_2(-i\eta,1,ik\zeta) \to \frac{-i}{\Gamma(-i\eta)}e^{\pi\eta/2}\frac{1}{k\zeta}e^{ik\zeta-i\eta\ln k\zeta}+\mathcal{O}(\zeta^{-2}),
\end{aligned}
\tag{7.191}
$$

Thus,

$$
\begin{aligned}
\phi_c(r,k\hat{z}) &= \exp(ik\frac{\xi-\zeta}{2})F(-i\eta,1,ik\zeta)\\
&\simeq \exp(ik\frac{\xi-\zeta}{2})\frac{1}{\Gamma(1+i\eta)}e^{\pi\eta/2+i\eta\ln(k\zeta)}\left\{1-\frac{i\eta^2}{k\zeta}\right\}+\exp(ik\frac{\xi-\zeta}{2})e^{ik\zeta-i\eta\ln k\zeta}\frac{-i}{\Gamma(-i\eta)}e^{\pi\eta/2}\frac{1}{k\zeta}+\mathcal{O}(\zeta^{-2}),\\
&\simeq \frac{e^{\pi\eta/2}e^{i\eta\ln(k\zeta)}}{\Gamma(1+i\eta)}\exp(ik\frac{\xi-\zeta}{2})\left\{1-\frac{i\eta^2}{k\zeta}\right\}+\frac{e^{\pi\eta/2}e^{-i\eta\ln k\zeta}}{\Gamma(-i\eta)}\frac{1}{ik\zeta}\exp(ik\frac{\xi+\zeta}{2})+\mathcal{O}(\zeta^{-2})
\end{aligned}
\tag{7.192}
$$

In short,

$$
\phi_c(\xi,k\zeta\gg 1)\sim\frac{(-ik\zeta)^{i\eta}}{\Gamma(1+i\eta)}\exp(ik\frac{\xi-\zeta}{2})+\frac{(ik\zeta)^{-1-i\eta}}{\Gamma(-i\eta)}\exp(ik\frac{\xi+\zeta}{2})
\tag{7.193}
$$

여기서, spherical coordinate로는

$$
\begin{aligned}
&\frac{\xi-\zeta}{2}=z=r\cos\theta,\quad \frac{\xi+\zeta}{2}=r,\quad \zeta=2r\sin^2\frac{\theta}{2},\\
&(-ik\zeta)^{i\eta}=e^{\frac{\pi\eta}{2}}e^{i\eta\ln k\zeta},\\
&(ik\zeta)^{-1-i\eta}=\frac{1}{ik\zeta}e^{\frac{\pi\eta}{2}}e^{-i\eta\ln k\zeta}=\frac{e^{\frac{\pi\eta}{2}}}{i2kr\sin^2\frac{\theta}{2}}\exp(-i\eta\ln(2kr))\exp(-2i\eta\ln\sin\frac{\theta}{2}),
\end{aligned}
\tag{7.194}
$$

One can use identity,

$$
\begin{aligned}
&(-i\eta)\Gamma(-i\eta)=\Gamma(1-i\eta)=\Gamma(1+i\eta)e^{-2i\sigma_0},\\
&\frac{\Gamma(1+i\eta)}{\Gamma(-i\eta)}=-i\eta\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\equiv -i\eta\exp(2i\sigma_0),
\end{aligned}
\tag{7.195}
$$

[13] Normalization is such that the unit flux comes in. Note that additional square root may be not necessary. In spherical coordinate,

$$
\psi_c^{\pm}(\boldsymbol{k},\boldsymbol{R})=e^{i\boldsymbol{k}\cdot\boldsymbol{R}}e^{-\pi\eta/2}\Gamma(1\pm i\eta)_1F_1(\mp i\eta;1;\pm i(kR-i\boldsymbol{k}\cdot\boldsymbol{R})).
\tag{7.186}
$$

where signs corresponds to asymptotic boundary condition

$$
\psi_c^{\pm}(\boldsymbol{k},\boldsymbol{R})\simeq e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\quad(\text{for }\boldsymbol{k}\cdot\boldsymbol{r}\to\mp\infty\ )
\tag{7.187}
$$

with relation,

$$
\psi_{\boldsymbol{k}}^{(+)}(r)=[\psi_{-\boldsymbol{k}}^{(-)}(r)]^*
\tag{7.188}
$$

Schiff's book gives

$$
C=v^{-\frac{1}{2}}\Gamma(1+i\eta)e^{-\frac{\eta\pi}{2}}
\tag{7.189}
$$

여기서, Coulomb phase shift σ_0 is defined as

$$\begin{aligned}
\sigma_0 &\equiv \frac{1}{2i}\ln\left(\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\right) = \arg\Gamma(1+i\eta), \\
\Gamma(1+i\eta) &= |\Gamma(1+i\eta)|e^{i\sigma_0}, \quad \Gamma(1-i\eta) = \Gamma(1+i\eta)^* = |\Gamma(1+i\eta)|e^{-i\sigma_0}, \\
\sigma_l &= \arg\Gamma(l+1+i\eta), \quad \exp(2i\sigma_l) = \frac{\Gamma(l+1+i\eta)}{\Gamma(l+1-i\eta)},
\end{aligned} \tag{7.196}$$

Usually, one evaluates σ_0 and obtain Coulomb phase shifts for higher partial waves from the series

$$\sigma_l = \sigma_0 + \sum_{s=0}^{l} \tan^{-1}(\frac{\eta}{s}). \tag{7.197}$$

Thus asymptotic form can be separated into incident wave and scattered wave,

$$\begin{aligned}
\phi_c(\xi, k\zeta \gg 1) &\simeq \frac{e^{\pi\eta/2}e^{i\eta\ln(k\zeta)}}{\Gamma(1+i\eta)}\left[\exp(ik\frac{\xi-\zeta}{2})(1-\frac{i\eta^2}{k\zeta}) + (-i\eta)e^{2i\sigma_0}\frac{e^{-2i\eta\ln k\zeta}}{ik\zeta}\exp(ik\frac{\xi+\zeta}{2})\right] \\
&= \frac{e^{\pi\eta/2}}{\Gamma(1+i\eta)}\left[e^{ikz+i\eta\ln k\zeta}(1-\frac{i\eta^2}{k\zeta}) + \frac{(-\eta)e^{2i\sigma_0}}{k\zeta}e^{ikr-i\eta\ln k\zeta}\right]
\end{aligned} \tag{7.198}$$

By replacing $\zeta = 2r\sin^2\frac{\theta}{2}$ and arrange terms, we get

$$\begin{aligned}
\phi_c(\xi, k\zeta \gg 1) &\simeq \frac{e^{\pi\eta/2}}{\Gamma(1+i\eta)}\left[e^{ikz+i\eta\ln k\zeta}(1-\frac{i\eta^2}{k\zeta}) + \frac{(-\eta)e^{2i\sigma_0}}{k\zeta}e^{ikr-i\eta\ln k\zeta}\right] \\
&\sim \frac{\exp(\frac{\pi}{2}\eta)}{\Gamma(1+i\eta)}\left[e^{ikz+i\eta\ln(k(r-z))} + \left(\frac{-\eta e^{2i\sigma_0}}{2kr\sin^2\frac{\theta}{2}}\right)e^{ikr-i\eta\ln(2kr\sin^2\frac{\theta}{2})}\right], \\
&= \frac{\exp(\frac{\pi}{2}\eta)}{\Gamma(1+i\eta)}\left[e^{i[kz+\eta\ln(k(r-z))]} + f_c(\theta)\frac{e^{i[kr-\eta\ln(2kr)]}}{r}\right],
\end{aligned} \tag{7.199}$$

We can choose normalization such that

$$\psi_k \sim e^{-\pi\eta/2}\Gamma(1+i\eta)\phi_c \sim \left[e^{i[kz+\eta\ln(k(r-z))]} + f_c(\theta)\frac{e^{i[kr-\eta\ln(2kr)]}}{r}\right] \tag{7.200}$$

$$\begin{aligned}
\boldsymbol{j}_{in} &\rightarrow \frac{\hbar k}{\mu}\hat{z} + \frac{\hbar\eta}{\mu}\frac{\hat{r}-\hat{z}}{2r\sin^2(\theta/2)}, \\
j_r r^2 &\rightarrow |f_C(\theta)|^2\frac{\hbar}{\mu}\left(k - \frac{\eta}{r}\right)
\end{aligned} \tag{7.201}$$

여기서 we get Coulomb scattering amplitude and cross section,

$$\begin{aligned}
f_c(\theta) &= -\frac{\eta}{2k\sin^2\frac{\theta}{2}}e^{-2i\eta\ln\sin\frac{\theta}{2}}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)} = -\frac{\eta}{2k\sin^2\frac{\theta}{2}}\exp(-2i\eta\ln\sin\frac{\theta}{2} + 2i\sigma_0), \\
\sigma_{Ruth}(\theta) &= |f_c(\theta)|^2 = \frac{\eta^2}{4k^2\sin^4(\theta/2)} = \left(\frac{Z_1Z_2e^2}{4E\sin^2(\theta/2)}\right).
\end{aligned} \tag{7.202}$$

Here, it is noteworthy that the scattering amplitude diverges when $1 - i\eta$ becomes zero or negative integer which corresponds to energy levels $\frac{1}{2\eta^2} = -\frac{1}{2n^2}$. Also, the asymptotic form is not valid for $\theta = 0$ because $k\zeta = 0$. Though there are additional logarithmic phase factors, there are additional terms in currents in incident current and scattered current, however, they are proportional to $1/r$ and vanish at large distance. Thus, still $f_c(\theta)$ can be considered as scattering amplitude. [14]

[14] In Schiff's book, $\psi_k(r) = C\phi_c$ with $C = v^{-1/2}\Gamma((1+i\eta)e^{-\eta/\pi/2}$. Thus, the particle density at $r = 0$ is proportional to

$$|\psi(0)|^2 = |C|^2 = \frac{2\eta\pi}{v(e^{2\eta\pi}-1)} \simeq \frac{2\pi\eta}{v}e^{-2\eta\pi} \quad \text{for repulsive small } \eta > 0. \tag{7.203}$$

The $e^{-2\eta\pi}$ is called Gamow factor.

Appendix: Confluent hypergeometric function

It is a special case of hypergeometric differential equation(Kumer-Laplace equation)

$$xf'' + (b-x)f' - af = 0. \tag{7.204}$$

해는 $z=0$ 에서 regular solution F 과 irregular solution G로 쓸 수 있다. 이 때, regular solution은 ${}_1F_1(a,b,z)$로도 쓰는데,

$$\begin{aligned} F(a,b,z) &= \frac{\Gamma(b)}{\Gamma(a)}\sum_{n=0}^{\infty}\frac{\Gamma(a+n)z^n}{\Gamma(b+n)n!} \\ &= 1+\frac{ax}{b1!}+\frac{a(a+1)}{b(b+1)}\frac{x^2}{2!}+\cdots \end{aligned} \tag{7.205}$$

이때, regular solution과 iregular solution을 Whittaker function, W_1과 W_2함수의 combination으로 나타내는 것이 편리한 경우가 있다.

$$\begin{aligned} F(a,b,z) &= W_1(a,b,z)+W_2(a,b,z), \quad G(a,b,z) = iW_1(a,b,z)-iW_2(a,b,z), \\ W_1(a,b,z) &= \frac{\Gamma(b)}{\Gamma(b-a)}(-z)^{-a}g(a,a-b+1,-z), \\ W_2(a,b,z) &= \frac{\Gamma(b)}{\Gamma(a)}e^z z^{a-b}g(1-a,b-a,z), \\ g(\alpha,\beta,z) &= \sum_n \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)}\frac{\Gamma(\beta+n)}{\Gamma(\beta)}\frac{1}{n!z^n} \\ &= 1+\frac{\alpha\beta}{z1!}+\frac{\alpha(\alpha+1)\beta(\beta+1)}{z^2 2!}+\cdots, \quad z\to\infty \end{aligned} \tag{7.206}$$

특별히 $b=1$ case, regular solution have asymptotic form,

$$F(a,1,x\gg 1) = \frac{(-x)^{-a}}{\Gamma(1-a)}+\frac{x^{a-1}}{\Gamma(a)}\exp(x) \tag{7.207}$$

$$F(a,b,z\ll 1) = 1+\frac{az}{b} \tag{7.208}$$

The integral form can be written as

$$F(a,b,z) = e^z F(b-a,b,-z) \tag{7.209}$$

$$\frac{d}{dz}F(a,b,z) = \frac{a}{b}F(a+1,b+1,z) \tag{7.210}$$

7.4.3 Coulomb wave function: Spherical Coordinates, partial wave

Previous section describes Coulomb wave function in cylindrical coordinates. But, it will be convenient to have a spherical coordinate solution. **This section needs to be cleaned up.**

In spherical coordinate, the solution can be written as

$$\begin{aligned} &\psi = \sum a_{l,m}\psi_{l,m}, \quad \psi_{l,m}(\eta,\rho) = \frac{1}{\rho}\chi_l(\eta,\rho)Y_{l,m}(\theta,\phi), \\ &\frac{d^2\chi_l(\eta,\rho)}{d\rho^2}+(1-\frac{2\eta}{\rho}-\frac{l(l+1)}{\rho^2})\chi_l(\eta,\rho) = 0 \end{aligned} \tag{7.211}$$

The regular and irregular normalized solution of Coulomb scattering , in Abramowitz and Stegun (1972), are

$$\chi_l(\eta,\rho) = aF_L(\eta,\rho) + bG_L(\eta,\rho), \tag{7.212}$$

where $\rho = \kappa r$, $\eta = \frac{\mu e_1 e_2}{\kappa} = \frac{Z_1 Z_2 \mu\alpha}{\kappa}$, [15] $\kappa = \sqrt{2\mu E}$.

Coulomb function $F_L(\eta,\rho)$

In terms of confluent hypergeometric function, the Coulomb function of the first kind is

$$F_L(\eta,\rho) = C_L(\eta)\rho^{L+1}e^{\mp i\rho}{}_1F_1(L+1\mp i\eta; 2L+2; \pm 2i\rho) \tag{7.213}$$

with $C_L(\eta)$ is Coulomb constant and ${}_1F_1(a;b;z) \equiv M(a,b,z)$ as the confluent hypergeometric function of the first kind. [16] Sign does does not change the function but may corresponds to different boundary condition. In limiting case $\rho \gg 1$,

$$\begin{aligned}
F_L(\eta,\rho) &\to C_L\rho^{L+1}e^{i\rho}\left[\frac{\Gamma(2L+2)}{\Gamma(L+1+i\eta)}e^{-2i\rho}(-2i\rho)^{-L-1+i\eta} + \frac{\Gamma(2L+2)}{\Gamma(L+1-i\eta)}e^{\pi i(L+1+i\eta)}(-2i\rho)^{-L-1-i\eta}\right] \\
&= C_L\left[\frac{\Gamma(2L+2)}{\Gamma(L+1+i\eta)}e^{-i\rho}\frac{2^{-L}}{(-2i)}(-i)^{-L+i\eta}e^{i\eta\ln 2\rho} + \frac{\Gamma(2L+2)}{\Gamma(L+1-i\eta)}e^{i\rho}\frac{2^{-L}}{2i}e^{-i\eta\ln 2\rho}(-i)^{L+i\eta}\right] \\
&= C_L\frac{\Gamma(2L+2)2^{-L}e^{\frac{\pi}{2}\eta}}{|\Gamma(L+1+i\eta)|}\left[\frac{-1}{2i}e^{-i\Theta_L} + \frac{1}{2i}e^{i\Theta_L}\right] = C_L\frac{\Gamma(2L+2)2^{-L}e^{\frac{\pi}{2}\eta}}{|\Gamma(L+1+i\eta)|}\sin\Theta_L, \\
\Theta_L &= \rho - \frac{\pi}{2}L + \sigma_L - \eta\ln 2\rho
\end{aligned} \tag{7.214}$$

Thus, by choosing normalization such that $F_L(0,\rho) = \rho j_L(\rho) \to \sin(\rho - \frac{\pi}{2}L)$, we can fix

$$C_L(\eta) \equiv \frac{2^L e^{-\frac{\pi}{2}\eta}|\Gamma(L+1+i\eta)|}{\Gamma(2L+2)}. \tag{7.215}$$

Also, this form implies the scattering amplitude have partial component of $\frac{e^{2i\sigma_L}-1}{2ik}$.

Partial wave expansion: method 1

Since we know the partial wave solution up to normalization, we can match the hyperbolic coordinate solution and fix the normalization

$$\begin{aligned}
\psi_c &= e^{-\frac{\pi}{2}\eta}\Gamma(1+i\eta)\exp(ikz){}_1F_1(-i\eta, 1, ik(r-z)) \\
&= \sum_L a_L(2L+1)i^L\frac{F_L(\eta,\rho)}{\rho}P_L(\cos\theta)
\end{aligned} \tag{7.216}$$

Then, from the orthogonality of Legendre polynomial,

$$R_l(r) = a_L(2L+1)i^L\frac{F_L(\eta,\rho)}{\rho} = \frac{2l+1}{2}\int_0^\pi P_l(\cos\theta)\psi_c(r,\theta)\sin\theta d\theta \tag{7.217}$$

Instead of doing full integration, we may only focus on the value at $r = 0$.[17] Then,

$$a_L = e^{i\sigma_L} \tag{7.218}$$

Note that $e^{i\sigma_L}$ factor comes from $\Gamma(l+1+i\eta) = |\Gamma(l+1+i\eta)|e^{i\sigma_l}$ and thus depends on the convention of $F_l(\eta,\rho)$.

[15] Note that the Coulomb interaction is written as $\frac{e_1e_2}{r}$ instead of $\frac{e_1e_2}{4\pi\epsilon_0 r}$ implying the electric charge are in cgs units and $\alpha = \frac{e^2}{\hbar c}$.

[16] ${}_1F_1(a;c;x) = \sum_{n=0}^\infty \frac{(a)_n x^n}{(c)_n n!}$ with $(a)_0 = 1$, $(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}$.
The normalization factor of C_L is chosen such that $\frac{1}{\rho}F_L(\eta=0,\rho) = j_L(\rho)$.

[17] **I need to check this!** It is simple to match for $L = 0$ only using $F_0(\eta,\rho \ll 1) = \rho$, ${}_1F_1(a,b,0) = 1$. This gives $a_0 = e^{i\sigma_0}$. In a similar way, we can show $a_1 = e^{i\sigma_1}$.

Partial wave expansion: method 2

Or, one can use the asymptotic form for matching, We may expand asymptotic form of ϕ_c explicitly to find the expansion coefficient and also the partial wave expansion of scattering amplitude,

$$\psi_k \sim e^{-\pi\eta/2}\Gamma(1+i\eta)\phi_c \sim \left[e^{i[kz+\eta\ln(k(r-z))]} + f_c(\theta)\frac{e^{i[kr-\eta\ln(2kr)]}}{r}\right] \tag{7.219}$$

By Legendre polynomial expansion of ϕ_c, (**Legendre Polynomial Expansion is not checked. equation comes from the book by I. Kaplan**)

$$\begin{aligned}
\phi_c(kr \gg 1, \theta) \quad &\sim \quad \frac{\exp(\frac{\pi}{2}\eta)}{\Gamma(1+i\eta)}\sum_{l=0}^{\infty}\frac{2l+1}{-2ikr}\Big[(-1)^l\exp(-ikr+i\eta\ln 2kr) \\
&\qquad -\exp(ikr - i\eta\ln 2kr + 2i\sigma_l)\Big]P_l(\cos\theta) \\
&\sim \quad \frac{\exp(\frac{\pi}{2}\eta)}{\Gamma(1+i\eta)}\sum_{l=0}^{\infty}(2l+1)\frac{i}{2}\frac{1}{\rho}\exp(i\sigma_l)i^l\Big[\exp(-i\Theta_L)-\exp(+i\Theta_L)\Big]P_l(\cos\theta), \\
&\sim \quad \frac{\exp(\frac{\pi}{2}\eta)}{\Gamma(1+i\eta)}\sum_{L=0}^{\infty}i^L(2L+1)e^{i\sigma_L}P_L(\cos\theta)\frac{1}{\rho}\frac{i}{2}[e^{-i\Theta_L}-e^{i\Theta_L}]
\end{aligned} \tag{7.220}$$

with $\Theta_L = \rho - \frac{\pi}{2}L - \eta\ln 2\rho + \sigma_L$ and we can identify Coulomb function, $\frac{1}{\rho}\frac{i}{2}[e^{-i\Theta} - e^{i\Theta}] \rightarrow \frac{F_L(\eta;\rho)}{\rho}$.

Thus,

$$\psi_c \quad = \quad v^{-1/2}\sum_L(2L+1)i^L e^{i\sigma_L}\frac{F_L(\eta,\rho)}{\rho}P_L(\cos\theta). \tag{7.221}$$

Coulomb functions

Regular solution $F_L(\eta,\rho=0)=0$ but, irregular solution $G_L(\eta,\rho=0)\neq 0$. They are related with Wronskian

$$W(G,F) = G\frac{dF}{dr} - \frac{dG}{dr}F = k \tag{7.222}$$

Two irregular functions have the corresponding definitions,

$$H_L^{\pm}(\eta,\rho) = G_L(\eta,\rho) \pm iF_L(\eta,\rho) = e^{\pm i\Theta}(\mp 2i\rho)^{1+L\pm i\eta}U(1+L\pm i\eta, 2L+2, \mp 2i\rho) \tag{7.223}$$

where $U(a,b,z)$ is the corresponding irregular confluent hypergeometric function.

$$\begin{aligned}
\Theta_L \quad &= \quad \rho - L\pi/2 + \sigma_L(\eta) - \eta\ln(2\rho), \\
\sigma_L(\eta) \quad &= \quad \arg\Gamma(1+L+i\eta)
\end{aligned} \tag{7.224}$$

is called the Coulomb phase shift.

Behavior near origin, $\rho \rightarrow 0$,

$$F_L(\eta,\rho) \sim C_L(\eta)\rho^{L+1}, \quad G_L(\eta,\rho) \sim [(2L+1)C_L(\eta)\rho^L]^{-1} \tag{7.225}$$

and

$$C_0(\eta) = \sqrt{\frac{2\pi\eta}{e^{2\pi\eta}-1}}, \quad C_L(\eta) = \frac{\sqrt{L^2+\eta^2}}{L(2L+1)}C_{L-1}(\eta) \tag{7.226}$$

A transition from small ρ power behavior to large ρ oscillatory behavior occurs outside the classical **turning point**(where $\dot{r} = 0$ classically at $R_{ca} = a + \sqrt{a^2+b^2}$, b is impact parameter and $a = q_p q_t/(2E)$ closest approach in head-on collision). This point is where $1 = 2\eta/\rho + L(L+1)/\rho^2$,

$$\rho_{tp} = \eta \pm \sqrt{\eta^2 + L(L+1)}. \tag{7.227}$$

Classically, $\rho_{tp} = kR_{near}$ with R_{near} is the distance of closest approach, when impact parameter satisfies $kb = \sqrt{L(L+1)} \simeq L + \frac{1}{2}$.

(when there is a nuclear interaction, the Coulomb barrier point and height is important. **Coulomb barrier** is defined as maximun of $\frac{l(l+1)}{2\mu r^2} + V_c(r) + V_N(r)$. The Coulomb barrier is important for resonance and we can roughly estimate the width of resonance which is proportional to tunneling probability is proportional to $\Gamma_l \propto (V_{B,l} - E_{r,l})^{-1}$. In other words, if resonance energy is deeper than Coulomb barrier its width will be narrower.)

On the other hand, in Quantum mechanics, overlap of two charged particle wave function is possible at $r = 0$. This probability is proportional to $|\psi(0)|^2 \sim C_0(\eta)^2 \sim \frac{\eta}{e^{2\pi\eta}-1}$. This **Coulomb penetration factor** becomes almost zero for low energy $p < 10$ MeV.

The asymptotic behavior of the Coulomb functions outside the turning point $(\rho) \gg \rho_{tp}$ is

$$F_L(\eta,\rho) \sim \sin\Theta_L, \quad G_L(\eta,\rho) \sim \cos\Theta_L, \quad H_L^{\pm}(\eta,\rho) \sim e^{\pm i\Theta_L}. \tag{7.228}$$

where Coulomb Hankel function are defined as

$$H_L^{(\pm)}(\eta,\rho) = G_L(\eta,\rho) \pm iF_L(\eta,\rho) \tag{7.229}$$

Asymptotically,

$$\begin{aligned} F_l(\eta,\rho) &\rightarrow \sin(\rho - \frac{\pi}{2}l - \eta\ln(2\rho) + \sigma_l), \quad \rho \to \infty \\ &= \frac{1}{2}(-i)^{l-1}e^{-i\sigma_l}[(-1)^l(2kr)^{i\eta}e^{-ikr} - (2kr)^{-i\eta}e^{i(kr+2\sigma_l)}], \\ \sigma_l(\eta) &= \arg\Gamma(l+1+i\eta), \end{aligned} \tag{7.230}$$

When $\eta = 0$, Coulomb functions becomes Bessel functions,

$$F_L(0,\rho) = \rho j_L(\rho), \quad G_L(0,\rho) = -\rho y_L(\rho) \tag{7.231}$$

Near origin, $\rho \ll L$,

$$\begin{aligned} F_L(0,\rho) &\sim \frac{1}{(2L+1)!!}\rho^{L+1}, \\ G_L(0,\rho) &\sim (2L-1)!!\rho^{-L} \end{aligned} \tag{7.232}$$

Asymptotically, $\rho \gg L$,

$$\begin{aligned} &F_L(0,\rho) \sim \sin(\rho - L\pi/2), \quad G_L(0,\rho) \sim \cos(\rho - L\pi/2), \\ &G_L(0,\rho) \pm iF_L(0,\rho) \sim e^{\pm i(\rho - L\pi/2)} = i^{\mp L}e^{\pm i\rho} \end{aligned} \tag{7.233}$$

Thus, $H_L^{\pm} = G_L(0,\rho) \pm iF_L(0,\rho)$ corresponds to outgoing and incoming wave.

7.4.4 Partial Wave expansion

$$\boxed{\psi_k^C(r) = \sqrt{\frac{\mathcal{N}}{(2\pi)^3}}\sum_L i^L(2L+1)e^{i\sigma_L}P_L(\cos\theta)\frac{F_L(\eta,\rho)}{\rho}} \tag{7.234}$$

From the phase difference in incoming wave and outgoing wave in F_L gives corresponding scattering amplitude in partial waves,

$$\boxed{f_c(\theta) = \sum_{l=0}^{\infty}(2l+1)\left(\frac{\exp(2i\sigma_l)-1}{2ik}\right)P_l(\cos\theta)} \tag{7.235}$$

However, this series does not converge well. It only useful for screened Coulomb function. For example, $\eta \to 0$ limit should give $f_c = 0$, but the expansion becomes

$$\lim_{\eta\to 0} f_c(\theta) = \frac{1}{2ik}\sum_l (2l+1)P_l(\cos\theta) = \frac{1}{2ik} \times 4\delta(1-\cos\theta) \tag{7.236}$$

Thus, $f_c(\theta)$ vanishes as $\eta \to 0$ for $\theta \neq 0$. However, it has singularity at $\theta = 0$, so that

$$\lim_{\eta\to 0}\int_0^{\theta_0} f_c(\theta)\sin\theta d\theta = -\frac{i}{k} \tag{7.237}$$

Partial wave expansion of Coulomb solution, we get[18]

$$\begin{aligned}
\psi_c &= \sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{F_L(\eta,kr)}{kr} \\
&= \sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{1}{kr}\frac{i}{2}[H_L^-(\eta,kr) - H_L^+(\eta,kr)]
\end{aligned} \tag{7.238}$$

With nuclear potential, we define S-matrix

$$\begin{aligned}
\psi &\to \sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{1}{kr}\frac{i}{2}[H_L^-(\eta,kr) - S_L H_L^+(\eta,kr)], \\
&= \sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{1}{kr}[F_L(\eta,kr) + T_L H_L^+(\eta,kr)]
\end{aligned} \tag{7.239}$$

with $S_L = 1 + 2iT_L$.

For non-central interaction, the wave function from initial L_i state is [19]

$$\psi_{L_i}^{(+)} = \sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{1}{kr}\frac{i}{2}[H_L^-(\eta,kr)\delta_{LL_i} - S_{LL_i}H_L^+(\eta,kr)], \tag{7.240}$$

Define R-matrix element at matching point $r = a$,

$$\boldsymbol{R}_L = \frac{1}{a}\frac{u_L(a)}{u_L'(a)} \tag{7.241}$$

By matching $\boldsymbol{R}_L$ at matching point with numerical solution from origin and asymptotic form of wave function, we can determine $\boldsymbol{S}_L$,

$$\boldsymbol{R}_L = \frac{1}{a}\frac{H_L^- - \boldsymbol{S}_L H_L^+}{H_L^{'-} - \boldsymbol{S}_L H_L^{'+}}, \text{ or } \boldsymbol{S}_L = \frac{H_L^- - a\boldsymbol{R}_L H_L^{'-}}{H_L^+ - a\boldsymbol{R}_L H_L^{'+}} \tag{7.242}$$

To get the expression for scattering amplitude and thus differential cross section, we need to match the partial wave expansion form with

$$\psi \to e^{ikz+\eta\ln(R-z)} + f(\theta)\frac{e^{ikR-\eta\ln 2kR}}{R} \tag{7.243}$$

where $f(\theta)$ includes both Coulomb scattering amplitude and nuclear scattering amplitude. Because we know the Coulomb scattering amplitude formally

$$f_c(\theta) = \frac{1}{2ik}\sum_L (2L+1)P_L(\cos\theta)(e^{2i\sigma_L(\eta)} - 1), \tag{7.244}$$

[18]Thompson's book is missing $e^{i\sigma_L}$ factor in partial wave expansion. In the limit $\eta \to 0$, $\psi_c \to e^{ikz}$, $\sigma_L \to 0$, $F_L(eta,\rho) \to \rho j_L(\rho)$.

[19]if the initial state was a plane wave state one have to expand initial state into partial waves.

we can rewrite

$$
\begin{aligned}
\psi &\rightarrow \sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{1}{kr}[F_L(\eta,kr)+T_L H_L^+(\eta,kr)], \\
&= e^{i[kz+\eta\ln(R-z)]}+f_c(\theta)\frac{e^{i(kR-\eta\ln 2kR)}}{r} \\
&\quad +\sum_{L=0}^{\infty}(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}\frac{1}{kr}[T_L H_L^+(\eta,kr)]
\end{aligned} \tag{7.245}
$$

From the asymptotic form,

$$
H_L^{(+)}(\eta,\rho)\rightarrow e^{i(\rho-\eta\ln 2\rho-\frac{L\pi}{2}+\sigma_L)} \tag{7.246}
$$

we get,

$$
\psi\rightarrow e^{i[kz+\eta\ln(R-z)]}+\left[f_c(\theta)+\sum_L(2L+1)i^L P_L(\cos\theta)e^{i\sigma_L}e^{-i\frac{L\pi}{2}}e^{i\sigma_L(\eta)}\frac{T_L}{k}\right]\frac{e^{i(kR-\eta\ln 2kR)}}{r} \tag{7.247}
$$

Because $e^{-i\frac{L\pi}{2}}=(-i)^L$, we get

$$
f(\theta)=f_c(\theta)+\sum_L(2L+1)P_L(\cos\theta)e^{2i\sigma_L(\eta)}\left(\frac{S_L-1}{2ik}\right) \tag{7.248}
$$

Asymptotic form of wave function

Just like spherical bessel functions, we can define Ricatti-Coulomb-Hankel functions and represent asymptotic wave function as

$$
\begin{aligned}
\psi_{\alpha',\alpha}(r;p)=\frac{w_{\alpha',\alpha}(r;p)}{r} &\rightarrow \frac{1}{2}[\delta_{\alpha',\alpha}H_{l'}^{(-)}(\eta,\rho)+S_{\alpha',\alpha}H_{l'}^{(+)}(\eta,\rho)] \\
&= \frac{i}{2}[\delta_{\alpha',\alpha}H_{l'}^{(2)}(\eta,\rho)-S_{\alpha',\alpha}H_{l'}^{(1)}(\eta,\rho)]
\end{aligned} \tag{7.249}
$$

with

$$
H_l^{(\pm)}(\eta,\rho)=\frac{1}{\rho}[F_l(\eta,\rho)\mp iG_l(\eta,\rho)],\quad H_l^{(1,2)}(\eta,\rho)=\frac{1}{\rho}[G_l(\eta,\rho)\pm iF_l(\eta,\rho)] \tag{7.250}
$$

Be careful that above H are Ricatti-Coulomb functions which is differnt from Coulomb Hankel function, $H_L^{\pm}$ in previous section.

We may define similar K-matrix from,

$$
\begin{aligned}
\frac{w_{\alpha',\alpha}(r;p)}{r} &\rightarrow \frac{1}{2}[\delta_{\alpha',\alpha}H_{l'}^{(-)}(\eta,\rho)+S_{\alpha',\alpha}H_{l'}^{(+)}(\eta,\rho)] \\
&= \frac{1}{2}[\frac{F_{l'}(\eta,\rho)}{\rho}(\delta_{\alpha'\alpha}+S_{\alpha'\alpha})+\frac{G_{l'}(\eta,\rho)}{\rho}i(\delta_{\alpha'\alpha}-S_{\alpha'\alpha}) \\
&= \sum_\beta\Big[\frac{F_{l'}(\eta,\rho)}{\rho}\delta_{\alpha'\beta}+\frac{G_{l'}(\eta,\rho)}{\rho}K_{\alpha'\beta}\Big](\frac{I+S}{2})_{\beta\alpha}
\end{aligned} \tag{7.251}
$$

with

$$
K=i(I-S)(I+S)^{-1} \tag{7.252}
$$

$$
\frac{1}{\rho}F_l(\eta,\rho)\rightarrow j_l(\rho),\quad \frac{1}{\rho}G_l(\eta,\rho)\rightarrow -n_l(\rho)\text{ as }\eta\rightarrow 0 \tag{7.253}
$$

Partial wave expansion for Coulomb wave,

$$\langle \boldsymbol{r}|\boldsymbol{p}\rangle_C^{(\pm)} = (factor)\sum_{\alpha} i^L e^{\pm i\sigma_L(\eta)}\frac{F_L(\eta;\rho)}{\rho}Y^*_{LM_L}(\hat{\boldsymbol{p}})Y_{LM_L}(\hat{\boldsymbol{r}}) \tag{7.254}$$

Partial wave expansion for scattering wave,

$$\langle \boldsymbol{r}|\boldsymbol{p}\rangle^{(+)} = (factor)\sum_{\alpha',\alpha} i^{L'} e^{\pm i\sigma_L(\eta)}\frac{w_{\alpha',\alpha}(\eta;\rho)}{r}\mathcal{Y}^*_{\alpha}(\hat{\boldsymbol{p}})\mathcal{Y}_{\alpha'}(\hat{\boldsymbol{r}}) \tag{7.255}$$

Be careful that L' and σ_L in the phase factor.

여기서, (factor)는 normalization convention 에 따라서,

$$\begin{aligned}
{}_C\langle \boldsymbol{p}|\boldsymbol{p}'\rangle_C &= (2\pi)^3\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}') &&\rightarrow (factor) = 4\pi,\\
{}_C\langle \boldsymbol{p}|\boldsymbol{p}'\rangle_C &= \delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}') &&\rightarrow (factor) = \sqrt{\tfrac{2}{\pi}},
\end{aligned}$$

이고, 중간의 $e^{\pm i\sigma_L}$ 은 $\eta\rightarrow 0(\alpha\rightarrow 0)$ limit 에서, 기존의 free particle solution 과 같은 phase를 가지도록 맞추어 주는 역할을 한다.

Originally, S-matrix is such that

$$\begin{aligned}
\psi_{out}(\boldsymbol{p}) &= \int d^3p'\langle \boldsymbol{p}|S|\boldsymbol{p}'\rangle\psi_{in}(\boldsymbol{p})\\
&= \psi_{in}(p) + \frac{ip}{2\pi}\int d\Omega_{p'} f(\boldsymbol{p}\leftarrow\boldsymbol{p}')\psi_{in}(\boldsymbol{p}')
\end{aligned} \tag{7.256}$$

For Coulomb wave becomes

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle_C^{(+)} \quad\rightarrow\quad (2\pi)^{-\frac{3}{2}}\left(\exp\{i[kz+\gamma\ln k(r-z)]\} + f_c(k\hat{r}\leftarrow\boldsymbol{k})\frac{\exp[i(kr-\eta\ln 2kr)]}{r}\right) \tag{7.257}$$

This shows that there is no scattering amplitude in conventional sense. However, we call f_C as Coulomb scattering amplitude.

Scattering amplitude

$$\begin{aligned}
f_C(\theta) &= \sum_{l=0}^{\infty}(2l+1)\left(\frac{e^{2i\sigma_l}-1}{2ik}\right)P_l(\cos\theta) = -\frac{e_1e_2\mu}{2k^2}\left(\sin\frac{\theta}{2}\right)^{-2}e^{2i(\sigma_0-\eta\ln[\sin(\theta/2)])},\\
\left(\frac{d\sigma}{d\Omega}\right)_C &= \frac{e_1^2e_2^2\mu^2}{4k^4\sin^4(\theta/2)}
\end{aligned} \tag{7.258}$$

Note that the partial wave summation does not converge well for finite l. Thus, we always have to use the final form of scattering amplitude.

7.4.5 Screening

There can be a screening of Coulomb field from electrons in an atom. Thus, the Coulomb field is cutoff at the radius R_{at}, but it influences only the very weakly scattered waves (i.e. into forward angles). For screening,

$$V_C^{screen}(r) = \frac{Z_1Z_2e^2}{r}e^{-r/R_{at}}. \tag{7.259}$$

$$f_C^{screen}(\theta) = -\frac{\mu}{2\pi\hbar^2}\int d^3r e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}V_C^{screen}(r) = -\frac{2\mu Z_1Z_2e^2/\hbar^2}{q^2+1/R_{at}^2} \tag{7.260}$$

where $q^2 = 4k^2\sin^2(\theta/2)$.

7.4.6 Strong interaction+Coulomb

Because of Coulomb interaction, usual phase shifts and total cross section concept have to be changed. It is common to define "nuclear" scattering amplitudes which is a Coulomb subtracted scattering amplitude.

$$f_{nuc} = f_{full} - f_C \tag{7.261}$$

However, note that this amplitude still includes Coulomb effects in itself.

If we consider phase shift by short range interaction, we modify σ_l by additional phase shift $\sigma_l + \delta_l$. So,

$$\begin{aligned} f(\theta) &= \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[\exp 2i(\sigma_l+\delta_l)-1]P_l(\cos\theta) \\ &= f_C(\theta) + \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\exp(2i\sigma_l)[\exp 2i\delta_l - 1]P_l(\cos\theta) \end{aligned} \tag{7.262}$$

With the definition of S-matrix as given in the asymptotic form

$$\begin{aligned} \psi_{\alpha',\alpha}(r;p) = \frac{w_{\alpha',\alpha}(r;p)}{r} &\to \frac{1}{2}[\delta_{\alpha',\alpha}H^{(-)}_{l'}(\eta,\rho) + S_{\alpha',\alpha}H^{(+)}_{l'}(\eta,\rho)] \\ &= \frac{i}{2}[\delta_{\alpha',\alpha}H^{(2)}_{l'}(\eta,\rho) - S_{\alpha',\alpha}H^{(1)}_{l'}(\eta,\rho)] \end{aligned} \tag{7.263}$$

For simplicity, let us consider only screened central potentials. with strong interaction

$$\begin{aligned} \psi_l(r) &\to (const)\times\sin(pr - \frac{l\pi}{2} - \eta\ln 2pr + \sigma_l + \nu_l), \\ \delta_l(p) &= \sigma_l + \nu_l - \eta\ln 2p\lambda, \quad , r > \lambda \end{aligned} \tag{7.264}$$

where, λ is a screening scale and ν_l is a "additional" phase shift from short range force. Thus, we have

$$\psi_{l,p} = \frac{i}{2}[\delta_{\alpha',\alpha}H^{(2)}_{l'}(\eta,\rho) - e^{2i\delta_l(p)}H^{(1)}_{l'}(\eta,\rho)] \tag{7.265}$$

Then, "change in radial function due to short range force" becomes

$$\begin{aligned} &= \frac{1}{2i}[e^{2i(\sigma_l+\nu_l-\eta\ln 2p\lambda)} - e^{2i(\sigma_l-\eta\ln 2p\lambda)}]H^{(1)}_{l'}(\eta,\rho) \\ &\to \frac{1}{2i}e^{2i(\sigma_l-\eta\ln 2p\lambda)}[e^{2i\nu_l}-1](-i)^l e^{ipr} \end{aligned} \tag{7.266}$$

Then, "change in full wave function" in $\psi^{(+)}$ by summing partial waves,

$$\to (2\pi)^{-\frac{3}{2}}\frac{1}{2ipr}e^{-2i\eta\ln 2p\lambda}\sum_l(2l+1)e^{2i\sigma_l}[e^{2i\nu_l}-1]P_l(\cos\theta)e^{ipr}, \tag{7.267}$$

so the "change in scattering amplitude" becomes

$$\frac{1}{2ip}e^{-2i\eta\ln 2p\lambda}\sum_l(2l+1)e^{2i\sigma_l}[e^{2i\nu_l}-1]P_l(\cos\theta) \tag{7.268}$$

Thus, "Nuclear" scattering amplitude is given as[20]

$$\boxed{f_{nuc}(\boldsymbol{k}', \boldsymbol{k}) = 4\pi \sum_{\alpha,\beta} i^{-l_\alpha + l_\beta} e^{i\sigma_{l_\alpha}} \left(\frac{S_{\alpha\beta} - \delta_{\alpha\beta}}{2ik}\right) e^{i\sigma_{l_\beta}} Y_{l_\alpha}(\hat{\boldsymbol{k}'}) Y^*_{l_\beta}(\hat{\boldsymbol{k}}).} \tag{7.270}$$

Here, the $i^{-L'+L}$ factor is necessary in the usual spherical harmonics convention.

The partial wave expansion of wave function with both Coulomb interaction and short range interaction,

$$\begin{aligned} \psi^{(+)} &= \phi_c + \psi_{sc}, \\ &= \sum_l C_l P_l(\cos\theta) \frac{u_l(k,r)}{kr} \end{aligned} \tag{7.271}$$

In one normalization,

$$\psi^{(+)} = A \sum_l (2l+1) i^l e^{i(\sigma_l + \delta_l)} P_l(\cos\theta) \frac{u_l(k,r)}{kr}, \quad u_l \to \frac{i}{2}[H_l^{(-)} - S_l H_l^{(+)}] e^{-i\delta_l} \tag{7.272}$$

Or

$$\psi^{(+)} = A \sum_l (2l+1) i^l e^{i\sigma_l} P_l(\cos\theta) \frac{u_l(k,r)}{kr}, \quad u_l \to \frac{i}{2}[H_l^{(-)} - S_l H_l^{(+)}] \tag{7.273}$$

In both case, scattering amplitude is

$$f(\theta) = f_c(\theta) + f_N(\theta), \quad f_N = \sum_l (2l+1) P_l(\cos\theta) e^{2i\sigma_l} \frac{S_l - 1}{2ik} \tag{7.274}$$

Conventions

Let us

7.4.7 Differential Cross Section

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \left(\frac{d\sigma}{d\Omega}\right)_C + \left(\frac{d\sigma}{d\Omega}\right)_{nuc} + \left(\frac{d\sigma}{d\Omega}\right)_{nuc-C} \\ &= |f_C(\theta)|^2 + |f_N(\theta)|^2 + 2\mathrm{Re}[f_C^*(\theta) f_N(\theta)] \end{aligned} \tag{7.275}$$

where, last term is a interference term between Coulomb and nuclear scattering amplitude. [21]

[20] One easy way to understand this form is

$$\begin{aligned} f_l &= \frac{e^{2i\delta_l} - 1}{2ip} = \frac{e^{2i(\sigma_l + \nu_l)} - e^{2i\sigma_l} + e^{2i\sigma_l} - 1}{2ip} \\ &= e^{2i\sigma_l} \frac{e^{2i\nu_l} - 1}{2ip} + \frac{e^{2i\sigma_l} - 1}{2ip} \end{aligned} \tag{7.269}$$

[21] Following is confusing: We can define "nuclear" total cross section and it is related with "nuclear" scattering amplitude by optical theorem,

$$\sigma_{nucl}(E) = \sigma_{full}(E) - \sigma_{Coul}(E) = \frac{4\pi}{k} \mathrm{Im}[f_{nuc}(E, \theta = 0)], \tag{7.276}$$

However, be careful that the differential cross section is not $|f_{nuc}|^2$

$$\sigma_{nuc}(E,\theta) = \sigma_{full}(E,\theta) - \sigma_C(E,\theta) = |f_{full}(E,\theta)|^2 - |f_C(E,\theta)|^2 \tag{7.277}$$

Since the partial wave expansion form of Coulomb scattering does not converge well for l, we have to use non-perturbative form of the partial wave summation.

Table 7.1: Relations between the wave functions and phase shifts, K,T and S-matrix for uncoupled channels. Notation is a bit different, so be careful. Hankel function is defined as $H_L^{\pm} = G_L \pm iF_L$.

Using:	δ	$\boldsymbol{K}$	$\boldsymbol{T}$	$\boldsymbol{S}$
$\chi(r) =$	$e^{i\delta}[F\cos\delta + G\sin\delta]$	$\frac{F+\boldsymbol{K}G}{1-i\boldsymbol{K}}$	$F + \boldsymbol{T}H^+$	$\frac{i}{2}[H^- - \boldsymbol{S}H^+]$
$\delta =$	δ	$\arctan \boldsymbol{K}$	$\arctan\frac{\boldsymbol{T}}{1+i\boldsymbol{T}}$	$\frac{1}{2i}\ln \boldsymbol{S}$
$\boldsymbol{K} =$	$\tan\delta$	$\boldsymbol{K}$	$\frac{\boldsymbol{T}}{1+i\boldsymbol{T}}$	$i\frac{1-\boldsymbol{S}}{1+\boldsymbol{S}}$
$\boldsymbol{T} =$	$e^{i\delta}\sin\delta$	$\frac{\boldsymbol{K}}{1-i\boldsymbol{K}}$	$\boldsymbol{T}$	$\frac{i}{2}(1-\boldsymbol{S})$
$\boldsymbol{S} =$	$e^{2i\delta}$	$\frac{1+i\boldsymbol{K}}{1-i\boldsymbol{K}}$	$1+2i\boldsymbol{T}$	$\boldsymbol{S}$

7.4.8 Identical particle scattering

Classical scattering의 경우, identical particle scattering은

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{d\sigma_1}{d\Omega}(\theta) + \frac{d\sigma_2}{d\Omega}(\theta) = \frac{d\sigma_1}{d\Omega}(\theta) + \frac{d\sigma_1}{d\Omega}(\pi-\theta) \tag{7.278}$$

However, this is not true for quantum scattering. There can be additional interference term.

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{d\sigma_1}{d\Omega}(\theta) + \frac{d\sigma_1}{d\Omega}(\pi-\theta) \pm 2\mathrm{Re}[f(\theta)^* f(\pi-\theta)] \tag{7.279}$$

where $f(\theta)$ is a scattering amplitude if particles are distinguishable.

When the projectile and target is identical, one have to use fully symmetric(anti-symmetric) wave function and this changes the scattering amplitude and also cross section formula.

Fully symmetric(anti-symmetric) wave function is written as

$$\begin{aligned}\psi_{\pm}(\boldsymbol{r}) &= \frac{1}{\sqrt{2}}[\psi(\boldsymbol{r}) \pm P_{12}\psi(\boldsymbol{r})], \\ &= \frac{1}{\sqrt{2}}[\psi(\boldsymbol{r}) \pm \psi(-\boldsymbol{r})], \quad \text{if spin part is symmetric}\end{aligned} \tag{7.280}$$

where $\psi(\boldsymbol{r})$ is a usual solution treating projectile and target is distinguishable. (When solving Schrodinger equation without taking into account identical particle, one gets this solution $\boldsymbol{r}$.) For convenience, let us use spin-symmetric case and focus on the spatial part. Asymptotic form is

$$\psi_{\pm}^{(+)}(\boldsymbol{r}) = \phi_{pm}(\boldsymbol{r}) + \psi_{\pm}^{sc}(\boldsymbol{r}), \tag{7.281}$$

with

$$\phi_{\pm}(\boldsymbol{r}) \to \frac{1}{(2\pi)^{3/2}}\left[\frac{e^{i\boldsymbol{k}_0\cdot\boldsymbol{r}} \pm e^{-i\boldsymbol{k}_0\cdot\boldsymbol{r}}}{\sqrt{2}}\right] \tag{7.282}$$

$$\psi_{\pm}^{sc}(\boldsymbol{r}) \to \frac{1}{(2\pi)^{3/2}}\left[\frac{f(\theta) \pm f(\pi-\theta)}{\sqrt{2}}\right]\frac{e^{ikr}}{r} \tag{7.283}$$

Now there are two incident currents which changes the incident flux($J = \hat{z}\cdot j_{in}$). Since the opposite signs of the currents are compensated by the opposite orientation of normals , the two contributions are identical. In this way, one gets a factor 2 that cancels the factor $\frac{1}{2}$ from extra $1/\sqrt{2}$ in the normalization of $\phi_+(\boldsymbol{r})$. Thus, the incident flux is unchanged. The flux scattered onto the detector, we needs to change

$$|f(\theta)|^2 \to |\frac{f(\theta) \pm f(\pi-\theta)}{\sqrt{2}}|^2 = \frac{1}{2}|f(\theta) \pm f(\pi-\theta)|^2 \tag{7.284}$$

The factor 1/2 cancels with factor 2 from the flux. Thus, we get the differential cross section,

$$\frac{d\sigma_\pm}{d\Omega}(\theta) = \sigma_\pm(\theta) = |f_\pm(\theta)|^2 = |f(\theta) \pm f(\pi-\theta)|^2, \tag{7.285}$$

which gives interference term unlike classical case.

7.4.9 identical fermion with spin scattering

In case of identical fermion particles like proton-proton scattering, the differential cross section have to be

$$\frac{d\sigma}{d\Omega} = |f \pm P_{12} f|^2 \tag{7.286}$$

For specific L, S, T channel of fermions, we would have (For bosons, $1 + (-1)^l$ factor)

$$\begin{aligned} P_{12} f_{S'S,T',T}(\theta) &= (-1)^{S'+T'} f_{S',S,T',T}(\pi-\theta) = (-1)^{L'+S'+T'} f_{S',S,T',T}(\theta), \\ \frac{d\sigma}{d\Omega} &= |\sum (1-(-1)^{L'+S'+T'}) f_{L',S',T'}|^2. \end{aligned} \tag{7.287}$$

This implies that, for boson-boson (or fermion-fermion spin-symmetric) collisions , this factor doubles the contribution from even waves(odd waves) and eliminates those from odd waves(even waves).

Thus, if we put anti-symmetrization condition to "nuclear" amplitude,

$$f^A_{nuc}(\boldsymbol{k}', \boldsymbol{k}) = 4\pi \sum_{\alpha,\beta} \left(\sqrt{2}\epsilon_{LST}\sqrt{2}\epsilon_{L'S'T'}\right) e^{i\sigma_{L'}} \left(\frac{S_{\alpha\beta} - \delta_{\alpha\beta}}{2ik}\right) e^{i\sigma_L} Y_\alpha(\hat{\boldsymbol{k}'}) Y^*_\beta(\hat{\boldsymbol{k}}) * i^{-L'+L}, \tag{7.288}$$

where anti-symmetrization gives additional $\sqrt{2}\epsilon_{LST}$ and $\sqrt{2}\epsilon_{L'S'T'}$ factors with $\epsilon_{LST} = \frac{1}{2}(1 - (-1)^{L+S+T})$. On the other hand, anti-symmetric Coulomb scattering amplitude with spins becomes

$$f^A_C(\theta, S', S) = \left(f_C(\theta) + (-1)^{S'} f_C(\pi-\theta)\right) \delta_{S'S} \tag{7.289}$$

Thus, differential cross section becomes

$$\frac{d\sigma}{d\Omega} = |f^A_{nuc}(\theta) + f^A_C(\theta)|^2 \tag{7.290}$$

If we consider two identical nucleus with spin I scattering, Coulomb scattering part

$$f_C(\theta) = -\frac{e_1 e_2 \mu}{2k^2} \left(\sin\frac{\theta}{2}\right)^{-2} e^{2i(\sigma_0 - \eta \ln \sin\frac{\theta}{2})}, \tag{7.291}$$

Then, from $k^2 = 2\mu E_C = \mu E_{lab}$,one gets

$$\left(\frac{d\sigma}{d\Omega}\right)_C = |f_C(\theta) + (-1)^S f_C(\pi-\theta)|^2 = \left(\frac{Z^2 e^2}{2E_{lab}}\right)^2 \left[\frac{1}{(\sin\frac{\theta}{2})^4} + \frac{1}{(\cos\frac{\theta}{2})^4} + (-1)^S \frac{2\cos(2\eta \ln\tan\frac{\theta}{2})}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}}\right], \tag{7.292}$$

for a total spin $S = s_1 + s_2$ states.

In case of unpolarized cross section by summing and averaging for each S, one gets, for identical particle of spin I, [22]

$$\frac{d\sigma^{unpol}}{d\Omega}(\theta) = \frac{d\sigma}{d\Omega}(\theta) + \frac{d\sigma}{d\Omega}(\pi-\theta) + \frac{(-1)^{2I}}{2I+1} 2\mathrm{Re}[f(\theta)^* f(\pi-\theta)] \tag{7.295}$$

[22] Unpolarized case the average comes as

$$\frac{1}{(2I+1)^2}\sum_{m1,m2} |f_{m1m2}|^2 = \frac{1}{(2I+1)^2}\sum_{S=0}^{2I}\sum_{M=-S}^{S} |\langle Im_1 Im_2|SM\rangle|^2 |f_S|^2 = \frac{1}{(2I+1)^2}\sum_{S=0}^{2I}(2S+1)|f_S|^2 \tag{7.293}$$

Thus, Mott formula of unpolarized coulomb scattering is

$$(\text{Unpolarized case}) \quad \Rightarrow \quad \left(\frac{Z^2e^2}{2E_{lab}}\right)^2 \left[\frac{1}{(\sin\frac{\theta}{2})^4} + \frac{1}{(\cos\frac{\theta}{2})^4} + \frac{2(-1)^{2I}}{(2I+1)} \frac{\cos(2\eta\ln\tan\frac{\theta}{2})}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}}\right]. \tag{7.296}$$

For a scattering by nuclear interaction, let us consider simplest S-wave scattering case,

$$\begin{aligned} f_{nuc}(\theta) &= e^{i\delta_0}\frac{\sin\delta_0}{k}e^{2i\sigma_0} \text{ for S-wave, note Coulomb phase factor,} \\ \left(\frac{d\sigma}{d\Omega}\right)_{nuc} &= (\text{average over spin})|f_{nuc}(\theta) + (-1)^S f_{nuc}(\pi-\theta)|^2 = \frac{\sin^2\delta_0}{k^2} \end{aligned} \tag{7.297}$$

Following expression is from Bertulani's book. **But it Need to be checked.**

$$\left(\frac{d\sigma}{d\Omega}\right)_{nuc-C} = -\frac{1}{2}(\frac{e^2}{E_p})^2\frac{\sin\delta_0}{\eta}\left[\frac{\cos[\delta_0+\eta\ln\sin^2\frac{\theta}{2}]}{\sin^2\frac{\theta}{2}} + \frac{\cos[\delta_0+\eta\ln\cos^2\frac{\theta}{2}]}{\cos^2\frac{\theta}{2}}\right] \tag{7.298}$$

Thus, if $f_S = (-1)^S f$ as like above, we can use

$$\sum_{S=0}^{2I}(2S+1)(-1)^S = (-1)^{2I}(2I+1) \tag{7.294}$$

Chapter 8

Cross Section

In this note, I try to check the relation between phase shifts and differential cross section of np scattering.

In http://nn-online.org/, we can find both phase shift table and differential cross section table. So I am doing consistency check.

8.1 S-matrix phase shift parametrization

- For np scattering with total angular momentum J, there are 5 possible phase shifts except $J = 0$ case. In ${}^{(2S+1)}L_J$ notation,

$$\delta({}^1J_J), \quad \delta({}^3J_J), \quad \delta({}^3(J-1)_J), \quad \epsilon_J, \quad \delta({}^3(J+1)_J) \tag{8.1}$$

  where last three angles are for coupled channels and ϵ_J is a mixing angle.

- $J = 0$ case, there are only two phase shifts for ${}^1S_0$ and ${}^3P_0$ because there is no other partial waves possible.

- In "Stapp-" or "bar"- parametrization, coupled S-matrix between $l = j-1$ and $l = j+1$ states is written as

$$S = \begin{pmatrix} \cos 2\bar{\epsilon} e^{2i\bar{\delta}_1} & i \sin 2\bar{\epsilon} e^{i(\bar{\delta}_1+\bar{\delta}_2)} \\ i \sin 2\bar{\epsilon} e^{i(\bar{\delta}_1+\bar{\delta}_2)} & \cos 2\bar{\epsilon} e^{2i\bar{\delta}_2} \end{pmatrix} \tag{8.2}$$

- we can find all phase shifts at given energy in partial wave analysis at

  http://nn-online.org/NN/?page=nnphs1.

8.2 S-matrix and scattering amplitude

- M-matrix in spin space is related to the unpolarized differential cross section,

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{1}{(2s_1+1)(2s_2+1)} \sum_{m_1',m_2',m_1,m_2} |M_{m_1',m_2',m_1,m_2}(\boldsymbol{q'} \leftarrow \boldsymbol{q})|^2 \\ &= \frac{1}{(2s_1+1)(2s_2+1)} \sum_{S',M'} \sum_{S,M} |M_{S'M',SM}(\boldsymbol{q'} \leftarrow \boldsymbol{q})|^2. \end{aligned} \tag{8.3}$$

- the relation between M-matrix to S-matrix can be found in the paper, eq.(17) of (Stoks+PRC48(1993)792).

$$\begin{aligned} M_{s'm',sm}(\theta,\phi) &= \sum_{l,J,l'} \sqrt{4\pi(2l+1)} Y_{l',m-m'}(\theta,\phi) \\ &\quad \times C^{Jm}_{l'm-m',s'm'} i^{l-l'} C^{Jm}_{l0,sm} \frac{\langle l',s'|S^J-1|l,s\rangle}{2ik} \end{aligned} \tag{8.4}$$

where, k is the relative momentum. However, be careful that this expression does not take into account iso-spins. If we take into account iso-spin, there should be a iso-spin C-G coefficients in $M^{T',T}_{S'M',SM}$ and $[1-(-1)^{l+s+t}]$ factors for anti-symmetrization. So that pp and nn have additional factor but np the iso-spin projection and anti-symmtrization factor cancels.

- Differential cross section data (and other scattering observables) can be found at

  `http://nn-online.org/NN/?page=nnobs1b`

- By using above relations, we should be able to compute differential cross sections once phase shifts are given.

- Note that the $i^{-l'+l}$ factor in M-matrix equation is important. We may absorb this factor to S-matrix or Spherical Harmonics. However, in that case, the definition of S-matrix can change!

- eq.(2.115) in "The Quantum mechanical Few-body Problem" by Glockle reads

$$\begin{aligned} M_{s'm',sm}(\theta,\phi) &= \sum_{l,J,l'} \sqrt{4\pi(2l+1)} Y_{l',m'-m}(\theta,\phi) \\ &\quad \times C^{Jm}_{l'm-m',s'm'} i^{l-l'} C^{Jm}_{l0,sm} \frac{\langle l',s'|S^J-1|l,s\rangle}{2ik} \end{aligned} \tag{8.5}$$

Note that $Y_{l',m'-m}$ is used instead of $Y_{l',m-m'}$! However, this should be a typo.

- Actually I found eq.(8.5) from eq.(2.115) in "The Quantum mechanical Few-body Problem" by Glockle.

$$\begin{aligned} M^{st}_{m'_s,m_s} &= \frac{1}{iq} \sum_{Jll'} i^{-l'+l} C^{Jm_s}_{l'm_s-m'_s,sm'_s} Y_{l'm'_s-m_s}(\hat{q}) \\ &\quad \times (S^J_{l's,ls} - \delta_{l'l}) C^{Jm_s}_{l0,sm_s} \sqrt{\pi(2l+1)} [1-(-)^{l+s+t}] \end{aligned} \tag{8.6}$$

- In case of np scattering, physical amplitude is

$$M_{pn\to pn} = \frac{1}{2}(M^{t=1} + M^{t=0}). \tag{8.7}$$

Thus, last $[1-(-)^{l+s+t}]$ cancels with $\frac{1}{2}$ and sums unrestricted over l and l'. If we include iso-spin projection factor $\frac{1}{2}$, we have to keep $[1-(-)^{l+s+t}]$ factor too.

8.3 pp scattering case

In case of pp- scattering, the scattering amplitude is a sum of nuclear and Coulomb scattering. Also, note that the pp-scattering case, the nuclear scattering amplitude have to include coulomb phase shift factors.

$$M^{nuc}_{s'm',sm}(\theta,\phi) = \sum_{l,J,l'} \sqrt{4\pi(2l+1)} Y_{l',m-m'}(\theta,\phi) \times C^{Jm}_{l'm-m',s'm'} C^{Jm}_{l0,sm} \times i^{l-l'} (2\epsilon_{LST}\epsilon_{L'S'T'}) \left(e^{i\sigma_{L'}} \frac{\langle l', s'|S^J - 1|l, s\rangle}{2ik} e^{i\sigma_L} \right) \tag{8.8}$$

And the total scattering amplitude includes Coulomb scattering amplitudes

$$M_{S'M'SM}(\theta,\phi) = M^{nuc}_{s'm',sm}(\theta,\phi) + (f^C(\theta,\phi) + (-1)^S f^C(\pi-\theta,\phi))\delta_{S'S}\delta_{M'M} \tag{8.9}$$

where, $\epsilon_{LST} = \frac{1}{2}(1-(-1)^{L+S+T})$ and $(-1)^S$ term for Coulomb scattering amplitude is required because of the identical particle scattering.

Mathematica file("PWA_NN_scattering_crosssection") shows that the relation between phase shift and differential cross section.

8.4 total cross section

The differential cross section of identical particle can be obtained from previous equation. In case of distinct particle scattering, total cross section is

$$\sigma_{tot}(\boldsymbol{p}) = \int d\Omega_{\boldsymbol{p}'} \frac{d\sigma}{d\Omega}(\boldsymbol{p}' \leftarrow \boldsymbol{p}). \tag{8.10}$$

But, for identical particle scattering, we define

$$\sigma_{tot}(\boldsymbol{p}) = \frac{1}{2}\int d\Omega_{\boldsymbol{p}'} \frac{d\sigma}{d\Omega}(\boldsymbol{p}' \leftarrow \boldsymbol{p}). \tag{8.11}$$

[1]

8.5 N-D scattering case

In case of n-d scattering, the phase shifts and S-matrix are defined as such

[1] Question: does this apply to the np-scattering in isospin formalism too?

Chapter 9

Numerical Method

practical guideline: Numerical solution of wave function.

- Choice of step size: Choose step size h at least $h \leq 0.2/k$ or $0.2a$ (minimal diffuseness of potential).
- Choice of starting point: Because of centrifugal force, we have to start integration other than zero for $L \neq 0$. $R_{min} \geq 2.0Lh$ is a practical guide. (L 이 커지더라도, centifugal force가 너무 커지는 것을 방지)

  According to the Melkanoff's paper, conservative estimation is $R_{min} = int(\sqrt{l(l+1)/12}+1)*h$.
- Maximum partial wave to be included may be guided by $kR_{max} \simeq L_{max}$ where R_{max} may be determined from the sum of maximal radius and diffuseness parameter of potentials.

9.1 Numerical method

자 two-body 문제의 경우, bound-state는 wave function에 대한 homogeneous LS equation 이나, Schrodinger eq.을 풀면되고, scattering 문제의 경우는 t-matrix에 대한 LS equation을 풀거나, Schrodinger eq.을 풀면 된다. Scattering의 phase shift는 t-matrix와 S-matrix의 관계로부터 구하거나, scattering wave function으로 부터 구할 수 있다. 따라서, 문제는 LS eq.이나 Scrodinger eq.을 어떻게 풀 것인가 이다.

9.1.1 Configuration space

Configuration space에서의 계산은 LS eq.보다는 Sch. eq.을 푸는 것이 편리하고, 이 경우 Sch. eq.은 coupled 2 차 미방 이므로, 적절한 boundary condition이 주어지면 Runge-Kutta method 방식으로 푼 다음 boundary 에서 matching을 시켜 주면 된다. Scattering wave의 경우는 주어진 에너지에서 미방을 진행 시켜 나가면 되고, Bound state의 경우는 에너지 값을 변화 시켜가면서, 적절한 boundary condition을 만족하는 에너지를 찾는다. 따라서, 미방을 풀어도 되고, 미방을 matrix equation으로 바꾸어 풀 수도 있다.

일반적인 연립 2차 미분 방정식을 다음과 같이 생각하자.

$$\mathcal{D} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \dots \\ u_N(r) \end{pmatrix} = \begin{pmatrix} J_1(r) \\ J_2(r) \\ \dots \\ J_N(r) \end{pmatrix}, \tag{9.1}$$

With boundary conditions

$$u_i(r_{min}) = a_i,\ u_i(r_{rmax}) = b_i \text{ for i=1,N} \tag{9.2}$$

대부분의 경우 적당한 matching point 안쪽에서의 해 $u_i^{(<)}$ 는 boundary condition을 만족하도록 다음과 같이 쓸 수 있다.

$$\begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(<)} = \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(<)}_{(sp)} + c^{(1)} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(<)(1)}_{(hm)} + c^{(2)} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(<)(2)}_{(hm)} + \cdots + c^{(N)} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(<)(N)}_{(hm)} \tag{9.3}$$

만약, vector and matrix notation을 도입하면, 위 식은

$$\mathcal{D}\boldsymbol{u}(r) = \boldsymbol{J}(r) \tag{9.4}$$

로 쓸 수 있다.

여기서, 각 해는 다음과 같은 boundary condition을 이용하여 얻는다.

$$\boldsymbol{u}(r_{min}) = 0,\ \boldsymbol{u}'(r_{min}) = 0, \quad \text{with source term } \rightarrow \boldsymbol{u}^{(<)}_{(sp)}(r) \tag{9.5}$$

$$\begin{aligned} & u_i(r_{min}) = a_i,\ u_i'(r_{min}) = a_i',\ u_{j\neq i}(r_{min}) = 0,\ u_{j\neq i}'(r_{min}) = 0 \text{ without source term} \\ \rightarrow \quad & \boldsymbol{u}^{(<)(i)}_{(hm)}(r) \end{aligned} \tag{9.6}$$

matching point 안 쪽에서 위의 함수는 boundary condition을 만족하는 미분 방정식의 해임을 알 수 있다. [1] Unknown N constants $c^{(i)}$ have to be fixed by matching.

In a similar way, we can write the solution at the outside of matching point as,

$$\begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(>)} = \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(>)}_{(sp)} + d^{(1)} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(>)(1)}_{(hm)} + d^{(2)} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(>)(2)}_{(hm)} + \cdots + d^{(N)} \begin{pmatrix} u_1(r) \\ u_2(r) \\ \cdots \\ u_N(r) \end{pmatrix}^{(>)(N)}_{(hm)} \tag{9.7}$$

where each $\boldsymbol{u}^{(>)}(r)$ are obtained from boundary conditions

$$\boldsymbol{u}(r_{max}) = 0,\ \boldsymbol{u}'(r_{max}) = 0, \quad \text{with source term } \rightarrow \boldsymbol{u}^{(>)}_{(sp)}(r) \tag{9.8}$$

$$\begin{aligned} & u_i(r_{max}) = b_i,\ u_i'(r_{min}) = b_i',\ u_{j\neq i}(r_{max}) = 0,\ u_{j\neq i}'(r_{max}) = 0 \text{ without source term} \\ \rightarrow \quad & \boldsymbol{u}^{(>)(i)}_{(hm)}(r) \end{aligned} \tag{9.9}$$

Now, we have 2N unnkowns and 2N matching equations.

$$\boldsymbol{u}^{(<)}(r_{match}) = \boldsymbol{u}^{(>)}(r_{match}), \quad \boldsymbol{u}'^{(<)}(r_{match}) = \boldsymbol{u}'^{(>)}(r_{match}) \tag{9.10}$$

In case of scattering the asymptotic wave function contains unknowns, but basically number of unknowns are the same. For fixed input channel,β, set of wave functions have $u_{\alpha,\beta}(r) \simeq u_\alpha(r) = r^{l_\alpha+1}$ at short distance and $u_{\alpha,\beta}(r) \simeq u_\alpha(r) = j_\alpha(r)\delta_{\alpha\beta} - K_{\alpha\beta}n_\alpha(r)$ at long distance. Thus, now we will have additional $\boldsymbol{u}^{(>)}_{(hm)}(r)$ corresponding to $u_\alpha(r) = j_\alpha(r)\delta_{\alpha\beta}$ and coefficients of homogeneous equation solutions $d^{(i)}$ corresponds to $K_{i\beta}$.

[1] If a_i' are not specified, usually we can use $u(r)\ r^{l+1}$, $u'(r)\ (l+1)r^l$ for boundary condition.

다시 쓰자면 initial channel 을 α_i 라고 쓰고, 모든 coupled final channel을 $u_{\alpha\alpha_i}$ 라고 쓰면,

$$\sum_\beta \mathcal{D}_{\alpha\beta}\boldsymbol{u}_{\beta\alpha_i}(r) = \boldsymbol{J}_{\alpha\alpha_i}(r) \text{ for each } \alpha \text{ and for given } \alpha_i \tag{9.11}$$

이 된다. 예를 들어 bound state라면 $\alpha_i = (bound)$로 하나가 되고 , scattering 이라면 α_i 가 여러가지 incmoing channel이 된다. General solution은

$$u_{\alpha\alpha_i} = u^{(sp)}_{\alpha\alpha_i} + \sum_\beta c^{(\beta)}_{\alpha_i} u^{(\beta)(hm)}_\alpha \tag{9.12}$$

With initial boundary condition $u^{(wp)}_{\alpha\alpha_i}(r) = 0$ and $u^{(\beta)}_\alpha(r) = \delta_{\alpha\beta} r^{l_\alpha+1}$ at small r. where $u^{(\beta)}_\alpha$ are linearly independent solutions. However, if the integration goes too large value of r, the linearly independence breaks down. Thus, in that case, it is better to integrates from both ways and match at midpoints.

9.1.2 How to solve differential equation: Homogeneous equation

Let us consider uncoupled 2nd order differential equation,

$$\frac{d^2y(x)}{dx^2} + P(x)\frac{dy(x)}{dx} + G(x)y(x) = R(x). \tag{9.13}$$

If the exact boundary conditions, $y(0)$ and $y'(0)$, are known, the solution of differential equation can be easily obtained by numerical integration. However, in physics, usual boundary condition is given in two limits, $y(r \ll 1)$ and $y(r \gg 1)$. Because of centrifugal force, usually it is not practical to use boundary condition at $r = 0$.

General solution of homogeneous 2nd order differential equation can be written as linear combination of two independent solutions.

$$y(x) = c_1 y_1(x) + c_2 y_2(x) \tag{9.14}$$

Thus, we may find the correct solution either (1) by searching correct initial condition to satisfy the boundary condition,(shooting method: solve differential equations for each initial condition changes), or (2) by solve linear matching equation with two independent solutions (Solve two differential equation with different boundary condition and make linear combination to satisfy the boundary condition.).

Because even small error in the initial condition can be larger because it picks up irregular solution as integrating, it is better to use inward and outward matching. (this is not just a matter of choice of algorithm. Use matching always!)

In homogeneous equation, we can set arbitrary overall normalization at first and fix it after getting the solution.

We can obtain inner(or outward) solutions at matching point $y_<(R;c)$ and $y'_<(R;c)$ with c is a parameter for initial condition.

- Bound state problem: This case we can set $c = 1$ or any arbitrary value because overall normalization is not a problem. However, we have another unknown eigenvalue E. Thus, inner solutions becomes $y_<(R;E)$ and $y'_<(R;E)$. On the other hand, outer solution contains two unknowns $y_>(R;E) \sim A * e^{-B(E)r}$. But, it is easy to remove overall constant from matching equation. Thus, we only have one unknown E. If we define function $f(E) = \frac{y_<(R;E)}{y'_<(R;E)} - \frac{y_>(R;E)}{y'_>(R;E)}$, the eigen value can be found by solving non-linear equation $f(E) = 0$ using Newton-Rapson or any other method. Once eiegenvalue is known, normalization can be fixed.

- Scattering problem: This case also we can set $c = 1$ or any arbitrary value because overall normalization is not a problem. Because energy is given, there is no unknowns in inner solutions, $y_<(R)$ and $y'_<(R)$. However, scattering case, the outer solution have unknown phase shift or K-(S-) matrix, $y_>(R;s)$ and $y'_>(R;s)$. If we define $f(s) = \frac{y_<(R)}{y'_<(R)} - \frac{y_>(R;s)}{y'_>(R;s)}$ and solve $f(s) = 0$, we get s matrix.(It is a linear equation.) Once s is fixed, we can fix normalization of solution.

- Coupled equation: In coupled channel, first prepare two solutions by using two independent initial conditions. $y^{(1)}_{<,\alpha}$ and $y^{(2)}_{<,\alpha}$ can be obtained by two initial conditions $y^{(1)}_{<,1} = r, y^{(1)}_{<,2} = 0$ and $y^{(2)}_{<,1} = 0, y^{(2)}_{<,2} = r$. Outer solution also can be obtained in similar way, $y^{(1)}_{>,\alpha}$ and $y^{(2)}_{>,\alpha}$. Then try to find the correct linear combination by using matching condition.

9.1.3 How to solve differential equation: Inhomogeneous equation

일반적인 inhomogeneous equation의 해는 special solution과 homogeneous equation의 두 해의 linear combination 으로 생각할 수 있다.

$$y(x) = y_{sp}(x) + c_1 y_1(x) + c_2 y_2(x) \tag{9.15}$$

Numerical solution은 주어진 boundary 에서의 solution $y(x)$ 만을 주고, y_{sp}, y_1, y_2를 구분하지 못한다. 하지만, 두개의 boundary condition을 이용하여, $y^{(1)}(x) = y_{sp}(x) + c^{(1)}_1 y_1(x) + c^{(1)}_2 y_2(x)$ 과 $y^{(2)}(x) = y_{sp}(x) + c^{(2)}_1 y_1(x) + c^{(2)}_2 y_2(x)$ 를 얻을 수 있다.

우리가 풀고자하는 inhomogeneous equation, $\mathcal{D}u(r) = J(r)$ 이 있고, boundary condition, $u(r_{min}) = cr^{l+1}_{min}$과 $u(r_{max}) = \beta\exp(-\kappa r_{max})$ 을 만족하도록 하는 해를 찾고자 한다고 하자. [2] 그러면, 다음과 같이 푼다.

- 먼저 initial condition $u(r_{min}) = 0$ and $u'(r_{min}) = 0$ 을 이용하여 inhomogeneous equation $\mathcal{D}u(r) = J(r)$을 풀고 이 해를 $u_{in,<}$ 이라고 하자. [3]

- initial condition $u(r_{min}) = r^{l+1}_{min}$ 과 $u'(r_{min}) = (l+1)r^l_{min}$ 을 이용하여 homogeneous equation $\mathcal{D}u(r) = 0$ 을 풀고, 이 해를 $u_{hm,<}$ 이라고 하자.

- 여기서 $u(r_{min}) = cr^{l+1}_{min}$를 만족하는 임의의 inhomogeneous equation의 해는 $u_<(r) = u_{in,<}(r) + cu_{hm,<}(r)$ 로 쓸 수 있다고 할 수 있다. 이로 부터 matching point 에서의 값을 $u_<(r_{match}) = u_{in,<}(r_{match}) + cu_{hm,<}(r_{match})$ 로 쓸수 있다. [4]

- 비슷하게 $u(r_{max}) = 0$, $u'(r_{max}) = 0$으로 두고 구한 inhomogeneous equation $\mathcal{D}u(r) = J(r)$의 해를 $u_{in,>}$ 이라고 두고,

- boundary condition을 $u(r_{max}) = \beta\exp(-\kappa r_{max})$ 으로 두고 구한 homogeneous equation의 해를 $u_{hm,>}$ 이라고 두면,

- $u(r_{max}) = \beta\exp(-\kappa r_{max})$을 만족하는 inhomogeneous equation의 해는 $u_>(r) = u_{in,>}(r) + \beta u_{hm,>}(r)$ 이라고 쓸 수 있고, matching point 에서의 값을 $u_>(r_{match}) = u_{in,>}(r_{match}) + \beta u_{hm,>}(r_{match})$ 라고 쓸 수 있다.

[2] But, is it correct boundary condition at small r? $u(r_{min}) = cr^{l+1}_{min}$ comes from the assumption that centrifugal force is the most singular term at short distances. However, if the source term is more singular, shouldn't we use different boundary condition? Well, we may use other form of $u(r_{min})$.

[3] Can we always have the inhomogeneous equation solution satisfying initial condition $u(r_{min}) = 0$ and $u'(r_{min}) = 0$ regardless the form of equation? I think it is possible. $y = y_{sp} + c_1 y_1 + c_2 y_2 = 0$ and $y' = y'_{sp} + c_1 y'_1 + c_2 y'_2 = 0$ have solution c_1 and c_2 as long as determinant is not zero.

[4] 처음 시작 조건에 unknown constant c를 바꾸어가면서 $u(r_{min}) = cr^{l+1}_{min}$ 에 대한 inhomogeneous solution을 구하는 것과 비슷하지만, 이 경우에는 $u_<(r_{match})$ 의 c 에 대한 dependence가 non-linear 하게 된다.

- 그러면, matching point에서의 matching condition을 이용하여,

$$\begin{aligned} u_{in,<}(r_{match}) + cu_{hm,<}(r_{match}) &= u_{in,>}(r_{match}) + \beta u_{hm,>}(r_{match}), \\ u'_{in,<}(r_{match}) + cu'_{hm,<}(r_{match}) &= u'_{in,>}(r_{match}) + \beta u'_{hm,>}(r_{match}). \end{aligned} \tag{9.16}$$

  c와 β를 구할 수 있다.

scattring 문제일 경우에는 $u(r) \sim j(r) - Kn(r)$ 을 boundary condition으로 이용하여야 한다. 따라서, $u_>(r) = u_{in,>}(r) + u_{hm,>}(r;K)$ 로 $u_{hm,>}(r;K)$ 은 $u(r) \sim j(r) - Kn(r)$을 만족하는 homogeneous equation 의 해이다. 이 것은 다시 $u(r) = j(r)$ 과 $u(r) = n(r)$을 boundary condition으로 만족하는 homogeneous equation의 두 해 $u_{j,>}$과 $u_{n,>}$를 구해서, $u_>(r) = u_{in,>}(r) + u_{j,>}(r) - Ku_{n,>}(r)$ 로 쓰고, matching equation 을 이용해서 c와 K 를 구할 수 있다.

9.1.4 Coupled Equation

예를 들어서, 2개의 coupled equation을 생각해보자. l_1 and l_2 is different but coupled states. Equation for wave function becomes

$$\begin{aligned} &[T_{l'}(x) - E]\Psi^J_{l',l}(x) + \sum_\beta V^J_{l'\beta}(x)\Psi^J_{\beta l}(x) = 0, \quad l', l, \beta = l_1, l_2, \\ &T_l(x) = -\frac{1}{2\mu}\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{d}{dx}\right) + \frac{1}{2\mu}\frac{l(l+1)}{x^2}, \\ &V^J_{l'\beta}(x) = \langle \mathcal{Y}^J_{l'}|V(x)|\mathcal{Y}^J_\beta\rangle \end{aligned} \tag{9.17}$$

여기서, $\Psi^J_{l'l}(x)$ 는 ingoing wave가 처음에 l 상태에서 interaction에 의해 l' 상태가 되었을 때의 wave function 이다. 위식에서 하나의 주어진 $l = l_1$ 에대해, $\Psi^J_{l_1l_1}$와 $\Psi^J_{l_2l_1}$ 의 두개의 해가 존재한다. 만약, $\Psi^J_{l'l} = \frac{u_{l'l}}{x}$로 바꿔쓰면,

$$\frac{1}{x}\left[-\frac{1}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2\mu}\frac{l'(l'+1)}{x^2} - E\right]u^J_{l'l}(x) + \sum_\beta V^J_{l'\beta}\frac{u^J_{\beta l}(x)}{x} = 0 \tag{9.18}$$

가 된다. 여기서 일반적으로 해는 두 개의 real valued solution의 linear combination이다.

$$\Psi^J_{l'l}(x) = \alpha^{(1)}_l\Phi^{(1)}_{l'} + \alpha^{(2)}_l\Phi^{(2)}_{l'} \tag{9.19}$$

Matrix element of potential 이 complex 가 아닌 이상, 슈뢰딩거 식의 해는 real-valued 인 것만 풀면 된다. 그리고, complex normalization factor를 곱하는 것으로 complex velued wave function 을 만들 수 있다. 한편,scattering wave는 asymptotically

$$\begin{aligned} \Psi^J_{l'l}(x) &= \frac{1}{2}[\delta_{l'l}h^{(-)}_{l'}(kr) + S^J_{l'l}h^{(+)}_{l'}(kr)], \\ &= \frac{i}{2}[\delta_{l'l}h^{(2)}_{l'}(kr) - S^J_{l'l}h^{(1)}_{l'}(kr)] \end{aligned} \tag{9.20}$$

with $h^{(\pm)}_l(z) = j_l(z) \pm in_l(z)$, $h^{(1,2)}_l(z) = (-n_l \pm ij_l)$.
  로 써지므로, 4개의 unknown complex numbers , α_{ls}, β_{ls}, and two $S^J_{l'sls}$, 를 알아야한다. 여기서 spherical Hankel function 은

$$h^{(1,2)}_l(qx) \rightarrow \frac{exp[\pm i(qx - \frac{1}{2}l\pi)]}{qx} \tag{9.21}$$

이다. How can we determine those constants? (Which is equivalent to solving the problem.)

2차 미방의 해는 continuous 해야한다는 조건으로 부터, 각각 2개의 boundary condition을 준다. 따라서, 2개의 boundary condition만 주면 모든 coefficient가 결정된다. 예를 들어 we can obtain S-matrix for uncoupled case from

$$S = \frac{\Phi_{ls}(x_2)h_l^{(2)}(qx_1) - \Phi_{ls}(x_1)h_l^{(2)}(qx_2)}{\Phi_{ls}(x_2)h_l^{(1)}(qx_1) - \Phi_{ls}(x_1)h_l^{(1)}(qx_2)} \tag{9.22}$$

여기서, regular solution Φ and analytically known hankel function $h_l^{(1,2)}$ at two points x_1, x_2가 알려지면, S-matrix가 얻어진다. Regular solution의 경우, $\Phi(r=0)$ 와 Logarithmic derivative continuation condition $\Phi'(r=r_N)/\Phi(r=r_N)$ 에 의해 solution이 결정된다.(Normalization은 중요하지 않음.) Coupled equation의 경우에는 위 식에 해당하는 식을 따로 이용해야 한다. Coupled equation의 경우 어떻게 해야할까?

좀 더 일반적으로 생각해 보자. M개의 연립된 N차 미분 방정식을 생각해 보자. 이 때, 필요한 boundary condition의 개수는 N*M 개가 된다. 따라서, 문제에서 N*M개의 independent boundary condition을 주면, N*M개의 linear independent solution이 얻어지고, 이 들의 combination에 의해 원하는 boundary condition을 만족하는 solution을 얻을 수 있다.

$$\Psi_{\alpha,\beta} = \sum_a M_{\alpha(a)}\Psi_\beta^{(a)}, \tag{9.23}$$

여기서 $\Psi_\beta^{(a)}$ 는 solution with quantum number β from (a) 번째 boundary condition. 이것은 inhomogeneous equation의 경우도 마찬가지 이다. 2차 미방이 2개의 homogeneous solution을 가진다면, 일반적인 해는 항상 $ah_1 + bh_2$ 로 쓸 수 있고, inhomogeneous equation의 경우엔 일반적인 해는 언제나 $ah_1 + bh_2 + h_{sp}$ 로 쓸 수 있다. 우리가 임의의 independent boundary condition 을 주어 두 해 x_1 과 x_2 을 얻었다면, 이들도 반드시 위 꼴로 써질 수 있다. 즉, $a'x_1 + b'x_2 = ah_1 + bh_2 + h_{sp}$ 이 되게 된다. 따라서 두 해 x_1,x_2 를 이용하여 원하는 boundary condition을 만족하는 solution 을 얻으면 이것은 h_1, h_2, h_{sp} 을 이용하여 구하는 것과 마찬가지 이다.

K-matrix

일반적으로 Wave function과 S-matrix 는 complex number 이다. 하지만, numerical solution은 real number 로 구하는 것이 편하다. Real matrix K를 도입하여, define Real valued solution $\hat{R}$ such that

$$\begin{aligned}
\Psi_{l',l}(x) &= R_{l',l}(x) \equiv \hat{R}_{l',\beta}(\frac{1+\hat{S}}{2})_{\beta,l} = \hat{R}_{l',\beta}(1-i\hat{K})^{-1}_{\beta,l}, \\
\hat{R}_{\alpha'\alpha}(k,r) &\to \left(\delta_{\alpha'\alpha}j_{L'}(kr) - \hat{K}_{\alpha'\alpha}n_{L'}(kr)\right)
\end{aligned} \tag{9.24}$$

Let us defined several matrix notations,

$$\begin{aligned}
(\hat{R})_{l'l} &= (\hat{J})_{l'l} - (\hat{N})_{l'\tilde{l}}(\hat{K})_{\tilde{l}l}, \\
(\hat{J})_{l'l} &\equiv j_{l'}(kr)\delta_{l'l}, \quad (\hat{N})_{l'l} \equiv n_{l'}(kr)\delta_{l'l}, \\
(\hat{\Phi})_{l'l} &\equiv \Phi_{l'}^{(l)}, \\
(\hat{\alpha})_{l'l} &\equiv \alpha_l^{(l')},
\end{aligned} \tag{9.25}$$

then in matrix equation,

$$\hat{R} = \hat{J} - \hat{N}\hat{K} = \hat{\Phi}\hat{\alpha} \tag{9.26}$$

If we put another point or derivative of wave function,

$$\hat{R}' = \hat{J}' - \hat{N}'\hat{K} = \hat{\Phi}'\hat{\alpha} \tag{9.27}$$

solution is [5]

$$
\begin{aligned}
\hat{K} &= (\hat{\Phi}'^{-1}\hat{N}' - \hat{\Phi}^{-1}\hat{N})^{-1}(\hat{\Phi}'^{-1}\hat{J}' - \hat{\Phi}^{-1}\hat{J}) \\
&= (\hat{N}' - \hat{\Phi}'\hat{\Phi}^{-1}\hat{N})^{-1}(\hat{J}' - \hat{\Phi}'\hat{\Phi}^{-1}\hat{J}), \\
\hat{\alpha} &= (\hat{N}'^{-1}\hat{\Phi}' - \hat{N}^{-1}\hat{\Phi})^{-1}(\hat{N}'^{-1}\hat{J}' - \hat{N}^{-1}\hat{J}) \\
&= (\hat{\Phi}^{-1})(\hat{J} - \hat{N}\hat{K}) \qquad (9.28)
\end{aligned}
$$

Once $\hat{K}$ is obtained,

$$
\begin{aligned}
\hat{R}(x) &= \hat{\Phi}(x)\hat{\alpha}, \\
R_{l'l}(x) &= \hat{\Phi}_{l'\beta}(x)(\hat{\alpha}(1-i\hat{K})^{-1})_{\beta l}, \\
\hat{S} &= (1-i\hat{K})^{-1}(1+i\hat{K}) \qquad (9.29)
\end{aligned}
$$

으로 S-matrix 와 complex wavefunction을 구할 수 있다. However, $\hat{J}$, $\hat{N}$,$\hat{J}^{-1}$ and $\hat{N}^{-1}$ may be numerically unstable at asymptotes.

Very low energy limit

For the case of very low energy, we have to use asymptotic form of spherical Bessel functions. We can rewrite the boundary condition as

$$
\frac{u_{l'l}(r)}{k^{l'}} = \sum_\beta \frac{1}{k^{l'}}\phi_{l'}^{(\beta)}\alpha_{(\beta)l} = \left(\delta_{l'l}\frac{rj_{l'}(kr)}{k^{l'}}\right) - \left(\delta_{l'l''}k^{l'+1}rn_{l'}(kr)\right)\left(\frac{K_{l''l}}{k^{2l''+1}}\right). \qquad (9.30)
$$

Let us define

$$
\begin{aligned}
(\tilde{u})_{l'l}(r) &\equiv u_{l'l}(r)/k^{l'}, \quad (\tilde{K})_{l'l} \equiv K_{l'l}/k^{2l'+1}, \\
(\phi)_{l'\beta}(r) &\equiv \phi_{l'}^{(\beta)}(r), \quad (\alpha)_{\beta l} \equiv \alpha_{(\beta)l}, \\
(\tilde{d})_{l'l} &\equiv \delta_{l'l}\frac{1}{k^{l'}}, \\
(\tilde{J})_{l'l}(r) &\equiv \delta_{l'l}\frac{krj_{l'}(kr)}{k^{l'+1}} \to \delta_{l'l}\frac{r^{l'+1}}{(2l'+1)!!} \\
(\tilde{N})_{l'l}(r) &\equiv \delta_{l'l}k^{l'}(kr)n_{l'}(kr) \to -\frac{(2l'-1)!!}{r^{l'}}\delta_{l'l} \qquad (9.31)
\end{aligned}
$$

Here note that we cannot redefine $\frac{1}{k^{l'}}\alpha_{(\beta)l} \neq \tilde{\alpha}_{(\beta)l}$ because it depends on l'. And if we use derivative of wave function as a boundary condition, let us define additionally,

$$
\begin{aligned}
(\phi')_{l'\beta} &\equiv \frac{d}{dr}\phi_{l'}^{(\beta)}, \\
(\tilde{J}')_{l'l} &\equiv \frac{d}{dr}(\tilde{J})_{l'l} = \delta_{l'l}\frac{1}{k^{l'}}\frac{d}{d(kr)}[(kr)j_{l'}(kr)] \to \delta_{l'l}\frac{(l'+1)r^{l'}}{(2l'+1)!!}, \\
(\tilde{N}')_{l'l} &\equiv \frac{d}{dr}(\tilde{N})_{l'l} = \delta_{l'l}k^{l'+1}\frac{d}{d(kr)}[(kr)n_{l'}(kr)] \to \delta_{l'l}\frac{(2l'-1)!!(l')}{r^{l'+1}} \qquad (9.32)
\end{aligned}
$$

Thus, we have to solve matrix equation,

$$
\begin{aligned}
(\tilde{d})(\phi)(\alpha) &= (\tilde{J}) - (\tilde{N})(\tilde{K}), \\
(\tilde{d})(\phi')(\alpha) &= (\tilde{J}') - (\tilde{N}')(\tilde{K}) \qquad (9.33)
\end{aligned}
$$

[5] Be careful that $\hat{\Phi}$ corresponds to $\hat{u}/x$. Thus if we use derivative of $\hat{u}$, there can be other factors. And again, if we use derivative of spherical Bessel functions, we have to note that argument of Bessel functions are kx.

Note that $\tilde{d}$, $\tilde{J}$, $\tilde{N}$, $\tilde{J}'$, and $\tilde{N}'$ are diagonal, thus they commutes with each other. Thus, multiplying $\tilde{d}^{-1}$ and $\tilde{d}$ to left- and right-side, equation becomes

$$\begin{aligned}(\phi)(\alpha)(\tilde{d}) &= (\tilde{J}) - (\tilde{N})(\mathcal{K}), \\ (\phi')(\alpha)(\tilde{d}) &= (\tilde{J}') - (\tilde{N}')(\mathcal{K}),\end{aligned} \tag{9.34}$$

where,

$$(\mathcal{K})_{l'l} \equiv \left[\tilde{d}^{-1}\tilde{K}\tilde{d}\right]_{l'l} = k^{l'}\frac{K_{l'l}}{k^{2l'+1}}\frac{1}{k_l} = \frac{K_{l'l}}{k^{l'+l+1}} \tag{9.35}$$

Thus, we can obtain

$$\begin{aligned}\mathcal{K} &= (\tilde{N}' - (\phi')(\phi^{-1})\tilde{N})^{-1}(\tilde{J}' - (\phi')(\phi^{-1})\tilde{J}), \\ (\alpha\tilde{d}) &= (\phi)^{-1}(\tilde{J} - \tilde{N}\mathcal{K})\end{aligned} \tag{9.36}$$

Once obtained, $\mathcal{K}$ and $(\alpha\tilde{d})$, we can get K-matrix and wave function by

$$\begin{aligned}K_{l'l} &= k^{l'+l+1}\mathcal{K}_{l'l}, \\ \frac{u_{l'l}(r)}{k^l} &= \sum_\beta \phi_{l'(\beta)}(\alpha\tilde{d})_{(\beta)l}\end{aligned} \tag{9.37}$$

다시 정리하자면, low energy limit을 생각할 때는, 원래의 matching equation,

$$\frac{u_{l'l}}{r} = \sum \frac{\phi_{l'}^{(n)}}{r}c_l^{(n)} = \delta_{l'l}j_l(kr) - K_{l'l}n_l(kr), \tag{9.38}$$

보다는 다음과 같은 matching equation을 이용하는 것이 편리하다. $\phi_{l'}^{(n)}$ 을 homogeneous equation의 solution이라고 할 때,

$$\frac{u_{l'l}}{k^l} = \sum_n \phi_{l'}^{(n)}\bar{c}_l^{(n)} = \delta_{l'l}\bar{j}_{l'} - \bar{K}_{l'l}\bar{n}_{l'}, \tag{9.39}$$

을 matching equation으로 $\bar{c}_l^{(n)}$ 과 $\bar{K}_{l'l}$을 구한다. 여기서,

$$\begin{aligned}\bar{j}_{l'}(r) &\equiv \frac{krj_{l'}(kr)}{k^{l'+1}}, \\ \bar{n}_{l'}(r) &\equiv k^{l'}(kr)n_{l'}(kr), \\ \bar{K}_{l'l} &\equiv \frac{K_{l'l}}{k^{l'+l+1}}, \\ \bar{c}_l^{(n)} &\equiv \frac{c_l^{(n)}}{k^l}.\end{aligned} \tag{9.40}$$

을 이용하여, 원래의 $c_l^{(n)}$ 과 $K_{l'l}$을 구할 수 있다. $\bar{j}_{l'}(kr)$, $\bar{n}_{l'}(kr)$, $\bar{K}_{l'l}$ 은 매우 작은 k value의 경우에도 잘 정의 된다.

하지만, inhomogeneous equation의 경우에는

$$\frac{u_{l'l}}{k^l} = \frac{\hat{u}_{l'l}^{(sp)}}{k^l} + \sum_n \phi_{l'}^{(n)}\bar{c}_l^{(n)} = \delta_{l'l}\bar{j}_{l'} - \bar{K}_{l'l}\bar{n}_{l'} \tag{9.41}$$

이고, $\bar{K}$ 는 $u_{l'l}^{sp}/k^l$ 이 잘 정의되는 경우에만 존재한다. (아마도 $u_{l'l}^{sp} \sim k^l$ 으로 예상할 수 있겠지만) 따라서, 이 경우에는 양쪽에 k^l 을 곱한 것을 계산하는 것이 나을지도...

In a similar way, Coulomb scattering case, we can use matching equation,

$$\frac{u_{l'l}}{k^l} = \sum_n \phi_{l'}^{(n)} \bar{c}_l^{(n)} = \bar{F}_{l'}(\eta,\rho)\delta_{l'l} - \bar{K}_{l'l}(-\bar{G}_{l'}(\eta,\rho)) \tag{9.42}$$

with

$$\begin{aligned} \bar{F}_{l'}(\eta,\rho) &\equiv \frac{F_{l'}(\eta,\rho)}{k^{l'+1}}, \\ \bar{G}_{l'}(\eta,\rho) &\equiv k^{l'} G_{l'}(\eta,\rho), \\ \bar{K}_{l'l} &\equiv \frac{K_{l'l}}{k^{l'+l+1}} \end{aligned} \tag{9.43}$$

Once K is obtained, S can be obtained with the same relation from K. However, there is an additional Coulomb phase factor for full complex wave function.

9.1.5 Bound state case

Bound state의 경우에는, wave function이 exponential 하게 감소해야 한다는 조건을 만족해야 하는데, 이 때 방정식의 E 는 unknown 이다. 임의의 E값에 대해서 (또는 $|q|$ 값에 대해서, $E = (i|q|)^2 < 0$ 2개의 regular solution을 풀 경우, 각각은 매우 먼 거리에서 exponential 하게 increasing 하는 해와 decreasing 하는 해를 모두 가진다.

$$\Phi_{l's}^{(i)} \to a_{l's}^{(i)} h_{l'}^{(2)}(i|q|x) + b_{l's}^{(i)} h_{l'}^{(1)}(i|q|x) \tag{9.44}$$

여기서 $a_{l's}$와 $b_{l's}$는 unknown 값이고, spherical Hankel function들은 $i|q|x$ 의 함수로 $h^{(1)}(i|q|x)$는 decreasing, $h^{(2)}(i|q|x)$는 increasing 함수 이다. 따라서, linear combination of the physical state는 asymptotic 하게

$$\Psi_{l's}^J(x) = (\alpha a_{l's}^{(1)} + \beta a_{l's}^{(2)}) h_{l'}^{(2)}(i|q|x) + (\alpha b_{l's}^{(1)} + \beta b_{l's}^{(2)}) h_{l'}^{(1)}(i|q|x) \tag{9.45}$$

로 쓸 수 있다. 이 때, wave function이 asymptotic 하게 감소해야 한다는 조건으로 부터,(square integrability condiion)

$$\alpha a_{l's}^{(1)} + \beta a_{l's}^{(2)} = 0 \tag{9.46}$$

또는

$$\begin{vmatrix} a_{l_1 s}^{(1)} & a_{l_1 s}^{(2)} \\ a_{l_2 s}^{(1)} & a_{l_2 s}^{(2)} \end{vmatrix} = 0 \tag{9.47}$$

이라는 조건이 얻어진다. 여기서 a vaue들은 regular solution $\Phi^{(i)}$ 의 numerical asymptotic value 를 asymptotic form과 matching 해서 얻어진다. 이 때 matching 을 origin 에서 바깥쪽으로만 가서, asymptotic form과 matching을 하기 보다는 양쪽에서 진행하여, 포텐셜의 중간에서 matching을 하는 것이 좋다.

9.1.6 Coupled channel bound state in reaction theory

Suppose a nuclei can be described as a core plus a valence particle. And the core can be excited with couplings with other states. Then, the full solution of bound state will be

$$|\psi\rangle = \sum_i \frac{\chi_i(r)}{r} |i\rangle \tag{9.48}$$

where R is a distance between core and valence particle, $|i\rangle$ contains the core state and angular information of valence particle, $\chi_i(r)$ is a core-valence wave relative function. We would like to obtain $\chi_i(r)$ with several core states $|i\rangle$. If we write the total energy of nucleus is E, core excitation energy ϵ_i, (Bound state의 경우, $E-\epsilon_i$ will be a binding energy. Scattering 의 경우 $E-\epsilon_i$ is a channel energy) and the projection of interaction $\hat{V}_{ij}(r) = \langle i|\hat{V}(\vec{r})|j\rangle$ which imply angular integration, the coupled equation becomes

$$\frac{d^2}{dr^2}u_i(r) - \frac{l_i(l_i+1)}{r^2}u_i(r) + (-\frac{2\mu}{\hbar^2})(\hat{V}_{ii}(r)+\epsilon_i - E)u_i(r) + \sum_{j\neq i}(-\frac{2\mu}{\hbar^2})\hat{V}_{ij}(r)u_j(r) = 0 \qquad (9.49)$$

In many case, either we may want to find eigenvalue E or find a appropriate potential to reproduce known binding energy E.

If we define fixed and variable potential parts as : (1) To find a eigenvalue for given potential, set

$$\begin{aligned} U_{ij}(r) &= -\frac{2\mu}{\hbar^2}\hat{V}_{ij}(r) - \delta_{ij}\frac{2\mu}{\hbar^2}(\epsilon_i - E_0), \\ \omega V_{ij}(r) &= -\delta_{ij}\frac{2\mu}{\hbar^2}(E-E_0) = -\delta_{ij}\frac{2\mu}{\hbar^2}\omega E_0 \end{aligned} \qquad (9.50)$$

(2) To find appropriate potential depth for a given energy, set

$$\begin{aligned} U_{ij}(r) &= -\delta_{ij}\frac{2\mu}{\hbar^2}(\epsilon_i - E), \\ \omega V_{ij}(r) &= \omega(-\frac{2\mu}{\hbar^2})\hat{V}_{ij}(r) \end{aligned} \qquad (9.51)$$

or $\hat{V}_{ij}$ can be separated into fixed parts and variable parts depending on the choice of variation. (Coulomb potential should be included in $U_{ij}(r)$)

Then, in both case, the equation becomes finding eigenvalue ω for equations

$$\frac{d^2}{dr^2}u_i(r) - \frac{l_i(l_i+1)}{r^2}u_i(r) + \sum_j (U_{ij}(r) + \omega V_{ij}(r))u_j(r) = 0. \qquad (9.52)$$

with boundary conditions

$$\begin{aligned} u_i(a) &= p_i W_{-\eta_i, l_i+\frac{1}{2}}(-2k_i a), \\ u_i(a+\delta R) &= p_i W_{-\eta_i, l_i+\frac{1}{2}}(-2k_i(a+\delta R)), \\ u_i(0) &= 0. \quad p_i \text{ are unknown yet.} \end{aligned} \qquad (9.53)$$

with

$$\begin{aligned} k_i^2 &\equiv \kappa_i^2 + \theta\omega, \quad \eta_i = \frac{\nu_i}{2k_i}, \quad \nu_i = \frac{2\mu Z_1 Z_2 e^2}{\hbar^2}, \\ \kappa_i^2 &\equiv \frac{2\mu|E-\epsilon_i|}{\hbar^2} \end{aligned} \qquad (9.54)$$

where θ is an asymptotic component of all the diagonal $V_{ii}(r)$.

Let the trial solutions of inside and outside as

$$\phi_i(r) = \begin{cases} \sum_j b_j f_{i,j}^{in}(r) \text{ for } r \le r_m \\ \sum_j c_j f_{i,j}^{out}(r) \text{ for } r \ge r_m \end{cases} \qquad (9.55)$$

With boundary conditions,

$$\begin{aligned} f_{i,j}^{in}(h) &= \delta_{ij}\frac{h^{l_i+1}}{(2l_i+1)!!}, \\ f_{i,j}^{out}(a) &= \delta_{ij}W_{-\eta_i, l_i+\frac{1}{2}}(-2k_i a). \end{aligned} \qquad (9.56)$$

We may set $c_1 = 1$. Then the $2M-1$ unknowns can be fixed by solving $2M-1$ matching conditions. ($u_i^{in}(r_m) = u_i^{out}(r_m)$ for $i = 1, ..M$, $u_i^{'in}(r_m) = u_i^{'out}(r_m)$ for $i = 2, ..M$) Remaining matching condition for $u_1'(r_m)$ can be used as a fitting function.

$$f(\omega) = u_1(r_m)(u_1^{'in}(r_m) - u_1^{'out}(r_m)) \tag{9.57}$$

One trick is to convert this function as a integral,

$$\begin{aligned} & \int_0^R \frac{d}{dr}(u_1 u_1') = \int_0^{r_m} \frac{d}{dr}(u_1 u_1') + \int_{r_m}^R \frac{d}{dr}(u_1 u_1') \\ = \;& u_1(r_m)u_1^{'in}(r_m) - u_1(r_m)u_1^{'out}(r_m) + u_1^{out}(R)u_1^{'out}(R), \\ & f(\omega) = \int_0^R \frac{d}{dr}(u_1 u_1') - u_1^{out}(R)u_1^{'out}(R) \end{aligned} \tag{9.58}$$

And from the Schrodinger equation,

$$\int_0^R dr \frac{d}{dr}(u_i u_i') - \int_0^R dr u_i' u_i' - \int_0^R dr \frac{l_i(l_i+1)}{r^2} u_i u_i + \sum_j \int_0^R u_i (U_{ij} + \omega V_{ij}) u_j = 0 \tag{9.59}$$

Thus, one may adopt a Newton's method or secant method for the next trial value of ω. Or, one may get following equation by integrating Schrodinger equation,

$$\begin{aligned} f(\omega) \;=\; & \int_0^R dr u_1' u_1' - \sum_{i \neq 1} \int_0^R dr u_i \frac{d^2}{dr^2} u_i + \sum_i \int_0^R dr \frac{l_i(l_i+1)}{r^2} u_i u_i \\ & - \sum_{ij} \int_0^R dr u_i (U_{ij} + \omega V_{ij}) u_j \end{aligned} \tag{9.60}$$

Thus, we may approximate (? only considering explicit ω dependence in the right hand side? But u will implicitly depends on ω)

$$\frac{d}{d\omega} f(\omega) \simeq - \sum_{ij} \int_0^R dr u_i V_{ij} u_j. \tag{9.61}$$

and get ,

$$\delta\omega \sum_{ij} \int_0^R u_i(r) V_{ij}(r) u_j(r) dr = u_1(r_m)[u_1^{'out}(r_m) - u_1^{'in}(r_m)] \tag{9.62}$$

However, I am not sure whether it is advantageous to use this than usual secant method

$$\omega_{n+1} = \frac{f(\omega_n)\omega_{n-1} - f(\omega_{n-1})\omega_n}{f(\omega_n) - f(\omega_{n-1})} \tag{9.63}$$

9.1.7 Numerov method

주어진 initial state는 바뀌지 않으므로 matrix notation 을 도입하면,

$$\begin{aligned} & \hat{\Psi}^{(l)}(x) = [\Psi^J_{l'l}(x)] = \frac{1}{x} \hat{u}^{(ls)}(x), \quad \hat{u}^{(ls)}(x) = \begin{pmatrix} u_{l_1,l}(x) \\ u_{l_2,l}(x) \end{pmatrix}, \\ & \sum_\beta \left[\frac{d^2}{dx^2} - \frac{l'(l'+1)}{x^2} + 2\mu E \right] \delta_{l'\beta} \hat{u}_\beta^{(ls)}(x) + \sum_\beta (-2\mu) V^J_{l'\beta} \hat{u}_\beta^{(ls)}(x) = 0 \end{aligned} \tag{9.64}$$

where $\mathcal{V}^J_{l'sls} \equiv \langle \mathcal{Y}^{JM}_{l's} | V | \mathcal{Y}^{JM}_{ls} \rangle$. 이 때, 두 regular solution 은 서로 다른 두개의 boundary condition을 $\hat{u}^{(ls)}(x)$ 에 주는 것으로 구할 수 있다.

Numerical 하게 미방을 푸는 방법으로는 Numerov 방법이 좋다. R.-K. ODE 는 general problem,

$$\frac{d}{dt}\boldsymbol{y}(t) = \boldsymbol{F}(\boldsymbol{y}, \dot{\boldsymbol{y}}, t) \tag{9.65}$$

form 으로 code에서는 $\boldsymbol{F}(\boldsymbol{y}, \dot{\boldsymbol{y}}, t)$ 가 $\boldsymbol{y}, \dot{\boldsymbol{y}}$를 포함하기 때문에 $\boldsymbol{y}$ 를 구하면서 $\boldsymbol{F}$를 매번 다시 계산해야 하기 때문에, $\boldsymbol{F}$를 구하는 subrouine이나 function을 정의해야 한다. 하지만, Numerov의 경우는 특별히

$$\frac{d^2}{dt^2}\boldsymbol{y}(t) = \boldsymbol{f}(t)\boldsymbol{y}(t) \tag{9.66}$$

꼴의 문제로 $\boldsymbol{f}(t)$를 한번에 모두 구해서 input 으로 사용할 수 있다. 특히, $\boldsymbol{f}(t)$중에 특정 변수(l,s,j 등)에 의존하지 않는 부분이 있는 경우에는 저장된 값을 여러 경우에 이용할 수 있다.

$$\begin{aligned}
\frac{d^2}{dx^2}\hat{u}^{(ls)}(x) &= \hat{\mathcal{F}}(x)\hat{u}^{(ls)}(x), \\
\hat{\mathcal{F}}(x)_{l'l} &= \left[\frac{l'(l'+1)}{x^2}\delta_{l'l} + 2\mu\hat{V}^J_{l'l}(x) - 2\mu E\delta_{l'l}\right]
\end{aligned} \tag{9.67}$$

형태가 되고, 여기서 $\mathcal{F}$는 centrigugal and energy terms and potential V를 포함한다.

Cowell method case,

$$u_{i+1} = \frac{[2 + 10\frac{h^2}{12}F_i]u_i - [1 - \frac{h^2}{12}F_{i-1}]u_{i-1}}{1 - \frac{h^2}{12}F_{i+1}} \tag{9.68}$$

with $u_0 = 0$, $u_1 = c$(arbitrary constant). But this case, denominator can be very small sometimes. Thus, to avoid such numerical problem, one may use modified Numerov method as follows.

Define auxiliary quantity

$$\xi(x) \equiv [1 - \frac{h^2}{12}\mathcal{F}(x)]u(x)$$

and let $F_i = \mathcal{F}(x_i)$, $u_i = u(x_i)$, $\xi_i = \xi(x_i)$,

$$\xi(i+2) = \left[2 + h^2\hat{\mathcal{F}}(i+1)[\hat{I} - \frac{h^2}{12}\hat{\mathcal{F}}(i+1)]^{-1}\right]\xi(i+1) - \xi(i) \tag{9.69}$$

or

$$\xi(i+1) = 12u_i - 10\xi(i) - \xi(i-1) \tag{9.70}$$

형태가 된다. 따라서, $\xi(i+1)$ 을 $\xi(i)$, $\xi(i-1)$ 로부터 얻으면, u_{i+1}을 $\xi(i+1)$로 부터 구할 수 있다. (각 i에서 $\xi(i)$와 u_i를 구하면, 두번째 식이 더 쉬워 보인다.)

With initial values (arbitrary constant c),

$$\begin{aligned}
&\xi_0 = 0, \quad \xi_1 = c, \quad \text{for } l \neq 1, \\
&\xi_0 = -\frac{1}{6}c, \quad \xi_1 = c, \quad \text{for } l = 1
\end{aligned} \tag{9.71}$$

[6] Original solution can be reverted from $u(x) = \xi(x)/[1 - \frac{h^2}{12}\mathcal{F}(x)]$ In coupled equation case, 2 개의 regular solution은

$$u^{(1)}(r \to 0) = \begin{pmatrix} r \\ 0 \end{pmatrix}, \text{ or } u^{(2)}(r \to 0) = \begin{pmatrix} 0 \\ r \end{pmatrix} \tag{9.72}$$

[6]The reason is because $u(r \to 0) \sim r^{l+1}$, and $F(r \to 0) = \frac{l(l+1)}{r^2}$ results $F(r)u(r) \to 0$ for $l \neq 0$, but $F(r)u(r) \to 2$ for $l = 1$.

로 구할 수 있다.

따라서, Coupled differential equation의 경우에 matrix inversion이 필요하다.

In case of inhomogeneous equation

$$\frac{d^2y}{dt^2} = f(t)y(t) + g(t) \tag{9.73}$$

we have

$$y_{i+1}(1-\frac{h^2}{12}f_{i+1}) - 2y_i(1+\frac{5h^2}{12}f_i) + y_{i-1}(1-\frac{h^2}{12}f_{i-1}) = \frac{h^2}{12}(g_{i+1}+10g_i+g_{i-1}) + O(h^6) \tag{9.74}$$

Derivation: From the taylor expansion,

$$\begin{aligned} y(x+h) &= y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \frac{h^3}{3!}y^{(3)}(x) + \frac{h^4}{4!}y^{(4)}(x) + \ldots, \\ y(x-h) &= y(x) - hy'(x) + \frac{h^2}{2!}y''(x) - \frac{h^3}{3!}y^{(3)}(x) + \frac{h^4}{4!}y^{(4)}(x) + \ldots, \\ y(x+h)+y(x-h) &= 2y(x) + h^2y^{(2)}(x) + \frac{h^4}{12}y^{(4)}(x) + \ldots \end{aligned} \tag{9.75}$$

Replacing

$$\begin{aligned} y^{(2)}(x) &= f(x)y(x) + g(x), \\ y^{(4)}(x) &= \frac{d^2}{dx^2}(f(x)y(x)+g(x)) \\ &\simeq \frac{1}{h^2}(f(x+h)y(x+h) + g(x+h) - 2(f(x)y(x)+g(x)) + f(x-h)y(x-h) + g(x-h)) \end{aligned} \tag{9.76}$$

gives the Numerov's method.

9.1.8 Short distance behavior in Schrodinger equation

The (Un)coupled Schrodinger equation can be written in matrix form as

$$-\boldsymbol{u}''(r) + \left[\hat{\boldsymbol{U}}(r) + \frac{\hat{\boldsymbol{l}}^2}{r^2}\right]\boldsymbol{u}(r) = k^2\boldsymbol{u}(r), \tag{9.77}$$

where $\hat{\boldsymbol{U}}(r) = 2\mu\hat{\boldsymbol{V}}(r)$, $k^2 = 2\mu E$. $\hat{\boldsymbol{l}}^2 = diag(l_1(l_1+1), \cdots)$. Boundary condition of $\boldsymbol{u}(r)$ can be written as

$$\boldsymbol{u}(r) \to \hat{\boldsymbol{h}}^{(-)}(r) - \hat{\boldsymbol{h}}^{(+)}(r)\hat{\boldsymbol{S}} \tag{9.78}$$

where $\hat{h}^{(\pm)}$ are reduced Hankel function. Let us consider the case,

$$\boldsymbol{U}(r) \to \frac{M\hat{\boldsymbol{C}}_n}{r^n}. \tag{9.79}$$

We may diagonalize the equation by using unitary transformation,

$$M\hat{\boldsymbol{C}}_n = \boldsymbol{G}\hat{\boldsymbol{D}}\boldsymbol{G}^{-1}, \quad \hat{\boldsymbol{D}} = diag(\pm R_1^{n-2}, \cdots) \tag{9.80}$$

where, R are constants with length dimension and sign represents repulsive(attractive) potential. We can get uncoupled equation for $\tilde{\boldsymbol{u}}(r) = \boldsymbol{G}\boldsymbol{u}(r)$. In usual case, either U or centrifugal force becomes dominant at short distance and we can ignore energy dependence. Thus,

$$-\tilde{\boldsymbol{u}}'' + \frac{\boldsymbol{D}}{r^n}\tilde{\boldsymbol{u}} \simeq 0, \quad r \to 0. \tag{9.81}$$

Thus, for regular potentials, $n \le 1$, we can set the boundary condition at short distance as

$$u(r \to 0) \sim r^{l+1}, \quad \frac{u'(r)}{u(r)} \to \frac{l+1}{r} \tag{9.82}$$

In case of singular potential, $n > 2$, we get,

$$\begin{aligned} u_-(r) &\to C_-(\frac{r}{R})^{n/4} \sin[\frac{2}{n-2}(\frac{R}{r})^{n/2-1} + \phi], \\ u_+(r) &\to C_+(\frac{r}{R})^{n/4} \sin[-\frac{2}{n-2}(\frac{R}{r})^{n/2-1}] \end{aligned} \tag{9.83}$$

where, ϕ is general energy dependent phase. [7]

9.2 Momentum space calculation

For general non-local potential, the Schrodinger equation becomes integro-differential equation,

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi_n(\boldsymbol{r}) + \int d^3r' V(\boldsymbol{r}, \boldsymbol{r}')\psi_n(\boldsymbol{r}') = E_n\psi_n(\boldsymbol{r}) \tag{9.86}$$

Though we can reduce the Schrodinger equation to differential equation for local potential, it is easier to solve momentum space equation.

$$(k^2 - k_0^2)\psi_n(\boldsymbol{k}) = \frac{2\mu}{\hbar^2}\int d\boldsymbol{k}' V(\boldsymbol{k}, \boldsymbol{k}')\psi_n(\boldsymbol{k}'), \tag{9.87}$$

where $2\boldsymbol{p} = \boldsymbol{p}_1 - \boldsymbol{p}_2$, $E_n = \frac{\hbar^2 k_0^2}{2\mu}$, n represent all quantum numbers. In case of scattering, we have

$$\psi_n(\boldsymbol{k}) = \delta(\boldsymbol{k} - \boldsymbol{k}_0)|SM_S, TT_3\rangle - \frac{m_N}{\hbar^2}\mathrm{P}\frac{1}{k^2 - k_0^2}\int d\boldsymbol{k}' V(\boldsymbol{k}, \boldsymbol{k}')\psi_n(\boldsymbol{k}'). \tag{9.88}$$

Instead of wave function in momentum space, we can solve R matrix, $R\phi_n = V\psi_n$,

$$\begin{aligned} R(\boldsymbol{k}, \boldsymbol{k}_0) &= V(\boldsymbol{k}, \boldsymbol{k}_0) - \frac{M}{\hbar^2}\mathrm{P}\int d\boldsymbol{k}' \frac{1}{k'^2 - k_0^2} V(\boldsymbol{k}, \boldsymbol{k}')R(\boldsymbol{k}', \boldsymbol{k}_0), \\ R^\alpha_{LL'}(k, k_0) &= V^\alpha_{LL'}(k, k_0) - \frac{2}{\pi}\mathrm{P}\sum_l \int_0^\infty \frac{dk' k'^2 V_{Ll}(k, k')R_{lL'}(k', k_0)}{k'^2 - k_0^2}. \end{aligned} \tag{9.89}$$

Once we solved R-matrix, we can obtain the wave function by

$$\begin{aligned} \psi^\alpha_{LL'}(k) &= \frac{1}{k^2}\delta(k - k_0)\delta_{LL'} - \frac{2}{\pi}\mathrm{P}\frac{R_{LL'}(k, k_0)}{k^2 - k_0^2}, \\ \psi^\alpha_{LL'}(r) &= j_L(k_0 r)\delta_{LL'} - \frac{2}{\pi}\int_0^\infty dk' \frac{k'^2 j_{L'}(k'r)R_{L'L}(k', k_0)}{k'^2 - k_0^2} \end{aligned} \tag{9.90}$$

[7] In some case, we may regularize the singular Schrodinger equation by introducing sharp cutoff distance r_c. In that case, we may fix the boundary condition at $r = r_c$ by inward integration from known asymptotic wave function at certain energy. Then use the same boundary condition for different energy.

$$\frac{u'_k(r_c)}{u_k(r_c)} = \frac{u'_0(r_c)}{u_0(r_c)} \tag{9.84}$$

In this case, we may use zero energy scattering length as an input boundary condition,

$$u_0(r) \to \frac{(2l-1)!!}{r^l} - \frac{1}{a_l}\frac{r^{l+1}}{(2l+1)!!} \tag{9.85}$$

In numerical calculation, $R_{max} = 15$ fm is adequate for large l.

The last equation gives asymptotic condition of wave function from the pole of integrand. Note that the asymptotic boundary condition is only restricted with on-shell R-matrix.

Momentum space wave function and its partial wave decomposition are

$$\begin{aligned} \psi_n(\boldsymbol{k}) &= (2\pi)^{-3/2} \int d^3 r e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \psi_n(\boldsymbol{r}), \\ V(\boldsymbol{k},\boldsymbol{k}') &= (2\pi)^{-3} \int d\boldsymbol{r} d\boldsymbol{r}' e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} V(\boldsymbol{r},\boldsymbol{r}') e^{i\boldsymbol{k}'\cdot\boldsymbol{r}'} \end{aligned} \tag{9.91}$$

$$\begin{aligned} \psi_n(\boldsymbol{k}) &= \sum_{\alpha L L' M} i^{L-L'} \psi^{\alpha}_{LL'}(k) Y_{LM_L}(\boldsymbol{k}_0) C^{JM}_{LM_L S M_S} \mathcal{Y}^{JM}_{L'S}(\boldsymbol{k}) |TT_3\rangle, \\ V(\boldsymbol{k},\boldsymbol{k}') &= \frac{2}{\pi}\frac{\hbar^2}{M_N} \sum i^{L-L'} V^{\alpha}_{LL'}(k,k') \mathcal{Y}^{JM}_{LS}(\boldsymbol{k}) \mathcal{Y}^{JM\dagger}_{L'S}(\boldsymbol{k}) P_T \end{aligned} \tag{9.92}$$

9.2.1 Momentum space LS equation

Momentum space 에서는 LS equation을 풀어 T-matrix를 얻어야한다.

Scattering 문제의 경우 구하고자 하는 것은

$$S^J_{l'sls} = \delta_{l'l} - 4i\mu q \sum_{l''} \langle \mathcal{Y}^{JM}_{l's} j_{l'} | V | \mathcal{Y}^{JM}_{l''s} \Psi^J_{l''sls} \rangle = \delta_{l'l} - 4i\mu q T^J_{l'sls} \tag{9.93}$$

여기서 K-matrix를 도입하는 것이 편리하다.

S-matrix 와 T-matrix는 momentum space에서 다음과 같이 정의되고,

$$\langle \boldsymbol{q}'|S|\boldsymbol{q}\rangle = {}^{-}\langle \boldsymbol{q}'|\boldsymbol{q}\rangle^{+} = \langle \boldsymbol{q}'|1 - iT|\boldsymbol{q}\rangle = \delta^3(\boldsymbol{q}'-\boldsymbol{q}) - 2\pi i \delta(E_q - E'_q) t_{\boldsymbol{q}'\boldsymbol{q}} \tag{9.94}$$

T는 LS -equation을 만족한다.

$$T_{\boldsymbol{q}\boldsymbol{q}'} = \langle \boldsymbol{q}|V|\boldsymbol{q}'\rangle + \int dq'' \lim \epsilon \to 0 \langle \boldsymbol{q}|V|\boldsymbol{q}''\rangle \frac{1}{E_{q'} + i\epsilon - E_{q''}} T_{q''q'} \tag{9.95}$$

여기서 K-matrix를 다음과 같이 정의하면,

$$K_{qq'} = \langle \boldsymbol{q}|V|\boldsymbol{q}'\rangle + \int d\boldsymbol{q}'' \langle \boldsymbol{q}|V|\boldsymbol{q}''\rangle \frac{P}{E_{q'} - E_{q''}} K_{q''q'} \tag{9.96}$$

이러한 K-matrix는 real이 되고, 적분에서의 pole에 의한 singularty도 없게 된다. 위 식을 풀어서 얻은 K-matrix와 T-matrix는 다음과 같은 관계를 가진다.

$$T_{qq'} = K_{qq'} - i\pi \int dq'' K_{qq''} \delta(E_{q'} - E_{q''}) T_{q''q'} \tag{9.97}$$

특히 external momentum 이 모두 on-shell인 경우 $E = p^2/(2m)$,

$$T_{qq'} = K_{qq'} - i\pi m q \int d\hat{q} K_{qq''} T_{q''q'} \tag{9.98}$$

으로 되어 on-shell K-matrix로 부터, on-shell T-matrix를 구할 수 있게 된다. Matrix notation을 사용하면,

$$\begin{aligned} T &= K(1 - 2i\mu q T) = (1 + 2i\mu q K)^{-1} K, \\ S &= 1 - 4i\mu q T = (1 + 2i\mu q K)^{-1}(1 - 2i\mu q K) \end{aligned} \tag{9.99}$$

K-matrix를 구하기 위해서 principal value singularity 를 취급해야 하는데, 이것은

$$\int_0^\infty \frac{P}{E_q - \frac{k^2}{2\mu}} dk = 0 \tag{9.100}$$

을 이용하여, singularity가 없어지도록 식을 변형하면, $E_q = q^2/2\mu$,

$$K^J_{l'sls}(q'q) = V^J_{l'sls}(q'q) + \frac{2}{\pi}\sum_{l''}\int_0^\infty \frac{dk}{q^2/2\mu - k^2/2\mu}[k^2 V^J_{l'sl''s}(q'k)K^J_{l''sls}(kq) - q^2 V^J_{l'sl''s}(q'q)K^J_{l''sls}(qq)] \quad (9.101)$$

로 만들어서 풀 수 있다. (integral equation은 적절한 quadrature 를 이용하여, discretise 시킨다음 algebraic equation을 푼다.)

Kowalski-Noyes method

또 다른 방법을 이용하여 K-matrix를 구할 수 있는데, Kowalski-Noyes 방법이다. matrix notation으로

$$K(q'q) = V(q'q) + \frac{2}{\pi}\int_0^\infty dk k^2 V(q'k)\frac{P}{E_q - k^2/2\mu}K(kq) \quad (9.102)$$

라고 쓰고,

$$\tau(q'q) = V(q'q)V^{-1}(qq) \quad (9.103)$$

를 정의하고 곱해준다음 $q = q'$인 경우를 빼주면,

$$K(q'q) = \tau(q'q)K(qq) + \frac{2}{\pi}\int_0^\infty dk k^2[V(q'k) - V(q'q)V^{-1}(qq)V(qk)]\frac{P}{E_q - k^2/2\mu}K(kq) \quad (9.104)$$

가 되고, auxiliary 함수 f를 도입하여

$$\begin{aligned} K(q'q) &= f(q'q)K(qq) \\ f(q'q) &= \tau(q'q) + \frac{2}{\pi}\int_0^\infty dk k^2[V(q'k) - V(q'q)V^{-1}(qq)V(qk)]1/(E_q - k^2/2\mu)^{-1}f(kq) \end{aligned} \quad (9.105)$$

를 풀면, on-shell K는

$$K(qq) = [1 - \frac{2}{\pi}\int_0^\infty dk k^2 V(qk)P/(E_q - k^2/2\mu)f(kq)]^{-1}V(qq) \quad (9.106)$$

를 quadrature 로 계산하면 얻어진다.

Numerical method in momentum space

Complex T-matrix 를 구해보자. T-matrix satisfies

$$T_{qq'} = \langle q|V|q'\rangle + \int dq''\langle q|V|q''\rangle\frac{P}{E_{q'} - E_{q''}}T_{q''q'} - i\pi\int dq''\langle q|V|q''\rangle\delta(E_{q'} - E_{q''})T_{q'q''} \quad (9.107)$$

이 된다. Partial wave projected T-matrix는

$$\begin{aligned} T^J_{l'sls} &= \sum_{l''}\langle\mathcal{Y}^M_{l'sJ}j_{l'}|V|\mathcal{Y}^M_{l''sJ}\Psi^J_{l''sls}\rangle, \\ T^J_{l'sls}(q'q) &= V^J_{l'sls}(q'q) + \frac{2}{\pi}\sum_{l''}\int_0^\infty dk\frac{k^2}{\frac{q^2}{2\mu} - \frac{k^2}{2\mu} + i\epsilon}V^J_{l'sl''s}(q'k)T^J_{l''sls}(kq), \\ &= V^J_{l'sls}(q'q) + \frac{2}{\pi}\sum_{l''}\left\{\int_0^\infty dkP\left(\frac{2\mu}{q^2 - k^2}\right)[k^2 V^J_{l'sl''s}(q'k)T^J_{l''sls}(kq) - q^2 V^J_{l'sl''s}(q'q)T^J_{l''sls}(qq)]\right. \\ &\left. -i\pi\frac{2\mu}{2}qV^J_{l'sl''s}(q'q)T^J_{l''sls}(qq)\right\} \end{aligned} \quad (9.108)$$

여기서, principle value integral 의 singularity 를 control 하기 위한 항이 추가되었다.

무한 적분 구간은 $\int_0^\infty dk$ 는 change of variable,

$$k = (const)\tan(\frac{\pi}{4}(x+1)), \quad w_k = (const)\frac{\pi}{4}\frac{w}{\cos^2(\frac{\pi}{4}(1+x))}$$

을 이용해서 유한 적분 $\int_{-1}^{+1} dx$ 로 바꿀 수 있다. $(const)$는 dimension 과 문제에 맞도록 결정한다. 실제로는 mesh point의 분포를 결정하는 역할을 한다. (전체 mesh points 중 절반이 $k_i \le (const)(?)$ 에 들어가도록 하도록 하는 역할을 한다. 따라서, 적어도 $C \sim 100$ MeV(?) 정도가 적절하다.)

만약, momentum space integration을 k_{max}까지로 한정하여 계산하는 경우라면, $\int_0^\infty dk \to \int_0^{k_{max}} dk$, 새로이 더해지는 항에 대한 추가 수정항이 필요해진다. 즉, 추가되는 항인

$$I = \int_0^{p_{max}} dp \frac{1}{k_0^2 - p^2} = \frac{1}{2}\ln|\frac{k_0 + p_{max}}{k_0 - p_{max}}| \tag{9.109}$$

이 $p_{max} \to \infty$가 아닌한 zero가 아니므로, singularity 를 regulate하기 위해서 I 항을 직접 추가해 주어야 한다.

${}^3P_0$를 제외하면, $S = 1$ 이고 $J \ne L$ 인 상태는 모두 coupled 이고, coupled 인 경우는 $L = J-1$ and $L = J+1$ 로 정해진다. 따라서, 주어진 , J 와 coupled 인지 여부에 의해서 모든 channel information 을 알 수 있다. $(2n+2)$ mesh points array를 다음과 같이 정한다.

$$k = (\underbrace{k_1, \ldots, k_n,}_{\text{for } L=J-1} \quad \underbrace{k_{n+1},}_{k_{n+1}=q} \quad \underbrace{k_{n+2}, \ldots, k_{2n+1},}_{\text{for } L=J+1} \quad \underbrace{k_{2n+1})}_{k_{2n+2}=q} \quad . \tag{9.110}$$

그러면 T-matrix 는 $(n+1)\times(n+1)$ matrix (또는 $(2n+2)\times(2n+2)$ matrix 로 표현된다. 그러면, 주어진 initial momentum q 에 대해서,

$$\begin{aligned} T(k_i, k_{n+1}) &= V(k_i, k_{n+1}) + \frac{2}{\pi}\left[\sum_{l=1}^{n}\left(w_l \frac{2\mu k_l^2}{k_{n+1}^2 - k_i^2}\right) V(k_i, k_l) T(k_l, k_{n+1})\right. \\ &\quad \left. + \left\{\left(\sum_{l=1}^{n} -w_l \frac{2\mu k_{n+1}^2}{k_{n+1}^2 - k_l^2}\right) - i\pi\frac{2\mu}{2}k_{n+1}\right\} V(k_i, k_{n+1}) T(k_{n+1}, k_{n+1})\right] \end{aligned} \tag{9.111}$$

Thus if define, vector u such that

$$\begin{aligned} u(i = 1:n) &\equiv \frac{2}{\pi} w_i \frac{2\mu k_i^2}{q^2 - k_i^2}, \\ u(i = n+1) &\equiv \frac{2}{\pi}\left\{\left(\sum_{l=1}^{n} -w_l \frac{2\mu k_{n+1}^2}{k_{n+1}^2 - k_l^2}\right) - i\pi\frac{2\mu}{2}k_{n+1}\right\} \end{aligned} \tag{9.112}$$

then, T-matrix equation becomes

$$\begin{aligned} T(k_i, k_{n+1}) &= V(k_i, k_{n+1}) + \sum_{l=1}^{n+1} V(k_i, k_l) u(k_l) T(k_l, k_{n+1}), \text{ for } i, j = 1 \ldots n+1, \\ \hat{T} &= [1 - (u\hat{V})]^{-1}\hat{V} \end{aligned} \tag{9.113}$$

We can solve the K-matrix equation in the same way except of the pole contribution of propagator and K-matrix is pure real.

Caution: The original equation for T-matrix or K-matrix are only valid for on-shell and half-on-shell matrix elements. Thus, originally the $T(k_i, j_{n+1})$ os $K(k_i, k_{n+1})$ are only vectors and also the right hand side $V(k_i, k_{n+1})$ is a vector not matrix. We may treat the right hand side V as $V(k_i, k_j)$ and obtain **full-off-shell** $K(k_i, k_j)$ matrix from the equation. However, because the inverted matrix depends on $q = k_{n+1}$, $K(k_i, k_j)$ also depends on q value. Thus, what actually calculated have to written as k-matrix for given on-shell energy E, $K(k_i, k_j; E)$. If k_i or $k-j$ satisfies on-shell condition, it becomes on-shell or half-on-shell K-matrix. Be careful that phase shifts are only calculated for on-shell matrices. Diagonal component of fully-off-shell amplitudes are not physical observables. We always have to use on-shell or half-on-shell K-matrix only for physical results. Note that time-reversal symmetric potential gives symmetric full-off-shell K-matrix $K(k_i, k_j; E) = K(k_j, k_i; E)$.

Bound state problem in momentum space

The bound state problem in momentum space is

$$\psi_n(\boldsymbol{k}) = -\frac{M_N}{\hbar^2}\frac{P}{k^2 + k_D^2}\int d\boldsymbol{k}' V(\boldsymbol{k}, \boldsymbol{k}')\psi_n(\boldsymbol{k}') \tag{9.114}$$

where , energy becomes negative, $E = -\frac{k_D^2}{M_N}$. We have to solve,

$$\sum_{i=1}^{2N} F_D(i,j)\psi(j) = 0, \tag{9.115}$$

with

$$F_D(i,j) = \delta_{ij} + \frac{2}{\pi}\frac{k_j^2\omega_j}{k_j^2 + k_D^2}V(i,j), \tag{9.116}$$

where i,j incorporate both orbital angular momentum and grid points $k_1, \dots k_N$. Thus, we have homogeneous $2N \times 2N$ matrix equation, $F\psi = 0$. The binding energy can be found by varying k_D so that the detF_D is zero. Once the binding energy is known, we can obtain $\psi(j)$. (Solution of a equation $\hat{F}\psi = 0$, with $\det F = 0$, means that not all vector $\psi(j)$ are independent. In this case, we may set the last term as $\psi(2N) = 1$ and solve the $(2N-1)$ dimensional inhomogeneous equation, $\sum_{j=1}^{2N-1} F_D(i,j)\psi(j) = -F_D(i,n)\psi(n)$. The last equation for $i = n$ can be used as a accuracy check.)

Another way to solve the problem is solving the bound state problem as an eigen-value problem, we may rewrite the equation as

$$\begin{aligned} k_D^2\psi_n(\boldsymbol{k}) &= -k^2\psi_n(\boldsymbol{k}) - m_N\int d\boldsymbol{k}' V(\boldsymbol{k}, \boldsymbol{k}')\psi_n(\boldsymbol{k}') \\ &= -m_N\int d\boldsymbol{k}'\left(\frac{k^2}{m_N}\delta^{(3)}(\boldsymbol{k}' - \boldsymbol{k}) + V(\boldsymbol{k}, \boldsymbol{k}')\right)\psi_n(\boldsymbol{k}') \end{aligned} \tag{9.117}$$

9.3 BHF(Bruckner Hartree-Fock) calculation for nuclear matter

This section was based on the Haftel and Tabakin, NPA158(1970)1-42.

Since the Brueckner-Bethe-Goldstone equation is similar to the LS equation, one can use similar method to obtain G-matrix except additional Pauli operator.

Now the discussion on BHF equation is moved to the note about Many-body.

9.4 Identical particles scattering

Antisymmetric wave function in NN scattering, : PRC70,044007(2004) by Schiavilla et.al.

- 지금까지 two nucleon state 의 anti-symmetrization 은 explicit 하게 formalism 에 포함 시키지 않았다. 만약 free two nucleon scattering state를 explicitly anti-symmetric 하도록 정의하면, formalism 이 약간 바뀌게 된다. Let us define anti-symmetric plane wave [8]

$$\begin{aligned}\langle \boldsymbol{r}|\boldsymbol{p}, SM_S, T\rangle^0 &= \phi_{\boldsymbol{p},SM_S,T}(\boldsymbol{r}) \\ &= \frac{1}{\sqrt{2}}[e^{i\boldsymbol{p}\cdot\boldsymbol{r}} - (-)^{S+T}e^{-i\boldsymbol{p}\cdot\boldsymbol{r}}]\chi^S_{M_S}\eta^T_{M_T=0} \\ &= 4\pi\sqrt{2}\sum_{JM_JL} i^L\epsilon_{LST}j_L(pr)[Z^{J,M_J}_{LSM_S}(\hat{\boldsymbol{p}})]^*\mathcal{Y}^M_{LSJ}(\hat{\boldsymbol{r}})\eta^T_0 \end{aligned} \tag{9.118}$$

where,

$$\epsilon_{LST} \equiv \frac{1}{2}(1-(-)^{L+S+T}), \quad Z^{J,M_J}_{LSM_S}(\hat{\boldsymbol{p}}) \equiv \sum_{M_L}\langle LM_L, SM_S|JM_J\rangle Y_{LM_L}(\hat{\boldsymbol{p}}) \tag{9.119}$$

Note that $\sqrt{2}\epsilon_{LST}$ appears in addition to usual plane wave explansion because of the anti-symmetrization. Thus, if they were not identical particles, these terms would disappear.

- The role of ϵ_{LST} serves to filter antisymmetric states ($L+S+T=(odd)$). Thus, if we always consider states antisymmetric only, ϵ_{LST} factor is not necessary.

- 여기서 주의 할 것은 위에서 정의되는 $|\boldsymbol{p}\rangle^{(+)}$ 나 $|\boldsymbol{p}\rangle_0$ 는 two nucleon의 anti-symmetrization 을 고려한 것으로 보통의 two nucleon relative state $|\boldsymbol{p}\rangle$와는 의미가 다르다는 것이다. 예를 들어, normalization은

$$\langle \boldsymbol{p}', S'M'_S, T'|\boldsymbol{p}, SM_S, T\rangle = \delta_{SS'}\delta_{M_SM'_S}\delta_{TT'}[(2\pi)^3\delta^{(3)}(\boldsymbol{p}'-\boldsymbol{p}) - (-1)^{S+T}(2\pi)^3\delta^{(3)}(\boldsymbol{p}+\boldsymbol{p}')] \tag{9.120}$$

이 된다. 따라서, completeness relation 은

$$\sum_{S,M_S,T}\frac{1}{2}\int\frac{d^3p}{(2\pi)^3}|\boldsymbol{p}, SM_S, T\rangle_{00}\langle\boldsymbol{p}, S, M_S, T| = 1. \tag{9.121}$$

- LS equation은

$$|\boldsymbol{p}, SM_S, T\rangle^{(\pm)} = |\boldsymbol{p}, SM_S, T\rangle^0 + \frac{1}{E-H_0\pm i\epsilon}v|\boldsymbol{p}, SM_S, T\rangle^{(\pm)}. \tag{9.122}$$

- T-matrix is defined as

$$T(\boldsymbol{p}', S'M'_S, T'; \boldsymbol{p}, SM_S, T) = {}_0\langle\boldsymbol{p}', S'M'_S, T'|v|\boldsymbol{p}, SM_S, T\rangle^{(+)} \tag{9.123}$$

LS eq.에 complete set $\sum_{S,M_S,T}\frac{1}{2}\int\frac{d^3p}{(2\pi)^3}|\boldsymbol{p}, SM_S, T\rangle^0\langle\boldsymbol{p}, SM_S, T|^0 = 1$을 넣으면,

$$|\boldsymbol{p}, SM_S, T\rangle^{(+)} = |\boldsymbol{p}, SM_S, T\rangle^0 + \sum_{S',M_{S'},T'}\frac{1}{2}\int\frac{d^3p'}{(2\pi)^3}|\boldsymbol{p}', S'M_{S'}, T'\rangle^0\frac{T(\boldsymbol{p}', S'M'_S, T'; \boldsymbol{p}, SM_S, T)}{E-p'^2/(2\mu)+i\epsilon} \tag{9.124}$$

[8]Particle Exchange gives, $\boldsymbol{p}\to-\boldsymbol{p}$, $\chi^S\to(-)^S\chi^S$,$\eta^T\to(-)^T\eta^T$.

potential matrix의 partial wave expansion은 다음과 같이 도입할 수 있다. local potential 의 경우 $\langle \boldsymbol{r}'|v|\boldsymbol{r}\rangle = v(\boldsymbol{r})\delta^{(3)}(\boldsymbol{r}'-\boldsymbol{r})$ 이므로

$$\begin{aligned}
& {}_0\langle \boldsymbol{p}', S'M_{S'}, T'|v|\boldsymbol{p}, SM_S, T\rangle_0 \\
= & \int d^3r {}_0\langle \boldsymbol{p}', S'M_{S'}, T'|\boldsymbol{r}\rangle v(\boldsymbol{r})\langle \boldsymbol{r}|\boldsymbol{p}, SM_S, T\rangle_0 \\
= & 2(4\pi)^2 \sum_{JM_J}\sum_{LL'} \epsilon_{L'S'T'}\epsilon_{LST} Z^{JM_J}_{L'S'M_{S'}}(\hat{\boldsymbol{p}}') Z^{JM_J}_{LSM_S}(\hat{\boldsymbol{p}})^* v^J_{L'S'T',LST}(p',p) \qquad (9.125)
\end{aligned}$$

$$v^J_{L'S'T',LST}(p',p) = i^{L-L'}\int d^3r j_{L'}(p'r)[\mathcal{Y}^{M_J}_{L'S'J}\eta^{T'}]^\dagger v(\boldsymbol{r}) j_{L'}(pr)[\mathcal{Y}^{M_J}_{LSJ}\eta^T] \qquad (9.126)$$

T-matrix에 대해서도

$$T(\boldsymbol{p}', S'M_{S'}, T', \boldsymbol{p}, SM_S, T) \equiv {}_0\langle \boldsymbol{p}', S'M_{S'}, T'|v|\boldsymbol{p}, SM_S, T\rangle^{(+)} = {}_0\langle \boldsymbol{p}', S'M_{S'}, T'|\hat{T}|\boldsymbol{p}, SM_S, T\rangle_0 \qquad (9.127)$$

로 생각하고, plane wave 의 partial wave expansion을 생각하면, potential의 식과 동일한 T-matrix의 partial wave component 를 얻을 수 있다.

- Let us introduce shorthand notation, $\bar{\alpha} = (S, M_S, T)$, $\alpha = (LSM_S, JM_J)$ and

$$Z^*_{\alpha,\bar{\alpha}}(\hat{p}) = \epsilon_{L'S'T'} Z^{JM_J}_{L'S'M'_S}(\hat{p})$$

. Then previous equations can be written as

$$\begin{aligned}
|\boldsymbol{p}, \bar{\alpha}\rangle_0 &= 4\pi\sqrt{2}\sum_\beta |p,\beta\rangle_0 Z^*_{\beta\bar{\alpha}}(\hat{p}), \\
\langle \boldsymbol{r}\alpha|p,\alpha\rangle_0 &= i^L j_L(pr)\mathcal{Y}^M_{LSJ}\eta^T_0, \\
{}_0\langle \boldsymbol{p}'\bar{\alpha}'|v|\boldsymbol{p}\bar{\alpha}\rangle_0 &= 2(4\pi)^2\sum_{\beta,\beta'} Z_{\bar{\alpha}'\beta'}(\hat{p}')Z^*_{\beta\bar{\alpha}}(\hat{p}) v_{\beta',\beta}(p',p) \qquad (9.128)
\end{aligned}$$

으로 쓸 수 있다. Note that

$$\sum_{\bar{\alpha}}\int d\Omega_p Z^*_{\bar{\alpha}\beta'}(\hat{p}) Z_{\bar{\alpha}\beta}(\hat{p}) = \delta_{\beta'\beta}\epsilon_{LST} \qquad (9.129)$$

- The LS equation in configuration space becomes

$$\begin{aligned}
\langle \boldsymbol{r}|\boldsymbol{p},\bar{\alpha}\rangle^{(+)} &= 4\pi\sqrt{2}\sum_\alpha Z^*_{\alpha\bar{\alpha}}(\hat{p})\langle r,\alpha|p,\alpha\rangle^{(+)} \\
&= 4\pi\sqrt{2}\sum_{\alpha,\beta}\delta_{\alpha,\beta} i^\beta Z^*_{\beta\bar{\alpha}}(\hat{p})\frac{w^j_{\beta,\alpha}(r;p)}{r}, \\
\langle \boldsymbol{r}|\boldsymbol{p},\bar{\alpha}\rangle_0 &= 4\pi\sqrt{2}\sum_\alpha Z^*_{\alpha\bar{\alpha}}(\hat{p})\langle r,\alpha|p,\alpha\rangle_0 \\
&= 4\pi\sqrt{2}\sum_{\alpha,\beta}\delta_{\alpha,\beta} i^\beta Z^*_{\beta\bar{\alpha}}(\hat{p}) j_\beta(pr), \qquad (9.130)
\end{aligned}$$

$$\begin{aligned}
& \sum_{\bar{\alpha}'}\frac{1}{2}\int\frac{d^3p'}{(2\pi)^3}\langle \boldsymbol{r}|\boldsymbol{p}',\bar{\alpha}'\rangle^0 \frac{1}{E-p'^2/(2\mu)+i\epsilon} T(\boldsymbol{p}'\bar{\alpha}',\boldsymbol{p}\bar{\alpha}) \\
= & \sum_{\bar{\alpha}'}\sum_{\beta'',\beta',\beta}\frac{1}{2}\frac{(4\pi\sqrt{2})^3}{(2\pi)^3}\int dp' p'^2\int d\Omega_{p'} Z^*_{\bar{\alpha}'\beta''}(\hat{p}') Z_{\bar{\alpha}'\beta'}(\hat{p}') Z^*_{\beta\bar{\alpha}}(\hat{p}) \\
& \times\langle r|p',\beta''\rangle_0 \frac{{}_0\langle p',\beta'|T|p,\beta\rangle_0}{E-p'^2/(2\mu)+i\epsilon} \\
= & (4\pi\sqrt{2})(\frac{(4\pi\sqrt{2})^2}{(2\pi)^3 2})\sum_{\beta',\beta} i^{\beta'}\epsilon_{\beta'} Z^*_{\beta\bar{\alpha}}(\hat{p}) j_{\beta'}(p'r)\frac{{}_0\langle p',\beta'|T|p,\beta\rangle_0}{E-p'^2/(2\mu)+i\epsilon} \qquad (9.131)
\end{aligned}$$

Thus, partial wave $\langle r, \alpha | p, \alpha \rangle^{(+)}$ can be written after factoring out common factors

$$\frac{w^j_{\alpha',\alpha}(r;p)}{r} = \delta_{\alpha',\alpha} j_{L'}(pr) + \frac{2}{\pi}\int_0^\infty dp' p'^2 j_{L'}(p'r) \frac{1}{E - p'^2/(2\mu) + i\epsilon} T^J_{\alpha',\alpha}(p';p) \tag{9.132}$$

This equation serves a way to obtain wave function in configuration space if T-matrix in momentum space is known.

- boundary condition is

$$\frac{w^j_{\alpha',\alpha}(r;p)}{r} \simeq \frac{1}{2}[\delta_{\alpha'\alpha} h^{(2)}_{L'}(pr) + h^{(1)}_{L'}(pr) S^J_{\alpha'\alpha}(p)] \tag{9.133}$$

where on-shell S-matrix is

$$S^J_{\alpha'\alpha}(p) = \delta_{\alpha'\alpha} - 4i\mu p T^J_{\alpha'\alpha}(p;p) \tag{9.134}$$

and

$$h^{(1,2)}_L(pr) = j_L(pr) \pm i n_L(pr) \tag{9.135}$$

- differential equation is

$$\left(-\frac{d^2}{dr^2} + \frac{L'(L'+1)}{r^2} - p^2\right) w^j_{\alpha'\alpha}(r;p) + \sum_\beta r v^J_{\alpha'\beta}(r) \frac{1}{r} w^j_{\beta,\alpha}(r;p) = 0 \tag{9.136}$$

where

$$v^J_{\alpha'\alpha}(r) = i^{L-L'}(2\mu)\int d\Omega \mathcal{Y}^\dagger_{\alpha'} \eta^\dagger_{\alpha'} v(\boldsymbol{r}) \eta_\alpha \mathcal{Y}_\alpha. \tag{9.137}$$

Note that (1) $v^J_{\alpha'\alpha}$ is different from $v^J_{\alpha'\alpha}(p', p)$. (2) Because of the property of potential, $\frac{1}{r}$ is not factored out in the last term. (3) $v^J_{\alpha'\alpha}(r)$ is defined in modified spherical harmonics convention such that parity violating potential matrix element to be pure real. (Parity conserving potential is real.) Thus, wave function have real solution. If equation is written in spherical harmonics convention, potential becomes pure imaginary and solutions also becomes complex number even at zero energy.

- scattering M-matrix can be related with T-matrix by

$$M_{S'M'_ST',SM_ST}(E,\theta) = -\frac{\mu}{2\pi} T(\boldsymbol{p}', S'M'_ST'; p\hat{z}, SM_ST). \tag{9.138}$$

In previous notation, $f_{S'M'T',SMT} = M_{S'M'T',SMT}$.

- **Be careful that results in this section was calculated in the normalization convention $\langle \boldsymbol{k}'|\boldsymbol{k}\rangle = (2\pi)^3\delta^{(3)}(\boldsymbol{k}' - \boldsymbol{k})$. Some equation depends on this convention.**

- **I am not sure about this part:** From this relations, scattering M-matrix is related with partial wave scattering S-matrix as

$$\begin{aligned} M_{S'M'_ST',SM_ST}(E,\theta) &= \sqrt{4\pi}\sum_{JLL'}\sqrt{2L+1}\left(\sqrt{2}\epsilon_{L'S'T'}\sqrt{2}\epsilon_{LST}\right) \\ &\quad \times\langle L'(M_S - M'_S), S'M'_S|JM_S\rangle\langle L0, SM_S|JM_S\rangle Y_{L'(M_S-M'_S)}(\theta) \\ &\quad \times\frac{S^J_{L'S',LS}(p) - \delta_{L'L}\delta_{S'S}}{2ip} \end{aligned} \tag{9.139}$$

Here note that $\sqrt{2}\epsilon_{LST}$ and $\sqrt{2}\epsilon_{L'S'T'}$ comes from anti-symmetrization factor in isospin formulation. This is equivalent to the anti-symmetrized scattering amplitude $f_A(\boldsymbol{p};S)$ for identical particle must be $f_A(\boldsymbol{p};S) = f(\boldsymbol{p}) \pm f(-\boldsymbol{p})$. In case of np, this additional $(\sqrt{2})^2$ cancels with isospin Clebsch-Gordan factor $C^{T'0}_{\frac{1}{2}\frac{1}{2},\frac{1}{2}-\frac{1}{2}} C^{T0}_{\frac{1}{2}\frac{1}{2},\frac{1}{2}-\frac{1}{2}}$, so that the final results is the same as non-identical particles.

Another point is that this expression is independent of normalization choice of state vector. So, scattering cross section expression

$$\frac{d\sigma_{\alpha,\beta}}{d\Omega} = |M_{\alpha,\beta}|^2 = (\text{S-matrix expression}) \tag{9.140}$$

in terms of S-matrix is independent of normalization choice.

- In the code, I computed the M-matrix as

$$\begin{aligned} M_{m_1' m_2', m_1 m_2} &= \sum_{L'S',LS,J,T,T',T_z} \sqrt{4\pi}\sqrt{2L+1}\left(\sqrt{2}\epsilon_{L'S'T'}\sqrt{2}\epsilon_{LST}\right) \\ &\quad \times \langle L'(M_S - M_S'), S'M_S'|JM_S\rangle\langle L0, SM_S|JM_S\rangle \\ &\quad \times \left(C^{T'T_z}_{t_1 t_1^z, t_2 t_2^z} C^{TT_z}_{t_1 t_1^z, t_2 t_2^z}\right)\langle \frac{1}{2}m_1' \frac{1}{2}m_2'|S'M_S'\rangle\langle \frac{1}{2}m_1 \frac{1}{2}m_2|SM_S\rangle \\ &\quad \times Y_{L'(M_S - M_S')}(\theta) i^{L-L'}\left(\frac{S(p)-\delta}{2ip}\right)^{(J)}_{L'S'T',LST} \end{aligned} \tag{9.141}$$

9.5 Spline method

미분 방정식을 푸는 방법에는 여러가지가 있지만, 3-body 이상의 partial differential equation의 경우에는 spline function을 이용하여 eq.을 discrete matrix linear algebra equation으로 바꾸는 것이 편리하다.

기본적으로 interpolation을 통해 함수를 basis spline function 의 linear combination으로 나타내고, 풀고자하는 식을 spline coefficient 에 대한 식으로 바꾸어 준다. 이를 위해서 필요한 것은 (1) 주어진 문제를 spline coefficient에 대한 식으로 바꾸기. (2) 얻어진 spline coefficient를 이용하여 임의의 점에서 함수의 값 구하기. 또는 주어진 함수의 값들로부터 spline coefficient 구하기 가 가능해야한다.

9.5.1 Cubic Hermite spline

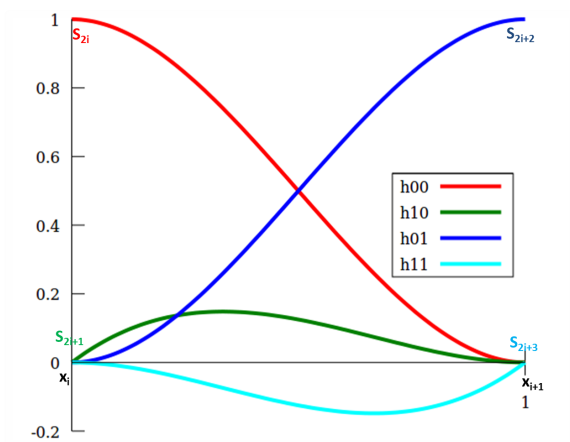

Figure 9.1: Cubic Hermite functions.

Spline method uses order k spline functions for interpolation of function and discretization of equation. This is better for interpolate function and its derivative, thus suitable for differential equation. Cubic Hermite spline interpolation in interval (x_i, x_{i+1}) can be written for function $y = f(x)$,

$$f(x) = h_{00}(t)y_i + h_{10}(t)(x_{i+1} - x_i)m_i + h_{01}(t)y_{i+1} + h_{11}(t)(x_{i+1} - x_i)m_{i+1} \tag{9.142}$$

where, $t = (x - x_i)/(x_{i+1} - x_i)$ (즉, t는 $x_i(t = 0)$와 $x_{i+1}(t = 1)$을 잇는 parameter) and m_i is a value of tangent function at point x_i. Basis functions are given as

	expanded	factorized
$h_{00}(t) = S_{2i}(t)$	$2t^3 - 3t^2 + 1$	$(1 + 2t)(1 - t)^2$
$h_{10}(t) = S_{2i+1}(t)$	$t^3 - 2t^2 + t$	$t(1 - t)^2$
$h_{01}(t) = S_{2i+2}(t)$	$-2t^3 + 3t^2$	$t^2(3 - 2t)$
$h_{11}(t) = S_{2i+3}(t)$	$t^3 - t^2$	$t^2(t - 1)$

(9.143)

여기서, tangent function m is not unique. Let us choose here $m_i = \frac{d}{dx}f(x = x_i)$ or numerically equivalent choices

$$m_i = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}, \text{ or } m_i = \frac{y_{i+1} - y_i}{2(x_{i+1} - x_i)} + \frac{y_i - y_{i-1}}{2(x_i - x_{i-1})}. \tag{9.144}$$

따라서, $x_i < x < x_{i+1}$ 에서의 함수값을 interpolate하기 위해서는, $y_{i-1}, y_i, y_{i+1}, y_{i+2}$ 또는, $y_i, y'_i, y_{i+1}, y'_{i+1}$ 의 4개의 함수 값이 필요하다.

In a form of matrix, for $x_i < x < x_{i+1}$ and $t = (x - x_i)/(x_{i+1} - x_i)$ (허? 이 식 맞나?)

$$\begin{aligned} f(t) &= \begin{pmatrix} t^3 & t^2 & t & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & -2 & 1 \\ -3 & -2 & 3 & -1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} y_i \\ y'_i \\ y_{i+1} \\ y'_{i+1} \end{pmatrix} \\ &= \begin{bmatrix} 2t^3 - 3t^2 + 1 \\ t^3 - 2t^2 + t \\ -2t^3 + 3t^2 \\ t^3 - t^2 \end{bmatrix}^T \begin{pmatrix} y_i \\ y'_i \\ y_{i+1} \\ y'_{i+1} \end{pmatrix} \end{aligned} \tag{9.145}$$

We may rename basis functions as $S_n(x)$. so that spline function $S_{2i}(x_i) = 1$ and $S'_{2i+1}(x_i) = 1$. 그러면, $x_i < x < x_{i+1}$ 에서

$$f(x) = C_{2i}S_{2i}(x) + C_{2i+1}S_{2i+1}(x) + C_{2i+2}S_{2i+2}(x) + C_{2i+3}S_{2i+3}(x) \tag{9.146}$$

으로 interpolation 하게 된다. 이 때, $S_{2i}(x)$ and $S_{2i+1}(x)$ 는 $x_{i-1} < x < x_{i+1}$ 사이에서 정의되는 함수이다.(단, 경계에서는 $S_{0,1}(x)$는 $x_0 < x < x_1$에서 정의된 함수.)이고, spline coefficient $C_{2i} = y_i$ and $C_{2i+1} = y'_i$ 로 결정된다.

즉,

$$f(x_i) = C_{2i}, \quad f'(x_i) = C_{2i+1}, \quad f(x_{i+1}) = C_{2i+2}, \quad f'(x_{i+1}) = C_{2i+3}. \tag{9.147}$$

문제는 보통 함수의 미분값이 알려져 있지 않다는 것.

Thus, $S_{2i}(x)$ and $S_{2i+1}(x)$ is defined as

	$x_{i-1} < x < x_i$	$x_i < x < x_{i+1}$	C
t	$\frac{x-x_{i-1}}{x_i-x_{i-1}},\ t=(0,1)$	$\frac{x-x_i}{x_{i+1}-x_i},\ t=(0,1)$	
$S_{2i}(x)$	$t^2(3-2t)$	$(1-t)^2(1+2t)$	$C_{2i} = y_i$
$S_{2i+1}(x)$	$-(x_i - x_{i-1})t^2(1-t)$	$(x_{i+1} - x_i)t(1-t)^2$	$C_{2i+1} = y'_i$

(9.148)

Thus, given list of break points and values of y_i and y'_i at break points determines all spline functions and its coefficients.

When the range of points are not the same, we need additional boundary conditions to convert one basis to the other in whole range. (Interpolation near the boundary would involve extrapolation without boundary condition.)

9.5.2 Discretizing Differential equation

미분 방정식

$$\hat{L}F(r) = 0$$

을 푸는 경우, $0 \le r \le r_N$ can be interpolated as

$$F(r) \simeq \sum_{j=0}^{k(N+1)-1} C_j S_j(r). \tag{9.149}$$

하지만, 동시에 미분 방정식을 matrix로 바꾸기 위해서는 r 을 mesh points로 나누어야 한다. 이 경우 mesh points를 각 break point 사이의 interval 에 대한 legendre quadrature로 잡는 것이 편리하다.

spline function 의 index는 전체 구간을 $x_0, .., x_N$ 의 break point로 나누었을 때, 각 break point마다 k 개의 spline function이 배당되는 식으로 정한다. 그리고, 각 interval,$[x_i, x_{i+1}]$, 에서 non-zero인 spline function은 break point x_i와 x_{i+1} 에 해당하는 spline function뿐이다. 그러면, differential equation은

$$\sum_{j=0}^{k(N+1)-1} C_j[\hat{L}S_j(r)] = 0 \tag{9.150}$$

으로 바뀌고, 우리는 total $k(N+1)$개의 unknown coefficient C_j를 구해야한다. 이 때, collocation point $col_1, ..col_{kN}$ point에서의 식들을 independent 하게 취급하여, KN 개의 식을 얻을 수 있다. 나머지, k 개의 조건은 boundary condition으로부터 얻을 수 있다. 예를 들어, $k = 2$ 인 경우 boundary condition 에 의해서, $C_0, C_1, ..., C_{2N}, C_{2N+1}$ 중에

$$\begin{aligned} F(r = 0) &= 0 = C_0 \\ F(r = r_N) &= C_{2N} \end{aligned} \tag{9.151}$$

으로 C_0와 C_{2N}가 미리 결정된다. 따라서, k-개의 boundary condition 을 포함하여,

$$\sum_{j=0}^{k(N+1)-1} C_j[\hat{L}S_j(r_i)] = 0,\ i \text{ 는 } 1, 2, \ldots, k(N+1) \tag{9.152}$$

의 식이 얻어진다. 그리고, $[\hat{L}S_j(r_i)] \to [A]_{i,j}$ 로 matrix로 나타내면,

$$[A]c = 0 \tag{9.153}$$

의 linear algebra problem 으로 바뀐다. 여기서, $[A]$ 와 c 는 dimension 이 $k(N+1)$ 으로 쓰거나, 이미 k 개의 C 가 결정되어 있으므로, kN 만의 식으로 쓸 수 있다. 단, kN 개 coefficient 만의 식을 쓸 경우, bound state라면, 나머지 모든 coefficient가 zero 이므로, 새로운 term 이 나타나지 않지만, scattering state의 경우에는 boundary condition에 의해서,

$$[A]c = b \tag{9.154}$$

와 같이 boundary 에서의 coefficient 에 비례하는 term 이 나타나게 된다. 이 때,

$$[b]_i = -\sum_{j=kN+1}^{k(N+1)-1} C_j[\hat{L}S_j(r_i)],\ \text{i 는 } kN+1, \ldots, k(N+1) \tag{9.155}$$

이고, C_j는 boundary 즉 last break point 에서의 $F(r_N)$ 및 그 derivative 에 의해서,

$$C_{kN} = F(r = r_N), \quad C_{kN+1} = F'(r = r_N), \ldots \tag{9.156}$$

결정된다.

실제 계산에서는 boundary condition 을 $r = 0$ 과 $r = r_{max}$ 에서의 값으로 주는 것이 보통이다. 이런경우에는 식을 어떻게 써야할까?

$$F(r) \simeq \sum_{j=0}^{k(N+1)-1} C_jS_j(r) = \sum_{j=1}^{kN} C_jS_j(r) + \sum_{j=kN+1}^{kN+k-1} C_jS_j(r) \tag{9.157}$$

이고, 특히 $k = 2$인 경우는, $C_0 = 0$인 경우 $(F(0) = 0)$

$$F(r) \quad = \quad \sum_{j=1}^{2N-1} C_jS_j(r) + C_{2N}S_{2N}(r) + C_{2N+1}S_{2N+1}(r) \tag{9.158}$$

로 쓸 수 있고, 이 중 C_{2N}은 boundary condition 에 의해서, $C_{2N} = F(r = r_N)$ 으로 이미 결정되어 있다. 따라서, 마지막 2개의 spline coefficient 및 spline function의 이름을 바꾸어,

$$F(r) = \sum_{j=1}^{kN} \tilde{C}_j\tilde{S}_j(r) + F(r_N)\tilde{S}_{2N+1}(r), \tag{9.159}$$

where

$$C_{2N}S_{2N}(x) = \tilde{C}_{2N+1}\tilde{S}_{2N+1}(x), \quad C_{2N+1}S_{2N+1}(x) = \tilde{C}_{2N}\tilde{S}_{2N}(x), \tag{9.160}$$

형식으로 쓸 수 있다. 단, 이경우, 마지막 spline function $\tilde{S}_{2N}(r), \tilde{S}_{2N+1}(r)$ 은 실제로는 $S_{2N+1}(r), S_{2N}(r)$ 이고, $\tilde{C}_{2N}$ 은 $F'(r_N)$에 해당한다는 점에 주의할 것. 만약, bound state 였다면, 위 식에서 마지막, $\tilde{S}_{2N+1}(r)$의 coefficient를 zero 로 둘 수 있게 된다. 따라서, $C_{1\ldots 2N}$ 의 unknown coefficients를 구하는 문제로 바뀐다. 따라서, collocation points $r_1, \ldots r_{2N}$ 에 대한 식은

$$\hat{L}F(r_i) = \sum_{j=1}^{2N} [\hat{L}\tilde{S}_j(r_i)]C_j + F(r_N)\hat{L}\tilde{S}_{2N+1}(r_i) = 0 \to \sum_j [A]_{ij}[C]_j + [B]_i = 0 \tag{9.161}$$

으로 쓸 수 있게 된다. 2차 미방의 경우, we can have two solutions, $[C^{(1)}]_j$ and $[C^{(2)}]_j$ 를 2개의 boundary condition 으로 부터 구할 수 있고, normalization factor는 boundary condition과의 matching 으로 구할 수 있다.

하지만, scattering problem 에서는 asymptotic wave function 의 phase shift/K-matrix 가 미리 알려져 있지 않기 때문에 $F(r_N)$ 을 미리 결정해서 줄 수가 없다. 만약 전체 미방이 homogeneous 라면, 미리, $F(r_N) = 1$ 으로 scale 된 문제를 푼 다음에, K-matrix 를 나중에 구해서 다시 보정할 할 수 있을 것이다.

$$\phi_\alpha(r) \sim \frac{[j_\alpha(kr)\delta_{\alpha\beta} - K_{\alpha\beta}n_\beta(kr)]}{[j_\alpha(kr_N)\delta_{\alpha\beta} - K_{\alpha\beta}n_\beta(kr_N)]} \to \ C_{2N} = 1 \tag{9.162}$$

$r_{match} < r_N$ 에서의 solution을 이용하여 matching 하면 K-matrix를 결정할 수 있고, 따라서, 거꾸로 $C_{2N} = F(r_N)$ 을 다시 보정해 줄 수 있다.

Inhomogeneous equation의 경우에도 풀어야하는 방정식 자체는 비슷하다. Scattering 문제의 경우에는 $[B]_j$ 안에 inhomogeneous term 이 포함되게 된다. 문제는 Inhomogeneous equation에서는 $F(r_N)$ 을 임의로 scale 할 수 없을 것이라는 점이다. Boundary condition을 어떻게 주어야 할까? 이 경우에는 asymptotic boundary conditiond르 이용하여 $F(r_N)$ 이 $F'(r_N)$의 함수가 되도록 만들면, equation에서 $F(r_N)$ 을 없앨 수가 있다. 예를 들어 asymptotic form 이 $S * g(r)$ 로 unknown S 를 포함하더라도 , logarithmic derivative continuous condition은

$$\frac{F'(r = r_N)}{F(r = r_N)} = \frac{g'(r = r_N)}{g(r = r_N)} \tag{9.163}$$

이 되어 matrix equation에서 $F(r_N)$ 대신 $F'(r_N)$을 사용할 수 있게 된다.

Converting collocation point values to spline coefficient

한편, 주어진 collocation points value들로 부터 spline coefficient를 역으로 구하는 것은

$$F(r_i) = \sum_{j=0}^{2N+1} C_j S_j(r_i) = \sum_{j=1}^{2N} \tilde{C}_j \tilde{S}_j(r_i) + F(r_N)\tilde{S}_{2N+1}(r_i) \tag{9.164}$$

로 쓸 수 있다. 따라서, matrix를 $S_{ij} = S_j(r_i)$ 로 정의하면,

$$C_j = \sum_{i=0}^{2N+1} [S^{-1}]_{ji} F(r_i), \text{ or } \tilde{C}_j = \sum_{i=1}^{2N} [\tilde{S}^{-1}]_{ji}[F(r_i) - F(r_N)\tilde{S}_{2N+1}(r_i)] \tag{9.165}$$

로 구할 수 있다.

예

간단한 예를 들어 보자. 문제를 단순히 하기 위해서, cubic hermite polynomial (k=2) 경우이고 구간이 단순히 x_0 와 x_1 인 경우만 생각해보자. 이 구간에서 임의의 함수값은

$$f(r) \simeq C_0 S_0(r) + C_1 S_1(r) + C_2 S_2(r) + C_3 S_3(r) \tag{9.166}$$

으로 정해진다. boudary condition에 의해서 4 개의 coefficient 중 오직 2개만이 unknown 이된다. 미분방정식도

$$[L]f(r) = C_0[L]S_0(r) + C_1[L]S_1(r) + C_2[L]S_2(r) + C_3[L]S_3(r) = [B](r) \tag{9.167}$$

로 주어진다. 경계 조간에 따라서, 풀어야하는 선형방정식이 달라지게 된다. 예를 들어 $f(x_0) = 0$, $f(x_1) = 0$(or $C_0 = C_2 = 0$ 의 2-boundary value가 주어지는 경우. 두 점 r_1, r_2 에서 다음을 풀면된다.

$$\begin{pmatrix} [L]S_1(r_1) & [L]S_3(r_1) \\ [L]S_1(r_2) & [L]S_3(r_2) \end{pmatrix} \begin{pmatrix} C_1 \\ C_3 \end{pmatrix} = \begin{pmatrix} [B](r_1) \\ [B](r_2) \end{pmatrix} \tag{9.168}$$

거꾸로 만약 함수의 collocation points 에서의 값이 주어져 있을 때, 정해진 knot 에서 정의된 spline basis function에 대한 spline coefficient는 다음과 같이 구할 수 있다.

$$\begin{aligned} f(r_1) &= C_1S_1(r_1) + C_3S_3(r_1), \\ f(r_2) &= C_1S_1(r_2) + C_3S_3(r_2) \end{aligned} \tag{9.169}$$

because $C_0 = 0$ and $C_2 = 0$ is already known. (즉, boundary condition을 이용해야한다.) 또는 collocation point들을 새로운 knot으로 생각하여, 새로 basis function을 만들어 interpolation하여 원래 knot에서의 함수값과 미분값을 계산하도록 할 수도 있다.

9.5.3 Explicit form of matrix equation

Differential equation we would like to solve is

$$\left[-\frac{1}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2\mu}\frac{l'(l'+1)}{x^2} - E\right] u_{l'l}(x) + \sum_{\beta} xV_{l'\beta}(x)\frac{u_{\beta l}(x)}{x} = 0 \tag{9.170}$$

With using last term exchanged spline function $\tilde{S}_j(x)$, we will interpolate

$$\begin{aligned} u_{\alpha\beta}(x) &= \sum_{j=0}^{2N+1} \tilde{C}^{\beta}_{\alpha,j}\tilde{S}_j(x) \\ &= \sum_{j=1}^{2N} \tilde{C}^{\beta}_{\alpha,j}\tilde{S}_j(x) + \tilde{C}^{\beta}_{\alpha,0}\tilde{S}_0(x) + \tilde{C}^{\beta}_{\alpha,2N+1}\tilde{S}_{2N+1}(x) \end{aligned} \tag{9.171}$$

Then, above equation becomes

$$\begin{aligned} &\sum_{\beta=1}^{N_s}\sum_{j=0}^{2N+1}\left[-\frac{1}{2\mu}\frac{d^2}{dx^2}\tilde{S}_j(x)\delta_{l',\beta} + \frac{1}{2\mu}\frac{l'(l'+1)}{x^2}\tilde{S}_j(x)\delta_{l',\beta} - E\tilde{S}_j(x)\delta_{l',\beta}\right]\tilde{C}^l_{\beta,j} \\ &+\sum_{\beta=1}^{N_s}\sum_{j=0}^{2N+1}\left[xV_{l'\beta}\frac{\tilde{S}_j(x)}{x}\right]\tilde{C}^l_{\beta,j} = 0 \end{aligned} \tag{9.172}$$

By choosing x_i points, $i \in [1, 2N]$, we can have $2N$ number of equations. Let us define vectors and matrices as

$$[\tilde{C}^l]_n \equiv \tilde{C}^l_{\beta,j}, \tag{9.173}$$

$$[\Delta]_{n'n} \equiv -\frac{1}{2\mu}\frac{d^2}{dx^2}\tilde{S}_j(x_i)\delta_{l',\beta} + \frac{1}{2\mu}\frac{l'(l'+1)}{x_i^2}\tilde{S}_j(x_i)\delta_{l',\beta}, \tag{9.174}$$

$$[B]_{n'n} \equiv \tilde{S}_j(x_i)\delta_{l'\beta}, \tag{9.175}$$

$$[V]_{n'n} \equiv x_i V_{l'\beta}(x_i)\frac{\tilde{S}_j(x_i)}{x_i}, \tag{9.176}$$

with

$$n' \equiv (l', i) \text{ and } n \equiv (\beta, j), \tag{9.177}$$

Then, above equation can be rewritten as matrix equation,

$$\sum_{\beta=1}^{N_s}\sum_{j=0}^{2N+1}[\Delta - EB + V]_{n'n}[\tilde{C}^l]_n = 0. \tag{9.178}$$

Note that number of index is different between n' and n. We have to use boundary conditions to make the above equation to be square.

Let us denote $n_0 \equiv (\beta, 0)$ and $n_f \equiv (\beta, 2N+1)$ and separate

$$\sum_{\beta=1}^{N_s}\sum_{j=1}^{2N}[\Delta - EB + V]_{n'n}[\tilde{C}^l]_n + \sum_{\beta=1}^{N_s}[\Delta - EB + V]_{n'n_0}[\tilde{C}^l]_{n_0} + \sum_{\beta=1}^{N_s}[\Delta - EB + V]_{n'n_f}[\tilde{C}^l]_{n_f} = 0 \tag{9.179}$$

For bound state problem, we can use boundary condition as

$$[\tilde{C}^l]_{n_0} = 0, \quad [\tilde{C}^l]_{n_f} = 0, \text{ for all } \beta. \tag{9.180}$$

and the matrix equation becomes eigenvalue problem

$$\sum_n{}'[\Delta + V]_{n'n}[\tilde{C}^l]_n = E\sum_n{}'[B]_{n'n}[\tilde{C}^l]_n, \quad \text{with } \sum_n{}' \equiv \sum_{\beta=1}^{N_s}\sum_{j=1}^{2N}. \tag{9.181}$$

For the scattering case, we have to use asymptotic form of wave function as boundary condition,

$$[\tilde{C}^l]_{n_0} = 0, \quad [\tilde{C}^l]_{n_f} = u_{\beta l}(r = r_N) = \frac{1}{2}r[\delta_{\beta l}h_\beta^{(-)}(kr) + S_{\beta l}h_\beta^{(+)}(kr)]. \tag{9.182}$$

and the matrix equation becomes

$$\sum_n{}'[\Delta + V - EB]_{n'n}[\tilde{C}^l]_n = [G^l]_{n'}, \quad [G^l]_{n'} \equiv -\sum_{\beta=1}^{N_s}[\Delta - EB + V]_{n'n_f}[\tilde{C}^l]_{n_f} \tag{9.183}$$

But, in fact, asymptotic form of $u_{\beta l}$ contains unknown complex S-matrix. Because of homogeneous form of the equation, we can change normalization of solution. However, still it does not completely fix boundary condition if it is a coupled equation. How should we solve the problem?

Possible answer?: M원 N차 연립 미분 방정식의 general solution은 M*N 개의 independent boundary condition을 통해 얻은 M*N개 solution들의 선형 결합으로 표현된다? 만약 이 주장이 옳다면, 위 문제에서 regular solution 에 한정해서, $[\tilde{C}^l]_{nf} = \delta_{\beta l}$ 로 모든 $l = 1..N_s$ 개의 different boundary condition으로 부터 N_s 개의 solution을 구한다음 이것들이 어떻게 결합하여 원하는 boundary condition 을 줄 수 있는지 구하면 된다. So, we will let

$$[G^l]_{n'} \equiv -\sum_{\beta=1}^{N_s}[\Delta - EB + V]_{n'n_f}\delta_{l\beta} = -[\Delta - EB + V]_{n'(l,2N+1)} \tag{9.184}$$

And solve for different l's and get N_s different solutions. Then, recombine them to obtain asymptotic boundary condition and fix the S-matrix.

Suppose we obtained $[\tilde{C}^{l=1..N_s}]_{i=1..2N}$. Then how can we find the correct normalization and S, K matrix?

9.5.4 Special case: perturbation

In case of inhomogeneous PV equation,

$$\left[-\frac{1}{2\mu}\frac{d^2}{dx^2}+\frac{1}{2\mu}\frac{l'(l'+1)}{x^2}-E\right]u^{PV}_{l'l}(x)+\sum_\beta xV^{PC}_{l'\beta}(x)\frac{u^{PV}_{\beta l}(x)}{x}+\sum_\beta xV^{PV}_{l'\beta}(x)\frac{u^{PC}_{\beta l}(x)}{x}=0,\tag{9.185}$$

we can transform the equation into matrix equation,

$$\begin{aligned}&\sum_{\beta=1}^{N_s}\sum_{j=1}^{2N}[\Delta-EB+V^{PC}]_{n'n}[\tilde{C}^{PV,l}]_n\\&+\sum_{\beta=1}^{N_s}[\Delta-EB+V^{PC}]_{n'n_0}[\tilde{C}^{PV,l}]_{n_0}+\sum_{\beta=1}^{N_s}[\Delta-EB+V^{PC}]_{n'n_f}[\tilde{C}^{PV,l}]_{n_f}\\&+\sum_{\beta=1}^{N_s}\sum_{j=0}^{2N+1}[V^{PV}]_{n'n}[\tilde{C}^{PC,l}]_n=0.\end{aligned}\tag{9.186}$$

Suppose we already solved the parity conserving wave function, the last term is already known and we can write as

$$[K^l]_{n'}\equiv-\sum_{\beta=1}^{N_s}x_iV^{PV}_{l'\beta}(x_i)\frac{u^{PC}_{\beta l}(x_i)}{x_i}\tag{9.187}$$

However, the boundary condition for u^{PV} as

$$[\tilde{C}^{PV,l}]_{n_0}=0,\quad[\tilde{C}^{PV,l}]_{n_f}=u^{PV}_{\beta l}(r=r_N),\tag{9.188}$$

is not directly applicable because it contains unknown scattering matrix and also cannot be arbitrarily scaled,

$$u^{PV}_{\beta l}(r)=\frac{1}{2}S^{PV}_{\beta l}h^{(+)}_\beta(kr),\tag{9.189}$$

where there is no $\delta_{\beta l}$ because $\beta\neq l$ for PV transition. But we can use logarithmic derivative continuous condition,

$$\frac{1}{u^{PV}_{\beta l}(r)}\frac{du^{PV}_{\beta l}(r)}{dr}=\frac{1}{h^{(+)}_\beta(kr)}\frac{dh^{(+)}_\beta(kr)}{dr}\tag{9.190}$$

Thus replace

$$u^{PV}_{\beta l}(r=r_N)=\frac{h^{(+)}_\beta(kr_N)}{\frac{d}{dr}h^{(+)}_\beta(kr_N)}\frac{du^{PV}_{\beta l}(r_N)}{dr}=\frac{h^{(+)}_\beta(kr_N)}{\frac{d}{dr}h^{(+)}_\beta(kr_N)}\tilde{C}^l{}_{\beta,2N}=\tilde{C}^l{}_{\beta,2N+1}\tag{9.191}$$

and change

$$\begin{aligned}&\sum_{\beta=1}^{N_s}[\Delta-EB+V]_{n'n_f}[\tilde{C}^{PV,l}]_{n_f}\\+\quad&\sum_{\beta=1}^{N_s}\sum_{j=1}^{2N}\left[\delta_{j,2N}[\Delta-EB+V^{PC}]_{n',n_f}\left(\frac{h^{(+)}_\beta(kr_N)}{\frac{d}{dr}h^{(+)}_\beta(kr_N)}\right)\right][\tilde{C}^{PV,l}]_n\\\equiv\quad&\sum_n{}'[X]_{n'n}[\tilde{C}^{PV,l}]_n\end{aligned}\tag{9.192}$$

And finally the equation becomes

$$\sum_n{}' [\Delta + V^{PC} - EB + X]_{n'n}[\tilde{C}^{PV,l}]_n = [K^l]_{n'} \tag{9.193}$$

After obtaining $[\tilde{C}^{PV,l}]_n$, we can obtain

$$S^{PV}_{\beta l} = \frac{2\tilde{C}^{PV,l}_{\beta,2N}}{\frac{d}{dr}h^{(+)}_\beta(kr_N)} \tag{9.194}$$

One subtle point in above expression is that β must contain both parity even and parity odd states. For example we choose $l' = 1$ and $l = 0$, $\sum_n$ in the above matrix equation must be parity odd states but $\sum_\beta$ in $[K]$ must be parity even states. Also, we have to solve the matrix equation for complex coefficients, unlike Parity conserving case.

9.5.5 Practical implementation

먼저, potential 이 real인 경우, complex normalization factor를 밖으로 빼어내서, 우리는 언제나 real-valued solution을 얻을 수 있다. scattering state의 경우에는 complex normalization factor 를

$$\begin{aligned} R_{\alpha',\alpha}(x) &= \sum_\beta \hat{R}_{\alpha',\beta}(x)[\frac{1+\hat{S}}{2}]_{\beta\alpha}, \\ \hat{R}_{\alpha',\beta}(x) &\to \delta_{\alpha',\beta}j_{L'}(kx) - \hat{K}_{\alpha'\beta}n_{L'}(kx) \end{aligned} \tag{9.195}$$

로 빼낼 수 있고, normalization 은

$$[\frac{1+\hat{S}}{2}]_{\beta\alpha} = [(1-i\hat{K})^{-1}]_{\beta,\alpha} \tag{9.196}$$

을 이용해 K-matrix로 나타낼 수 있다.

한편, 실제 계산에서 우리가 다루는 것은 spline coefficient 에 관한 equation이다. 따라서,

$$\hat{R}_{\alpha,\beta}(x) = \sum_{j=1}^{2N_x} \tilde{C}^\beta_{\alpha,j}\tilde{S}_j(x) + \tilde{C}^\beta_{\alpha,2N_x+1}\tilde{S}_{2N_x+1}(x) \tag{9.197}$$

이것은 위의 K-matrix 와 다음 식을 만족해야 한다.

$$\begin{aligned} \tilde{C}^\beta_{\alpha,2N+1} &= \hat{R}_{\alpha,\beta}(x_N) = \delta_{\alpha,\beta}j_\alpha(kx_N) - \hat{K}_{\alpha\beta}n_\alpha(kx_N), \\ \tilde{C}^\beta_{\alpha,2N} &= \hat{R}'_{\alpha,\beta}(x_N) = \delta_{\alpha,\beta}j'_\alpha(kx_N) - \hat{K}_{\alpha\beta}n'_\alpha(kx_N). \end{aligned} \tag{9.198}$$

따라서,

$$\begin{aligned} K_{\alpha\beta} &= \left[\frac{\delta_{\alpha\beta}j'_\alpha(kx_N) - \tilde{C}^\beta_{\alpha,2N}}{n'_\alpha(kx_N)}\right], \\ \tilde{C}^\beta_{\alpha,2N+1} &= \left[\delta_{\alpha,\beta}j_\alpha(kx_N) - \delta_{\alpha\beta}\frac{n_\alpha(kx_N)}{n'_\alpha(kx_N)}j'_\alpha(kx_N)\right] + \tilde{C}^\beta_{\alpha,2N}\frac{n_\alpha(kx_N)}{n'_\alpha(kx_N)} \end{aligned} \tag{9.199}$$

으로 $\tilde{C}^\alpha_{\beta,(2N)}$ 값으로 모두 나타낼 수 있다. 따라서, linear algebra 문제를 푸는데 두 가지 접근을 생각해 볼 수 있다. eq.(9.195)에 eq.(9.199)를 대입하여, 식을 $\tilde{C}^\alpha_{\beta,1:2N}$ 에 대한 inhomogeneous equation으로 만들어서 풀면, normalization condition까지 고려한 결과 $\tilde{C}^\alpha_{\beta,1:2N}$를 한 번에 얻게 된다. 한 편, 위와 같이 푸는 대신, $\tilde{C}^\beta_{\alpha,2N+1} = \delta_{\alpha,\beta}$의 boundary condition 을 주어 모든 β 에 대한 solution을 얻은 뒤

다시 normalization을 restore 해주는 방볍이다. 이렇게 구해진 spline coefficient solution을 $D^{\beta}_{\alpha,j}$ 라고 하자. 즉, 우리는

$$\tilde{C}^{\beta}_{\alpha,j} = \sum_{\gamma} M_{\alpha\gamma} \tilde{D}^{\gamma}_{\beta,j}, \quad \tilde{D}^{\beta}_{\alpha,2N+1} = \delta_{\alpha,\beta}, \tag{9.200}$$

인 solutions $\tilde{D}^{\beta}_{\alpha,j}$ 를 얻었다고 하자. Conversion factor or Normalization factor $M_{\alpha\gamma}$ can be obtained from the comparison with eq.(9.199), $M_{\alpha\beta} = \tilde{C}^{\beta}_{\alpha,2N+1}$. 하지만, $\tilde{C}$ 는 미리 알려진 것이 아니므로, M 을 D로 나타내어 주면,[9]

$$\sum_{\gamma} M_{\alpha\gamma} \left[\tilde{D}^{\gamma}_{\beta,2N+1} - \tilde{D}^{\gamma}_{\beta,2N} \frac{n_\alpha(kx_N)}{n'_\alpha(kx_N)} \right] = \left[\delta_{\alpha,\beta} j_\alpha(kx_N) - \delta_{\alpha\beta} \frac{n_\alpha(kx_N)}{n'_\alpha(kx_N)} j'_\alpha(kx_N) \right] \tag{9.201}$$

으로부터 , $M_{\alpha\gamma}$를 구할 수 있다. Note here $\gamma = 1 : N_{ch}$ but $\alpha, \beta = 1 : N_s$.

In summary, the steps we need to takes are

1. Solve and obtain solutions for coupled channels $\tilde{D}^{\gamma}_{\alpha,j}$ for $j = 1 : 2N$ with boundary conditions $\tilde{D}^{\beta}_{\alpha,2N+1} = \delta_{\alpha,\beta}$.
2. Obtain conversion matrix M from eq.(9.201).
3. Obtain $\tilde{C}$ from eq. (9.200).
4. Obtain K-matrix and last spline coefficients from eq.(9.199)
5. Obtain complex normalization and S-matrix from eq.(9.196)
6. Finally, full wave function can be obtained by multiplying complex normlaization to real valued solutions.

Until now we used notation $n = (\beta, j)$ to represent both partial wave quantum number and spatial coordinate ot spline index. In practical implementation, it would be better to introduce 1-D index

$$k = (\beta - 1) * (kN_x) + j, \quad \beta = 1 \dots N_s, \quad j = 1 \dots kN_x, \tag{9.202}$$

so that the wave function $F_{\alpha,i}(x)$ can be written as 1-D array $F_i(k = 1 \dots N_s kN_x)$ with only external index for initial channel i. If we have coupled channels, we would want match

$$F^{full}_i(1 : N_s kN_x) = \sum_j N_{ij} F^{num}_j(1 : N_s KN_x), \tag{9.203}$$

where, $F^{full}_i(1 : N_s kN_x)$ is a full complex wave function with correct normalization and asymptotic form in channel i, $F^{num}_j(1 : N_s KN_x)$ is a numerical solution with boundary condition of $[\tilde{C}^j]_{nf} = \delta_{\beta j}$ and N_{ij} is a complex normalization matrix to match F^{full}_i.

9.5.6 Lanczos method: iteration method

앞에서 3-body 문제를 spline method를 이용하여 linear algebra 문제로 바꾸는 것을 살펴보았다. 여기서는 linear algebra problem 특히 bound state의 경우에 large matrix에 대해 효율적으로 푸는 방법을 살펴보자. 이것은 다음 3-body 노트에서 이야기하자.

[9] It is possible that the number of interested coupled channels is less than the number of internal partial wave states. In that case, matrix M can be non-square. But, nonetheless the equation can be solved. $[M(N_s \times N_{ch})[D(N_{ch} \times N_s)] = [N_s \times N_s]$, which can be changed into the form of $Ax = b$ by transpose the equation.

9.6 T-amplitude with two different potential (Alternate derivation of DWBA)

Let us call there are two potentials $\hat{V} = \hat{V}_Y + \hat{C}$. In operator form, the T matrix will be written as

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_0\hat{T} = \hat{V} + \hat{V}\hat{G}\hat{V} \tag{9.204}$$

We introduce Green's functions and $\hat{T}_Y$ as

$$\begin{aligned}
&\hat{G}^{(+)} = \frac{1}{E - \hat{H}_0 - \hat{V} + i\epsilon}, \quad \hat{G}_0^{(+)} = \frac{1}{E - \hat{H}_0 + i\epsilon}, \quad \hat{G}_Y^{(+)} = \frac{1}{E - \hat{H}_0 - \hat{V}_Y + i\epsilon}, \\
&\hat{T}_Y = \hat{V}_Y + \hat{V}_Y\hat{G}_0\hat{T}_Y = \hat{V}_Y + \hat{V}_Y\hat{G}_Y\hat{V}_Y
\end{aligned} \tag{9.205}$$

From the relation between Green's functions, we get formal relations [10]

$$\begin{aligned}
\hat{G}^{-1} &= \hat{G}_Y^{-1} - \hat{C}, \\
\hat{G} &= (\hat{G}_Y - \hat{C})^{-1} = (1 - \hat{G}_Y\hat{C})^{-1}\hat{G}_Y = \hat{G}_Y(1 - \hat{C}\hat{G}_Y)^{-1}, \\
\hat{C}\hat{G} &= (1 - \hat{C}\hat{G}_Y)^{-1} - 1 = (1 - \hat{C}\hat{G}_Y)^{-1}\hat{C}\hat{G}_Y.
\end{aligned} \tag{9.207}$$

Then,

$$\begin{aligned}
\hat{T} &= (\hat{V}_Y + \hat{C}) + (\hat{V}_Y + \hat{C})\hat{G}(\hat{V}_Y + \hat{C}) \\
&= \hat{V}_Y + \hat{C} + \hat{V}_Y\hat{G}\hat{V}_Y + \hat{C}\hat{G}\hat{V}_Y + \hat{V}_Y\hat{G}\hat{C} + \hat{C}\hat{G}\hat{C}
\end{aligned} \tag{9.208}$$

we can replace

$$\begin{aligned}
\hat{V}_Y\hat{G}\hat{V}_Y &= \hat{V}_Y\hat{G}_Y(1 - \hat{C}\hat{G}_Y)^{-1}\hat{V}_Y = \hat{V}_Y\hat{G}_Y[1 + \hat{C}\hat{G}_Y(1 - \hat{C}\hat{G}_Y)^{-1}]\hat{V}_Y \\
&= \hat{V}_Y\hat{G}_Y\hat{V}_Y + \hat{V}_Y\hat{G}_Y(1 - \hat{C}\hat{G}_Y)^{-1}\hat{C}\hat{G}_Y\hat{V}_Y, \\
\hat{C}\hat{G}\hat{C} &= (1 - \hat{C}\hat{G}_Y)^{-1}\hat{C} - \hat{C}, \\
\hat{C}\hat{G}\hat{V}_Y &= (1 - \hat{C}\hat{G}_Y)^{-1}\hat{C}\hat{G}_Y\hat{V}_Y, \\
\hat{V}_Y\hat{G}\hat{C} &= \hat{V}_Y\hat{G}_Y(1 - \hat{C}\hat{G}_Y)^{-1}\hat{C}
\end{aligned} \tag{9.209}$$

Thus, we get

$$\hat{T} = \hat{T}_Y + (1 + \hat{V}_Y\hat{G}_Y)(1 - \hat{C}\hat{G}_Y)^{-1}\hat{C}(1 + \hat{G}_Y\hat{V}_Y) \tag{9.210}$$

We define $|\chi_{\boldsymbol{p}}\rangle$ such that $|\chi_{\boldsymbol{p}}\rangle$ is a solution of Schrodinger equation for $\hat{V}_Y$:

$$\begin{aligned}
|\chi_{\boldsymbol{p}}\rangle^{(\pm)} &\equiv (1 + \hat{G}_Y^{(\pm)}\hat{V}_Y)|\boldsymbol{p}\rangle, \\
\hat{G}_Y(E_p)^{-1}|\chi_{\boldsymbol{p}}\rangle &= (E_p - \hat{H}_0 - \hat{V}_Y)|\chi_{\boldsymbol{p}}\rangle = (\hat{G}_Y^{-1}(E_p) + \hat{V}_Y)|\boldsymbol{p}\rangle = (E_p - \hat{H}_0)|\boldsymbol{p}\rangle = 0
\end{aligned} \tag{9.211}$$

Thus,

$$\langle\boldsymbol{p}'|\hat{T}(E)|\boldsymbol{p}\rangle = \langle\boldsymbol{p}'|\hat{T}_Y(E)|\boldsymbol{p}\rangle + {}^{(-)}\langle\chi_{\boldsymbol{p}'}|(1 - \hat{C}\hat{G}_Y(E))^{-1}\hat{C}|\chi_{\boldsymbol{p}}\rangle^{(+)} \tag{9.212}$$

where E is not neccessarily E_p or $E_{p'}$ when they are not on-shell. If $\hat{C}$ is perturbative case, we may approximate $(1 - \hat{C}\hat{G}_Y)^{-1} \simeq 1$, and we get DWBA approximation. Above equation corresponds to the equation (4.5) in **D.B.Kaplan etal., NPB478(1996)629.**

[10] In general, we can use matrix relations

$$B(1 - AB)^{-1} = (1 - BA)^{-1}B, \quad (1 - A)^{-1} = 1 + A(1 - A)^{-1}, \quad A(1 - A)^{-1} = (1 - A)^{-1}A \tag{9.206}$$

We may express rewrite the operators in terms of $\hat{G}_0$ and $\hat{T}_Y$ from relation,

$$\begin{aligned}\hat{T}_Y &= \hat{V}_Y + \hat{V}_Y\hat{G}_0\hat{T}_Y = \hat{V}_Y + \hat{V}_Y\hat{G}_Y\hat{V}_Y,\\ 1+\hat{G}_Y\hat{V}_Y &= \hat{G}_Y\hat{G}^{-1},\end{aligned}\tag{9.213}$$

$$\begin{aligned}|\chi_{\boldsymbol{p}}\rangle &= (1+\hat{G}_Y\hat{V}_Y)|\boldsymbol{p}\rangle = (1+\hat{G}_0\hat{T}_Y)|\boldsymbol{p}\rangle,\\ (1-\hat{C}\hat{G}_Y)^{-1}\hat{C} &= (\hat{C}^{-1}-(1+\hat{G}_YV_Y)\hat{G}_0)^{-1}.\end{aligned}\tag{9.214}$$

This corresponds to the equation (9) of **Long and Yang, PRC86(2012)024001.**

9.7 Chiral EFT potential up to NLO

Machleidt potential in momentum space has form,

$$\begin{aligned}V(\boldsymbol{p}',\boldsymbol{p}) &= V_C + \tau_1\cdot\tau_2 W_C\\ &+ [V_S+\tau_1\cdot\tau_2W_S]\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\\ &+ [V_{LS}+\tau_1\cdot\tau_2W_{LS}]\,(-i\boldsymbol{S}\cdot(\boldsymbol{q}\times\boldsymbol{k}))\\ &+ [V_T+\tau_1\cdot\tau_2W_T]\,\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}\\ &+ [V_{\sigma L}+\tau_1\cdot\tau_2W_{\sigma L}]\,\boldsymbol{\sigma}_1\cdot(\boldsymbol{q}\times\boldsymbol{k})\boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k})\end{aligned}\tag{9.215}$$

where,

$$\begin{array}{rcl}\boldsymbol{q}= & \boldsymbol{p}'-\boldsymbol{p} & \text{momentum transfer },\\ \boldsymbol{k}= & \frac{1}{2}(\boldsymbol{p}'+\boldsymbol{p}) & \text{average momentum },\\ \boldsymbol{S}= & \frac{1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) & \text{total spin}\end{array}\tag{9.216}$$

The LO(Q^0) chiral EFT potential involves one-pion exchange and contact terms.

$$V_{1\pi}(\boldsymbol{p}',\boldsymbol{p}) = -\frac{g_A^2}{4f_\pi^2}\tau_1\cdot\tau_2\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2},\quad V^{(0)} = C_S + C_T\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2.\tag{9.217}$$

The NLO(Q^2) chiral EFT,

$$\begin{aligned}W_C &= -\frac{L(q)}{384\pi^2f_\pi^4}\left[4m_\pi^2(5g_A^4-4g_A^2-1)+q^2(23g_A^4-10g_A^2-1)+\frac{48g_A^4m_\pi^4}{\omega^2}\right],\\ V_T &= -\frac{1}{q^2}V_S = -\frac{3g_A^4L(q)}{64\pi^2f_\pi^4},\end{aligned}\tag{9.218}$$

where,

$$L(q)\equiv\frac{\omega}{q}\ln\frac{\omega+q}{2m_\pi},\quad \omega\equiv\sqrt{4m_\pi^2+q^2}.\tag{9.219}$$

NLO contact potentials

$$\begin{aligned}V^{(2)}(\boldsymbol{p}',\boldsymbol{p}) &= C_1q^2+C_2k^2+(C_3q^2+C_4k^2)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\\ &+C_5(-i\boldsymbol{S}\cdot(\boldsymbol{q}\times\boldsymbol{k}))+C_6(\boldsymbol{\sigma}_1\cdot\boldsymbol{q})(\boldsymbol{\sigma}_2\cdot\boldsymbol{q})+C_7(\boldsymbol{\sigma}_1\cdot\boldsymbol{k})(\boldsymbol{\sigma}_2\cdot\boldsymbol{k})\end{aligned}\tag{9.220}$$

Partial wave representation of the potential can be obtained by,

$$V_{L'L}(p',p) = \int d\Omega_{\boldsymbol{p}'}\int d\Omega_{\boldsymbol{p}}Y_{L'}^*(\hat{\boldsymbol{p}}')V(\boldsymbol{p}',\boldsymbol{p})Y_L(\hat{\boldsymbol{p}})\tag{9.221}$$

Thus, if we do not include regulator, potentials in each partial wave are

$$
\begin{aligned}
V^{(0)}({}^1S_0) &= 4\pi(C_S - 3C_T) = \widetilde{C}_{{}^1S_0}, \\
V^{(0)}({}^3S_1) &= 4\pi(C_S + C_T) = \widetilde{C}_{{}^3S_1}, \\
V^{(2)}({}^1S_0) &= C_{1S_0}(p^{'2} + p^2) = 4\pi(C_1 + \frac{1}{4}C_2 - 3C_3 - \frac{3}{4}C_4 - C_6 - \frac{1}{4}C_7)(p^{'2} + p^2), \\
V^{(2)}({}^3P_0) &= C_{{}^3P_0} pp' = \ldots, \\
V^{(2)}({}^1P_1) &= C_{{}^1P_1} pp' = \ldots, \\
V^{(2)}({}^3P_1) &= C_{{}^3P_1} pp' = \ldots, \\
V^{(2)}({}^3S_1) &= C_{{}^3S_1}(p^2 + p^{'2}) = \ldots, \\
V^{(2)}({}^3S_1 -{}^3 D_1) &= C_{{}^3S_1 - {}^3D_1} p^2 = \ldots, \\
V^{(2)}({}^3P_2) &= C_{{}^3P_2} pp' = \ldots
\end{aligned} \tag{9.222}
$$

Chapter 10

Semi-classical scattering

In the semiclassical approximation the dynamics of the scattering is classical, and is described in terms of classical notions like trajectories, impact parameters, turning points, and so on. The classical dynamical quantities enter in the calculation of the amplitude and phase of the wave function. Typical quantal interference effects are preserved in the semiclassical approximation.

10.1 Classical scattering

10.1.1 deflection function

Trajectory $\boldsymbol{r} = \boldsymbol{r}(t)$.

From two equations

$$
\begin{aligned}
E &= \frac{\mu}{2}(\frac{dr}{dt})^2 + \frac{L^2}{2\mu r^2} + V(r), \\
L &= \mu r^2 \frac{d\phi}{dt}
\end{aligned}
\tag{10.1}
$$

we get

$$
\frac{d\phi}{dr} = \frac{L}{r^2\sqrt{2\mu[E - V(r) - L^2/(2\mu r^2)]}} \tag{10.2}
$$

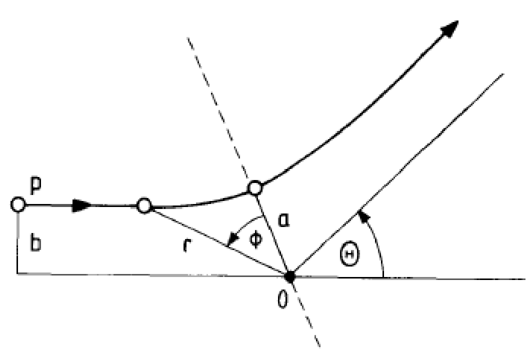

Figure 10.1: Classical trajectory

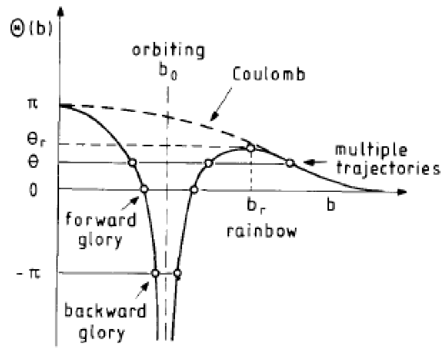

Figure 2.5 Schematic deflection function $\Theta(b)$ for scattering by a real Coulomb-plus-nuclear potential. The Coulomb deflection function is shown for comparison (dashed curve).

Figure 10.2: classical deflection function in both attraction and repulsion

At turning point, $r = a$,

$$E - V(a) - \frac{L^2}{2\mu a^2} = 0. \tag{10.3}$$

and

$$\phi(r) = \int_a^r dr' \frac{L}{r'^2\sqrt{2\mu[E - V(r') - L^2/(2\mu r'^2)]}} \tag{10.4}$$

Deflection angle Θ from the solution at $r \to \infty$ gives deflection function

$$\begin{aligned} \Theta(b) &= \pi - 2\phi(\infty) \\ &= \pi - 2\int_a^\infty dr \frac{b}{r^2\sqrt{1 - V(r)/E - b^2/r^2}} \end{aligned} \tag{10.5}$$

Postive deflection $\Theta > 0$ implies net repulsion, $\Theta < 0$ imples net attraction.

In case of classical scattering, one can tell near-side and far-side scattering.

We can identify deflection as scattering angle for $\Theta = \theta > 0$ for repulsion. In case of attraction, $\theta = |\Theta \mod 2\pi|$. scattering cross section is

$$\frac{d\sigma}{d\Omega} = \frac{bdbd\phi}{|\sin\Theta d\Theta|d\phi} = \frac{b}{\sin\theta|d\Theta/db|} \tag{10.6}$$

Rutherford scattering

$$\Theta(b) = 2\arctan(\frac{\eta}{kb}), \to b = \frac{\eta}{k}\cot(\frac{\Theta}{2}) \tag{10.7}$$

turning point,

$$a = \frac{\eta}{k} + \sqrt{(\frac{\eta}{k})^2 + b^2} \tag{10.8}$$

attraction and repulsion

Coulomb은 언제나 repulsive하지만, 일반적으로는 attraction과 repulsion이 모두 있다. 이런 경우는 다양한 trajectory를 가질 수 있다.

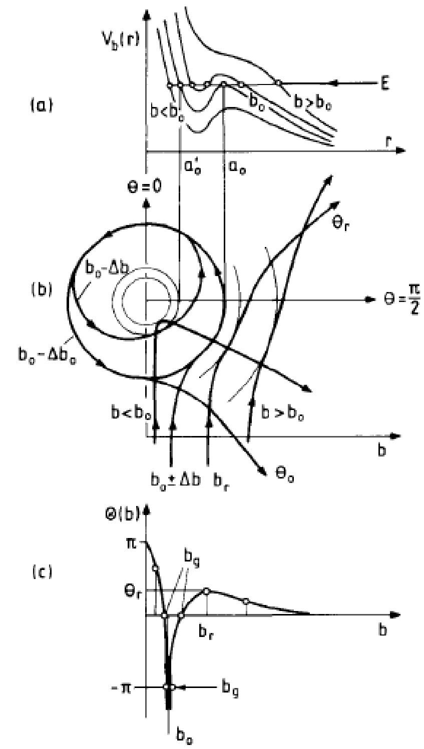

Figure 2.6 Particle scattering at energy E. (a) Effective potential $V_b(r)$ for various impact parameters b and the associated turning points. (b) The corresponding trajectories in the scattering plane. (c) The deflection function.

Figure 10.3

그림에서 같은 scattering angle θ 를 주는 impact parameter가 여러개 있는 경우는 multiple trajectory의 경우.

cross section is singular at $\sin(\Theta(b_g)) = 0$ or $\Theta(b_g) = \pi - m\pi$. These are called glories. 즉, 이를 만족시키는 impact parameter의 경우 마치 scattering을 하지 않은 것 같은 효과를 준다. (예를 들어 사람의 뒷쪽에서 빛이 비추는 경우 특정 impact parameter는 deflection이 없으므로 밝게 보일 것이다.)

cross section is also singular when $d\Theta/db = 0$, 즉 deflection function의 maxima. This defines rainbow.(즉, rainbow 처럼, scattering angle의 끝부분이 있음.)

deflection function itself can be singular at certain b_o, which is orbiting.

10.2 Semiclassical (WKB)

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l} - 1)P_l(\cos\theta) \tag{10.9}$$

- (1) phase shift are calculated in WKB approximation (difference of the full and free classical actions)
- (2) Legendre polynomial are replaced with asymptotic forms for large l values
- (3) sum over angular momentum into integral
- (4) whole expression evaluated in stationary phase.

The δ_l^{WKB} phase shift of WKB approximation can be obtained as

$$\delta_l^{WKB} = \frac{\pi}{2}(l+\frac{1}{2}) + \int_a^\infty [p_l(r)/\hbar - k] - ka. \tag{10.10}$$

Note here that $p_l(r)$ is a classical quantity. Also, the expression can be considered as

$$\delta_l^{WKB} = \lim_{r\to\infty} \frac{1}{\hbar}[s_l(r) - s_l^0(r)] \tag{10.11}$$

where, WKB phase shift is a difference between radial action $s_l(r)$

$$s_l(r) = \int_a^r p_l(r')dr', \quad p_l(r) = \sqrt{2\mu[E - V_l(r)]} \tag{10.12}$$

and free radial action $s_l^0(r)$

$$s_l^0(r) = \int_{(l+1/2)/k}^r p_l^0(r')dr' \to \hbar[kr - \frac{\pi}{2}(l+\frac{1}{2})], \text{ for } r\to\infty \tag{10.13}$$

which both are classical quantities.

Alternative WKB(?): instead of integration, one can obtain WKB phase shift by solving differential equation. In other words, solve following equations from $t = t_i$ with radius $r = r_i$ to $r = r_f$ outside of interaction range,

$$\begin{aligned} \dot{r} &= p_l(r)/\mu, \\ \dot{p}_l(r) &= -V_l'(r), \\ \dot{\delta}_l(r) &= \frac{1}{\hbar}[p_l(r) - p_l^0(r)]\dot{r} \end{aligned} \tag{10.14}$$

to get WKB phase shift as $\delta_l^{WKB} = \delta_l(r_f)$. (This method can be used for complex potential. complex trajectory and momentum?.)

After additional steps for Legendre polynomials, stationary approximation, scattering amplitude and differential cross section can be approximated as

$$\begin{aligned} f_0^+(\theta) &= -\frac{i}{k}\frac{\sqrt{\lambda_0}}{\sqrt{\sin\theta}} \exp\left[i\left(\phi_+(\lambda_0) + \frac{\pi}{4} - \frac{1}{2}\arg\frac{d\Theta}{d\lambda}|_{\lambda_0}\right)\right] |\frac{d\Theta(\lambda)}{d\lambda}|_{\lambda_0}^{-1/2}, \\ \phi_\pm(\lambda) &= 2\delta^{WKB}(\lambda) \pm \lambda\theta \mp \frac{\pi}{4} + 2m\pi\lambda - m\pi \end{aligned} \tag{10.15}$$

where setting $m = 0$, $\lambda_0 = \lambda_0(\theta)$ at angle θ is determined by solution of

$$\Theta(b = \lambda_0/k) = \mp\theta - m2\pi, \quad \text{for } f_m^\pm(\theta) \tag{10.16}$$

where

$$2\frac{d\delta_l^{WKB}}{dl} = \Theta(b) \quad \text{with} \quad b = (l+\frac{1}{2})/k \tag{10.17}$$

Semiclassical approximations are employed mainly to interpret the features of the cross section in terms of classical trajectories and their interferences.

Chapter 11

Supplements

11.1 Common special functions

11.1.1 Coulomb functions

From Abramowitz and Stegun,

- Differential equation:

$$\frac{d^2w}{d\rho^2} + \left(1 - \frac{2\eta}{\rho} - \frac{l(l+1)}{\rho^2}\right) w = 0 \tag{11.1}$$

  solution of above differential equation are regular Coulomb and irregular Coulomb function.

$$w(\rho) = c_1 F_L(\eta, \rho) + c_2 G_L(\eta, \rho) \tag{11.2}$$

- Regular Coulomb function

$$\begin{aligned} F_L(\eta,\rho) &= C_L(\eta)\rho^{L+1}e^{-i\rho}M(L+1-i\eta, 2L+2, 2i\rho), \\ C_L(\eta) &= \frac{2^L e^{-\pi\eta/2}|\Gamma(L+1+i\eta)|}{\Gamma(2L+2)}, \quad C_0^2(\eta) = \frac{2\pi\eta}{e^{2\pi\eta}-1} \end{aligned} \tag{11.3}$$

- relation with spherical Bessel functions

$$\begin{aligned} F_L(0,\rho) &= \rho j_L(\rho), \\ G_L(0,\rho) &= -\rho y_L(\rho) = -\rho n_L(\rho) \end{aligned} \tag{11.4}$$

- Wronskian Relation

$$\begin{aligned} &F_L' G_L - F_L G_L' = 1, \\ &F_{L-1}G_L - F_L G_{L-1} = L(L^2+\eta^2)^{-1/2} \end{aligned} \tag{11.5}$$

- Asymptotic Expansion: large ρ limit.

$$\begin{aligned} &\theta_l \equiv \rho - \eta \ln 2\rho - L\frac{\pi}{2} + \sigma_L, \\ &\sigma_L \equiv arg\Gamma(L+1+i\eta), \\ &G_L(\eta,\rho) \pm iF_L(\eta,\rho) \to exp(\pm i\theta_l) \quad , \rho \gg 1, \\ &F_L(\eta, \rho \gg 1) = \frac{e^{i\theta_l} - e^{-i\theta_l}}{2i}, \\ &G_L(\eta, \rho \gg 1) = \frac{e^{i\theta_l} + e^{-i\theta_l}}{2} \end{aligned} \tag{11.6}$$

- Asymptotic Expansion for $\eta = 0$

$$\begin{aligned} F_L(0, \rho \gg 1) &= \rho j_L(\rho \gg 1) \\ &= \frac{i}{2}\left(e^{-i(\rho - l\pi/2)} - e^{i(\rho - l\pi/2)}\right) \\ &= \frac{i}{2}\left(i^l e^{-i\rho} - (-i)^l e^{i\rho}\right) \end{aligned} \tag{11.7}$$

- Asymptotic form

$$\begin{aligned} \frac{F_L(\eta,\rho)}{\rho} &\rightarrow \frac{e^{i\theta_l} - e^{-i\theta_l}}{2i} = \frac{i}{2}\frac{1}{\rho}\left(e^{-i(\rho - l\pi/2 + \sigma_l - \eta\ln 2\rho)} - e^{i(\rho - l\pi/2 + \sigma_l - \eta\ln 2\rho)}\right) \\ &= e^{-i\sigma_l}\frac{i}{2}\left(\frac{e^{-i(\rho - l\pi/2 - \eta\ln 2\rho)}}{\rho} - e^{2i\sigma_l}\frac{e^{i(\rho - l\pi/2 - \eta\ln 2\rho)}}{\rho}\right) \\ &= e^{-i\sigma_l}\frac{i}{2}\left(\frac{e^{-i(\rho - l\pi/2 - \eta\ln 2\rho)}}{\rho} - \frac{e^{i(\rho - l\pi/2 - \eta\ln 2\rho)}}{\rho}\right) \\ &\quad + e^{-i\sigma_l} i^{-l}\left(\frac{e^{2i\sigma_l} - 1}{2ik}\right)\frac{e^{i(\rho - \eta\ln 2\rho)}}{r} \end{aligned} \tag{11.8}$$

Note that the wave function cannot be separated as a free incident wave and scattered wave. Also, the phase factor $e^{-i\sigma_l}$ is present in both terms. Thus, for Coulomb wave, the beam in the direction $\boldsymbol{k}$ is no longer $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$.

- near the origin,

$$\begin{aligned} F_L(0,\rho) &= \rho j_L(\rho) \xrightarrow{\rho\to 0} \frac{\rho^{(L+1)}}{(2l-1)!!}, \\ G_L(0,\rho) &= -\rho n_L(\rho) \xrightarrow{\rho\to 0} (2l+1)!!\rho^{-L} \end{aligned} \tag{11.9}$$

11.1.2 Spherical Bessel functions

11.1.3 Spherical Harmonics and Legendre Polynomial