Scattering Theory Note: Three body

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Faddeev equation을 공부해보자.

1 Jacobi coordinates

3-body에서 center of mass motion을 제외한 relative motion을 기술하기 위해서는 Jacobi coordinate를 도입하는 것이 편하다. In many case, we assume equal mass particles.

It is very important to fix our notation for particular meaning.

Let us first define ket state $|\boldsymbol{x}_i\boldsymbol{y}_i\rangle_j$. This vector means in configuration 'j', the distance vector between i pairs is $\boldsymbol{x}$ and i-particles distance from i-pair is $\boldsymbol{y}$. The configuration implies not just 3-particles, but interactions and thus channels(like two-particle makes a bound state or three-particle bound state or three particle break up..).

Thus, Jacobi coordinates and three particle coordinates are related as in configuration space, with center of mass $\boldsymbol{R} = (\boldsymbol{x}_1 + \boldsymbol{x}_2 + \boldsymbol{x}_3)/3$

$$\left(\begin{array}{c}\boldsymbol{x}_1 = \boldsymbol{r}_2 - \boldsymbol{r}_3 \\ \boldsymbol{y}_1 = \boldsymbol{r}_1 - \frac{1}{2}(\boldsymbol{r}_2 + \boldsymbol{r}_3)\end{array}\right), \quad \left(\begin{array}{c}\boldsymbol{x}_2 = \boldsymbol{r}_3 - \boldsymbol{r}_1 \\ \boldsymbol{y}_2 = \boldsymbol{r}_2 - \frac{1}{2}(\boldsymbol{r}_3 + \boldsymbol{r}_1)\end{array}\right), \quad \left(\begin{array}{c}\boldsymbol{x}_3 = \boldsymbol{r}_1 - \boldsymbol{r}_2 \\ \boldsymbol{y}_3 = \boldsymbol{r}_3 - \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2)\end{array}\right) \tag{1}$$

But, they are related with each other(the same configuration can be described in terms of each $(\boldsymbol{x}_i, \boldsymbol{y}_i)$ pairs.)

$$\left(\begin{array}{c}\boldsymbol{x}_2 = -\frac{1}{2}\boldsymbol{x}_1 - \boldsymbol{y}_1 \\ \boldsymbol{y}_2 = \frac{3}{4}\boldsymbol{x}_1 - \frac{1}{2}\boldsymbol{y}_1\end{array}\right), \quad \left(\begin{array}{c}\boldsymbol{x}_3 = -\frac{1}{2}\boldsymbol{x}_1 + \boldsymbol{y}_1 \\ \boldsymbol{y}_3 = -\frac{3}{4}\boldsymbol{x}_1 - \frac{1}{2}\boldsymbol{y}_1\end{array}\right) \tag{2}$$

In momentum space, with $\boldsymbol{K} = (\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3)$

$$\left(\begin{array}{c}\boldsymbol{p}_1 = \frac{1}{2}(\boldsymbol{k}_2 - \boldsymbol{k}_3) \\ \boldsymbol{q}_1 = \frac{2}{3}[\boldsymbol{k}_1 - \frac{1}{2}(\boldsymbol{k}_2 + \boldsymbol{k}_3)]\end{array}\right), \quad \left(\begin{array}{c}\boldsymbol{p}_2 = \frac{1}{2}(\boldsymbol{k}_3 - \boldsymbol{k}_1) \\ \boldsymbol{q}_2 = \frac{2}{3}[\boldsymbol{k}_2 - \frac{1}{2}(\boldsymbol{k}_3 + \boldsymbol{k}_1)]\end{array}\right), \quad \left(\begin{array}{c}\boldsymbol{p}_3 = \frac{1}{2}(\boldsymbol{k}_1 - \boldsymbol{k}_2) \\ \boldsymbol{q}_3 = \frac{2}{3}[\boldsymbol{k}_3 - \frac{1}{2}(\boldsymbol{k}_1 + \boldsymbol{k}_2)]\end{array}\right) \tag{3}$$

Also, each Jacobi momentums are convertible,

$$\left(\begin{array}{c}\boldsymbol{p}_2 = -\frac{1}{2}\boldsymbol{p}_1 - \frac{3}{4}\boldsymbol{q}_1 \\ \boldsymbol{q}_2 = \boldsymbol{p}_1 - \frac{1}{2}\boldsymbol{q}_1\end{array}\right), \quad \left(\begin{array}{c}\boldsymbol{p}_3 = -\frac{1}{2}\boldsymbol{p}_1 + \frac{3}{4}\boldsymbol{q}_1 \\ \boldsymbol{q}_3 = -\boldsymbol{p}_1 - \frac{1}{2}\boldsymbol{q}_1\end{array}\right) \tag{4}$$

All state vectors are normalized as

$$\begin{aligned}
&\int d\boldsymbol{k}_1 d\boldsymbol{k}_2 d\boldsymbol{k}_3 |\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\rangle\langle\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3| = 1 \\
&\langle\boldsymbol{k}'_1\boldsymbol{k}'_2\boldsymbol{k}'_3|\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\rangle = \delta^{(3)}(\boldsymbol{k}'_1 - \boldsymbol{k}_1)\delta^{(3)}(\boldsymbol{k}'_2 - \boldsymbol{k}_2)\delta^{(3)}(\boldsymbol{k}'_3 - \boldsymbol{k}_3) \\
&\int d\boldsymbol{p}_\alpha d\boldsymbol{q}_\alpha d\boldsymbol{K} |\boldsymbol{p}_\alpha\boldsymbol{q}_\alpha\boldsymbol{K}\rangle\langle\boldsymbol{p}_\alpha\boldsymbol{q}_\alpha\boldsymbol{K}| = 1 \\
&\langle\boldsymbol{p}'_\alpha\boldsymbol{q}'_\alpha\boldsymbol{K}'|\boldsymbol{p}_\alpha\boldsymbol{q}_\alpha\boldsymbol{K}\rangle = \delta^{(3)}(\boldsymbol{p}'_\alpha - \boldsymbol{p}_\alpha)\delta^{(3)}(\boldsymbol{q}'_\alpha - \boldsymbol{q}_\alpha)\delta^{(3)}(\boldsymbol{K}'_\alpha - \boldsymbol{K}_\alpha)
\end{aligned} \tag{5}$$

Asymptotic channel states can be written for channel α as

$$|\phi_{\boldsymbol{q}_\alpha}\rangle = |\varphi_\alpha\rangle|\boldsymbol{q}_\alpha\rangle \tag{6}$$

and break up channel as[1]

$$|\phi_\alpha\rangle^{(+)} = |\boldsymbol{p}_\alpha\rangle^{(+)}|\boldsymbol{q}_\alpha\rangle \tag{7}$$

————————- very confusing arguments following————————

Three identical boson particle의 경우에는 [2]

$$\begin{aligned} &|\boldsymbol{xy}\rangle = |\boldsymbol{x}_1\boldsymbol{y}_1\rangle_1 = |\boldsymbol{x}_2\boldsymbol{y}_2\rangle_2 = |\boldsymbol{x}_3\boldsymbol{y}_3\rangle_3 \\ &\Psi(\boldsymbol{x}_1,\boldsymbol{y}_1) = {}_1\langle\boldsymbol{x}_1\boldsymbol{y}_1|\Psi\rangle = {}_2\langle\boldsymbol{x}_2\boldsymbol{y}_2|\Psi\rangle = {}_3\langle\boldsymbol{x}_3\boldsymbol{y}_3|\Psi\rangle \end{aligned} \tag{8}$$

$|\Psi\rangle$는 permutation에 대해 symmetric 해야한다.

$$\begin{aligned} \Psi(\boldsymbol{x}_1\boldsymbol{y}_1) &= {}_1\langle\boldsymbol{x}_1\boldsymbol{y}_1|\Psi\rangle = {}_1\langle\boldsymbol{x}_1\boldsymbol{y}_1|P_{12}P_{23}|\Psi\rangle \\ &= {}_1\langle\boldsymbol{x}_1\boldsymbol{y}_1|P_{12}P_{23}|\Psi\rangle \end{aligned} \tag{9}$$

$$\begin{aligned} &|\boldsymbol{x}_1\boldsymbol{y}_1\rangle_2 = |\boldsymbol{x}_2\boldsymbol{y}_2\rangle_3 = |\boldsymbol{x}_3\boldsymbol{y}_3\rangle_1 \\ &|\boldsymbol{x}_1\boldsymbol{y}_1\rangle_3 = |\boldsymbol{x}_2\boldsymbol{y}_2\rangle_1 = |\boldsymbol{x}_3\boldsymbol{y}_3\rangle_2 \end{aligned} \tag{10}$$

where, $|\boldsymbol{xy}\rangle$ only states that distance between one-pair is $\boldsymbol{x}$ and other distance is $\boldsymbol{y}$ without specifying particle index.

Permutation operator defined $P^+ = P_{12}P_{23}$, $P^- = P_{23}P_{12}$ change these ket vectors. In above convention[3] we have

$$P^+|\boldsymbol{xy}\rangle_i = |\boldsymbol{xy}\rangle_{i+1}(?)$$

, where $i+1$ is considered in a cyclic order. Thus

$$P^+|\boldsymbol{xy}\rangle_1 = |\boldsymbol{xy}\rangle_2 = |\boldsymbol{x}_2\boldsymbol{y}_2\rangle_2 = |\boldsymbol{x}_1\boldsymbol{y}_1\rangle_1(?)$$

and $\boldsymbol{x}_1^{(1)} = \boldsymbol{x}_2^{(2)}$, $\boldsymbol{y}_1^{(1)} = \boldsymbol{y}_2^{(2)}$.

According to Glockle,[4]

$$\begin{aligned} P^+|\boldsymbol{x}_i\boldsymbol{y}_i\rangle_j &= |\boldsymbol{x}_i\boldsymbol{y}_i\rangle_{j+1}, \quad \text{in a cyclic notation for } j+1, \\ P^-|\boldsymbol{x}_i\boldsymbol{y}_i\rangle_j &= |\boldsymbol{x}_i\boldsymbol{y}_i\rangle_{j-1}, \quad \text{in a cyclic notation for } j-1 \end{aligned} \tag{11}$$

And we have relation $(P^+)^\dagger = P^-$ which make it possible to act permutation on bra state.

(For example, $P^+|\boldsymbol{x}_1\boldsymbol{y}_1\rangle_2 = |\boldsymbol{x}_1\boldsymbol{y}_1\rangle_3 = |\boldsymbol{x}_2\boldsymbol{y}_2\rangle_1$)

We can define full Faddeev state vector $|\Psi\rangle$ as sum of Faddeev components $|\psi\rangle_1 + |\psi\rangle_2 + |\psi\rangle_3$. This full Faddeev wave function is invariant under permutation so that

$$\Psi(\boldsymbol{x}_1\boldsymbol{y}_1) = \Psi(\boldsymbol{x}_2\boldsymbol{y}_2) = \Psi(\boldsymbol{x}_3\boldsymbol{y}_3) = {}_1\langle\boldsymbol{x}_1\boldsymbol{y}_1|\Psi\rangle \tag{12}$$

[1] It is noted by (+) because in special case, we have to consider pair interaction even in break up channel.

[2] We can imagine three particles in space. And name them, (123) or (231) or (312). This do not change actual distance between them. Only changes names of them.

[3] **NOTE:** It is very confusing notation and seems contradicting by looking $|\boldsymbol{x}_2\boldsymbol{y}_2\rangle_2 = |\boldsymbol{x}_1\boldsymbol{y}_1\rangle_2$. I am not sure how to resolve this.

[4] In fact, I am not sure this convention or relation is correct or not.

We can think permutation acts to Faddeev component as $|\psi\rangle_2 = P^+|\psi\rangle_1$, $|\psi\rangle_3 = P^-|\psi\rangle_1$. [5]

And write projection of Faddeev component on position space as

$$ {}_i\langle \boldsymbol{x}\boldsymbol{y}|\psi\rangle_i = \psi_i(\boldsymbol{x},\boldsymbol{y}) \tag{13} $$

We will use wave function form when bra and ket are in the same configuration.

Then first use permutation acting on bra vector and acts on ket

$$ {}_1\langle \boldsymbol{x}_1\boldsymbol{y}_1|\psi\rangle_1 = {}_2\langle \boldsymbol{x}_2\boldsymbol{y}_2|\psi\rangle_1 = {}_3\langle \boldsymbol{x}_2\boldsymbol{y}_2|P^+|\psi\rangle_1 = {}_3\langle \boldsymbol{x}_2\boldsymbol{y}_2|\psi\rangle_2 = {}_2\langle \boldsymbol{x}_1\boldsymbol{y}_1|\psi\rangle_2 \tag{14} $$

In terms of wave function, we get

$$ \psi_1(\boldsymbol{x}_1,\boldsymbol{y}_1) = \psi_2(\boldsymbol{x}_1,\boldsymbol{y}_1) \tag{15} $$

And similar method gives also $\psi_1(\boldsymbol{x}_1,\boldsymbol{y}_1) = \psi_3(\boldsymbol{x}_1,\boldsymbol{y}_1)$. This means that Faddeev wave function have the same functional form.

Some book use notation,

$$ \psi(\boldsymbol{x}_2,\boldsymbol{y}_2) = P^+\psi(\boldsymbol{x}_1,\boldsymbol{y}_1) \tag{16} $$

This corresponds to the relation in the notation here,

$$ {}_2\langle \boldsymbol{x}_2\boldsymbol{y}_2|\psi\rangle_2 = {}_1\langle \boldsymbol{x}_1\boldsymbol{y}_1|P^+|\psi\rangle_1 \tag{17} $$

[6] We can also have

$$ {}_1\langle \boldsymbol{x}_1\boldsymbol{y}_1|P^+|\psi\rangle_1 = {}_3\langle \boldsymbol{x}_1\boldsymbol{y}_1|\psi\rangle_1 = {}_1\langle \boldsymbol{x}_2\boldsymbol{y}_2|\psi\rangle_1 = {}_2\langle \boldsymbol{x}_2\boldsymbol{y}_2|\psi\rangle_2 = \psi_2(\boldsymbol{x}_2,\boldsymbol{y}_2). \tag{20} $$

To reduce confusion, let us use every matrix or element wave function in terms of configuration '1', Faddeev component and coordinates.

1.1 Jacobi coordinates for unequal mass particles

For particles with unequal mass $m_{1,2,3}$ and coordinate $\boldsymbol{r}_1 1, 2, 3$ or momentum $\boldsymbol{p}_{1,2,3}$, Jacobi coordinate becomes,

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[5] This definition of permutation operator is the same as above defined permutation operator?

[6] **However**, I am confused in the equation

$$ {}_1\langle \boldsymbol{x}_1\boldsymbol{y}_1|\psi_1\rangle = {}_2\langle \boldsymbol{x}_1\boldsymbol{y}_1|\psi_2\rangle \tag{18} $$

because $\boldsymbol{x}_1$ and $\boldsymbol{y}_1$ in left-hand side and right-hand side seems not the same one. Thus How can we get the conclusion from following equation?

$$ \psi_1(\boldsymbol{x}_1^{(1)},\boldsymbol{y}_1^{(1)}) = \psi_2(\boldsymbol{x}_1^{(2)},\boldsymbol{y}_1^{(2)}) \tag{19} $$

2 Problem in L-S equation for scattering with more than two particles

3개의 입자로 이루어진 시스템을 생각하자. CM motion을 제외하면, 시스템 전체의 Hamiltonian은 Jacobi coordinate로 다음과 같이 나타낼 수 있다.

$$H = H_0 + V_1 + V_2 + V_3, \tag{21}$$

여기서, $V_i = V_{jk}$ 는 i 를 제외한 나머지 입자 사이의 interaction을 나타낸다. 새로운 notation $V^i = V_{ij} + V_{ik}$를 도입하면,

$$H = H_0 + V_\alpha + V^\alpha = H_\alpha + V^\alpha \tag{22}$$

라고 쓸 수 있다. (여기서, H_0는 free 3-body term으로 $\frac{p_l^2}{2\mu_l} + \frac{q_l^2}{2M_l}$ 으로 나타낼 수 있다.
3개의 입자가 만들수 있는 asymptotic configuration은

$$\begin{aligned}
Bd &: (123), \quad E_{bd} < 0 \\
1 &: 1,(23), \quad E_1 = \epsilon_1 + \frac{q_1^2}{2M_1}, \quad |\phi_1\rangle = |\varphi_1\rangle|\boldsymbol{q}_1\rangle \\
2 &: 2,(31), \quad E_2 = \epsilon_2 + \frac{q_2^2}{2M_2}, \quad |\phi_2\rangle = |\varphi_2\rangle|\boldsymbol{q}_2\rangle \\
3 &: 3,(12), \quad E_3 = \epsilon_3 + \frac{q_3^2}{2M_3}, \quad |\phi_3\rangle = |\varphi_3\rangle|\boldsymbol{q}_3\rangle \\
0 &: 1,2,3, \quad E_0 = \frac{p_l^2}{2\mu_l} + \frac{q_l^2}{2M_l}, \quad |\phi_0\rangle = |\boldsymbol{p}_l\rangle|\boldsymbol{q}_l\rangle
\end{aligned} \tag{23}$$

으로 쓸 수 있다. (여기서, $H_i|\varphi_i\rangle = \epsilon_i|\varphi_i\rangle$는 실제로는 excited state일 수 있다. $\epsilon_i^{(n)}$) 우리는 산란에 의해서, 예를 들어 특정 boundary condition의 "free"-state $|\phi_1\rangle$ 가 scattering state $|\Psi_1^{(+)}\rangle$를 unique 하게 결정하기를 원한다. ($|\Psi_1^{(+)}\rangle$는 다른 channel(2,3)로의 outgoing state를 포함한다.) Formal theory of scattering, introduced Möller channel operator such that

$$\begin{aligned}
&\lim_{t\to-\infty} ||\Psi_\alpha^{(+)}(t) - \phi_\alpha(t)|| = 0, \\
&|\psi_\alpha^{(+)}(0)\rangle = \lim_{t\to-\infty} e^{iHt}e^{-iH_\alpha t}|\phi_\alpha(0)\rangle, \\
&\Omega_\alpha^{(+)} = \lim_{t\to-\infty} e^{iHt}e^{-iH_\alpha t}
\end{aligned} \tag{24}$$

This can be re-written in ϵ limit,

$$|\Psi_{q_\alpha}^{(+)}\rangle = \lim_{\epsilon\to0} \frac{i\epsilon}{E_{q_\alpha} + i\epsilon - H}|\phi_{q_\alpha}\rangle, \tag{25}$$

By defining channel resolvent operators, we get identity

$$\begin{aligned}
G_\alpha(z) &= \frac{1}{z - H_\alpha}, \\
G(z) &= G_\alpha(z) + G_\alpha(z)V^\alpha G(z) \\
&= G_\alpha(z) + G(z)V^\alpha G_\alpha(z)
\end{aligned} \tag{26}$$

Unlike two-body case, we have several ways to write the identity with α.

Applying this identity, we get, LS like equations with different α and β,

$$|\Psi^{(+)}_{q_\alpha}\rangle = \lim_{\epsilon\to 0}\frac{i\epsilon}{E_\alpha + i\epsilon - H_\beta}|\phi_\alpha\rangle + \lim_{\epsilon\to 0}\frac{1}{E_\alpha + i\epsilon - H_\beta}V^\beta|\Psi^{(+)}_\alpha\rangle \tag{27}$$

From the Lippmann's identity, (증명은 생략)

$$\lim_{\epsilon\to 0}\frac{i\epsilon}{E_\alpha + i\epsilon - H_\beta}|\phi_\alpha\rangle = \delta_{\alpha\beta}|\phi_\alpha\rangle, \tag{28}$$

We will have three relations for $\alpha = 1$,

$$\begin{aligned}
|\Psi^{(+)}_1\rangle &= |\phi_1\rangle + \lim_{\epsilon\to 0}\frac{1}{E_1 + i\epsilon - H_1}V^1|\Psi^{(+)}_1\rangle, \\
|\Psi^{(+)}_1\rangle &= \lim_{\epsilon\to 0}\frac{1}{E_1 + i\epsilon - H_2}V^2|\Psi^{(+)}_1\rangle, \\
|\Psi^{(+)}_1\rangle &= \lim_{\epsilon\to 0}\frac{1}{E_1 + i\epsilon - H_3}V^3|\Psi^{(+)}_1\rangle.
\end{aligned} \tag{29}$$

이 중에서 첫번째 식이 Lippmann-Schwinger equation이 된다. 그러나 문제는 첫번째 식인 LS equation을 푸는 것으로는 $|\Psi^{(+)}_1\rangle$의 unique solution 을 얻을 수 없다는 것이다. 예를 들어, 위 식에서 $\alpha = 2$인 경우에대해서도 비슷한 식을 얻는다.

$$\begin{aligned}
|\Psi^{(+)}_2\rangle &= |\phi_2\rangle + \lim_{\epsilon\to 0}\frac{1}{E_2 + i\epsilon - H_2}V^2|\Psi^{(+)}_2\rangle, \\
|\Psi^{(+)}_2\rangle &= \lim_{\epsilon\to 0}\frac{1}{E_2 + i\epsilon - H_1}V^1|\Psi^{(+)}_2\rangle, \\
|\Psi^{(+)}_2\rangle &= \lim_{\epsilon\to 0}\frac{1}{E_2 + i\epsilon - H_3}V^3|\Psi^{(+)}_2\rangle.
\end{aligned} \tag{30}$$

이로부터 $|\Psi^{(+)}_2\rangle$ 도 $|\Psi^{(+)}_1\rangle$ 에 대한 LS equation의 homogeneous part 에 대한 solution이 됨을 알 수 있다. 즉, $|\Psi^{(+)}_1 - N\Psi^{(+)}_2\rangle$ 도 LS equation의 해가 됨을 알 수 있다. 따라서, LS equation 만으로는 $|\Psi^{(+)}_1\rangle$ 를 unique하게 결정하지 못한다.

반면, Eq(29)의 첫번째 식뿐 아니라 나머지 식까지 모두 고려하면 (즉 triad LS equations), $|\Psi^{(+)}_1$를 unique하게 결정할 수 있다. (triad LS 를 모두 고려하면, 위의 예에서 $|\Psi^{(+)}_1 - N\Psi^{(+)}_2\rangle$ 가 해를 만족하지 않음을 알 수 있다.) 따라서, 3-body 의 경우에는 LS equation 만을 푸는 것이 아니라, triad LS equations을 풀어야 한다.

이것은 동등하게, Faddeeve equation또는 AGS equation을 푸는 것으로 바꾸어 생각할 수 있다. Resolvent 로부터 우리는 다음과 같은 identity를 얻을 수도 있다.

$$G(z) = G_0(z) + G_0(z)VG(z) = G_0(z) + G(z)VG_0(z), \quad G_0(z) = \frac{1}{z - H_0} \tag{31}$$

Lippmann identity를 적용하면,

$$|\Psi^{(+)}_\alpha\rangle = G_0V|\Psi^{(+)}_\alpha\rangle = \sum_{i=1}^{3} G_0V_i|\Psi^{(+)}_\alpha\rangle = \sum_{i=1}^{3}|\psi_{\alpha,i}\rangle \tag{32}$$

여기서, Fadeeve component를 정의하면,

$$|\psi_{\alpha,i}\rangle \equiv G_0V_i|\Psi^{(+)}_\alpha\rangle, \tag{33}$$

Then, LS equation을 적용하면, (Use $G_0V_\alpha G_\alpha = G_\alpha V_\alpha G_0$ and $G_0V_\beta|\phi_\beta\rangle = |\phi_\beta\rangle$),

$$\begin{aligned} |\psi_{\alpha,\alpha}\rangle &= G_0V_\alpha(|\phi_\alpha\rangle + G_\alpha V^\alpha|\Psi_\alpha^{(+)}\rangle) \\ &= G_0V_\alpha|\phi_\alpha\rangle + G_\alpha V_\alpha(G_0V_\beta + G_0V_\gamma)|\Psi_\alpha^{(+)}\rangle \\ &= |\phi_\alpha\rangle + G_\alpha V_\alpha(|\psi_{\alpha,\beta}\rangle + |\psi_{\alpha,\gamma}\rangle), \end{aligned} \tag{34}$$

Thus, we get Faddeeve equation,

$$\begin{aligned} |\psi_{\alpha,\alpha}\rangle = \quad |\phi_\alpha\rangle + \quad & G_\alpha V_\alpha(|\psi_{\alpha,\beta}\rangle + |\psi_{\alpha,\gamma}\rangle), \\ |\psi_{\alpha,\beta}\rangle = \quad & G_\beta V_\beta(|\psi_{\alpha,\gamma}\rangle + |\psi_{\alpha,\alpha}\rangle), \\ |\psi_{\alpha,\gamma}\rangle = \quad & G_\gamma V_\gamma(|\psi_{\alpha,\alpha}\rangle + |\psi_{\alpha,\beta}\rangle), \end{aligned} \tag{35}$$

만약 식을 3-body space에서의 transition amplitude 에 관한 식으로 바꾸어 쓰면, AGS (Alt-Grassberger-Sandhas) equation이 얻어진다.

$$\langle\phi_\beta|U_{\beta\alpha}|\phi_\alpha\rangle \equiv \langle\phi_\alpha|V^\beta|\Psi_\alpha^{(+)}\rangle \tag{36}$$

From the triad equation, $|\Psi_1^{(+)}\rangle = G_2V^2|\Psi_1^{(+)}\rangle = G_2U_{21}|\phi_1\rangle$,

$$\begin{aligned} U_{11}|\phi_1\rangle &= V^1|\Psi_1^{(+)}\rangle = (V_2+V_3)|\Psi_1^{(+)}\rangle = V_2U_{21}|\phi_1\rangle + V_3U_{31}|\phi_1\rangle, \\ U_{21}|\phi_1\rangle &= V^2|\Psi_1^{(+)}\rangle = (V_3+V_1)|\Psi_1^{(+)}\rangle = V_3G_3U_{31}|\phi_1\rangle + V_1|\phi_1\rangle + V_1G_1U_{11}|\phi_1\rangle, \\ U_{31}|\phi_1\rangle &= V^3|\Psi_1^{(+)}\rangle = (V_1+V_2)|\Psi_1^{(+)}\rangle = V_1|\phi_1\rangle + V_1G_1U_{11}|\phi_1\rangle + V_2G_2U_{21}|\phi_1\rangle \end{aligned} \tag{37}$$

Thus, we get AGS equation, from $V_1|\phi_1\rangle = (E_1 - H_0)|\phi_1\rangle = G_0^{-1}|\phi_1\rangle$,

$$U_{\beta\alpha} = \bar{\delta}_{\alpha\beta}G_0^{-1} + \sum_\gamma \bar{\delta}_{\gamma\beta}V_\gamma G_\gamma U_{\gamma\alpha}, \quad \bar{\delta}_{\alpha\beta} = 1 - \delta_{\alpha\beta} \tag{38}$$

Be careful that the energy in the resolvent are given as E_1($G_i = 1/(E_1 + i\epsilon - H_i)$) for half on-shell U-matrix.

When all particles are identical, we would have relations for bosons and fermions,

$$P_{ij}|\Psi\rangle = \pm|\Psi\rangle, \tag{39}$$

from the definition of Faddeeve components

$$\begin{aligned} |\psi_2\rangle &= G_0V_2|\Psi\rangle = G_0V_2(P_{12}P_{23})^\dagger P_{12}P_{23}|\Psi\rangle = P_{12}P_{23}G_0V_1|\Psi\rangle \\ &= P_{12}P_{23}|\psi_1\rangle, \\ |\psi_3\rangle &= P_{23}P_{12}|\psi_1\rangle \end{aligned} \tag{40}$$

Thus,[7]

$$|\Psi\rangle = (1 + P^+ + P^-)|\psi_1\rangle \tag{41}$$

[7]We can verify that this satisfies the condition for both bosons and fermions, $P_{ij}|\Psi\rangle = \pm|\Psi\rangle$

3 Derivation of Faddeev equation: Skip

3-body system의 wave function or state $|\Psi\rangle$ would satisfy Schrodinger equation,

$$i\frac{\partial}{\partial t}|\Psi\rangle = (H_0 + V)|\Psi\rangle \tag{42}$$

Energy eigenstate 라고 생각하면, LS equation 의 kernel은

$$K(z) = G(z)V = G_0(z)V + G_0(z)VG_0(z)V + \dots \tag{43}$$

으로 마지막 식은 Born series 전개로 생각할 수 있다. 그러나, 이러한 전개는 비 실용적이며 (Born series가 diverge 할 수도 있다.), Faddeev의 의하면, unique solution 을 주지도 못한다. Three body system의 경우 kernel $G_0(z)V$는 δ-function을 momentum space에서 가지게 되어 singular 하게 된다.

2-body 의 경우는 T-matrix가 바로 scattering amplitude 및 cross section과 연관이 있지만, 3-body 에서의 T-matrix는 scattering cross section과 직접 연결되지 못한다.

$$T(z) = V + VG(z)V \tag{44}$$

여기서, 3-body T-matrix, $V = V_1 + V_2 + V_3$, $G(z) = 1/(z - H)$. 이식을 LS equation 형식으로 바꾸면,

$$T(z) = V + VG_0(z)T(z) \tag{45}$$

그러나, 이 경우도 여전히 singular한 문제가 있다. 만약 bound-state가 있는 경우는 Born-series 는 올바른 bound-state pole을 주지 못하므로, re-sum을 해야한다.(즉 non-perturvative 하다.)

Faddeev는 $T(z)$를 분해했다.

$$\begin{aligned} T(z) &= T^{(1)}(z) + T^{(2)}(z) + T^{(3)}(z), \\ T^{(k)}_{ij}(z) &= V_{ij} + V_{ij}G_0(z)T_{ij}(z) \end{aligned} \tag{46}$$

이 식을 다시 rearrange하면,

$$[1 - V_{ij}G_0](z)T^{(k)}(z) = V_{ij} + V_{ij}G_0(z)[T^{(i)}(z) + T^{(j)}(z)] \tag{47}$$

이 되고 , $T_{ij}(z) = V_{ij} + V_{ij}G_0(z)T_{ij}(z)$ 를 이용하면(즉, T_{ij}는 V_{ij} interaction 만이 포함된다. 또한 $T^{(k)}(z)$와 $T_{ij}(z)$ 는 다르다. $T_{ij}(z)$는 two-body interaction 만을 포함하는 3-body 에서의 two-body sector 인반면에 , $T^{(k)}(z)$ 는 disconneted diagram 이 포함되지 않는 3-body matrix 이다. ,

$$T^{(k)}(z) = T_{ij}(z) + T_{ij}(z)G_0(z)[T^{(i)}(z) + T^{(j)}(z)] \tag{48}$$

가 얻어진다.

정리하면, In terms of Faddeev component of wave function, (anti-)symmetrized wave function can be represented by

$$|\Psi\rangle_{S,A} = |\Psi\rangle_1 + |\Psi\rangle_2 + |\Psi\rangle_3 \tag{49}$$

where Ψ represent all physical quantum numbers. This implies that all three $|\Psi\rangle_i$ have the same quantum numbers and only have different naming for particles. And each $|\Psi\rangle_{i;jk}$ is already (anti-)symmetrized for jk exchange.

• **Bound state** 의 경우: Bound state problem 의 경우는

$$|\psi^{(k)}\rangle = G_0(z)T_{ij}(z)[|\psi^{(i)}\rangle + |\psi^{(j)}\rangle] \tag{50}$$

의 homogeneous eq.을 만족시킨다.

• **Scattering**의 경우, 만약 particle 1 scattering on a bound state of 2 and 3,

$$\begin{aligned} |\psi^{(1)}\rangle &= \Phi_1 + G_0(z)T_{23}(z)[|\psi^{(2)}\rangle + |\psi^{(3)}\rangle], \\ |\psi^{(2)}\rangle &= G_0(z)T_{31}(z)[|\psi^{(3)}\rangle + |\psi^{(1)}\rangle], \\ |\psi^{(3)}\rangle &= G_0(z)T_{12}(z)[|\psi^{(1)}\rangle + |\psi^{(2)}\rangle] \end{aligned} \tag{51}$$

with

$$\begin{aligned} T^{(k)}(z) &= T_{ij}(z) + T_{ij}(z)G_0(z)[T^{(i)}(z) + T^{(j)}(z)], \\ T_{ij}(z) &= V_{ij} + V_{ij}G_0(z)T_{ij}(z) \end{aligned} \tag{52}$$

where $z = E \pm i\epsilon$ and $G_0(z) = (z - H_0)^{-1}$. 특히 two-body t-matrix in three body space는

$$G_\alpha V_\alpha = G_0 t_\alpha$$

를 만족시킨다. 따라서, two-body potential 대신 two-body t-matrix 를 이용하여 식을 쓸 수도 있다.

• **Schrodinger equation form:** bound state나 scattering state나 모두

$$\begin{aligned} (E - H_0 - V_{23})|\psi^{(1)}\rangle &= V_{23}[|\psi^{(2)}\rangle + |\psi^{(3)}\rangle], \\ (E - H_0 - V_{31})|\psi^{(2)}\rangle &= V_{31}[|\psi^{(3)}\rangle + |\psi^{1)}\rangle], \\ (E - H_0 - V_{12})|\psi^{(3)}\rangle &= V_{12}[|\psi^{(1)}\rangle + |\psi^{(2)}\rangle] \end{aligned} \tag{53}$$

또는

$$(E - H_0 - V_i)|\psi^{(i)}\rangle = V_i[|\psi^{(j)}\rangle + |\psi^{(k)}\rangle] \tag{54}$$

의 형식이 된다.

4 Explicit form of Faddeev equation in momentum space and configuration space: None partial wave form

Faddeev eq.은 momentum space, configuration space 에서 LS form and Schrodinger form 으로 쓸 수 있다. 또한, potential 대신, two-body t-matrix를 이용하여 식을 쓸 수도 있다. 또한 wave function에 대한 식을 푸는 대신 scattering amplitude에 대한 식을 풀 수도 있다.

어떤 경우나 integral equation 형식으로 쓰건, integro differential equation 으로 쓰건, 위 식들을 projection 시키기만 하면 얻어진다. partial wave state로의 projection은 다음 section 에서 살펴보도록 하자.

• **Momentum space LS form:** momentum space에서는 t-matrix를 이용한 식이 편리하다.

$$|\psi_i\rangle = |\phi_i\rangle\delta_{i,1} + G_0 t^{(i)}(|\psi_j\rangle + |\psi_k\rangle) \tag{55}$$

where, I set the asymptotic state is '1' configuration. Then, projection to momentum space gives

$$\langle \boldsymbol{pq}|\psi_i\rangle = \langle \boldsymbol{pq}|\psi_i\rangle\delta_{i,1} + \int d\boldsymbol{p}'d\boldsymbol{q}'\langle \boldsymbol{pq}|G_0t^{(i)}|\boldsymbol{p}'\boldsymbol{q}'\rangle(\langle \boldsymbol{p}'\boldsymbol{q}'|\psi_j\rangle + \langle \boldsymbol{p}'\boldsymbol{q}'|\psi_k\rangle) \tag{56}$$

여기서,

$$\begin{aligned}
\langle \boldsymbol{pq}|G_0(E)t^{(i)}(E)|\boldsymbol{p}'\boldsymbol{q}'\rangle &= \frac{1}{E - E_{\boldsymbol{pq}} + i\epsilon}\langle \boldsymbol{pq}|t^{(i)}|\boldsymbol{p}'\boldsymbol{q}'\rangle \\
\langle \boldsymbol{pq}|t^{(i)}(E)|\boldsymbol{p}'\boldsymbol{q}'\rangle &= \langle \boldsymbol{qq}|V_i|\boldsymbol{p}'\boldsymbol{q}'\rangle + \langle \boldsymbol{pq}|VG_0t^{(i)}(E)|\boldsymbol{p}'\boldsymbol{q}'\rangle \\
&= \delta^{(3)}(\boldsymbol{q}-\boldsymbol{q}')\langle \boldsymbol{p}|V_i|\boldsymbol{p}'\rangle + \int d^3p''\langle \boldsymbol{p}|V|\boldsymbol{p}''\rangle\frac{1}{E - E_{\boldsymbol{p}''\boldsymbol{q}''} + i\epsilon}\langle \boldsymbol{p}''\boldsymbol{q}'|t^{(i)}(E)|\boldsymbol{p}'\boldsymbol{q}'\rangle
\end{aligned}$$

로 쓸 수 있고, 만약 two-body t-matrix in 2-body system 을 아는 경우에는 해를

$${}_i\langle \boldsymbol{pq}|t^{(i)}(E)|\boldsymbol{pq}\rangle_i = \delta^{(3)}(\boldsymbol{q}-\boldsymbol{q}')\langle \boldsymbol{p}|\hat{t}(E - E_{q'})|\boldsymbol{p}'\rangle \tag{58}$$

로 쓸 수 있다.[8] 따라서, Faddeev equation은

$$\langle \boldsymbol{qq}|\psi_i\rangle = \langle \boldsymbol{pq}|\phi_i\rangle\delta_{i,1} + \int d^3\boldsymbol{p}'d^3p''d^3q''\frac{1}{E - E_{p'q} + i\epsilon}\langle \boldsymbol{p}|\hat{t}(E - E_q)|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'\boldsymbol{q}|P|\boldsymbol{p}''\boldsymbol{q}''\rangle\langle \boldsymbol{p}''\boldsymbol{q}''|\psi_i\rangle \tag{59}$$

Bound state 의 경우는 위식의 free term을 없애면 된다.

•**Schrodinger form in configuration space:** Projecting on configuration space gives,

$$(E - H_0)\langle \boldsymbol{xy}|\psi_i\rangle = \int d^3\boldsymbol{x}'d^3\boldsymbol{y}'d^3\boldsymbol{x}''d^3\boldsymbol{y}''\langle \boldsymbol{xy}|V_i|\boldsymbol{x}'\boldsymbol{y}'\rangle\langle \boldsymbol{x}'\boldsymbol{y}'|(1+P)|\boldsymbol{x}''\boldsymbol{y}''\rangle\langle \boldsymbol{x}''\boldsymbol{y}''|\psi_i\rangle \tag{60}$$

If potential is local, we can write

$$(E - H_0)\langle \boldsymbol{xy}|\psi_i\rangle = \int d^3\boldsymbol{x}'d^3\boldsymbol{y}'V_i(\boldsymbol{x})\langle \boldsymbol{xy}|(1+P)|\boldsymbol{x}'\boldsymbol{y}'\rangle\langle \boldsymbol{x}'\boldsymbol{y}'|\psi_i\rangle \tag{61}$$

5 Partial wave decomposition of Faddeev component

Let us write a complete set,

$$\sum_\alpha \int dx x^2 \int dy y^2 |\alpha xy\rangle\langle \alpha xy| = 1 \tag{62}$$

and define,

$$\langle \boldsymbol{x}'\boldsymbol{y}'|\alpha xy\rangle = \frac{\delta(x'-x)}{x'x}\frac{\delta(y'-y)}{y'y}\mathcal{Y}_\alpha(\hat{x}'\hat{y}') \tag{63}$$

where, $\mathcal{Y}_\alpha(\hat{x}\hat{y})$ can be thought as generalized bipolar spherical Harmonics. [9]

[8] 예를 들어 하나의 covention 에서 $E_{pq} = \frac{p^2}{m} + \frac{3}{4m}q^2$이다.

[9] Bipolar spherical harmonics is

$$\mathcal{Y}^{LM}_{l_1l_2}(\hat{x}\hat{y}) \equiv [Y_{l_1}(\hat{x}) \otimes Y_{l_2}(\hat{y})]_{LM} \equiv \sum_{m_1,m_2}\langle LM|l_1m_1, l_2m_2\rangle Y_{l_1m_1}(\hat{x})Y_{l_2m_2}(\hat{y}) \tag{64}$$

Thus, configuration space representation of state, $|\psi\rangle = \sum_\alpha \int dx x^2 dy y^2 |\alpha xy\rangle\langle\alpha xy|\psi\rangle$,

$$\langle \boldsymbol{xy}|\psi\rangle = \sum_\alpha \langle \boldsymbol{xy}|\alpha xy\rangle\langle\alpha xy|\psi\rangle \tag{65}$$

and write

$$\begin{aligned} \langle\alpha xy|\psi\rangle &= \frac{F_\alpha(x,y)}{xy} \\ \langle \boldsymbol{xy}|\alpha xy\rangle &= \mathcal{Y}_\alpha(\hat{x}\hat{y}) = \langle\alpha\hat{x}\hat{y}|\alpha\rangle \end{aligned} \tag{66}$$

Thus, one component of Faddeev Wave function can be written

$$\psi^{(k)}(\boldsymbol{x},\boldsymbol{y}) = \sum_\alpha \frac{F^{(k)}_\alpha(x,y)}{xy}\mathcal{Y}_\alpha(\hat{x}\hat{y}) \tag{67}$$

From now, let us assume that radial function $F_\alpha(x,y)$ is known. [10]

5.1 Momentum space in LS form

$$\langle\alpha pq|\psi_i\rangle = \langle\alpha pq|\phi_i\rangle\delta_{i1} + \langle\alpha pq|G_0 t^{(i)} P|\psi_i\rangle \tag{69}$$

Using

$$\begin{aligned} \langle\alpha pq|G_0(E)|\alpha' p' q'\rangle &= \delta_{\alpha\alpha'}\frac{\delta(p-p')}{pp'}\frac{\delta(q-q')}{qq'}\frac{1}{E-\frac{p^2}{m}-\frac{3}{4m}q^2+i\epsilon} \\ {}_i\langle\alpha pq|t^{(i)}(E)|\alpha' p' q'\rangle_i &= \frac{\delta(q-q')}{qq'}\delta_{\alpha_y\alpha'_y}\hat{t}_{\alpha_x,\alpha'_x}(pp', E-\frac{3}{4m}q^2) \end{aligned} \tag{70}$$

Thus,

$$\begin{aligned} \langle\alpha pq|\psi_i\rangle = \langle\alpha pq|\phi_i\rangle\delta_{i1} &+ \frac{1}{E-\frac{p^2}{m}-\frac{3}{4m}q^2+i\epsilon}\sum_{\alpha'}\int dp' p'^2 \delta_{\alpha_y\alpha'_y}\hat{t}_{\alpha_x,\alpha'_x}(pp', E-\frac{3}{4m}q^2) \\ &\times\sum_{\alpha''}\int dp'' p''^2\int dq'' q''^2\langle\alpha' p' q'|P|\alpha'' p'' q''\rangle\langle\alpha'' p'' q''|\psi_i\rangle \end{aligned} \tag{71}$$

5.2 Configuration space in Schrodinger form

Projecting $\langle\alpha xy|$,

$$\langle\alpha xy|E-H_0-V_i|\psi^i\rangle = \langle\alpha xy|V_i P|\psi_i\rangle \tag{72}$$

[10] In fact, implicitly there is another index $|\boldsymbol{p},\alpha_i\rangle$ for incoming states before scattering. Thus, we may further decompose

$$\psi^{(k)}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\alpha',\alpha}\frac{F^{(k)}_{\alpha',\alpha}(x,y)}{xy}\mathcal{Y}_\alpha(\hat{x}\hat{y})\langle\alpha,\hat{p}|\boldsymbol{p},\alpha_i\rangle \tag{68}$$

If we let $\langle xy\alpha|\psi^i\rangle \equiv \frac{F^{(i)}_\alpha(x,y)}{xy}$ and if potential does not contain any derivatives,

$$\langle xy\alpha|H_0+V_i|\psi^i\rangle = \sum_{\alpha'}\frac{1}{xy}[-\Delta^{(\alpha)}(x,y)\delta_{\alpha\alpha'}+\hat{V}_{\alpha\alpha'}(x)]F^{(i)}_{\alpha'}(x,y) \tag{73}$$

with [11]

$$\begin{aligned}\langle\alpha xy|H_0|\alpha' x'y'\rangle &= \delta_{\alpha\alpha'}\frac{\delta(x-x')}{xx'}\frac{\delta(y-y')}{yy'}(-\Delta^{(\alpha)}(x,y))\\ \langle\alpha xy|V_i|\alpha' x'y'\rangle &= \hat{V}_{\alpha\alpha'}(x)\frac{\delta(x-x')}{xx'}\frac{\delta(y-y')}{yy'} \quad \text{if local potential}\end{aligned} \tag{79}$$

Thus,

$$\frac{1}{xy}\sum_{\alpha'}[(E+\Delta^{(\alpha)}(x,y))\delta_{\alpha\alpha'}-\hat{V}_{\alpha\alpha'}(x)]F^{(i)}_{\alpha'}(x,y) = \sum_{\alpha'}\hat{V}_{\alpha\alpha'}(x)\sum_{\alpha''}\int dx'x'^2dy'y'^2\langle\alpha' xy|P|\alpha'' x'y'\rangle\frac{F^{(i)}_{\alpha''}(x',y')}{x'y'} \tag{80}$$

If using the h function in the following section, we can write

$$\sum_{\alpha'}[(E+\Delta^{(\alpha)}(x,y))\delta_{\alpha\alpha'}-\hat{V}_{\alpha\alpha'}(x)]F^{(i)}_{\alpha'}(x,y) = 2\sum_{\alpha'}\hat{V}_{\alpha\alpha'}(x)\sum_{\alpha''}\int dz\hat{h}_{\alpha'\alpha''}(x,y,z)F^{(i)}_{\alpha''}(x',y') \tag{81}$$

6 Permutation

The representation of permutation operator is in the heart of three body calculation. Permutation operator gives

$${}_1\langle xy\alpha|P_{12}P_{23}+P_{13}P_{23}|x'y'\alpha'\rangle_1 = {}_1\langle xy\alpha|x'y'\alpha'\rangle_2 + {}_1\langle xy\alpha|x'y'\alpha'\rangle_3 \tag{82}$$

[11] For two-body case, Schrodinger equation for full wave function is written as

$$T_l(x) \equiv \frac{-1}{2\mu}\frac{1}{x^2}\frac{d}{dx}(x^2\frac{d}{dx}) + \frac{1}{2\mu}\frac{l(l+1)}{x^2} \tag{74}$$

And

$$[T_{l'}(x)-E]\Psi^J_{l'sls}(x) + \sum_{l''}\mathcal{V}^J_{l'sl''s}(x)\Psi^J_{l''sls}(x) = 0 \tag{75}$$

with

$$\mathcal{V}^J_{l'sl''s}(x) \equiv \langle\mathcal{Y}^{JM}_{l's}|V(x)|\mathcal{Y}^{JM}_{ls}\rangle \tag{76}$$

Using $\Psi^J_{l''sls}(x) = \frac{u^J_{l''sls}(x)}{x}$, above equation can be rewritten as

$$[\tilde{T}_{l'}(x)-E]u^J_{l'sls}(x) + \sum_{l''}\mathcal{V}^J_{l'sl''s}(x)u^J_{l''sls}(x) = 0 \tag{77}$$

with

$$\tilde{T}_{l'}(x) = -\frac{1}{2\mu}\frac{d^2}{dx^2} \tag{78}$$

Be careful that if there was a derivative in the potential the last term should written as $x\sum_{l''}\mathcal{V}^J_{l'sl''s}(x)\frac{u^J_{l''sls}(x)}{x}$

where, the meaning of above amplitude is that overlap matrix element betwen the state with relative position is x, y and quantum numbers α in 1(23) configuration and the state with relative position x', y' and quantum numbers α' in 2(31) or 3(12) configuration.

By using $P_{13}P_{23} = P_{23}P_{12}P_{23}P_{23}$ and

$$ {}_1\langle xy\alpha|x'y'\alpha'\rangle_3 = {}_1\langle xy\alpha|P_{13}P_{23}|x'y'\alpha'\rangle_1 = (-1)^{l+s+t}(-1)^{l'+s'+t'}{}_1\langle xy\alpha|P_{12}P_{23}|x'y'\alpha'\rangle_1 = {}_1\langle xy\alpha|x'y'\alpha'\rangle_2 \quad (83) $$

where we use $(-1)^{l+s+t} = -1$ from the anti-symmetrization of (23) pair in $|xy\alpha\rangle_1$. Thus, we only have to consider ${}_1\langle xy\alpha|x'y'\alpha'\rangle_2$.

6.1 Explicit form of permutation operator

There are different representation of permutation operator. Here, let us use $h_{\alpha\alpha'}$ form. Assume that

$$ \begin{pmatrix} \boldsymbol{x}' \\ \boldsymbol{y}' \end{pmatrix} = \begin{pmatrix} c_1 & s_1 \\ s_2 & c_2 \end{pmatrix} \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{pmatrix} \quad (84) $$

Thus,

$$ {}_1\langle \boldsymbol{x}_1\boldsymbol{y}_1|P^{\pm}|\boldsymbol{x}'_1\boldsymbol{y}'_1\rangle_1 = \delta^{(3)}(\boldsymbol{x}'_1 - c_1\boldsymbol{x}_1 - s_1\boldsymbol{y}_1)\delta^{(3)}(\boldsymbol{y}'_1 - s_2\boldsymbol{x}_1 - c_2\boldsymbol{y}_1) \quad (85) $$

Thus finally we have

$$ \begin{aligned} & {}_1\langle xy(l_xl_y)LM|x'y'(l'_xl'_y)LM\rangle_2 = {}_1\langle xy(l_xl_y)LM|P^+|x'y'(l'_xl'_y)LM\rangle_1 \\ \equiv & \int_{-1}^{1} dz\delta(x' - |x'_1|)\delta(y' - |y'_1|)\hat{h}^{LM}_{l_xl_y,l'_xl'_y}(x,y,z)\frac{1}{xyx'y'} \end{aligned} \quad (86) $$

where,

$$ \begin{aligned} |x'_1| &= \sqrt{(c_1x)^2 + (s_1y)^2 + 2c_1s_1xyz} \\ |y'_1| &= \sqrt{(s_2x)^2 + (c_2y)^2 + 2s_2c_2xyz} \end{aligned} \quad (87) $$

with

$$ \begin{aligned} \hat{h}^{LM}_{l_xl_y,l'_xl'_y}(x,y,z) = & \sum_k \frac{\hat{k}\sqrt{\hat{l}_x\hat{l}_y\hat{l}'_x\hat{l}'_y}}{2} P_k(z) \sum_{l_1+l_2=l'_x} \sum_{l_3+l_4=l'_y} \sqrt{\frac{(2l'_x+1)!(2l'_y+1)!}{(2l_1)!(2l_2)!(2l_3)!(2l_4)!}} \\ & \times \frac{x^{l_1+l_3+1}y^{l_2+l_4+1}}{(x')^{l'_x+1}(y')^{l'_y+1}} c_1^{l_1}c_2^{l_4}s_1^{l_2}s_2^{l_3} \sum_{l_5} \hat{l}_5 \begin{pmatrix} k & l_x & l_5 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_3 & l_5 \\ 0 & 0 & 0 \end{pmatrix} \\ & \times \sum_{l_6} \hat{l}_6(-1)^{l_6+l_x+L} \begin{pmatrix} k & l_y & l_6 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2 & l_4 & l_6 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l_x & l_y & L \\ l_6 & l_5 & k \end{Bmatrix} \\ & \times \begin{Bmatrix} l_1 & l_3 & l_5 \\ l_2 & l_4 & l_6 \\ l'_x & l'_y & L \end{Bmatrix} \end{aligned} \quad (88) $$

form is useful to obtain full wave function in a form [12]

$$\begin{aligned}(xy)_1\langle\alpha xy|(1+P)|\psi\rangle_1 &= (xy)_1\langle\alpha xy|\psi\rangle_1 + 2(xy)_1\langle\alpha xy|P^+|\psi\rangle_1 \\ &= F^1_\alpha(x,y) + 2\sum_{\alpha'}\int_{-1}^{1} dz\hat{h}_{\alpha\alpha'}(x,y,z)F^1_{\alpha'}(x',y') \end{aligned} \quad (90)$$

$$\int\int d\hat{x}d\hat{y}\mathcal{Y}^*_\alpha(\hat{x}\hat{y})\frac{xy}{x'y'}F_{\alpha'}(x',y')\mathcal{Y}_{\alpha'}(\hat{x}',\hat{y}') = \int_{-1}^{+1} du\hat{h}_{\alpha\alpha'}(x,y,u)F_{\alpha'}(x',y') \quad (91)$$

7 Numerical realization of the Faddeev equation

The first thing to do is to make the equation discrete. Let us use spline interpolation.

$$F_\alpha(x,y) = \sum_{m_x,m_y} C^\alpha_{m_x,m_y}S^x_{m_x}(x)S^y_{m_y}(y) \quad (92)$$

We can choose collocation point's such that the same m_x and m_y index can be used also for collocation points. Then, we can represent wave function at collocation points by indexes $n = (\alpha, m_x, m_y)$, $n' = (\alpha', m'_x, m'_y)$. This makes,

$$F_\alpha(x_{m_x}, y_{m_x}) \to F_n = \sum_{n'}[B]_{nn'}C_{n'} \quad (93)$$

with

$$[B]_{nn'} = \delta_{\alpha\alpha'}S^x_{m'_x}(x_{m_x})S^y_{m'_y}(y_{m_y}) \quad (94)$$

- **identity:** Then, we can convert

$$E\delta_{\alpha\alpha'}F_{\alpha'}(x_{m_x}, y_{m_x}) \to E[B]_{nn'}C_{n'} \quad (95)$$

- **potential:**

$$V_{\alpha,\alpha'}F_{\alpha'}(x_{m_x}, y_{m_x}) \to [V]_{nn'}C_{n'} = ([\tilde{V}][B])_{nn'}C_{n'} \quad (96)$$

where,

$$\begin{aligned}[V]_{nn'} &= V_{\alpha\alpha'}(x_{m_x})S^x_{m'_x}(x_{m_x})S^y_{m'_y}(y_{m_y}) = ([\tilde{V}][B])_{nn'} \\ \left[\tilde{V}\right]_{nn'} &= V_{\alpha\alpha'}(x_{m_x})\delta_{m_x,m'_x}\delta_{m_y,m'_y} \end{aligned} \quad (97)$$

- **kinetic term:**

$$\Delta^\alpha(x,y)\delta_{\alpha\alpha'}F_\alpha(x,y) \to [\Delta]_{nn'}C_{n'} \quad (98)$$

[12] We may think

$$(xy)\langle\alpha xy|P^+|\psi\rangle_1 = \sum_{\alpha'}\int_{-1}^{+1} du\hat{h}_{\alpha\alpha'}(x,y,u)F_{\alpha'}(x',y') \quad (89)$$

where,

$$[\Delta]_{nn'} = \delta_{\alpha\alpha'}\frac{1}{m}\left[S''^{x}_{m'_x}(x_{m_x})S^{y}_{m'_y}(x_{m_y}) - \frac{l_x(l_x+1)}{x^2_{m_x}}S^{x}_{m'_x}(x_{m_x})S^{y}_{m'_y}(y_{m_y}) + S^{x}_{m'_x}(x_{m_x})S''^{y}_{m'_y}(x_{m_y}) - \frac{l_y(l_y+1)}{y^2_{m_y}}S^{x}_{m'_x}(x_{m_x})S^{y}_{m'_y}(y_{m_y})\right] \quad (99)$$

• **Integral operators** For integration, we can use Gaussian quadrature

$$\int dz F(z) \simeq \sum_i w_i F(z_i) \quad (100)$$

Then, integral part of the equation become

$$\begin{aligned} & 2\sum_{\tilde{\alpha}}\hat{V}_{\alpha\tilde{\alpha}}(x)\sum_{\alpha'}\int dz h_{\tilde{\alpha}\alpha'}(x,y,z)F_{\alpha'}(x',y') \\ \to\ & 2\sum_{\tilde{\alpha}}\hat{V}_{\alpha\tilde{\alpha}}(x)\sum_{\alpha'}\sum_{i_z} w_{i_z} h_{\tilde{\alpha}\alpha'}(x,y,z_i)F_{\alpha'}(x',y') \\ \to\ & 2\sum_{\tilde{\alpha}}\hat{V}_{\alpha\tilde{\alpha}}(x)\sum_{\alpha'}\sum_{i_z} w_{i_z} h_{\tilde{\alpha}\alpha'}(x,y,z_i)\sum_{n''}\delta_{\alpha'\alpha''}S_{m''_x}(x')S_{m''_y}(y')C_{n''} \\ \to\ & 2\sum_{n''}\sum_{\tilde{\alpha}}\hat{V}_{\alpha\tilde{\alpha}}(x)\sum_{i_z} w_{i_z} h_{\tilde{\alpha}\alpha''}(x,y,z_i)S_{m''_x}(x')S_{m''_y}(y')C_{n''} \\ =\ & 2\sum_{n''}[H]_{nn''}C_{n''} \end{aligned} \quad (101)$$

where, $[H]_{nn''}$ can be written as

$$[H]_{nn''} = \sum_{\tilde{\alpha}}\hat{V}_{\alpha\tilde{\alpha}}(x_{m_x})\sum_{i_z} w_{i_z} h_{\tilde{\alpha}\alpha''}(x_{m_x},y_{m_y},z_i)S_{m''_x}(x';m_x,m_y,z_i)S_{m''_y}(y';m_x,m_y,z_i) \quad (102)$$

for given $n=(\alpha,m_x,m_y)$, $n''=(\alpha'',m''_x,m''_y)$. and x' and y' are function of m_x,m_y,z_i. We can separate $[H]_{nn'}=\sum_{\tilde{n}}[\tilde{V}]_{n\tilde{n}}[\tilde{H}]_{\tilde{n}n'}$ with

$$[\tilde{H}]_{\tilde{n}n''} = \sum_{i_z} w_{i_z} h_{\tilde{\alpha}\alpha''}(x_{\tilde{m}_x},y_{\tilde{m}_y},z_i)S^{x}_{m''_x}(x^h(m_x,m_y,z_i))S^{y}_{m''_y}(y^h(m_x,m_y,z_i)) \quad (103)$$

• **Faddeev equation for bound state:** In abstract matrix notation we have

$$(E[B]+[\Delta]-[V])[C] = 2[H][C] \to [A][C] = ([V]-[\Delta]+2[H])[C] = E[B][C] \quad (104)$$

Though the whole equation is to be $k(N+1)$ dimension for each coordinate, bound state vanishes at large separation, thus, in actual calculation we only need kN dimension.

• **scattering state:** Scattering problem is different in the fact that the wave function does not vanish at large separation. Thus, if we want to express the equation in kN dimension, there is a term coming from boundary condition. Let us say the wave function as

$$\begin{aligned} F_\alpha(x,y) &= \sum_{m'_x=0}^{k(N_x+1)-1}\sum_{m'_y=0}^{k(N_y+1)-1} C_{\alpha,m'_x,m'_y}S_{m'_x}(x)S_{m'_y}(y) \\ &= \sum_{m'_x=1}^{kN_x}\sum_{m'_y=1}^{kN_y} C_{\alpha,m'_x,m'_y}S_{m'_x}(x)S_{m'_y}(y) + \sum_{m'_x=1}^{k(N_x+1)-1}\sum_{m'_y=kN_y+1}^{k(N_y+1)-1} C_{\alpha,m'_x,m'_y}S_{m'_x}(x)S_{m'_y}(y) \end{aligned} \quad (105)$$

If C_{α,m'_x,m'_y} outside of the boundary is known by the boundary condition, then acting $\hat{L}$ makes the first term as the same form as Faddeev equation of bound state and remaining terms as additional terms.

For example, if $k = 2$ and boundary condition was $C_{m_x,m_y=2N_y} = 1$. Then , by renaming last two spine function and its coefficient as $2N_y + 1 \leftrightarrow 2N_y$ makes,

$$F_\alpha(x,y) = \sum_{m'_x=1}^{2N_x}\sum_{m'_y=1}^{2N_y} C_{\alpha,m'_x,m'_y} S_{m'_x}(x) S_{m'_y}(y) + \sum_{m'_x=1}^{2N_x} C_{\alpha,m'_x} C^y_{\alpha,m'_y=2N_y+1} S_{m'_x}(x) S_{2N_y+1}(y) \quad (106)$$

where C_α, m_x is a spline coefficients of asymptotic 2-body bound state wave function and the last spline index for y is actually for $S_{2N_y}(y)$. Then applying $\hat{L}$ gives usual Faddeev equation of form $[A]C$ and additional boundary condition term

$$[b]_n = \sum_{m'_x=1}^{2N_x} C_{\alpha,m'_x} C^y_{\alpha,m'_y=2N_y+1} \hat{L} S_{m'_x}(x_{m_x}) S_{2N_y+1}(y_{m_y}) \quad (107)$$

For example, explicit form of $[b]$ term gives

$$\begin{aligned} b_n = & \sum_{\alpha' j'_x} C_{\alpha' j'_x} \Big[(E - V_{\alpha\alpha'}(x_{j_x})) S^x_{j'_x}(x_{j_x}) S^y_{2N_y+1}(y_{j_y}) \\ & - \frac{\hbar^2}{m} \delta_{\alpha\alpha'} \left(S''_{j'_x}(x_{j_x}) S_{2N_y+1}(y_{j_y}) - \frac{l_x(l_x+1)}{x^2_{j_x}} S_{j'_x}(x_{j_x}) S_{2N_y+1}(y_{j_y}) \right. \\ & \left. + S_{j'_x}(x_{j_x}) S''_{2N_y+1}(y_{j_y}) - \frac{l_y(l_y+1)}{y^2_{j_y}} S_{j'_x}(x_{j_x}) S_{2N_y+1}(y_{j_y}) \right) \\ & + V_{\alpha\alpha'}(x_{j_x}) \sum_{i_u=1}^{N_u} \cdots \end{aligned} \quad (108)$$

Thus, equation looks like, $[A]c = b$.

$$([V] - [\Delta] - E[B] + [H])[C] = [b] \quad (109)$$

8 Linear Algebra in numerical method

The problem is now to solve linear algebra problem of either $[A]c = E[B]c$ or $[A]c = b$. However, because of the large dimension of matrix $[A]$, we cannot use direct inversion of matrix $[A]$. We need some iterative algorithm to solve this problem.

8.1 Bound state problem

According to Rimas, there is two iterative algorithm to solve $[A]x = E[B]x$ type equation. Both are some variation of Lanczo's algorithm using eq. of form $[B]^{-1}[A]x = Ex$.

(1) Inverse iteration method using equation of form

$$(E_0 - [B]^{-1}[A])\psi = (E_0 - E)\psi \quad (110)$$

(2) Power method using equation of form

$$([V] - [\Delta] + [H])\psi = E[B]\psi \rightarrow (E_0[B] - [V] + [\Delta])^{-1}[H]\psi = \lambda(E_0)\psi \quad (111)$$

8.2 Scattering problem

For $Ax = b$ type equation can be solves by
(1) GMRES algorithm
(2) BICGSTAB algorithm
These method requires good preconditioning M such that

$$M^{-1}Ax = M^{-1}b, \quad \text{or , } AM^{-1}x = M^{-1}b \tag{112}$$

8.3 TENSOR inversion trick

Thus, we need either $[B]^{-1}[A]$ or $(E_0[B]-[V]+[\Delta])^{-1}[H]$ for bound state problem and also they an be used as a preconditioning for scattering problem. Because of the block diagonal property of matrix, we may use $[L][U]$ factorization for each block diagonal matrices to obtain inverse of a matrix. However, it is not effective. Thus, we need to use tensor inversion trick which uses the tensor structure of matrices.

Matrix $[M] = (E_0[B] - [V] + [\Delta])$ can be grouped as follows:

$$\begin{aligned}[M]_{n,n'} &= \delta_{\alpha,\alpha'}\left(\left[(E_0 - V_{\alpha,\alpha'} - \frac{\hbar^2}{m}\frac{l_x(l_x+1)}{x_{j_x}^2})S_{j'_x}(x_{j_x}) + \frac{\hbar^2}{m}S''_{j'_x}(x_{j_x})\right]S^y_{j'_y}(y_{j_y})\right. \\ &\left. + S^x_{j'_x}(x_{j_x})\left[-\frac{\hbar^2}{m}\frac{l_y(l_y+1)}{y_{j_y}^2})S_{j'_y}(y_{j_y}) + \frac{\hbar^2}{m}S''_{j'_y}(y_{j_y})\right]\right)\end{aligned} \tag{113}$$

이 식은 central potential 인 경우에만 성립한다. $[V]$는 partial wave 에 대해서, 일반적으로 diagonal 이 아니므로, 그 경우에는 완전한 tensor decomposition 은 불가능하다.

Introducing matrices

$$\begin{aligned}
[1^\alpha]_{\alpha,\alpha'} &= \delta_{\alpha,\alpha'} && \text{(of dimension } N_\alpha \times N_\alpha) \\
[\delta^a_{\alpha_0}]_{\alpha,\alpha'} &= \delta_{\alpha_0,\alpha}\delta_{a,\alpha'} && \text{(of dimension } N_\alpha \times N_\alpha) \\
& && N_\alpha \text{ distinct matrices} \\
[N^X]_{j_x,j'_x} &= S^x_{j'_x}(x_{j_x}) && \text{(of dimension } k_xN_x \times k_xN_x) \\
[N^Y]_{j_y,j'_y} &= S^y_{j'_y}(y_{j_y}) && \text{(of dimension } k_yN_y \times k_yN_y) \\
[D^X_{\alpha_0}]_{j_x,j'_x} &= \left(E_0 - V_{\alpha_0,\alpha_0}(x_{j_x}) - \frac{\hbar^2}{m}\frac{l_x(l_x+1)}{x_{j_x}^2}\right)S_{j'_x}(x_{j_x}) + \frac{\hbar^2}{m}S''_{j'_x}(x_{j_x}) && \text{(of dimension } k_xN_x \times k_yN_y) \\
& && N_\alpha \text{ distinct matrices} \\
[D^Y]_{j_x,j'_x} &= -\frac{\hbar^2}{m}\frac{l_x(l_x+1)}{x_{j_x}^2}S_{j'_x}(x_{j_x}) + \frac{\hbar^2}{m}S''_{j'_x}(x_{j_x}) && \text{(of dimension } k_xN_x \times k_yN_y)
\end{aligned} \tag{114}$$

In terms of these matrices, which decomposes partial wave state, x-space and y-space, $[B]$ becomes,

$$[B]_{nn'} = [[1^\alpha]_{\alpha\alpha'} \otimes [N^X]_{j_x,j'_x} \otimes [N^Y]_{j_y,j'_y}] \tag{115}$$

and its inversion

$$[B]^{-1} = [[1^\alpha] \otimes [N^X]^{-1} \otimes [N^Y]^{-1}] \tag{116}$$

where, $[N^X]^{-1}$, $[N^Y]^{-1}$ can be obtained by direct methods. We can have

$$\delta_{\alpha,\alpha'}\left[(E_0 - V_{\alpha,\alpha'} - \frac{\hbar^2}{m}\frac{l_x(l_x+1)}{x_{j_x}^2})S_{j'_x}(x_{j_x}) + \frac{\hbar^2}{m}S''_{j'_x}(x_{j_x})\right] \rightarrow \sum_{\alpha_0}[\delta_{\alpha_0}]_{\alpha\alpha'} \otimes [D^X_{\alpha_0}]_{j_x,j'_x} \quad (117)$$

Then,

$$[M] = \left[\sum_{\alpha_0}[\delta_{\alpha_0}]_{\alpha\alpha'} \otimes [D^X_{\alpha_0}]_{j_x j'_x} \otimes [N^Y]_{j_y j'_y}\right] + \left[[1]_{\alpha\alpha'} \otimes [N^X]_{j_x j'_x} \otimes [D^Y]_{j_y j'_y}\right] \quad (118)$$

Matrix inversion of $[M]$ can be done if we factor out interpolation matrix $[B]$ and introduce diagonal matrices by similarity transformation,

$$\begin{aligned} \left[N^X\right]^{-1}[D^X_{\alpha_0}] &= [U^X_{\alpha_0}][d^X_{\alpha_0}][U^X_{\alpha_0}]^{-1} \\ \left[N^Y\right]^{-1}[D^Y] &= [U^Y][d^Y][U^Y]^{-1} \end{aligned} \quad (119)$$

$$\begin{aligned} [M] &= [B]\left[\sum_{\alpha_0}[1^\alpha] \otimes [U^X_\alpha]^{-1} \otimes [U^Y]^{-1}\right]\left(\left[\sum_{\alpha_0}[\delta_{\alpha_0}] \otimes [d^X_{\alpha_0}] \otimes [1^Y]\right] + \left[[1] \otimes [1^X] \otimes [d^Y]\right]\right) \\ &\quad \left[\sum_{\alpha_0}[1^\alpha] \otimes [U^X_\alpha] \otimes [U^Y]\right] \\ [M]^{-1} &= \left[\sum_{\alpha_0}[1^\alpha] \otimes [U^X_\alpha] \otimes [U^Y]\right]^{-1}\left(\left[\sum_{\alpha_0}[\delta_{\alpha_0}] \otimes [d^X_{\alpha_0}] \otimes [1^Y]\right] + \left[[1] \otimes [1^X] \otimes [d^Y]\right]\right)^{-1} \\ &\quad \left[\sum_{\alpha_0}[1^\alpha] \otimes [U^X_\alpha]^{-1} \otimes [U^Y]^{-1}\right]^{-1}[B]^{-1} \end{aligned} \quad (120)$$

9 Krylov space technique: Iterative Orthonormal Vectors

Suppose we change the bound state equation into a coupled equations as

$$K(-E_b)|\psi\rangle = |\psi\rangle \quad (121)$$

This equation holds only when energy is at the correct value. In most case, we don't know E_b and try to find the E_b by trial of various E. Then, for a given trial energy E, the trial equation becomes

$$K(E)|\psi\rangle = \lambda(E)|\psi\rangle, \quad (122)$$

so that the $\lambda(E)$ eigenvalues will be different from 1 in most case. Only at the correct energy, λ becomes 1. Problem is that even for the trial equation is too large in dimension. (For example, 3-body problem will have dimension

$$N = N_\alpha \times N_p \times N_q,$$

where N_α is total number of partial waves, N_p and N_q are number of mesh in momentum p and q) Thus, we need a different way to solve trial equation to obtain eigenvalue λ and find a value of E such that largest eigenvalue becomes 1.

One idea is to use some basis functions up to $\mathcal{N} \ll N$ such that the eigenvalue problem can be solved by using standard method. How can find such basis functions?

Suppose we can write states in terms of orthonormal basis functions,

$$|\psi\rangle = \sum_{i=0}^{\mathcal{N}} c_i |\bar{\varphi}_i\rangle \tag{123}$$

Then, the original problem changes into $\mathcal{N}$-dimensional matrix equation ,

$$\sum_{j=0}^{\mathcal{N}} B_{ij}(E) c_j = \lambda(E) c_i, \tag{124}$$

where

$$B_{ij} = \langle \bar{\varphi}_i | K | \bar{\varphi}_j \rangle \tag{125}$$

If most of eigenvalues are smaller than 1, then the state $K^n|\phi_0\rangle$ which is a combination of all basis states, but only the dominant state contribution will be important as increasing n. Thus, if we make a basis functions in terms of $K^n|\phi_0\rangle$, only first small n basis functions will be enough to describe the largest eigenvalue states.

(a) start from arbitrary normalized state vector $|\bar{\varphi}_0\rangle$. generate state $|\varphi_1\rangle$ by,

$$|\varphi_1\rangle = K|\bar{\varphi}_0\rangle \tag{126}$$

(b) After Orthogonalization and normalization, we get $|\tilde{\varphi}_1\rangle$ and $|\bar{\varphi}_1\rangle$

$$\begin{aligned} |\tilde{\varphi}_1\rangle &= |\varphi_1\rangle - |\bar{\varphi}_0\rangle\langle\bar{\varphi}_0|\varphi_1\rangle, \\ |\bar{\varphi}_1\rangle &= \frac{|\tilde{\varphi}_1\rangle}{||\tilde{\varphi}_1||} \end{aligned} \tag{127}$$

Note that $|\tilde{\varphi}_1\rangle$ and $|\bar{\varphi}_1\rangle$ are orthogonal to $|\bar{\varphi}_0\rangle$. (c) repeat (a) and (b). Then, in each time, we generate

$$\begin{aligned} |\varphi_{i+1}\rangle &= K|\bar{\varphi}_i\rangle, \\ |\tilde{\varphi}_{i+1}\rangle &= |\varphi_{i+1}\rangle - \sum_{n=0}^{i} |\bar{\varphi}_n\rangle\langle\bar{\varphi}_n|\varphi_{i+1}\rangle, \\ |\bar{\varphi}_{i+1}\rangle &= \frac{|\tilde{\varphi}_{i+1}\rangle}{||\tilde{\varphi}_{i+1}||}. \end{aligned} \tag{128}$$

Note that $|\tilde{\varphi}_{i+1}\rangle$ and $|\bar{\varphi}_{i+1}\rangle$ are orthogonal to all $|\bar{\varphi}_n\rangle$ with $n \leq i$. And we can express state vector

$$|\varphi_{i+1}\rangle = \sum_{n=0}^{i+1} |\bar{\varphi}_n\rangle\langle\bar{\varphi}_n|\varphi_{i+1}\rangle, \quad \langle\bar{\varphi}_{i+1}|\varphi_{i+1}\rangle = ||\tilde{\varphi}_{i+1}||. \tag{129}$$

(d) The matrix element B_{ij} can be computed as

$$\begin{aligned} B_{ij} &= \langle\bar{\varphi}_i|K|\bar{\varphi}_j\rangle = \langle\bar{\varphi}_i|\varphi_{j+1}\rangle \\ &= 0 \quad \text{for } i > j+1 \\ &= ||\tilde{\varphi}_{j+1}|| \quad \text{for } i = j+1 \\ &= \langle\bar{\varphi}_i|\varphi_{j+1}\rangle \quad \text{for } i < j+1 \end{aligned} \tag{130}$$

If kernel K is a hermitian, we may get

$$\begin{aligned} B_{ij} &= \langle\bar{\varphi}_i|K|\bar{\varphi}_j\rangle = \langle\varphi_{i+1}|\bar{\varphi}_j\rangle \\ &= 0 \quad \text{for } j > i+1 \end{aligned} \tag{131}$$

In this case, the matrix B will be block-diagonal(?) form.

(e) Now use the standard numerical methods to solve the matrix eigenvalue equation,

$$Bc = \lambda c \tag{132}$$

since $\mathcal{N} \ll N$.

In practice, the $\mathcal{N}$ is not known a priori. Thus, we need to check convergence of the eigenvalue by increasing $\mathcal{N}$ values. (i.e. compare the eigenvalue $\lambda^{(n)}$ and $\lambda^{(n+1)}$ by increasing n until no eigenvalue change occurs.) In fact, we also need to test convergence of λ to 1 by changing trial energy E.

This is similar to the Lanczos method for

$$Ax = Bx, \rightarrow Ax = \lambda Bx \rightarrow A^{-1}Bx = \frac{1}{\lambda}x \rightarrow Hx = \Lambda x \tag{133}$$

where $\Lambda = 1/\lambda \rightarrow 1$ for correct energy. (Also, $\Lambda = 1$ will be the largest eigenvalue for the equation $Hx = \Lambda x$.

In case of scattering problem, the matrix equation of form $A \cdot x = b$ have to be solved.

For example, 2-body T-matrix equation basically looks like

$$t(k, k_0; E) = V(k, k_0) + \int K(k, k'; E)t(k', k_0; E) \tag{134}$$

For given half-on-shell momentum k_0, we can expand in terms of orthonormal basis functions (similarily for potential and kernel), [13]

$$|W\rangle = \hat{t}(E)|\phi_0\rangle = \sum_{i=0}^{\mathcal{N}} c_i|\bar{\varphi}_i\rangle \tag{135}$$

$$\langle\bar{\varphi}_i|W\rangle = c_i = \langle\bar{\varphi}_i|V(E)|\phi_0\rangle + \sum_{j=0}^{\mathcal{N}}\langle\bar{\varphi}_i|K(E)|\bar{\varphi}_j\rangle c_j \tag{136}$$

We may set starting vector $|\tilde{\varphi}_0\rangle = V(E)|\phi_0\rangle$ and define normalized vector [14]

$$|\bar{\varphi}_0\rangle = \frac{|\tilde{\varphi}_0\rangle}{||\tilde{\varphi}_0||}. \tag{137}$$

[13] We may consider,

$$\langle k|W\rangle = \langle k|\hat{t}(E)|k_0\rangle = \sum_{i=0}^{\mathcal{N}} c_i\bar{\varphi}_i(k)$$

[14] In practice, we would need partial wave expression for each state vectors. For a case $|\phi_0\rangle$ is a $|^1S_0; k_0\rangle$ state case, its partial wave expression will be $\alpha, k_i|\phi_0\rangle = \delta_{\alpha,^1S_0}\delta_{k_i,k_0}$. And, $\langle\alpha, k_i|\tilde{\phi}_0\rangle = \sum_\beta\sum_j w_{\beta,j}\langle\alpha k_i|V|\beta k_j\rangle\langle\beta k_j|\phi_0\rangle$

Then,

$$\begin{aligned} c_i &= \langle\bar{\varphi}_i|\bar{\varphi}_0\rangle||\tilde{\varphi}_0|| + \sum_{j=0}^{\mathcal{N}} B_{ij}c_j \\ &= \delta_{i0}||\tilde{\varphi}_0|| + \sum_{j=0}^{\mathcal{N}} B_{ij}c_j \end{aligned} \tag{138}$$

We get the matrix equation ,

$$\sum_{j=0}^{\mathcal{N}} A_{ij}c_j = f_i, \tag{139}$$

where

$$\begin{aligned} &A_{ij} = \delta_{ij} - B_{ij}, \\ &f_i = \delta_{i0}||\tilde{\varphi}_0||. \end{aligned} \tag{140}$$

The procedure to obtain orthonormal vectors are the same as previous case,
(a) get $|\bar{\varphi}_0\rangle$
(b) get $|\varphi_1\rangle$,$|\tilde{\varphi}_1\rangle$,$|\bar{\varphi}_1\rangle$,

$$\begin{aligned} |\varphi_1\rangle &= K|\bar{\varphi}_0\rangle \\ |\tilde{\varphi}_1\rangle &= |\varphi_1\rangle - |\bar{\varphi}_0\rangle\langle\bar{\varphi}_0|\varphi_1\rangle = |\bar{\varphi}_1\rangle||\tilde{\varphi}_1|| \end{aligned} \tag{141}$$

(c) repeat to get $|\varphi_{i+1}\rangle$,$|\tilde{\varphi}_{i+1}\rangle$,$|\bar{\varphi}_{i+1}\rangle$,

$$\begin{aligned} |\varphi_{i+1}\rangle &= K|\bar{\varphi}_i\rangle \\ |\tilde{\varphi}_{i+1}\rangle &= |\varphi_{i+1}\rangle - \sum_{n=0}^{i} |\bar{\varphi}_n\rangle\langle\bar{\varphi}_n|\varphi_{i+1}\rangle \\ |\bar{\varphi}_{i+1}\rangle &= \frac{|\tilde{\varphi}_{i+1}\rangle}{||\tilde{\varphi}_{i+1}||} \end{aligned} \tag{142}$$

(d) solve $\sum_{j=0}^{\mathcal{N}} A_{ij}c_j = f_i$ for c_j
(e) Convergence test as increasing $\mathcal{N}$: first check $|c_{\mathcal{N}}|$ is small enough. And then, test for the original integral equation,

$$\epsilon = \max(|\langle k_i|W\rangle - \langle k_i|\tilde{\varphi}_0\rangle - \langle k_i|K|W\rangle|), \quad \text{for } i = 1, \ldots, N$$

momentum quadrature may be chosen such that $k_N = k_0$ on-shell momentum.

Note: Notation $|k_i\rangle$ in fact includes all momentum mesh points and partial wave indices. For example,

9.1 Another explanation

General eigenvalue problem,

$$A \cdot v = \lambda \cdot v, \tag{143}$$

with A is a $n \times n$ matrix. Eigen vector v can be rewritten in the basis of the power-iterated subspace, $\{q, Aq, A^2q, A^3q, \cdots\}$. Then one could use a finite number of m vectors to orthogonally transform the matrix A into a Hessenberg matrix H_m, from which the eigenvalues and vectors are calculated faster than a general matrix. (Hessenberg matrix have matrix elements zero for upper or lower part.) After orthogonalization, basis is given by $p_1, \cdots, p_m$ and applied to the general matrix A, we get the $m \times m$ Hessenberg matrix,

$$H_m = \begin{pmatrix} h_{1,1} & h_{1,2} & \dots & h_{1,m} \\ h_{2,1} & h_{2,2} & \dots & h_{2,m} \\ 0 & h_{3,2} & \dots & h_{3,m} \\ 0 & 0 & \dots & h_{4,m} \\ & & \dots & \\ & & \dots & h_{m,m} \end{pmatrix} \tag{144}$$

10 RGM and GCM

Reference: Microscopic Cluster Models by P. Descouvemont and M. Dufour.

Cluster Model은 핵을 일종의 클러스터들의 합으로 생각하여 문제를 단순화 시킨다. 당연히, 이때 사용되는 클러스터들 간의 힘은 유효핵력이 된다. miscroscopic 방법은 클러스터의 내부 구조까지 고려하여, anti-symmetrization을 생각한다. 단, 같은 핵이라고 해도, 핵의 상태에 따라 서로 다른 클러스터링으로 취급하는 것이 좋을 수 있다.

Resonating group method(RGM) wave function for two-cluster 는

$$\Psi = \mathcal{A}\phi_1\phi_2 g(\boldsymbol{\rho}) \tag{145}$$

where, $\mathcal{A}$ is an anti-symmetrization operator including the internal degree of freedom in clusters and $g(\boldsymbol{\rho})$ is unknown relative wave function which should be obtained by cluster Schrodinger equation.

Basically, Generator coordinate method(GCM)은 RGM과 같지만, relative wave function을 Gaussian basis function으로 expand 하는 것이다. 일반적으로는 total wave function에 여러가지 종류의 clustering 이 포함된다.

RGM, GCM의 microscopic 계산에는 계산의 편리함때문에 보통 Volkov, Minesotta 타입의 단순화된 핵력을 이용한다.

10.1 RGM equation

Let us consider two cluster system. Coordinates of clusters are defined as

$$\boldsymbol{R}_{cm,1} = \frac{1}{A_1}\sum_{i=1}^{A_1} \boldsymbol{r}_i, \quad \boldsymbol{R}_{cm,2} = \frac{1}{A_2}\sum_{i=A_1+1}^{A} \boldsymbol{r}_i \tag{146}$$

$$\boldsymbol{R}_{cm} = \frac{1}{A}(A_1\boldsymbol{R}_{cm,1} + A_2\boldsymbol{R}_{cm,2}), \quad \boldsymbol{\rho} = \boldsymbol{R}_{cm,2} - \boldsymbol{R}_{cm,1}. \tag{147}$$

각각의 클러스터의 wave function은 $\phi_1(\xi_{1i})$ 와 $\phi_2(\xi_{2i})$ 로 나타내진다.

$$\xi_{1,i} = \boldsymbol{r}_i - \boldsymbol{R}_{cm,1}, \quad \xi_{2,i} = \boldsymbol{r}_i - \boldsymbol{R}_{cm,2}. \tag{148}$$

But, note that not all ξ_i are independent.

$$\sum_{i=1}^{A_1} \xi_{1i} = \sum_{i=A_i+1}^{A} \xi_{2i} = 0. \tag{149}$$

RGM wavf function,

$$\Psi(\xi_{1i}, \xi_{2i}, \boldsymbol{\rho}) = \mathcal{A}\phi_1(\xi_{1i})\phi_2(\xi_{2i})g(\boldsymbol{\rho}) \tag{150}$$

where, anti-symmetrization operator is with Permutation operator P_p,

$$\mathcal{A} = \sum_{p=1}^{A!} \epsilon_p P_p \tag{151}$$

Note that $\mathcal{A}$ is not a projector,

$$\mathcal{A}^2 = A!\mathcal{A} \tag{152}$$

Re-writing,

$$\Psi = \mathcal{A}\phi_1\phi_2 g(\boldsymbol{\rho}) = \int d\boldsymbol{r}\mathcal{A}\phi_1\phi_2\delta(\boldsymbol{\rho} - \boldsymbol{r})g(\boldsymbol{r}) \tag{153}$$

The Schrödinger equation in CM coordinate,(CM motion is removed)

$$\begin{aligned}
&(H - E_T)\Psi = 0 \to \int d\boldsymbol{\rho}' \left[\mathcal{H}(\boldsymbol{\rho}, \boldsymbol{\rho}') - E_T\mathcal{N}(\boldsymbol{\rho}, \boldsymbol{\rho}')\right] g(\boldsymbol{\rho}') \\
&\mathcal{N}(\boldsymbol{\rho}, \boldsymbol{\rho}') = \langle\phi_1\phi_2\delta(\boldsymbol{\rho} - \boldsymbol{r})|1|\mathcal{A}\phi_1\phi_2\delta(\boldsymbol{\rho}' - \boldsymbol{r})\rangle, \\
&\mathcal{H}(\boldsymbol{\rho}, \boldsymbol{\rho}') = \langle\phi_1\phi_2\delta(\boldsymbol{\rho} - \boldsymbol{r})|H|\mathcal{A}\phi_1\phi_2\delta(\boldsymbol{\rho}' - \boldsymbol{r})\rangle.
\end{aligned} \tag{154}$$

where integration over internal coordinates ξ and relative coordinates $\boldsymbol{r}$ are implied. One can simplify the equation by writing,

$$\begin{aligned}
\mathcal{A} &= 1 + \mathcal{A}', \\
H &= H_1 + H_2 + H_{rel}.
\end{aligned} \tag{155}$$

여기서, $\mathcal{A}'$은 다른 클러스터 사이에서의 exchange terms 만, H_i는 internal Hamiltonians of the clusters,

$$\begin{aligned}
H_{rel} &= -\frac{\hbar^2}{2\mu}\Delta_\rho + \sum_{i=1}^{A_1}\sum_{j=A_1+1}^{A} v_{ij}, \quad \mu = \mu_0 m_N, \quad \mu_0 = \frac{A_1 A_2}{A_1 + A_2}, \\
E_i &= \langle\phi_i|H_i|\phi_i\rangle, \\
E_{rel} &= E_T - E_1 - E_2.
\end{aligned} \tag{156}$$

(각 cluster wavr function의 antisymmetrization은 ? 이미 wave function에 고려되어 있기 때문에 쓰지 않는다인가?) Now non-local Kernels are

$$\begin{aligned}
\mathcal{N}(\boldsymbol{\rho}, \boldsymbol{\rho}') &= \delta(\boldsymbol{\rho} - \boldsymbol{\rho}') + \mathcal{N}_E(\boldsymbol{\rho}, \boldsymbol{\rho}'), \\
\mathcal{N}_E(\boldsymbol{\rho}, \boldsymbol{\rho}') &= \langle\phi_1\phi_2\delta(\boldsymbol{\rho} - \boldsymbol{r})|\mathcal{A}'\phi_1\phi_2\delta(\boldsymbol{\rho}' - \boldsymbol{r})\rangle, \\
\mathcal{H}(\boldsymbol{\rho}, \boldsymbol{\rho}') &= (E_1 + E_2)\delta(\boldsymbol{\rho} - \boldsymbol{\rho}') \\
&\quad + \langle\phi_1\phi_2\delta(\boldsymbol{\rho} - \boldsymbol{r})|H'|\phi_1\phi_2\delta(\boldsymbol{\rho}' - \boldsymbol{r})\rangle + \langle\phi_1\phi_2\delta(\boldsymbol{\rho} - \boldsymbol{r})|H'|\mathcal{A}'\phi_1\phi_2\delta(\boldsymbol{\rho}' - \boldsymbol{r})\rangle \\
&= \left(-\frac{\hbar^2}{2\mu}\Delta_\rho + V_D(\boldsymbol{\rho}) + E_1 + E_2\right)\delta(\boldsymbol{\rho} - \boldsymbol{\rho}') + \mathcal{H}_E(\boldsymbol{\rho}, \boldsymbol{\rho}'),
\end{aligned} \tag{157}$$

$$V_D(\boldsymbol{\rho}) = \langle \phi_1 \phi_2 | \sum_{i=1}^{A_1} \sum_{j=A_1+1}^{A} v_{ij} | \phi_1 \phi_2 \rangle \tag{158}$$

Thus RGM equation is

$$\left(-\frac{\hbar^2}{2\mu} \Delta_\rho + V_D(\boldsymbol{\rho}) \right) g(\boldsymbol{\rho}) + \int K(\boldsymbol{\rho}, \boldsymbol{\rho}') g(\boldsymbol{\rho}') d\boldsymbol{\rho}' = E g(\boldsymbol{\rho}), \tag{159}$$

with

$$K(\boldsymbol{\rho}, \boldsymbol{\rho}') = \mathcal{H}_E(\boldsymbol{\rho}, \boldsymbol{\rho}') - E_T \mathcal{N}_E(\boldsymbol{\rho}, \boldsymbol{\rho}'). \tag{160}$$

따라서, 일단 Kernel이 준비되면, RGM equation을 통해 $g(\boldsymbol{\rho})$ 를 얻을 수 있다. RGM에서 어려운 부분은 이러한 overlap과 Hamiltonian 을 준비하는 것이다.

10.1.1 Example, $\alpha + n$ system

Suppose α and neutron system,

$$\begin{aligned} \phi_1 &= \Phi_\alpha(\xi_1, \xi_2, \xi_3) | n_1 \downarrow n_1 \uparrow p_1 \downarrow p_1 \uparrow \rangle, \\ \phi_2 &= | n_2 \downarrow \rangle, \end{aligned} \tag{161}$$

여기서, n_1, p_1 은 1st cluster 에 속한다는 것을 나타낸다. ($\phi_{1,2}$는 이미 antisymmetrization이 이루어져 있다고 볼 수 있다.) Simple approximation,

$$\Phi_\alpha(\xi_1, \xi_2, \xi_3) = \frac{1}{N} \exp(-\nu \sum_{i=1}^{4} \xi_i^2) \tag{162}$$

with normalization

$$\langle \Phi_\alpha | \Phi_\alpha \rangle = 1 = \frac{1}{N^2} (\frac{\pi^3}{32\nu^3})^{3/2}. \tag{163}$$

The only exchange operator P_{15} contribute to the antisymmetrization. (Because external neutron is spin down. 허어??)

Note that in CM coordinate,

$$\boldsymbol{r}_{i=1,2,3,4} = -\frac{1}{5}\boldsymbol{\rho} + \xi_i, \quad \boldsymbol{r}_5 = \frac{4}{5}\boldsymbol{\rho}. \tag{164}$$

From

$$\begin{aligned} P_{15}\xi_1 &= P_{15}\left(\boldsymbol{r}_1 - \frac{1}{4}\sum_{i=1}^{4} \boldsymbol{r}_i \right) = \boldsymbol{r}_5 - \frac{1}{4}(\boldsymbol{r}_5 + \boldsymbol{r}_2 + \boldsymbol{r}_3 + v r_4) = \frac{3}{4}\boldsymbol{\rho} + \frac{1}{4}\xi_1, \\ P_{15}\xi_2 &= -\frac{1}{4}\boldsymbol{\rho} + \frac{1}{4}\xi_1 + \xi_2, \\ P_{15}\xi_3 &= -\frac{1}{4}\boldsymbol{\rho} + \frac{1}{4}\xi_1 + \xi_3, \\ P_{15}\boldsymbol{\rho} &= -\frac{1}{4}\boldsymbol{\rho} + \frac{5}{4}\xi_1, \end{aligned} \tag{165}$$

we get

$$P_{15}\Phi_\alpha\delta(\boldsymbol{\rho}-\boldsymbol{r}) = \Phi_\alpha \exp\left[-\frac{4\nu}{5}(r^2-(P_{15}\boldsymbol{\rho})^2)\right]\delta(P_{15}\boldsymbol{\rho}-\boldsymbol{r}) \tag{166}$$

By using

$$\int |\Phi_\alpha(\xi_1,\xi_2,\xi 3)|^2 d\xi_2 d\xi_3 = \left(\frac{\sqrt{3}\pi}{6\nu}\right)^3 \exp(-\frac{8\nu}{3}\xi_1^2), \tag{167}$$

$$\begin{aligned}
\mathcal{N}_E(\boldsymbol{\rho},\boldsymbol{\rho}') &= -\int d\boldsymbol{r} d\xi_1 d\xi_2 d\xi_3 \Phi_\alpha(\xi_1,\xi_2,\xi_3)\delta(\boldsymbol{\rho}-\boldsymbol{r})P_{15}\Phi_\alpha(\xi_1,\xi_2,\xi_3)\delta(\boldsymbol{\rho}'-\boldsymbol{r}) \\
&= -(\frac{4}{5})^3(\frac{8\nu}{3\pi})^{3/2}\exp\left[-\frac{4\nu}{75}(17\rho^2+17\rho'^2+16\boldsymbol{\rho}\cdot\boldsymbol{\rho}')\right].
\end{aligned} \tag{168}$$

10.1.2 Generator Coordinate Method

Expand the radial function $g(\boldsymbol{\rho})$ over Gaussian functions centered at different locations, called the **generator coordinates**.

Let us define one-center Slater determinant,

$$\Phi_1(\boldsymbol{r}_1\cdots\boldsymbol{r}_{A_1};\boldsymbol{S}_1) = \frac{1}{\sqrt{A_1!}}\det\{\hat{\varphi}(\boldsymbol{S}_1)\ldots\hat{\varphi}(\boldsymbol{S}_1)\}, \tag{169}$$

where

$$\begin{aligned}
\hat{\varphi}_i(\boldsymbol{S}) &= \varphi_i(\boldsymbol{r},\boldsymbol{S})|m_{s_i}\rangle|m_{t_i}\rangle, \\
\varphi_i(\boldsymbol{r},\boldsymbol{S}) &= \varphi_{0s}(\boldsymbol{r},\boldsymbol{S}) = (\pi b^2)^{-3/4}\exp(-\frac{(\boldsymbol{r}-\boldsymbol{S})^2}{2b^2}) \text{ for s-orbital,} \\
&= \varphi_{1p\mu}(\boldsymbol{r},\boldsymbol{S}) = \frac{\sqrt{2}}{b}(\boldsymbol{r}_\mu-\boldsymbol{S}_\mu)\varphi_{0s}(\boldsymbol{r},\boldsymbol{S}) \text{ for p-orbital}
\end{aligned} \tag{170}$$

By using translation invariant determinant, ϕ_1

$$\phi_1(\xi_{1i}), \quad \xi_{1i} = \boldsymbol{r}_i - \boldsymbol{R}_{cm,1}. \tag{171}$$

We may express, one-center Slater determinant as [15]

$$\Phi(\boldsymbol{r}_i;\boldsymbol{S}) = \exp\left(-\frac{A_1}{2b^2}(\boldsymbol{R}_{cm,1}-\boldsymbol{S})^2\right)\phi_1(\xi_{1i}) \tag{173}$$

We may express full $A-$body Slater determinant by using two kinds of basis functions with different center, $\varphi_i(\boldsymbol{r},\boldsymbol{S}_1)$ and $\varphi_i(\boldsymbol{r},\boldsymbol{S}_2)$. We may set the origin along the $\boldsymbol{R}=\boldsymbol{S}_2-\boldsymbol{S}_1$. In other words, we can choose coordinates as $\boldsymbol{S}_1=-\lambda\boldsymbol{R}$, $\boldsymbol{S}_2=(1-\lambda)\boldsymbol{R}$. However, note that $\boldsymbol{S}_i$ does not necessarily the same as the center of mass of each cluster $\boldsymbol{R}_i$.

[15] One can simply show this by

$$\sum_i \frac{(\boldsymbol{r}_i-\boldsymbol{S})^2}{2b^2} = \sum_i \frac{(\xi_{1,i}+\boldsymbol{S}-\boldsymbol{R}_{cm,1})^2}{2b^2} = \left(\sum_i \frac{\xi_{1,i}^2}{2b^2}\right) + \frac{A_1}{2b^2}(\boldsymbol{S}-\boldsymbol{R}_{cm,1})^2 \tag{172}$$

Define two-cluster Slater determinant as

$$\begin{aligned}\Phi(\boldsymbol{r}_i;\boldsymbol{R}) &= \frac{1}{\sqrt{A!}}\det\{\hat{\varphi}(\boldsymbol{r}_1,-\lambda\boldsymbol{R})\ldots\hat{\varphi}(\boldsymbol{r}_{A_1},-\lambda\boldsymbol{R})\ldots\hat{\varphi}(\boldsymbol{r}_A,(1-\lambda)\boldsymbol{R})\} \\ &= \frac{1}{\sqrt{N_0}}\mathcal{A}\Phi_1(\boldsymbol{r}_i;-\lambda\boldsymbol{R})\Phi_2(\boldsymbol{r}_i;(1-\lambda)\boldsymbol{R}), \quad N_0=\frac{A!}{A_1!A_2!} \end{aligned} \tag{174}$$

This can be rewritten as

$$\Phi(\boldsymbol{r}_i;\boldsymbol{R}) = \frac{1}{\sqrt{N_0}}\Phi_{cm}(\boldsymbol{R}_{cm};\boldsymbol{R})\mathcal{A}\phi_1(\xi_{1i})\phi_2(\xi_{2i})\Gamma(\rho,\boldsymbol{R}) \tag{175}$$

where[16]

$$\begin{aligned}\Phi_{cm}(\boldsymbol{R}_{cm};\boldsymbol{R}) &= (\frac{A}{\pi b^2})^{3/4}\exp\left(-\frac{A}{2b^2}[\boldsymbol{R}_{cm}+\boldsymbol{R}(\lambda-\frac{A_2}{A})]^2\right), \\ \Gamma(\rho,\boldsymbol{R}) &= (\frac{\mu_0}{\pi b^2})^{3/4}\exp(-\frac{\mu_0}{2b^2}(\rho-\boldsymbol{R})^2). \end{aligned} \tag{177}$$

This expression makes the c.m. and radial coordinates uncoupled. In other words, the two-cluster Slater determinant can be treated separately for the c.m. and radial part though the wave function itself is not translation invariant. Then, two-cluster Slater determinant is

$$\Phi(\boldsymbol{r}_i;\boldsymbol{R}) = \Phi_{cm}\bar{\Phi}(\xi;\boldsymbol{R}), \tag{178}$$

where $\bar{\Phi}(\xi,\boldsymbol{R})$ is independent of c.m. coordinate. Note that $\Phi(\boldsymbol{r}_i;\boldsymbol{R})$ is good for numerical calculation because it is a Slater determinant. The overlap of Slater determinant is

$$\begin{aligned}\langle\Phi(\boldsymbol{R})|\Phi(\boldsymbol{R}')\rangle &= \langle\Phi_{cm}|\Phi_{cm}\rangle\langle\bar{\Phi}(\boldsymbol{R})|\bar{\Phi}(\boldsymbol{R})\rangle, \\ \langle\Phi_{cm}|\Phi_{cm}\rangle &= \exp\left(-\frac{A(\lambda-A_2/A)^2}{4b^2}(\boldsymbol{R}-\boldsymbol{R}')^2\right). \end{aligned} \tag{179}$$

In other words, one can obtain overlap between basis functions $\bar{\Phi}(\boldsymbol{R})$.

We may consider $\frac{1}{\Phi_{cm}}\Phi(\boldsymbol{r}_i;\boldsymbol{R})$ as a kind of basis function for the radial function of RGM. In other words,

$$\Psi = \Phi_{cm}^{-1}\int f(\boldsymbol{R})\Phi(\boldsymbol{R})d\boldsymbol{R} \tag{180}$$

where Ψ is invariant under translation and generator function is to be determined from Hamiltonian.

중요: Actually, the difference between Ψ and Φ is the main message from GCM. While Ψ is the RGM wave function which describes internal structure of a nuclei, it is difficult to use because of the complication from anti-symmetrization operator. On the other hand, Φ is easier to manipulate and make calculation, while it contains additional center of mass motion. By using GCM, one can separate internal degrees of freedom and the center of mass from Slater determinant.

[16]This can be shown from

$$\begin{aligned}& A_1(\boldsymbol{R}_{cm,1}-(-\lambda\boldsymbol{R}))^2+A_2(\boldsymbol{R}_{cm,2}-(1-\lambda)\boldsymbol{R})^2 \\ =\ & A_1(\boldsymbol{R}_{cm,1}+\boldsymbol{R}(\lambda-\frac{A_2}{A})+\frac{A_2}{A}(\boldsymbol{R}-\boldsymbol{\rho}))^2+A_2(\boldsymbol{R}_{cm,1}+\boldsymbol{R}(\lambda-\frac{A_2}{A})-\frac{A_1}{A}(\boldsymbol{R}-\boldsymbol{\rho}))^2 \end{aligned} \tag{176}$$

This can be expressed as

$$\Psi = \mathcal{A}\phi_1\phi_2 g(\rho), \tag{181}$$

with

$$g(\rho) = \int f(\boldsymbol{R})\Gamma(\rho, \boldsymbol{R})d\boldsymbol{R}. \tag{182}$$

Generally speaking A-body Slater determinant wave function made from s.p. wave functions are not translation invariant. However, by using the GCM basis with c.m. correction, we may express,

$$\Phi(\boldsymbol{r}_i) \simeq \sum_{\boldsymbol{R}_n} f(\boldsymbol{R}_n)\Phi_{cm}(\boldsymbol{R}_n)\bar{\Phi}(\boldsymbol{R}_n) \tag{183}$$

where $\bar{\Phi}(\boldsymbol{R}_n)$ is translation invariant.

The generator function $f(\boldsymbol{R})$ can be obtained by solving

$$\int [H(\boldsymbol{R}, \boldsymbol{R}') - E_T N(\boldsymbol{R}, \boldsymbol{R}')] f(\boldsymbol{R}')d\boldsymbol{R}' = 0, \tag{184}$$

where GCM kernels are

$$\begin{aligned} N(\boldsymbol{R}, \boldsymbol{R}') &= \langle\bar{\Phi}(\boldsymbol{R})|\bar{\Phi}(\boldsymbol{R}')\rangle, \\ H(\boldsymbol{R}, \boldsymbol{R}') &= \langle\bar{\Phi}(\boldsymbol{R})|H|\bar{\Phi}(\boldsymbol{R}')\rangle. \end{aligned} \tag{185}$$

Note that one can use the Slater determinant wave functions to compute the matrix elements with cm correction. For example, overlap kernel can be computed as $\langle\bar{\Phi}(\boldsymbol{R})|\bar{\Phi}(\boldsymbol{R}')\rangle/\langle\Phi_{cm}|\Phi_{cm}\rangle$. Thus, GCM simplifies the calculation of Kernels and by discretization

$$g(\rho) \simeq \sum_n f(\boldsymbol{R}_n)\Gamma(\rho, \boldsymbol{R}_n) \tag{186}$$

the equation for generator function becomes a diagonalization of a matrix.