

A study of the Omega-Omega interaction using the  
central potential in Lattice QCD

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# Chapter 1

## Introduction

Classification of natural science, it is due to scale. In order scale is large, the scale of the universe is described in astrophysics, the scale of the earth is described in earth planetary science, the molecular scale is described in biology, the atomic scale is described in the chemical, the nuclei scale is described in nuclear physics and the smallest scale is described in particle physics. At present, there are fundamental particles as the fermion which make up the matter, the boson which mediate the interaction. Further fermions are classified into six quarks ( $u, d, c, s, t, b$ ) and six leptons ( $e, \nu_e, \mu, \nu_\mu, \tau, \nu_\tau$ ). Bosons are classified into the gauge boson ( $\gamma, W^\pm, Z, g, G$  which is unconfirmed) and the Higgs boson  $H^0$  which is confirmed in 2012 [1, 2]. We believe that everything is made from the interactions of these fundamental particles.

At recent years, people try the numerical calculation across the scale, because the connection between different scale is not apparent. As a first step, we study the nuclear potential which is the input of nuclear physics from quarks and gluons. In Standard model (SM), the origin of the nuclear potential is quarks and gluons interaction, and dynamics of quarks and gluons is described Quantum Chromodynamics (QCD) which is  $SU(3)$  Yang-Mills theory. Therefore we calculate QCD to estimate the nuclear interaction. In fact, the perturbative QCD is successful in predicting the phenomena in high energy region, on the other hand, it is difficult to calculate the QCD in low energy region. This is caused that the coupling constant of QCD is large in low energy region called confinement, in contrast the coupling constant is small in high energy region called asymptotic freedom. Therefore perturbative calculation is unreliable.

Lattice QCD is a powerful tool to calculate the QCD in non-perturbative region. To calculate in non-perturbative region, Lattice QCD runs the path integral numerically using the high performance computer. For numerical calculation, Lattice QCD is described on Euclidian space-time which is discretized with a finite lattice spacing  $a$ , and it is well defined. Quantum field theory in continuum space-time has an uncountable infinite number of degrees of freedom, on the other hand, Lattice QCD has countable infinite number of degrees of freedom. Since the momentum has the upper limit  $\frac{\pi}{a}$  which arises from a finite lattice spacing  $a$ , it does not appear the ultraviolet divergence. So Lattice QCD is a theory that has been regularized. In addition, the Lattice QCD calculation in finite volume, it is equivalent to quantum mechanics that has a finite degree of freedom, and we can calculate it. Of course the reality of space-time is believed that it is continuous, we estimate the physical value in the limit of the continuum  $a \rightarrow 0$ . Basically input parameters in the lattice QCD are the hopping parameter  $\kappa$  which corresponds to the quark mass which is an input parameter of SM and the  $\beta$  which corresponds to the coupling constant in QCD.

The first principle calculation using the LatticeQCD, it can estimate the hadronic spectrum, the condensates and chiral symmetry breaking, the properties of QCD finite temperature or density. The hadron mass is a single hadron quantity which is estimated from 2-pt correlator which is successful to predict the physical mass. CP-PACS Collaboration studied the light hadron mass with quenched approximation [3, 4] which ignores the dynamical effects of the sea quarks, and PACS-CS Collaboration estimated in 2+1 flavor full QCD toward the physical point [5] which used nature of quark mass. Furthermore some

simulation includes the effect of (Quantum electrodynamics) QED [6, 7], and 1+1+1 flavor full QCD + QED simulation at physical point [8]. Because of the theory and computer development, Lattice QCD can calculate the hadrons interaction that is estimated from 4-pt correlator. There are two ways as the calculation of hadron interactions. One is the traditional approach called Lüscher method [9], which estimate the phase shift from the interaction energy which is measured in finite box. Other one called HAL QCD potential method has been developed in recent years [10, 11]. It calculates the phase shift via the nuclear potential which is calculated from the equal time Nambu-Behte-Salpeter wave function (NBS wave function). This method can be applied not only to the nuclear potential [10, 11, 12] but also to other interactions such as baryon-baryon interactions [13, 14, 15], meson-meson interactions [16, 17], the LS force [18, 19], the anti-symmetric LS force [20], and three-body force [21]. See [12] for a recent review of this method.

Hyperons (baryons including strange quarks) are expected to appear in extremely high density such as a core of neutron stars, so that the equation of state (EoS) in dense matters is affected. To determine the EoS of neutron stars precisely, information on their interaction is necessary. Experimentally, however, it is difficult to determine them due to the short lifetime of hyperons. Therefore, theoretical determinations of hyperon interactions are crucially important. Indeed the HAL QCD method has been employed to investigate hyperon interactions in various channels [13, 14, 15]. Considering the hyperon system, it has an approximate flavor  $SU(3)$  symmetry between the mass of  $u$ ,  $d$ , and  $s$  quarks. The flavor  $SU(3)$  derives the irreducible representations ( $3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10$ ). The 8 called octet baryon and the 10 called decuplet baryon. HAL QCD potential method investigations so far are limited to octet-octet baryons interactions. Quiet recently, an octet-decuplet interaction has been investigated by the HAL QCD method using the nucleon-Omega system, since only Omega is stable decuplet baryon under QCD interaction. The result suggests an existence of the bound state in this system [22].

In this paper, we investigate interactions in the Omega-Omega system, which has the highest strangeness among two baryon systems, as a first step to understand the decuplet-decuplet interaction. In the past studies, there is a possibility that some decuplet baryons have a bound state. However, almost all decuplet baryons are unstable due to decays via the strong interaction. An exception is the Omega baryon, which is stable against the strong decays, so its interaction is suitable to be investigated. The quark model predict which is used the quark model [23] the Omega-Omega interaction is strongly attractive [24]. It is, however, still difficult to investigate the Omega-Omega interaction experimentally because Omega decay via weak interaction. Therefore, the lattice QCD study for the Omega-Omega interaction is necessary and important. As previously mentioned, it is difficult to estimate the Omega-Omega interaction in the experiment, the model calculation has an ambiguity. So Chiral Quark Model model calculation [25] predicted the strong attraction [24] but the other model (Quark Disloc./Color-screen Model) did the weak repulsive force [26, 27]. In addition, the lattice QCD investigation on the Omega-Omega interaction by the Lüscher method found the weak repulsion but with large errors [28]. They used two simulation using two different volumes with  $L \sim 2.5$  and  $3.9$  fm on anisotropic clover lattices at  $m_\pi \sim 390$  MeV with a lattice spacing of  $a_s \sim 0.123$  fm in the spatial direction and  $a_t \sim a_s/3.5$  in the temporal direction. Using it, the estimate the scattering length  $a = 0.16 \pm 0.22$  fm in  $J = 0$ .

HAL QCD method study of the octet-octet system interaction about hadron-hadron, hadron-hyperon and hyperon-hyperon, its qualitative nature of which is consistent with the results of the quark model. If we believe the quark model results, it can expect that Omega-Omega simulation results in Lattice QCD consistent with the qualitative results of the quark model which suggests that Omega-Omega interaction is strongly attractive, but the results of Lüscher method is not so strong interaction [28]. As mentioned in the introduction, Since the Omega baryon is stable in QCD, the method has been used in the HAL QCD Collab. can be safely applied.

This paper is organized as follows. In chapter 2, we explain the method to determine the nuclear potential in lattice QCD. In chapter 3, for calculation of the Omega-Omega interaction, we show some topics particularly Omega operator and spin and angular momentum projections. In chapter 4, we explain

the Okubo-marshark decomposition [29] for decuplet-decuplet system in first order. In chapter 5 we show the numerical simulation results and discussion, Finally we summarize this work in chapter 6.

## Chapter 2

# Nuclear Force in Lattice QCD

In this chapter, we show how to extract Nuclear potential from QCD. In quantum mechanics, we calculate wave function by using the Schrödinger equation. In HAL QCD potential method, however, we inversely use the Schrödinger equation to extract a potential. There are two important points.

- Can we extract energy independent potential?
- What is the wave function in QCD?

We first explain Lattice gauge theory. We then define an energy independent potential. Finally we explain what kind of properties the wave function should have.

### 2.1 Lattice gauge theory

We consider actions in Lattice gauge theory. One of the guiding principles of our construction is the requirement that in the limit  $a \rightarrow 0$  the lattice action approaches the continuum form.

#### 2.1.1 Gauge field

The lattice formulation provides the only possible framework at present to study QCD non-perturbatively. We consider a four-dimensional Euclidean space. In lattice QCD, we introduce gauge field on a space-time lattice  $(n, \mu)$ .

$$A_\mu(n) = A_\mu^a(n)T^a \in SU(N) \quad (2.1)$$

where  $T^a$  is  $N \times N$  matrix and

$$\text{Tr}T^a = 0 \quad , (T^a)^\dagger = T^a, \quad (2.2)$$

$$\text{Tr}(T^a T^b) = \frac{1}{2}\delta^{ab} \quad , [T^a, T^b] = if^{abc}T^c \quad (2.3)$$

is satisfied. We define link variable  $U(x, x + \hat{\mu}a)$  as

$$U_{n,\mu} \equiv U(x, x + \hat{\mu}a) = \exp(igaA_\mu(n + \frac{\hat{\mu}}{2})), \quad (2.4)$$

$$U_{n,\mu}^\dagger \equiv U_{n+\hat{\mu},-\mu}, \quad (2.5)$$

where  $\hat{\mu}$  is unit vector of space-time.  $U_{n,\mu}$  is gauge transformed at  $V_n \in SU(N)$  as

$$U_{n,\mu} \rightarrow V_n U_{n,\mu} V_{n+\hat{\mu}}^\dagger. \quad (2.6)$$

We define gauge invariant object. We consider the product of link variables around an elementary square, called the plaquette. Let this plaquette lie in the  $\mu - \nu$  plane. We then define  $U_{\mu\nu}(n)$

$$U_{\mu\nu}(n) \equiv U_{n,\mu} U_{n+\mu,\nu} U_{n+\nu,\mu}^\dagger U_{n,\nu}^\dagger. \quad (2.7)$$

It is possible to write down the gauge action as

$$S_G = \sum_{n,\mu \neq \nu} \beta \text{tr}[U_{n,\mu} U_{n+\mu,\nu} U_{n+\nu,\mu}^\dagger U_{n,\nu}^\dagger] = \sum_{n,\mu > \nu} 2\beta \text{Re} \text{tr}[U_{\mu\nu}(n)], \quad (2.8)$$

where  $\beta = \frac{1}{g^2}$ .  $\beta$  is the inverse of the coupling constant squared.

### 2.1.2 Dirac field

We introduce matter field. The matter part in continuum is written as

$$S_F = \int d^4x \bar{\psi}(x) (\gamma_\mu D^\mu + m) \psi(x), \quad (2.9)$$

where  $D_\mu = \partial_\mu + igA_\mu$ . It is easy to show that  $S_F$  is invariant under the gauge transformation. We can define Lattice action

$$S_F = \frac{1}{2} \sum_{n,\mu} [\bar{\psi}'_n \gamma_\mu U_{n,\mu} \psi'_{n+\hat{\mu}} - \bar{\psi}'_{n+\hat{\mu}} \gamma_\mu U_{n,\mu}^\dagger \psi'_n] + M \sum_n \bar{\psi}'_n \psi'_n, \quad (2.10)$$

where  $\psi'_n, \bar{\psi}'_n, M$  are dimensionless as  $\bar{\psi}'_n = a^{\frac{3}{2}} \bar{\psi}_n, \psi'_n = a^{\frac{3}{2}} \psi_n, M = ma$ .

This naive lattice action, however, has a problem. We consider free case ( $\forall U_{n,\mu} = 1$ ) to show this problem. This propagator becomes

$$G_F(p) = \frac{-i \sum_\mu \gamma_\mu \sin(p_\mu a) + M}{(\sum_\mu \gamma_\mu \sin(p_\mu a))^2 + M^2}. \quad (2.11)$$

The pole of the propagator is given by

$$\sin^2(p_\mu a) + M^2 = 0. \quad (2.12)$$

When we consider the continuum limit ( $a \rightarrow 0$ ), the pole must satisfy

$$\sin(p_\mu a) = \begin{cases} \hat{p}_\mu a & , p_\mu = \hat{p}_\mu \\ -\hat{p}_\mu a & , p_\mu = \hat{p}_\mu + \frac{\pi}{a} \end{cases}. \quad (2.13)$$

This shows that two possibilities appears for each direction  $\mu$ . Since a pole of the propagator is corresponds to a particle in quantum field theory, one propagator describes  $2^d = 16$  particles in four dimensional lattice filed theory. This problem is called doubling problem.

In order to avoid this problem, we introduce the Wilson fermion action as

$$S_W = S_F + S_{\text{Willson}}, \quad (2.14)$$

where Willson term  $S_{\text{Willson}}$  is given by



$$S_{\text{Willson}} = -\frac{ar}{2} \int d^4x \bar{\psi} D^2 \psi. \quad (2.15)$$

The parameter  $r$  is constant and is called Willson parameter. Since the Willson term is proportional to the lattice space  $a$ , it vanishes in continuum limit. It is possible to separate physical particles and doubler particles. We consider Willson action in momentum space as

$$S_W = \bar{\psi}(-p) \left[ i \sum_{\mu} \gamma_{\mu} \sin(p_{\mu}a) + M + r \sum_{\mu} (1 - \cos(p_{\mu}a)) \right] \psi(p), \quad (2.16)$$

where  $M(p)$  behaves like a mass term.

$$M(p) \equiv M + r \sum_{\mu} (1 - \cos(p_{\mu}a)). \quad (2.17)$$

Then the propagator for the Wilson fermion is given by

$$G_F(p) = \frac{-i \sum_{\mu} \gamma_{\mu} \sin(p_{\mu}a) + M(p)}{\sin^2(p_{\mu}a) + M(p)^2}. \quad (2.18)$$

In  $a \rightarrow 0$  limit,  $M(p)$  behaves as

$$M(p) = \begin{cases} ma & \text{physical pole} \\ ma + 2r|\delta| & \text{doublers} \end{cases}, \quad (2.19)$$

where  $|\delta|$  counts the number of  $\pi$ 's for the doubler momentum. The mass in the physical unit thus becomes

$$m_{\text{phys}} = m, \quad (2.20)$$

$$m_{\text{doubler}} = m + \frac{2r}{a} |\delta| \rightarrow \infty. \quad (2.21)$$

All doublers decouple since they become infinitely heavy in the continuum limit. In this way the Wilson fermion action can avoid the doubling problem.

We define the hopping parameter

$$K \equiv \frac{1}{2(M + 4r)}. \quad (2.22)$$

The Wilson fermion action is written as

$$S_W = \sum_n \bar{\psi}_n \psi_n - K \sum_{n,\mu} [\bar{\psi}_n (r - \gamma_{\mu}) U_{n,\mu} \psi_{n+\hat{\mu}} + \bar{\psi}_{n-\hat{\mu}} (r + \gamma_{\mu}) U_{n-\hat{\mu},\mu}^{\dagger} \psi_n]. \quad (2.23)$$

The gauge action is

$$S_G = \sum_{n,\mu \neq \nu} \beta \text{Tr}[U_{n,\mu} U_{n+\mu,\nu} U_{n+\nu,\mu}^{\dagger} U_{n,\nu}^{\dagger}] = \sum_{n,\mu > \nu} 2\beta \text{ReTr}[U_{\mu\nu}(n)]. \quad (2.24)$$

We have used an improved Wilson fermion action in [30]. in our numerical simulations.

## 2.2 Effective mass

To calculate the potential of the Omega-Omega system, we first determine the Omega mass in the simulation set up. In this section, we show how to measure the effective mass in Lattice QCD. For simplicity, we use the scalar field. The 2-point correlator is defined by

$$G(t) = \sum_x \langle 0 | \phi(x) \phi(0) | 0 \rangle, \quad (2.25)$$

where  $t \equiv x^0$ . Using completeness relation  $1 = \sum_{k=0} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_k} |E_k(p)\rangle \langle E_k(p)|$

$$\begin{aligned} &= \sum_x \sum_{k=0} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(x) | E_k(p) \rangle \langle E_k(p) | \phi(0) | 0 \rangle \\ &= \sum_x \sum_{k=0} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | e^{-i\hat{p}x} \phi(0) e^{i\hat{p}x} | E_k(p) \rangle \langle E_k(p) | \phi(0) | 0 \rangle \\ &= \sum_x \sum_{k=0} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(0) e^{ipx} | E_k(p) \rangle \langle E_k(p) | \phi(0) | 0 \rangle \\ &= \sum_x \sum_{k=0} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(0) | E_k(p) \rangle \langle E_k(p) | \phi(0) | 0 \rangle e^{ipx} \\ &= \sum_x \sum_{k=0} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_k} |\langle 0 | \phi(0) | E_k(p) \rangle|^2 e^{-i\vec{p}\vec{x}} e^{-E_k(\vec{p})x_0} \\ &= \sum_{k=0} \int d^3 p \frac{1}{2E_k} |\langle 0 | \phi(0) | E_k(p) \rangle|^2 e^{-E_k(\vec{p})x_0} \delta^3(\vec{p}) \\ &= \sum_{k=0} \frac{1}{2E_k} |\langle 0 | \phi(0) | E_k(0) \rangle|^2 e^{-E_k(0)x_0}. \end{aligned} \quad (2.26)$$

We take  $t \equiv x_0 \gg 1$  to extract the ground state contribution ( $k = 0$ ) (excited states are suppressed exponentially at large  $t$ ).

$$\begin{aligned} &\sim \frac{1}{2E_0} |\langle 0 | \phi(0) | E_0(p) \rangle|^2 e^{-E_k(0)x_0} \\ &\sim \frac{1}{2m_0} |Z_0|^2 e^{-m_0 t}, \end{aligned} \quad (2.27)$$

where  $m_k = E_k(0)$  is the mass of the  $k$ -th one-particle state and  $Z_k \equiv \langle 0 | \phi(0) | E_k(p) \rangle$ . The effective mass is defined as

$$m_0(t) = \log \frac{G(t)}{G(t+1)}. \quad (2.28)$$

We plot  $m(t)$  and fit the plateau to determine the mass  $m_0$ . We show periodic boundary condition case Appendix A.

## 2.3 HAL QCD method

In this section, we show how to extract the potential. The potential method was originally introduced by HAL QCD collaboration [10, 11].

To show the basic concept of the non-local potential in a finite box with the size  $L \times L \times L$ . The Schrödinger equation is given by

$$\left(\frac{1}{2\mu}\nabla^2 + E_n\right)\psi_n(r) = \int d^3r' U(r, r')\psi_n(r'), \quad (2.29)$$

where  $r$  is relative coordinate and  $\mu$  is a reduced mass

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}, \quad (2.30)$$

where  $E_n$  is the discrete energy eigenvalues  $E_n = \frac{k_n^2}{2\mu} \{n|n \in \mathbb{Z}, 0 \leq n\}$ . It's important that the potential  $U(r, r')$  is not depend on  $n$ . In general, we show that the energy independent non-local potential and the energy depend local potential are equivalent. First we consider a Schrödinger equation used a local potential.

$$\left(\frac{1}{2\mu}\nabla^2 + E_n\right)\psi_n(r) = V_n(r)\psi_n(r), \quad (2.31)$$

where  $V_n$  is depend on  $n$ . We use the bracket

$$V_n(r) = (E_n - (-\frac{1}{2\mu}\nabla^2))\psi_n(r) = \langle r | E_n - H_0 | n \rangle, \quad (2.32)$$

where  $H_0$  is a free hamiltonian  $\langle r | H_0 | n \rangle = -\frac{1}{2\mu}\nabla^2\psi_n(r)$ . The non-local potential can write

$$U(r, r') = \langle r | E_n - H_0 | r' \rangle \quad (2.33)$$

$$= \sum_{n, n'} \langle r | (E_n - H_0) | n \rangle \langle n | n' \rangle \langle n' | r' \rangle \quad (2.34)$$

$$= \sum_{n, n'} V_n(r)\psi_n(r)N_{n, n'}^{-1}\psi_n^*(r'), \quad (2.35)$$

where  $N_{n, n'}^{-1}$

$$N_{n, n'}^{-1} \equiv \langle n | n' \rangle. \quad (2.36)$$

Since taking the sum of  $n$  and  $n'$ ,  $U(r, r')$  is independent on  $n$  and  $n'$ . So, we was able to rewrite the energy depend local potential to the energy independent non-local potential. Now we can define the energy independent potential. Therefore, we can extract a general potential from the wave-function  $\psi_n(r)$ .

### 2.3.1 Nambu-Behte-Salpeter wave function and phase shift

We discuss what is the wave function in QCD. In scattering theory, wave function must have the correct phase shift in asymptotic state. We try to keep this property when we consider the QCD wave function.

We first introduce the equal time NBS wave function as

$$\Psi_{n\alpha'\beta';\alpha\beta}(\vec{r}, t) = \langle 0 | N_{\alpha'}(x, t)N_{\beta'}(y, t) | N_{\alpha}(k_n)N_{\beta}(-k_n); in \rangle, \quad (2.37)$$

where  $\vec{r} = \vec{x} - \vec{y}$ ,  $\alpha'\beta'\alpha\beta$  are spin indices,  $\langle 0 | =_{\text{out}} \langle 0 | =_{\text{in}} \langle 0 |$  is the QCD vacuum,  $|N_{\alpha}(k_n)N_{\beta}(-k_n); in\rangle$  is asymptotic in-state of two nucleon with the energy  $W_n = 2\sqrt{m_N^2 + k_n^2}$  and  $N(x)$  is the local Nucleon operator. Explicitly, we have

$$n_{\beta}(y) \equiv \varepsilon^{abc}(u_{\alpha}^a(y)(C\gamma_5)_{\alpha\delta}d_{\delta}^b(y))d_{\beta}^c(y), \quad (2.38)$$

$$p_\alpha(x) \equiv \varepsilon^{abc}(u_\beta^a(x)(C\gamma_5)_{\beta\delta}d_\delta^b(x))u_\alpha^c(x), \quad (2.39)$$

where  $C \equiv \gamma^4\gamma^0$  is the charge conjugate matrix,  $a, b, c$  are color indices.

One of the most important properties here is that the NBS wave function at large  $|\vec{r}|$  in QCD has the same asymptotic form of the scattering wave in quantum mechanics. We show asymptotic form of NBS wave function in Appendix B.

### 2.3.2 How to measure Nambu-Behte-Salpeter wave function in Lattice QCD

In previous sub section, we define the NBS wave function as the wave function of QCD. In this subsection, we explain how to measure the NBS wave function on the Lattice. Fig. 2.1 shows the image of the NBS wave function on the lattice.

we start with the 4-point correlator

$$C_{NN}(\vec{x}, \vec{y}, t, t_0) \equiv \langle 0 | n_\beta(y, t) p_\alpha(x, t) J_{pn}(t_0) | 0 \rangle \quad (2.40)$$

We insert the completeness relation system  $1 = \sum_m |m\rangle \langle m|$

$$\begin{aligned} &= \sum_m \langle 0 | n_\beta(y) p_\alpha(x) | m \rangle e^{-E_m(t-t_0)} \langle m | J_{pn} | 0 \rangle \\ &= \sum_m A_m e^{-E_m(t-t_0)} \phi(\vec{x} - \vec{y}, m) + \text{inelastic state} \end{aligned} \quad (2.41)$$

where we define

$$A_m \equiv \langle m | J_{pn} | 0 \rangle, \quad (2.42)$$

$$\psi(\vec{x} - \vec{y}, m) \equiv \langle 0 | n_\beta(y) p_\alpha(x) | m \rangle. \quad (2.43)$$

$\psi(\vec{x} - \vec{y}, m)$  is the NBS wave function. So the 4-point correlator includes the NBS wave function. Taking the large  $t-t_0$ , we can get the NBS wave function of the ground state, because excited states are suppressed exponentially at large  $t-t_0$ .

Here  $J_{pn}$  is a source operator which creates the two-nucleon state. For example, the wall source is given by

$$J_{pn}(t_0) \equiv [\bar{p}_\alpha^{\text{wall}}(t_0) \bar{n}_\beta^{\text{wall}}(t_0)], \quad (2.44)$$

where  $\bar{p}^{\text{wall}}$  and  $\bar{n}^{\text{wall}}$  are Dirac-conjugate of  $p^{\text{wall}}$  and  $n^{\text{wall}}$ , which are defined as

$$n_\beta^{\text{wall}}(t_0) \equiv \varepsilon^{abc} \left( \sum_y u_\alpha^a(y, t_0) (C\gamma_5)_{\alpha\delta} \sum_{y'} d_\delta^b(y', t_0) \right) \sum_{y''} d_\beta^c(y'', t_0), \quad (2.45)$$

$$p_\alpha^{\text{wall}}(t_0) \equiv \varepsilon^{abc} \left( \sum_x u_\beta^a(x, t_0) (C\gamma_5)_{\beta\delta} \sum_{x'} d_\delta^b(x', t_0) \right) \sum_{x''} u_\alpha^c(x'', t_0). \quad (2.46)$$

Since  $p^{\text{wall}}$  and  $n^{\text{wall}}$  are not gauge invariant, we should fix the gauge. The wall source create only states with zero total momentum.

On the other hand, the Gaussian source operator is given by

$$J_{pn}(x_0, t_0) \equiv [\bar{p}_\alpha^{\text{Gaussian}}(x_0, t_0) \bar{n}_\beta^{\text{Gaussian}}(x_0, t_0)], \quad (2.47)$$

where  $\bar{p}^{\text{Gaussian}}$  and  $\bar{n}^{\text{Gaussian}}$  are defined as

$$n_{\beta}^{\text{Gaussian}}(x_0, t_0) \equiv \varepsilon^{abc} \left( \sum_y e^{-\frac{(y-x_0)^2}{r^2}} u_{\alpha}^a(y, t_0) (C\gamma_5)_{\alpha\delta} \sum_{y'} e^{-\frac{(y'-x_0)^2}{r^2}} d_{\delta}^b(y', t_0) \right) \sum_{y''} e^{-\frac{(y''-x_0)^2}{r^2}} d_{\beta}^c(y'', t_0), \quad (2.48)$$

$$p_{\alpha}^{\text{Gaussian}}(x_0, t_0) \equiv \varepsilon^{abc} \left( \sum_x e^{-\frac{(x-x_0)^2}{r^2}} u_{\beta}^a(x, t_0) (C\gamma_5)_{\beta\delta} \sum_{x'} e^{-\frac{(x'-x_0)^2}{r^2}} d_{\delta}^b(x', t_0) \right) \sum_{x''} e^{-\frac{(x''-x_0)^2}{r^2}} u_{\alpha}^c(x'', t_0). \quad (2.49)$$

When we calculate the NBS wave function on the lattice, we apply the projection operator to fix quantum numbers at source and sink. We explain it in section 3.

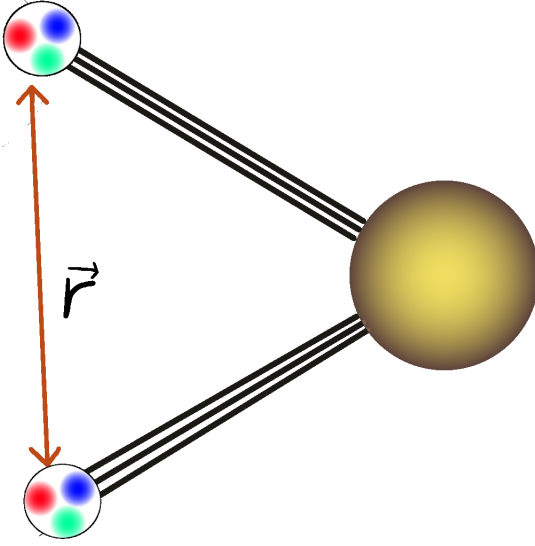


Figure 2.1: Image of the NBS wave function on the lattice. We extract the information of the Omega-Omega interaction at sink.

### 2.3.3 Time dependence method

We have described how to determine the NBS wave function in the lattice simulation, and it need large  $t - t_0$  where excited states are suppressed. The signal-to-noise ratio, however, becomes worse at large time [31]. The signal-to-noise ratio of the correlation for  $n$ -nucleons is

$$\left(\frac{S}{N}\right)_n \sim e^{-n(m_N - \frac{3}{2}m_{\pi})t}. \quad (2.50)$$

The signal-to-noise ratio becomes worse in the many-body system. This is a fatal problem to calculate interactions between hadrons in lattice QCD.

Fortunately, there is a good method, called time dependence method [32], which avoids this signal-to-noise problem to extract potentials. The time dependent method can derive the QCD potential without ground state saturation. For simplicity, we ignore the spin indices and take  $t_0 = 0$ .

First, we define R-correlator as

$$R(t, r) \equiv \sum_n \frac{C_n(r, t)}{e^{-2mt}} \quad (2.51)$$

where  $C_n(r, t)$  is 4-point correlator, given by

$$\begin{aligned}
C_n(t, r) &\equiv \langle 0 | N(x, t) N(y, t) J(0) | 0 \rangle \\
&= \sum_n \langle 0 | N(x) N(y) | n \rangle \langle n | J(0) | 0 \rangle e^{-E_n t} \\
&= \sum_n A_n \psi_n(r) e^{-E_n t}
\end{aligned} \tag{2.52}$$

where  $\vec{r} = \vec{x} - \vec{y}$ ,  $E_n = 2\sqrt{m_N^2 - k_n^2}$ ,

$$A_n \equiv \langle n | J(0) | 0 \rangle, \tag{2.53}$$

$$\psi(r) \equiv \langle 0 | N(x) N(y) | n \rangle. \tag{2.54}$$

Therefore

$$\begin{aligned}
R(t, r) &= \sum_n A_n \psi_n(r) e^{-E_n t} \frac{1}{e^{-2m_N t}} \\
&= \sum_n A_n \psi_n(r) e^{-W_n t},
\end{aligned} \tag{2.55}$$

where  $W_n \equiv 2(\sqrt{m_N^2 - k_n^2} - m_N)$ .

$W_n$  have an identity

$$W(\vec{k}_n) = \frac{\vec{k}_n^2}{m_N} - \frac{(W(k_n))^2}{4m_N}, \tag{2.56}$$

which can be shown as

$$\begin{aligned}
\frac{(W(\vec{k}_n))^2}{4m_N} &= \frac{1}{4m_N} (4m_n^2 + 4\vec{k}_n^2 + 4m_N^2 - 8m_N \sqrt{m_N^2 + \vec{k}_n^2}) \\
&= 2m_N + \frac{\vec{k}_n^2}{m_N} - 2\sqrt{m_N^2 + \vec{k}_n^2}.
\end{aligned} \tag{2.57}$$

We then perform a time derivative of R-correlator as follows

$$\begin{aligned}
-\frac{\partial}{\partial t} R(t, r) &= \sum_n W(\vec{k}_n) \psi_n(\vec{r}) A_n e^{-W(\vec{k}_n) t} \\
&= \sum_n \left( \frac{\vec{k}_n^2}{m_N} - \frac{(W(k_n))^2}{4m_N} \right) \psi_n(\vec{r}) A_n e^{-W(\vec{k}_n) t} \\
&= \sum_n \left( \frac{\vec{k}_n^2}{m_N} - \frac{1}{4m_N} \frac{\partial^2}{\partial t^2} \right) \psi_n(\vec{r}) A_n e^{-W(\vec{k}_n) t}
\end{aligned} \tag{2.58}$$

We have used the identity  $W(\vec{k}_n) = \frac{\vec{k}_n^2}{m_N} - \frac{(W(k_n))^2}{4m_N}$  in the second line.

Finally we use Eq. (2.29), we can get the time-dependent Schrödinger-like equation

$$\left( \frac{1}{m_N} \nabla^2 - \frac{\partial}{\partial t} + \frac{1}{4m_N} \frac{\partial^2}{\partial t^2} \right) R(t, t_0, r) = \int dr' U(r, r') R(t, t_0, r') dr'. \tag{2.59}$$

Via this equation, we can derive  $U(r, r')$  from  $R(t, r)$ . Since the R-correlator does not depend on the energy, we can derive the potential without ground state saturation. A condition necessary for this method to work is that  $t - t_0$  should be large enough to suppress both inelastic contributions in the two-Omega system and excited states in the single-Omega correlation function. In the non-relativistic limit, the time-dependent Schrödinger-like equation is reduced to

$$\left(\frac{1}{m_N}\nabla^2 - \frac{\partial}{\partial t}\right)R(t, t_0, r) = \int dr' U(r, r')R(t, t_0, r')dr', \quad (2.60)$$

since  $\frac{1}{4m_N}\frac{\partial^2}{\partial t^2}$  is corresponding to the relativistic effect.

# Chapter 3

## $\Omega - \Omega$ case

### 3.1 Charge conjugation of the Omega baryon

We introduce to Omega baryon operator's properties which is defined as

$$\Omega_{k_1 g}(x) \equiv \varepsilon^{c_1 c_2 c_3} \delta_{g_3 g} (C \gamma_{k_1})_{g_1 g_2} s_{g_1}^{c_1}(x) s_{g_2}^{c_2}(x) s_{g_3}^{c_3}(x). \quad (3.1)$$

It's not  $\text{spin} \frac{3}{2}$  baryon, so we need spin projection to  $\text{spin} \frac{3}{2}$ . The operator is satisfied these properties

- spin (Lorentz symmetry)
- parity
- $U(1)$  charge
- $SU(3)$  gauge symmetry (singlet)
- flavor symmetry

In Omega baryon case, favor is only s quarks,  $\text{spin} = \frac{3}{2}$ , parity =  $-$ ,  $U(1)$  charge is  $-1$  and  $SU(3)$  gauge symmetry is singlet. We will check the properties of Omega baryon operator. First, we check that  $\varepsilon^{abc} q_a q_b q_c$  is gauge invariant.

$$\begin{aligned} \varepsilon^{abc} q_a q_b q_c &\rightarrow \varepsilon^{abc} U_{aa'} q_{a'} U_{bb'} q_{b'} U_{cc'} q_{c'} \\ &= \det U \varepsilon^{a'b'c'} q_{a'} q_{b'} q_{c'} \\ &= \varepsilon^{a'b'c'} q_{a'} q_{b'} q_{c'} \end{aligned} \quad (3.2)$$

Second, we check spin symmetry. we define quarks as

$$q = \begin{pmatrix} \varepsilon_\alpha \\ \eta^{\dot{\beta}} \end{pmatrix} \quad (3.3)$$

where dot is complex representation in  $SL(2C)$ . We show the  $q^T C$  is a similar transformation to the  $\bar{q}$ . The Lorentz transformation of  $q^T C$  is



$$\begin{aligned}
q^T C &= \begin{pmatrix} (\xi_\alpha)^T & (\eta^{\dot{\beta}})^T \end{pmatrix} \begin{pmatrix} \varepsilon_{\alpha\beta} & 0 \\ 0 & \varepsilon^{\dot{\beta}\dot{\alpha}} \end{pmatrix} \\
&= \begin{pmatrix} (\xi^T)^\alpha & (\eta^T)_{\dot{\beta}} \end{pmatrix} \begin{pmatrix} \varepsilon_{\alpha\beta} & 0 \\ 0 & \varepsilon^{\dot{\beta}\dot{\alpha}} \end{pmatrix} \\
&= \begin{pmatrix} (\xi^T)_\beta & (\eta^T)^{\dot{\alpha}} \end{pmatrix}.
\end{aligned} \tag{3.4}$$

On the other hands, transformation of the  $\bar{q}$  as

$$\begin{aligned}
\bar{q} &= q^\dagger \gamma^0 \\
&= \begin{pmatrix} (\xi_\alpha)^\dagger & (\eta^{\dot{\beta}})^\dagger \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} (\xi_\alpha^*)^T & (\eta^{*\beta})^T \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} (\xi^\dagger)^{\dot{\alpha}} & (\eta^\dagger)_\beta \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} (\eta^\dagger)_\beta & (\xi^\dagger)^{\dot{\alpha}} \end{pmatrix}.
\end{aligned} \tag{3.5}$$

These transformation properties are equivalent, because these indices are same. Therefore the  $q^T C \gamma_k q$  is a Lorentz vector. Finally we use spin projection from  $\text{spin}1 \oplus \text{spin}\frac{1}{2}$  operator ( $q^T C \gamma_k q$ ) to  $\text{spin}\frac{3}{2}$  operator  $\Omega_{\frac{3}{2}}$ . We explain it in 3.1.1.

We can check parity= + in Omega operator.

$$\begin{aligned}
q^T C \gamma_k q &\Rightarrow q^T \gamma_0 C \gamma_k \gamma_0 q \\
&= -q^T \gamma_0 C \gamma_0 \gamma_k q \\
&= q^T C \gamma_k q
\end{aligned} \tag{3.6}$$

We used following equation

$$q \Rightarrow P q(x, t) P^{-1} = \gamma_0 q(-x, t) \tag{3.7}$$

$$q^T \Rightarrow P q(x, t)^T P = q^T(-x, t) \gamma_0^T = q^T(-x, t) \gamma_0 \tag{3.8}$$

where  $C$  is

$$C^* = C, \tag{3.9}$$

$$C \equiv i\gamma_2 \gamma_0 = -C^{-1} = -C^T = -C^\dagger \quad \text{Minkowski,} \tag{3.10}$$

$$C \equiv \gamma_0 \gamma_2 = -C^{-1} = -C^T = -C^\dagger \quad \text{Euclid.} \tag{3.11}$$

When we use only strange quarks, U(1) charge is  $-1$  and flavor symmetry is satisfied. Next we define anti-Omega operator.

$$\begin{aligned}
\bar{\Omega}_{k_1 g}(x) &\equiv \Omega^\dagger \gamma^0 = \varepsilon^{c_1 c_2 c_3} \delta_{g'_3 g} ((C \gamma_{k_1})_{g_1 g_2} (s_{g_1}^{c_1})^T s_{g_2}^{c_2} s_{g_3}^{c_3})^\dagger (\gamma_0)_{g_3 g'_3} \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g'_3 g} ((\gamma_{k_1}^\dagger C^\dagger)_{g_2 g_1} s_{g_3}^{c_3 \dagger} s_{g_2}^{c_2 \dagger} (s_{g_1}^{c_1 \dagger})^T) (\gamma_0)_{g_3 g'_3} \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g'_3 g} ((\gamma_0 \gamma_{k_1} \gamma_0 C^\dagger)_{g_2 g_1} (s^{c_3 \dagger} \gamma_0)_{g'_3} s_{g_2}^{c_2 \dagger} (s_{g_1}^{c_1 \dagger})^T) \\
&= -\varepsilon^{c_1 c_2 c_3} \delta_{g'_3 g} ((\gamma_0 \gamma_{k_1} C^\dagger \gamma_0)_{g_2 g_1} (s^{c_3 \dagger} \gamma_0)_{g'_3} s_{g_2}^{c_2 \dagger} (s_{g_1}^{c_1 \dagger})^T) \\
&= -\varepsilon^{c_1 c_2 c_3} \delta_{g'_3 g} ((\gamma_{k_1} C^\dagger)_{g_2 g_1} (s^{c_3 \dagger} \gamma_0)_{g'_3} (s_{g_2}^{c_2 \dagger} \gamma_0) (\gamma_0 (s_{g_1}^{c_1 \dagger})^T)) \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g'_3 g} (\gamma_{k_1} C)_{g_2 g_1} \bar{s}_{g'_3}^{c_3} \bar{s}_{g_2}^{c_2} (\bar{s}_{g_1}^{c_1})^T \\
&= -\varepsilon^{c_3 c_2 c_1} \delta_{g'_3 g} (\gamma_{k_1} C)_{g_2 g_1} \bar{s}_{g'_3}^{c_3} \bar{s}_{g_2}^{c_2} (\bar{s}_{g_1}^{c_1})^T \\
&= -\varepsilon^{c_3 c_2 c_1} \delta_{g'_3 g} \bar{s}_{g'_3}^{c_3} \bar{s}_{g_2}^{c_2} (\bar{s}_{g_1}^{c_1})^T C (\bar{s}_{g_1}^{c_1})^T
\end{aligned} \tag{3.12}$$

To increase the statistics, we consider charge conjugation of the Omega baryon. The charge conjugation is define as

$$\psi \rightarrow \psi_{\text{anti}} = \hat{C} \psi \hat{C}^{-1} = i \gamma_2 \psi^* = C(\bar{\psi})^T, \tag{3.13}$$

$$\psi^T \rightarrow (\hat{C} \psi \hat{C}^{-1})^T = \hat{C} \psi^T \hat{C}^{-1} = (C(\bar{\psi})^T)^T = \bar{\psi} C^T = \bar{\psi} C^{-1}, \tag{3.14}$$

$$\bar{\psi} \rightarrow \hat{C} \psi^\dagger \gamma_0 \hat{C}^{-1} = (\hat{C} \psi^T \hat{C}^{-1})^* \gamma_0 = (\psi^\dagger \gamma_0)^* C^{-1} \gamma_0 = \psi^T C, \tag{3.15}$$

$$\bar{\psi}^T \rightarrow \hat{C} \bar{\psi}^T \hat{C}^{-1} = (\hat{C} \bar{\psi} \hat{C}^{-1})^T = (\psi^T C)^T = C^{-1} \psi, \tag{3.16}$$

where  $\hat{C}$  is operator of charge conjugation. Let's try to charge conjugation in Proton and Omega.

For Proton case,

$$\begin{aligned}
P_\alpha &\rightarrow \hat{C} P_\alpha \hat{C}^{-1} = \hat{C} \varepsilon^{c_1 c_2 c_3} \delta_{g_3, \alpha} (q_{g_1}^{c_1})^T (C \gamma_5)_{g_1 g_2} q_{g_2}^{c_2} q_{g_3}^{c_3} \hat{C}^{-1} \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g_3, \alpha} \hat{C} (q_{g_1}^{c_1})^T \hat{C}^{-1} (C \gamma_5)_{g_1 g_2} \hat{C} q_{g_2}^{c_2} \hat{C}^{-1} \hat{C} q_{g_3}^{c_3} \hat{C}^{-1} \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g_3, \alpha} \bar{q}_{g_1}^{c_1} C^{-1} (C \gamma_5)_{g_1 g_2} C (q_{g_2}^{c_2})^T C (\bar{q}_{g_3}^{c_3})^T \\
&= C \varepsilon^{c_1 c_2 c_3} \delta_{g_3, \alpha} \bar{q}_{g_1}^{c_1} C^{-1} (C \gamma_5)_{g_1 g_2} C (\bar{q}_{g_2}^{c_2})^T (\bar{q}_{g_3}^{c_3})^T \\
&= C \varepsilon^{c_1 c_2 c_3} \delta_{g_3, \alpha} (\bar{q}_{g_1}^{c_1})^T (\gamma_5 C)_{g_1 g_2}^T (\bar{q}_{g_2}^{c_2})^T (\bar{q}_{g_3}^{c_3})^T \\
&= -C \varepsilon^{c_1 c_2 c_3} \delta_{g_3, \alpha} (\bar{q}_{g_3}^{c_3} \bar{q}_{g_2}^{c_2} (\gamma_5 C)_{g_2 g_1}^T (\bar{q}_{g_1}^{c_1})^T)^T \\
&(\gamma_5 C)^T = -\gamma_5 C = -C \gamma_5 \\
&= -C \varepsilon^{c_3 c_2 c_1} \delta_{g_3, \alpha} (\bar{q}_{g_3}^{c_3} \bar{q}_{g_2}^{c_2} (C \gamma_5)_{g_2 g_1} (\bar{q}_{g_1}^{c_1})^T)^T \\
&= C_{\alpha \alpha'} (\bar{P}_{\alpha'})^T
\end{aligned} \tag{3.17}$$

For Omega case, It is similar to Proton.

$$\begin{aligned}
\Omega_{k_1 g}(x) &\rightarrow \hat{C}\Omega\hat{C}^{-1} \equiv \hat{C}\varepsilon^{c_1 c_2 c_3} \delta_{g_3, g}(s_{g_1}^{c_1})^T (C\gamma_{k_1})_{g_1 g_2} s_{g_2}^{c_2} s_{g_3}^{c_3} \hat{C}^{-1} \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g_3, g} \hat{C}(s_{g_1}^{c_1})^T \hat{C}^{-1} \hat{C}(C\gamma_{k_1})_{g_1 g_2} \hat{C}^{-1} \hat{C} s_{g_2}^{c_2} C^{-1} \hat{C} s_{g_3}^{c_3} \hat{C}^{-1} \\
&= \varepsilon^{c_1 c_2 c_3} \delta_{g_3, g} \bar{s}_{g_1}^{c_1} C^{-1} (C\gamma_{k_1})_{g_1 g_2} C(\bar{s}_{g_2}^{c_2})^T C(\bar{s}_{g_3}^{c_3})^T \\
&= C\varepsilon^{c_1 c_2 c_3} \delta_{g_3, g} \bar{s}_{g_1}^{c_1} (\gamma_{k_1} C)_{g_1 g_2} (\bar{s}_{g_2}^{c_2})^T (\bar{s}_{g_3}^{c_3})^T \\
&= -C\varepsilon^{c_1 c_2 c_3} \delta_{g_3, g} (\bar{s}_{g_3}^{c_3} \bar{s}_{g_2}^{c_2} ((\gamma_{k_1} C)^T)_{g_2 g_1} (\bar{s}_{g_1}^{c_1})^T)^T \\
&= -C\varepsilon^{c_1 c_2 c_3} \delta_{g_3, g} (\bar{s}_{g_3}^{c_3} \bar{s}_{g_2}^{c_2} (\gamma_{k_1} C)_{g_2 g_1} (\bar{s}_{g_1}^{c_1})^T)^T \\
&= C\varepsilon^{c_3 c_2 c_1} \delta_{g_3, g} (\bar{s}_{g_3}^{c_3} \bar{s}_{g_2}^{c_2} (\gamma_{k_1} C)_{g_2 g_1} (\bar{s}_{g_1}^{c_1})^T)^T \\
&= -C_{g g'} \bar{\Omega}_{g' k_1}^T
\end{aligned} \tag{3.18}$$

We used this relation  $(\gamma_\mu C)^T = \gamma_\mu C$ .

Now we have the rules of the charge conjugation in Omega baryon, we can increase statics of the 4-point correlator which defined as

$$\begin{aligned}
G_{\alpha\beta\mu\nu; \alpha'\beta'\mu'\nu'}(x, y, t, x', y') &\equiv \langle 0 | T \{ \Omega_{\alpha\mu}(x, t) \Omega_{\beta\nu}(y, t) \bar{\Omega}_{\alpha'\mu'}(x', 0) \bar{\Omega}_{\beta'\nu'}(y', 0) \} | 0 \rangle \\
&\equiv \theta(t) \langle 0 | \Omega_{\alpha\mu}(x, t) \Omega_{\beta\nu}(y, t) \bar{\Omega}_{\alpha'\mu'}(x', 0) \bar{\Omega}_{\beta'\nu'}(y', 0) | 0 \rangle \\
&\quad - \theta(-t) \langle 0 | \bar{\Omega}_{\alpha'\mu'}(x', 0) \bar{\Omega}_{\beta'\nu'}(y', 0) \Omega_{\alpha\mu}(x, t) \Omega_{\beta\nu}(y, t) | 0 \rangle.
\end{aligned} \tag{3.19}$$

For simplicity we consider  $t > 0$ . To reduce noise we consider 4-point correlator

$$\begin{aligned}
G_{\alpha\beta\mu\nu; \alpha'\beta'\mu'\nu'}(x, y, t, x', y') &= \langle 0 | T \{ \Omega_{\alpha\mu}(x, t) \Omega_{\beta\nu}(y, t) \bar{\Omega}_{\alpha'\mu'}(x', 0) \bar{\Omega}_{\beta'\nu'}(y', 0) \} | 0 \rangle \\
&= \langle 0 | \Omega_{\alpha\mu}(x, t) \Omega_{\beta\nu}(y, t) \bar{\Omega}_{\alpha'\mu'}(x', 0) \bar{\Omega}_{\beta'\nu'}(y', 0) | 0 \rangle.
\end{aligned} \tag{3.20}$$

Using the vacuum is invariance under charge conjugation  $\langle 0 | C = \langle 0 |, C^{-1} | 0 \rangle = | 0 \rangle$ .

$$\begin{aligned}
&G_{\alpha\beta\mu\nu; \alpha'\beta'\mu'\nu'}(x, y, t, x', y') \\
&= \langle 0 | \hat{C} \Omega_{\alpha\mu}(x, t) \Omega_{\beta\nu}(y, t) \bar{\Omega}_{\alpha'\mu'}(x', 0) \bar{\Omega}_{\beta'\nu'}(y', 0) C^{-1} | 0 \rangle \\
&= \langle 0 | \hat{C} \Omega_{\alpha\mu}(x, t) \hat{C}^{-1} \hat{C} \Omega_{\beta\nu}(y, t) \hat{C} \hat{C} \bar{\Omega}_{\alpha'\mu'}(x', 0) \hat{C} \hat{C} \bar{\Omega}_{\beta'\nu'}(y', 0) C^{-1} | 0 \rangle \\
&= C_{\alpha\bar{\alpha}} C_{\beta\bar{\beta}} \langle 0 | \bar{\Omega}_{\bar{\alpha}\mu}^T(x, t) \bar{\Omega}_{\bar{\beta}\nu}^T(y, t) \Omega_{\bar{\alpha}'\mu'}^T(x', 0) \Omega_{\bar{\beta}'\nu'}^T(y', 0) | 0 \rangle C_{\bar{\alpha}'\alpha'} C_{\bar{\beta}'\beta'} \\
&= C_{\alpha\bar{\alpha}} C_{\beta\bar{\beta}} \langle 0 | (\Omega_{\bar{\alpha}\mu}^\dagger(x, -t) \gamma_0)^T (\Omega_{\bar{\beta}\nu}^\dagger(y, -t) \gamma_0)^T \bar{\Omega}_{\bar{\alpha}'\mu'}^*(x', 0) \bar{\Omega}_{\bar{\beta}'\nu'}^*(y', 0) \gamma_0 | 0 \rangle C_{\bar{\alpha}'\alpha'} C_{\bar{\beta}'\beta'} \\
&= (C\gamma_0)_{\alpha\bar{\alpha}} (C\gamma_0)_{\beta\bar{\beta}} \langle 0 | \Omega_{\bar{\alpha}\mu}^*(x, -t) \Omega_{\bar{\beta}\nu}^*(y, -t) \bar{\Omega}_{\bar{\alpha}'\mu'}^*(x', 0) \bar{\Omega}_{\bar{\beta}'\nu'}^*(y', 0) | 0 \rangle (\gamma_0 C)_{\bar{\alpha}'\alpha'} (\gamma_0 C)_{\bar{\beta}'\beta'} \\
&= (C\gamma_0)_{\alpha\bar{\alpha}} (C\gamma_0)_{\beta\bar{\beta}} \langle 0 | \Omega_{\bar{\alpha}\mu}(x, -t) \Omega_{\bar{\beta}\nu}(y, -t) \bar{\Omega}_{\bar{\alpha}'\mu'}(x', 0) \bar{\Omega}_{\bar{\beta}'\nu'}(y', 0) | 0 \rangle^* (\gamma_0 C)_{\bar{\alpha}'\alpha'} (\gamma_0 C)_{\bar{\beta}'\beta'} \\
&= (C\gamma_0)_{\alpha\bar{\alpha}} (C\gamma_0)_{\beta\bar{\beta}} \langle 0 | T \{ \bar{\Omega}_{\bar{\alpha}'\mu'}(x', 0) \bar{\Omega}_{\bar{\beta}'\nu'}(y', 0) \Omega_{\bar{\alpha}\mu}(x, -t) \Omega_{\bar{\beta}\nu}(y, -t) \} | 0 \rangle^* (\gamma_0 C)_{\bar{\alpha}'\alpha'} (\gamma_0 C)_{\bar{\beta}'\beta'} \\
&= (C\gamma_0)_{\alpha\bar{\alpha}} (C\gamma_0)_{\beta\bar{\beta}} G_{\alpha\beta\mu\nu; \alpha'\beta'\mu'\nu'}(x', y', x, y, -t)^* (\gamma_0 C)_{\bar{\alpha}'\alpha'} (\gamma_0 C)_{\bar{\beta}'\beta'}
\end{aligned} \tag{3.21}$$

In 4th line we used these relation as

$$\bar{\Omega}(x, t) = e^{tH} \Omega^\dagger(x) e^{-tH} \gamma_0 = (e^{-tH} \Omega(x) e^{tH})^\dagger \gamma_0 = \Omega^\dagger(x, -t) \gamma_0, \tag{3.22}$$

$$\Omega^T(x, t) = (e^{tH} \Omega(x) e^{-tH})^T = e^{-tH} \Omega^T(x) e^{tH} = (e^{-tH} \Omega^\dagger(x) \gamma_0 e^{tH} \gamma_0)^* = \bar{\Omega}^*(x, -t) \gamma_0. \tag{3.23}$$

As a results we can increase statistics, because we can calculate the 4-point correlator  $G_{\alpha\beta\mu\nu; \alpha'\beta'\mu'\nu'}(x, y, t, x', y')$  from back propagate  $G_{\alpha\beta\mu\nu; \alpha'\beta'\mu'\nu'}(x', y', x, y, -t)^*$ .

### 3.1.1 Quantum numbers of the two-Omega baryon system

We consider the quantum number with the Omega baryon as a local operator. This operator have the total spin( $S$ ), the orbital angular momentum( $L$ ), the total angular momentum( $J$ ). The two fermion state must change a sign under an exchange of them, while the asymptotic Omega-Omega state with given  $L$  and  $S$  has a factor  $(-1)^{S+L+1}$  by the exchange, so that we should have  $S + L = \text{even}$ . In table 3.1, we show the combination of  $L$  and  $S$  such as to reproduce the conserved quantum numbers  $J^P$  in QCD. For flavor structure, we consider only two-Omega baryon in initial and final state, because it doesn't couple another baryon in QCD. In this paper, we use the wall source, thus  $L = 0$  in source. We can construct only  $S = 0$  state, because symmetry of Omega operator and wall source. We show it in Appendix C. Hence we calculate only  $J^P = 0^+(L = 0, S = 0)$  in which the bound state is the most expected.

	$P = +$	$P = -$
$J = 0$	$^1S_0, ^5D_0$	$^3P_0, ^7F_0$
$J = 1$	$^5D_1$	$^3P_1, ^7F_1$
$J = 2$	$^5S_2, ^1D_2, ^5D_2, ^5G_2$	$^3P_2, ^7P_2, ^3F_2, ^7F_2, ^7H_2$
$J = 3$	$^5D_3, ^5G_3$	$^7P_3, ^3F_3, ^7F_3, ^7H_3$
$J = 4$	$^5D_4, ^1G_4, ^5G_4, ^5I_4$	$^7P_4, ^3F_4, ^7F_4, ^3H_4, ^7H_4, ^7K_4$

Table 3.1: Condition of the quantum number in Omega-Omega system. Set of S, L change each other in same cell, because Parity and J is conserved. It's taking into account constraints due to Pauli principle.

Let us consider the total spin and the angular momentum projection to the  $J^P = 0^+$  state. We first define spin 3/2 operator to perform total spin projection.

$$\Omega_{\frac{3}{2}, \frac{3}{2}} = -(\psi\Gamma_+\psi)\psi_{\frac{1}{2}} \quad (3.24)$$

$$\Omega_{\frac{3}{2}, \frac{1}{2}} = \frac{1}{\sqrt{3}}[\sqrt{2}(\psi\Gamma_Z\psi)\psi_{\frac{1}{2}} + (\psi\Gamma_+\psi)\psi_{-\frac{1}{2}}] \quad (3.25)$$

$$\Omega_{\frac{3}{2}, -\frac{1}{2}} = \frac{1}{\sqrt{3}}[\sqrt{2}(\psi\Gamma_Z\psi)\psi_{-\frac{1}{2}} + (\psi\Gamma_-\psi)\psi_{\frac{1}{2}}] \quad (3.26)$$

$$\Omega_{\frac{3}{2}, -\frac{3}{2}} = (\psi\Gamma_-\psi)\psi_{-\frac{1}{2}} \quad (3.27)$$

where  $\Gamma_{\pm} \equiv \frac{1}{2}(C\gamma^2 \pm iC\gamma^1)$ ,  $\Gamma_Z \equiv \frac{-i}{\sqrt{2}}C\gamma^3$  are spin 1 di-quark operator, in non-relativistic limit. Linear combining single-Omega operator, we construct spin 3, spin 2, spin 1, spin 0 states of two-Omega. These state is given by

$$(\Omega\Omega)_{3,0} = \frac{1}{\sqrt{20}}(\Omega_{\frac{3}{2}, \frac{3}{2}}\Omega_{\frac{3}{2}, -\frac{3}{2}} + 3\Omega_{\frac{3}{2}, \frac{1}{2}}\Omega_{\frac{3}{2}, -\frac{1}{2}} + 3\Omega_{\frac{3}{2}, -\frac{1}{2}}\Omega_{\frac{3}{2}, \frac{1}{2}} + \Omega_{\frac{3}{2}, -\frac{3}{2}}\Omega_{\frac{3}{2}, \frac{3}{2}}), \quad (3.28)$$

$$(\Omega\Omega)_{2,0} = \frac{1}{2}(\Omega_{\frac{3}{2}, \frac{3}{2}}\Omega_{\frac{3}{2}, -\frac{3}{2}} + \Omega_{\frac{3}{2}, \frac{1}{2}}\Omega_{\frac{3}{2}, -\frac{1}{2}} - \Omega_{\frac{3}{2}, -\frac{1}{2}}\Omega_{\frac{3}{2}, \frac{1}{2}} - \Omega_{\frac{3}{2}, -\frac{3}{2}}\Omega_{\frac{3}{2}, \frac{3}{2}}), \quad (3.29)$$

$$(\Omega\Omega)_{1,0} = \frac{1}{\sqrt{20}}(3\Omega_{\frac{3}{2}, \frac{3}{2}}\Omega_{\frac{3}{2}, -\frac{3}{2}} - \Omega_{\frac{3}{2}, \frac{1}{2}}\Omega_{\frac{3}{2}, -\frac{1}{2}} - \Omega_{\frac{3}{2}, -\frac{1}{2}}\Omega_{\frac{3}{2}, \frac{1}{2}} + 3\Omega_{\frac{3}{2}, -\frac{3}{2}}\Omega_{\frac{3}{2}, \frac{3}{2}}), \quad (3.30)$$

$$(\Omega\Omega)_{0,0} = \frac{1}{2}(\Omega_{\frac{3}{2}, \frac{3}{2}}\Omega_{\frac{3}{2}, -\frac{3}{2}} - \Omega_{\frac{3}{2}, \frac{1}{2}}\Omega_{\frac{3}{2}, -\frac{1}{2}} + \Omega_{\frac{3}{2}, -\frac{1}{2}}\Omega_{\frac{3}{2}, \frac{1}{2}} - \Omega_{\frac{3}{2}, -\frac{3}{2}}\Omega_{\frac{3}{2}, \frac{3}{2}}). \quad (3.31)$$

We derive it Appendix D.

Secondly, we consider a projection of orbital angular momentum using cubic group which show Appendix E. we employ the cubic group projection defined by

$$P_\nu^a = \frac{d_a}{g} \sum_i^g D_{\nu\nu}^a(R_i)^* R_i, \quad (3.32)$$

where  $a$  represents an irreducible representation of the cubic group, whose dimension is  $d_a$ ,  $R_i$  is an element of the cubic group and acts on  $\vec{r}$  the sink operator.  $D^a(R_i)$  is the corresponding matrix in the irreducible representation acting on spin components, and  $g$  is the order of the cubic group. We use  $A_1$  corresponding the  $L = 0$  and the  $L = 4$  state, but the  $L = 4$  component is small.

### 3.2 2pt-correlator and 4pt-correlator in Omega-Omega system.

We show wick contraction of the Omega-Omega system for calculating the effective mass and NBS wave function. We need mass information to calculate Potential Eq. (2.59). We need 2pt-correlator to measure the effective mass in Eq. (2.28). The Omega baryon operator and the anti-Omega baryon operator is defined as

$$\Omega_{k_1 g}(x) \equiv \varepsilon^{c_1 c_2 c_3} \delta_{g_3 g} (C \gamma_{k_1})_{g_1 g_2} s_{g_1}^{c_1}(x) s_{g_2}^{c_2}(x) s_{g_3}^{c_3}(x) \quad (3.33)$$

,

$$\bar{\Omega}_{k_1 g}(x) \equiv -\varepsilon^{c_3 c_2 c_1} \delta_{g_3 g} (\gamma_{k_1} C)_{g_2 g_1} \bar{s}_{g_3}^{c_3}(x) \bar{s}_{g_2}^{c_2}(x) \bar{s}_{g_1}^{c_1}(x) \quad (3.34)$$

So 2pt time correlator is given as

$$\begin{aligned} G(t) &= - \sum_x \langle \Omega_{k g}(t, x) \bar{\Omega}_{k' g'}(0, 0) \rangle \\ &= \sum_x \varepsilon^{c_1 c_2 c_3} \varepsilon^{c'_3 c'_2 c'_1} \delta_{g_3 g} \delta_{g'_3 g'} (C \gamma_{k_1})_{g_1 g_2} (\gamma_{k'_1} C)_{g'_2 g'_1} \left\langle s_{g_1}^{c_1}(x) s_{g_2}^{c_2}(x) s_{g_3}^{c_3}(x) \bar{s}_{g'_3}^{c'_3}(0) \bar{s}_{g'_2}^{c'_2}(0) \bar{s}_{g'_1}^{c'_1}(0) \right\rangle, \end{aligned} \quad (3.35)$$

where factor  $-1$  which does not contribute the physics is the definition of the anti-Omega operator. We define  $s(\xi_1) \equiv s_{g_1}^{c_1}(x)$  and  $\bar{s}(\xi'_1) \equiv \bar{s}_{g'_1}^{c'_1}(0)$ . We calculate the bracket part

$$\begin{aligned} \left\langle s_{g_1}^{c_1}(x) s_{g_2}^{c_2}(x) s_{g_3}^{c_3}(x) \bar{s}_{g'_3}^{c'_3}(0) \bar{s}_{g'_2}^{c'_2}(0) \bar{s}_{g'_1}^{c'_1}(0) \right\rangle &= \langle s(\xi_1) s(\xi_2) s(\xi_3) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \rangle \\ &= \langle s(\xi_1) \bar{s}(\xi'_1) \rangle \langle s(\xi_2) \bar{s}(\xi'_2) \rangle \langle s(\xi_3) \bar{s}(\xi'_3) \rangle \\ &\quad - \langle s(\xi_1) \bar{s}(\xi'_1) \rangle \langle s(\xi_2) \bar{s}(\xi'_3) \rangle \langle s(\xi_3) \bar{s}(\xi'_2) \rangle \\ &\quad - \langle s(\xi_1) \bar{s}(\xi'_2) \rangle \langle s(\xi_2) \bar{s}(\xi'_1) \rangle \langle s(\xi_3) \bar{s}(\xi'_3) \rangle \\ &\quad + \langle s(\xi_1) \bar{s}(\xi'_2) \rangle \langle s(\xi_2) \bar{s}(\xi'_3) \rangle \langle s(\xi_3) \bar{s}(\xi'_1) \rangle \\ &\quad + \langle s(\xi_1) \bar{s}(\xi'_3) \rangle \langle s(\xi_2) \bar{s}(\xi'_1) \rangle \langle s(\xi_3) \bar{s}(\xi'_2) \rangle \\ &\quad - \langle s(\xi_1) \bar{s}(\xi'_3) \rangle \langle s(\xi_2) \bar{s}(\xi'_2) \rangle \langle s(\xi_3) \bar{s}(\xi'_1) \rangle \end{aligned} \quad (3.36)$$

Finally we get 2pt-correlator as

$$\begin{aligned} G(t) &= \sum_x \varepsilon^{c_1 c_2 c_3} \varepsilon^{c'_3 c'_2 c'_1} \delta_{g_3 g} \delta_{g'_3 g'} (C \gamma_{k_1})_{g_1 g_2} (\gamma_{k'_1} C)_{g'_2 g'_1} \\ &\quad [\langle s(\xi_1) \bar{s}(\xi'_1) \rangle (\langle s(\xi_2) \bar{s}(\xi'_2) \rangle \langle s(\xi_3) \bar{s}(\xi'_3) \rangle - \langle s(\xi_2) \bar{s}(\xi'_3) \rangle \langle s(\xi_3) \bar{s}(\xi'_2) \rangle) \\ &\quad + \langle s(\xi_1) \bar{s}(\xi'_2) \rangle (-\langle s(\xi_2) \bar{s}(\xi'_1) \rangle \langle s(\xi_3) \bar{s}(\xi'_3) \rangle + \langle s(\xi_2) \bar{s}(\xi'_3) \rangle \langle s(\xi_3) \bar{s}(\xi'_1) \rangle)) \\ &\quad + \langle s(\xi_1) \bar{s}(\xi'_3) \rangle (\langle s(\xi_2) \bar{s}(\xi'_1) \rangle \langle s(\xi_3) \bar{s}(\xi'_2) \rangle - \langle s(\xi_2) \bar{s}(\xi'_2) \rangle \langle s(\xi_3) \bar{s}(\xi'_1) \rangle)]. \end{aligned} \quad (3.37)$$

where  $\langle s(\xi)\bar{s}(\xi') \rangle$  is the quark propagator from 0 to  $x$ . In this way, we can calculate the 2pt-correlator quark propagators are given.

Next we consider 4pt-correlator defined as

$$\begin{aligned}
W_{\alpha k_1 \beta k_2, \beta' k'_2 \alpha' k'_1}(r) &\equiv \sum_x \left\langle \Omega_{\alpha k_1}(x+r) \Omega_{\beta k_2}(x) \bar{\Omega}_{\beta k'_2} \bar{\Omega}_{\alpha' k'_1} \right\rangle \\
&= \sum_x \left\langle \Omega_{\alpha k_1}(x+r) \Omega_{\beta k_2}(x) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \right\rangle \\
&\quad \epsilon^{c'_4 c'_5 c'_6} \epsilon^{c'_1 c'_2 c'_3} \delta_{\alpha' g'_3} \delta_{\beta' g'_6} (\gamma_{k'_1} C)_{g'_2 g'_1} (\gamma_{k'_2} C)_{g'_5 g'_4}
\end{aligned} \tag{3.38}$$

We calculate the bracket part as

$$\begin{aligned}
&\langle \Omega_{\alpha k_1}(x+r) \Omega_{\beta k_2}(x) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \rangle \\
&= \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_6) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_1) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_5) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_2) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_1) \bar{s}(\xi'_5) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_2) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \bar{s}(\xi'_5) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \\
&- \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_2) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_5) \bar{s}(\xi'_1) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_1) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_6) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_5) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_4) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_2) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_2) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_1) \bar{s}(\xi'_5) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_5) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \bar{s}(\xi'_6) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_6) \bar{s}(\xi'_4) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \bar{s}(\xi'_5) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_3) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \bar{s}(\xi'_4) \rangle \\
&+ \langle \Omega_{\alpha k_1}(x+r) \bar{s}(\xi'_2) \bar{s}(\xi'_6) \bar{s}(\xi'_5) \rangle \langle \Omega_{\beta k_2}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_1) \bar{s}(\xi'_4) \rangle,
\end{aligned} \tag{3.39}$$

where  $\langle \Omega(x) \bar{s}(\xi') \bar{s}(\xi') \bar{s}(\xi') \rangle$  is called “sub diagram” which is calculated

$$\begin{aligned}
\langle \Omega_{\alpha k_1}(x) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \rangle &= \varepsilon^{c_1 c_2 c_3} (C \gamma_{k_1})_{g_1 g_2} \delta_{\alpha g_3} \langle s(\xi_1) s(\xi_2) s(\xi_3) \bar{s}(\xi'_3) \bar{s}(\xi'_2) \bar{s}(\xi'_1) \rangle \\
&= \varepsilon^{c_1 c_2 c_3} (C \gamma_{k_1})_{g_1 g_2} \delta_{\alpha g_3} \\
&\quad [\langle s(\xi_1) \bar{s}(\xi'_1) \rangle \langle s(\xi_2) \bar{s}(\xi'_2) \rangle \langle s(\xi_3) \bar{s}(\xi'_3) \rangle \\
&\quad - \langle s(\xi_1) \bar{s}(\xi'_1) \rangle \langle s(\xi_2) \bar{s}(\xi'_3) \rangle \langle s(\xi_3) \bar{s}(\xi'_2) \rangle \\
&\quad - \langle s(\xi_1) \bar{s}(\xi'_2) \rangle \langle s(\xi_2) \bar{s}(\xi'_1) \rangle \langle s(\xi_3) \bar{s}(\xi'_3) \rangle \\
&\quad + \langle s(\xi_1) \bar{s}(\xi'_2) \rangle \langle s(\xi_2) \bar{s}(\xi'_3) \rangle \langle s(\xi_3) \bar{s}(\xi'_1) \rangle \\
&\quad + \langle s(\xi_1) \bar{s}(\xi'_3) \rangle \langle s(\xi_2) \bar{s}(\xi'_1) \rangle \langle s(\xi_3) \bar{s}(\xi'_2) \rangle \\
&\quad - \langle s(\xi_1) \bar{s}(\xi'_3) \rangle \langle s(\xi_2) \bar{s}(\xi'_2) \rangle \langle s(\xi_3) \bar{s}(\xi'_1) \rangle].
\end{aligned} \tag{3.40}$$

The 4pt correlator has 6 s-quarks at sink and 6  $\bar{s}$ -quarks at source, thus the number of the contraction is  $6! = 720$ , Using the symmetry of the quarks in sub diagrams, we can reduce the number of the contraction  $6!/(3!3!) = 20$ . Due to this, there is 20 terms in Eq. (3.39).

For reduction of the computational cost, we consider momentum space using Fourier transform. We note that we used FFTW library which is very fast using the butterfly computation in our simulation.

$$f(x) = \frac{1}{V} \sum_q \tilde{f}(q) e^{iq \cdot x} \tag{3.41}$$

$$\tilde{f}(q) = \sum_x f(x) e^{-iq \cdot x} \tag{3.42}$$

We can remove sum of  $x$  in the 4pt-correlator as

$$\begin{aligned}
W(r) &\equiv \sum_x f(x+r) g(x) \\
&= \sum_x \frac{1}{V^2} \sum_q \sum_k \tilde{f}(q) e^{iq(x+r)} \tilde{g}(k) e^{ikx} \\
&= \frac{1}{V} \sum_q \sum_k \tilde{f}(q) \tilde{g}(k) e^{iqr} \delta(q+k) \\
&= \frac{1}{V} \sum_q \tilde{f}(q) \tilde{g}(-q) e^{iqr}.
\end{aligned} \tag{3.43}$$

As a results, we perform follow step for calculate the NBS wave function.

- calculate quark propagator
- contracted sub diagrams at sink part
- Fourier transform of sub diagrams
- contracted diagram at source part
- inverse Fourier transform of diagrams

Finally we show the contraction of the diagram in source part in Fig. 3.1 and Fig. 3.2.

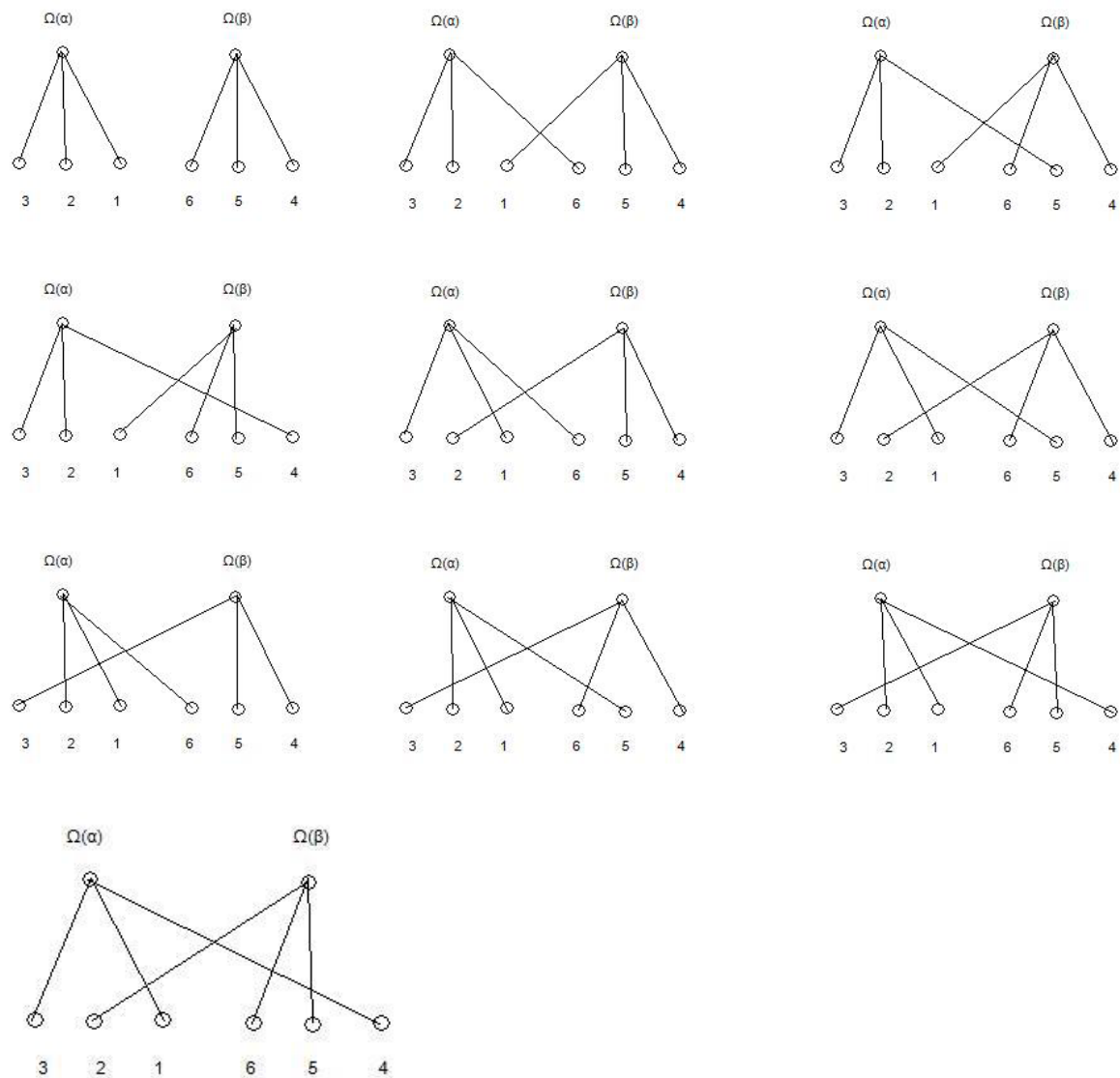


Figure 3.1: Diagram of the Omega-Omega system at the first half of part.



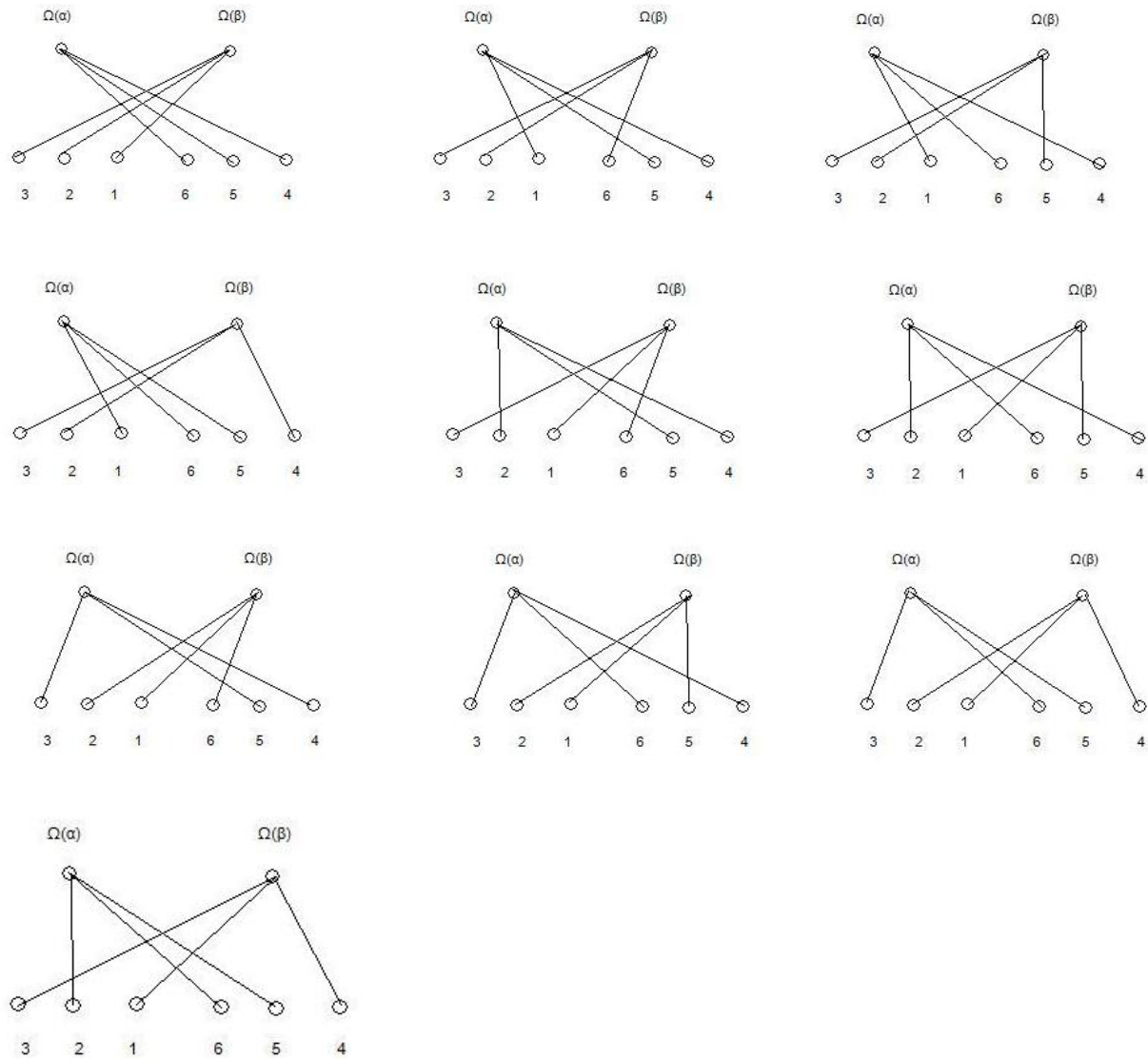


Figure 3.2: Diagram of the Omega-Omega system at the second half of part.

## Chapter 4

# Okubo-marshark decomposition

We derive the general form of the baryon-baryon potential. There are several symmetries of the potential.

- Because of Probability conservation, potential have hermitian symmetry.  $V^\dagger = V$
- Energy-momentum conservation. Energy conservation demand that the potential does not depend on time. Momentum conservation deduce the translation invariance of potential.
- Galilei invariance. We can use the center of mass momentum of the two-body system.

This is a general form of potential used translational symmetry and Galilei invariance

$$V_{\alpha'\beta':\alpha\beta}(\vec{r}, \vec{v}), \quad (4.1)$$

where  $\vec{r} = \vec{r}_1 - \vec{r}_2$ ,  $\vec{v} = \vec{v}_1 - \vec{v}_2$ .

- Flavor symmetry. For example  $8 \otimes 8 = 27 \oplus 10 \oplus \bar{10} \oplus 8$ ,  $10 \otimes 8 = 35 \oplus 8 \oplus 10 \oplus 27$ ,  $10 \otimes 10 = 28 \oplus 27 \oplus 35 \oplus \bar{10}$

$$V_{\alpha'\beta':\alpha\beta}(\vec{r}, \vec{v}, \vec{S}_1, \vec{S}_2) = \sum_R V^{(R)}(\vec{r}, \vec{v}, \vec{S}_1, \vec{S}_2) \cdot P_{\alpha'\beta':\alpha\beta}^{(R)}, \quad (4.2)$$

where  $P_{\alpha'\beta':\alpha\beta}^{(R)}$  is projection matrix onto irreducible representation  $R$ ,  $\alpha, \beta$  are spin indices.

- T-symmetry.  $x \longleftrightarrow x$ ,  $p \longleftrightarrow -p$ ,  $S \longleftrightarrow -S$
- P-symmetry.  $x \longleftrightarrow -x$ ,  $p \longleftrightarrow -p$ ,  $S \longleftrightarrow S$
- Rotation symmetry. We consider rotation symmetry

$$V_{\alpha'\beta':\alpha\beta}(\vec{r}_1, \vec{r}_2, \vec{v}_1, \vec{v}_2) = U_{\alpha'\bar{\alpha}'}(g)U_{\beta'\bar{\beta}'}(g)V_{\bar{\alpha}'\bar{\beta}':\bar{\alpha}\bar{\beta}}(g^{-1}\vec{r}_1, g^{-1}\vec{r}_2, g^{-1}\vec{v}_1, g^{-1}\vec{v}_2)U_{\bar{\alpha}\alpha}(g^{-1})U_{\bar{\beta}\beta}(g^{-1}), \quad (4.3)$$

where  $\alpha, \beta, \alpha', \beta'$  is spinor indices and  $U(g)$  is representation matrix for  $\text{spin}\frac{1}{2}$  and  $\text{spin}\frac{3}{2}$  for  $g \in SO(3)$ .

- Particle exchange  $x \longleftrightarrow -x$ ,  $p \longleftrightarrow -p$ ,  $S_1 \longleftrightarrow S_2$ , if we consider a potential between same particles.

The potential is constrained by theses conditions.

## 4.1 Octet-Octet baryon

Okubo and Marshak derived the general form of the octet-octet baryon potential in the space of the two-component spinors. It's derived by [29].

## 4.2 Decuplet-Decuplet baryon

In this chapter we derive the Okubo-Marshak decomposition for decuplet-decuplet system. Note that we show general form of potentials except 6th order 3rd and 4th term, Considering only 0th order of derivative expansion.

As a strategy, we make  $SU(2)$  matrix for spin  $\frac{3}{2}$ . Because of  $4 \times 4$  matrix, We need 16 linearly independent bases.

$$B^{(0)}, B^{(1)}, \dots, B^{(15)} \quad (4.4)$$

We can decompose spin of the potential by using these bases

$$V_{\alpha'\beta':\alpha\beta} = \sum_{i,j=0}^{15} V^{(i,j)} B_{\alpha'\alpha}^{(i)} B_{\beta'\beta}^{(j)} \quad (4.5)$$

$SU(2)$  matrix for spin  $\frac{3}{2}$

$$S^1 = \frac{1}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \quad S^2 = \frac{1}{2} \begin{pmatrix} 0 & -i\sqrt{3} & 0 & 0 \\ i\sqrt{3} & 0 & -2i & 0 \\ 0 & 2i & 0 & -i\sqrt{3} \\ 0 & 0 & i\sqrt{3} & 0 \end{pmatrix}$$

$$S^3 = \frac{1}{2} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \quad (4.6)$$

These matrix satisfy this commutation relation as

$$[S^i, S^j] = i\varepsilon^{ijk} S^k. \quad (4.7)$$

We make non-abelian traceless symmetric tensor for  $SU(2)$

$$P^{(0)}(\vec{S}) \equiv 1, \quad (4.8)$$

$$P_i^{(1)}(\vec{S}) \equiv S_i, \quad (4.9)$$

$$P_{ij}^{(2)}(\vec{S}) \equiv \frac{1}{2}\{S_i, S_j\} - \frac{1}{3}S^2\delta_{ij}, \quad (4.10)$$

$$P_{ijk}^{(3)}(\vec{S}) \equiv A_{ijk} - \frac{2}{15}B_{ijk} - \frac{1}{15}C_{ijk}$$

$$= A_{ijk} + \frac{1-3\vec{S}^2}{15}(\delta_{ij}S_k + \delta_{ik}S_j + \delta_{jk}S_i), \quad (4.11)$$

where

$$A^{ijk} \equiv \frac{1}{3!}(S^i S^j S^k + S^i S^k S^j + S^j S^i S^k + S^j S^k S^i + S^k S^i S^j + S^k S^j S^i) \quad (4.12)$$

$$B^{ijk} \equiv \vec{S}^2(\delta^{ij} \cdot S^k + \delta^{ik} \cdot S^j + \delta^{jk} \cdot S^i), \quad (4.13)$$

$$C^{ijk} \equiv \sum_{l=1}^3 (\delta^{ij} S^l S^k S^l + \delta^{ik} S^l S^j S^l + \delta^{jk} S^l S^i S^l). \quad (4.14)$$

Theses are base of Spherical harmonics which show Appendix F.

We can check traceless. Traceless of  $P_i^{(1)}$  is trivial.

$P_{ij}^{(2)}$  is satisfied

$$\delta_{ij} P_{ij}^{(2)} = \delta_{ij} \left( \frac{1}{2} \{S_i, S_j\} - \frac{1}{3} S^2 \delta_{ij} \right) = 0 \quad (4.15)$$

$P_{ijk}^{(3)}$  is satisfied

$$\delta_{ij} P_{ijk}^{(3)}(\vec{S}_2) = 0 \quad (4.16)$$

We check it.

$$\begin{aligned} \delta_{ij} P_{ijk}^{(3)}(\vec{S}_2) &= \delta_{ij} \left( A^{ijk} + \frac{1 - 3\vec{S}_2^2}{15} (\delta^{ij} S_2^k + \delta^{ik} S_2^j + \delta^{jk} S_2^i) \right) \\ &= A^{ijk} + \frac{1 - 3\vec{S}_2^2}{3} S_2^k \end{aligned} \quad (4.17)$$

$$A_{iik} \equiv \frac{1}{3!} (4S^2 S_k + 2S_i S_k S_i) = \frac{1}{3!} (4S^2 S_k + 2(S^2 - 1)S_k) = -\frac{1}{3} (1 - 3S^2) S_k \quad (4.18)$$

So Eq. (4.16) is satisfied.

Therefore these are traceless.  $S_i$  is satisfied

$$U(g) S_i U(g^{-1}) = R_{ij}(g) S_j. \quad (4.19)$$

Therefore  $P$  is transformed as

$$U(g) P^{(0)} U(g^{-1}) = P^{(0)}, \quad (4.20)$$

$$U(g) P_i^{(1)} U(g^{-1}) = R_{ii'}(g) P_{i'}^{(1)}, \quad (4.21)$$

$$U(g) P_{ij}^{(2)} U(g^{-1}) = R_{ii'}(g) R_{jj'}(g) P_{i'j'}^{(2)}, \quad (4.22)$$

$$U(g) P_{ijk}^{(3)} U(g^{-1}) = R_{ii'}(g) R_{jj'}(g) R_{kk'}(g) P_{i'j'k'}^{(3)}. \quad (4.23)$$

The potential is imposed a rotation symmetry by using scalar product about spin indices  $i, j$

$$V_{\alpha'\beta':\alpha\beta}(\vec{r}, \vec{v}, \vec{S}_1, \vec{S}_2) = \sum_{n,m=0} V_{i_1, \dots, i_n; j_1, \dots, j_m}^{(n,m)}(\vec{r}, \vec{v}) \cdot (P_{i_1, \dots, i_n}^{(n)}(\vec{S}_1)) (P_{j_1, \dots, j_m}^{(m)}(\vec{S}_2)). \quad (4.24)$$

Origin of the spin indices in the  $V_{i_1, \dots, i_n; j_1, \dots, j_m}^{(n,m)}(\vec{r}, \vec{v})$  are  $r_i$  and  $\nabla_i$ . Finally, the potential have rotational symmetry, because right hand side is scalar.

These 16matrices are linear independence

- 0-order: 1 matrix

$$P^{(0)} \quad (4.25)$$

- 1st-order: 3 matrices

$$P_1^{(1)}, P_2^{(1)}, P_3^{(1)} \quad (4.26)$$

- 2nd-order: 5 matrices

$$P_{12}^{(2)}, P_{23}^{(2)}, P_{31}^{(2)}, P_{11}^{(2)}, P_{22}^{(2)} \quad (4.27)$$

- 3rd-order: 7 matrices

$$P_{123}^{(3)}, P_{112}^{(3)}, P_{113}^{(3)}, P_{221}^{(3)}, P_{223}^{(3)}, P_{331}^{(3)}, P_{332}^{(3)} \quad (4.28)$$

It is not enough, however in these 16 matrices. Since we decompose the  $r$  dependent part, we need up to 6th-order abelian traceless symmetric tensor for scalar product. We know traceless symmetric tensors are base of the spherical harmonics which show Appendix F, therefore we can decompose the  $r$  dependent part using the traceless symmetric tensors.

- 4th-order:

$$P_{ijkl}^{(4)}(r) = (r_i r_j r_k r_l - \frac{\vec{r}^2}{7} (r_i r_j \delta_{kl} + r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik} + r_k r_l \delta_{ij})) + \frac{\vec{r}^4}{35} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (4.29)$$

5th-order is not used, because order of spin is only even, but we show

- 5th-order:

$$\begin{aligned} P_{ijkmn}^{(5)}(r) = & (r_i r_j r_k r_m r_n \\ & - \frac{1}{9} (r_i r_j r_k \delta_{mn} + r_i r_j r_m \delta_{kn} + r_i r_k r_m \delta_{jn} + r_j r_k r_m \delta_{in} + r_i r_j r_n \delta_{km} \\ & + r_i r_k r_n \delta_{jm} + r_j r_k r_n \delta_{im} + r_i r_m r_n \delta_{jk} + r_j r_m r_n \delta_{ik} + r_k r_m r_n \delta_{ij}) \\ & + \frac{1}{63} (r_i [\delta_{ij} \delta_{mn} + \delta_{jm} \delta_{kn} + \delta_{jn} \delta_{km}] + r_j [\delta_{ik} \delta_{mn} + \delta_{im} \delta_{kn} + \delta_{in} \delta_{km}] + r_k [\delta_{ij} \delta_{mn} + \delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}] \\ & + r_m [\delta_{ji} \delta_{kn} + \delta_{ik} \delta_{jn} + \delta_{in} \delta_{jk}] + r_n [\delta_{ij} \delta_{km} + \delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk}]) \end{aligned} \quad (4.30)$$

- 6th-order:

$$\begin{aligned}
P_{ijk mnl}^{(6)}(\vec{r}) &= r_i r_j r_k r_m r_n r_l \\
&- \frac{1}{11} \{ r_i r_j r_k r_m \delta_{nl} + r_i r_j r_k r_n \delta_{ml} + r_i r_j r_m r_n \delta_{kl} + r_i r_k r_m r_n \delta_{jl} + r_j r_k r_m r_n \delta_{il} \\
&+ r_i r_l r_k r_l \delta_{mn} + r_i r_j r_m r_l \delta_{kn} + r_i r_k r_m r_l \delta_{jn} + r_j r_k r_m r_l \delta_{in} + r_i r_j r_n r_l \delta_{km} \\
&+ r_i r_k r_n r_l \delta_{jm} + r_j r_k r_n r_l \delta_{im} + r_i r_m r_n r_l \delta_{jk} + r_j r_m r_n r_l \delta_{ik} + r_k r_m r_n r_l \delta_{ij} \} \\
&+ \frac{1}{99} (r_i r_j \delta_{km} \delta_{nl} + r_i r_j \delta_{kn} \delta_{ml} + r_i r_j \delta_{mn} \delta_{kl} + r_i r_k \delta_{jm} \delta_{nl} + r_i r_k \delta_{jn} \delta_{ml} \\
&+ r_i r_k \delta_{mn} \delta_{jl} + r_i r_m \delta_{jk} \delta_{nl} + r_i r_m \delta_{jn} \delta_{kl} + r_i r_m \delta_{kn} \delta_{jl} + r_i r_n \delta_{jk} \delta_{ml} \\
&+ r_i r_n \delta_{jm} \delta_{kl} + r_i r_n \delta_{km} \delta_{jl} + r_i r_l \delta_{jk} \delta_{mn} + r_i r_l \delta_{jm} \delta_{kn} + r_i r_l \delta_{km} \delta_{jn} \\
&+ r_j r_m \delta_{kn} \delta_{il} + r_j r_n \delta_{ik} \delta_{ml} + r_j r_n \delta_{im} \delta_{kl} + r_j r_n \delta_{km} \delta_{il} + r_j r_l \delta_{ik} \delta_{mn} \\
&+ r_j r_l \delta_{im} \delta_{kn} + r_j r_l \delta_{km} \delta_{in} + r_k r_m \delta_{ij} \delta_{nl} + r_k r_m \delta_{in} \delta_{jl} + r_k r_m \delta_{jn} \delta_{il} \\
&+ r_k r_n \delta_{ij} \delta_{ml} + r_k r_m \delta_{im} \delta_{jl} + r_k r_n \delta_{jm} \delta_{il} + r_k r_l \delta_{ij} \delta_{mn} + r_k r_l \delta_{im} \delta_{jn} \\
&+ r_k r_l \delta_{jm} \delta_{in} + r_m r_n \delta_{ij} \delta_{kl} + r_m r_n \delta_{ik} \delta_{jl} + r_m r_n \delta_{jk} \delta_{il} + r_m r_l \delta_{ij} \delta_{kn} \\
&+ r_m r_l \delta_{ik} \delta_{jn} + r_m r_l \delta_{jk} \delta_{in} + r_n r_l \delta_{ij} \delta_{km} + r_n r_l \delta_{ik} \delta_{jm} + r_n r_l \delta_{jk} \delta_{im} \\
&- \frac{1}{693} (\delta_{ij} \delta_{km} \delta_{nl} + \delta_{ij} \delta_{kn} \delta_{ml} + \delta_{ij} \delta_{mn} \delta_{kl} + \delta_{ik} \delta_{jm} \delta_{nl} + \delta_{ik} \delta_{jn} \delta_{ml} \\
&+ \delta_{ik} \delta_{mn} \delta_{jl} + \delta_{jk} \delta_{im} \delta_{nl} + \delta_{im} \delta_{jn} \delta_{kl} + \delta_{im} \delta_{kn} \delta_{jl} + \delta_{jk} \delta_{in} \delta_{ml} \\
&+ \delta_{jm} \delta_{in} \delta_{kl} + \delta_{km} \delta_{in} \delta_{jl} + \delta_{jk} \delta_{il} \delta_{mn} + \delta_{jm} \delta_{il} \delta_{kn} + \delta_{km} \delta_{il} \delta_{jn})
\end{aligned} \tag{4.31}$$

These have useful reduction formula as

$$\begin{aligned}
S^i S^j S^i &= ([S^i, S^j] + S^j S^i) S^i \\
&= (i \varepsilon^{ijk} S^k + S^j S^i) S^i \\
&= \frac{1}{2} i \varepsilon^{ijk} [S^k, S^i] + S^j S^2 \\
&= \frac{1}{2} i i \varepsilon^{ijk} \varepsilon^{kil} S^l + S^j S^2 \\
&= -\delta_{jl} S^l + S^j S^2 \\
&= (\vec{S}^2 - 1) S^j.
\end{aligned} \tag{4.32}$$

Now that we are ready, we start to decompose a potential between decuplet baryon and decuplet baryon.

- Polynominal-degrees of spin matrices = 0, 2, 4, 6, because of T-symmetry.

$$x \rightarrow -x, \quad p \rightarrow -p \quad S \rightarrow -S \quad i \rightarrow -i \tag{4.33}$$

- Potential have symmetry of  $S_1 \longleftrightarrow S_2$ , if we consider a potential between same particles. Now we consider  $\Omega - \Omega$  system. Because of spatial reflection and particle exchange.

$$x \rightarrow x, \quad p \rightarrow p \quad S_1 \rightarrow S_2 \tag{4.34}$$

- Possible forms of potentials can be expressed as products of spin-matrix structure and coordinate function structure, because a potential have rotational symmetry.

$$V_{\alpha'\beta':\alpha\beta}(\vec{r}, \vec{v}, \vec{S}_1, \vec{S}_2) = \sum_{n,m=0} V_{i_1, \dots, i_n; j_1, \dots, j_m}^{(n,m)}(\vec{r}, \vec{v}) \cdot (P_{i_1, \dots, i_n}^{(n)}(\vec{S}_1))(P_{j_1, \dots, j_m}^{(m)}(\vec{S}_2)) \quad (4.35)$$

order(index)	spin-matrix	coordinate function
0	$\frac{1}{2}(P^{(0)}(\vec{S}_1) + P^{(0)}(\vec{S}_2))$	$V_C(r)$
2(i,j)	$\frac{1}{2}(P_i^{(1)}(\vec{S}_1)P_j^{(1)}(\vec{S}_2) + P_i^{(1)}(\vec{S}_2)P_j^{(1)}(\vec{S}_1))$	$V_{C_2}(r)\delta_{ij}$
	$\frac{1}{2}(P_{ij}^{(2)}(\vec{S}_1) + P_{ij}^{(2)}(\vec{S}_2))$	$V_T(r)P_{ij}^{(2)}(\vec{r})$
4(i,j,k,l)	$\frac{1}{2}(P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2) + P_{ij}^{(2)}(\vec{S}_2)P_{kl}^{(2)}(\vec{S}_1))$	$V_{C_4}(r)\delta_{ij}\delta_{kl}$
	$\frac{1}{2}(P_{ijk}^{(3)}(\vec{S}_1)P_l^{(1)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2)P_l^{(1)}(\vec{S}_1))$	$V_{T_4}(r)P_{ij}^{(2)}(\vec{r})\delta_{kl}$
		$V_Q(r)P_{ijkl}^{(4)}(\vec{r})$
6(i,j,k,l,m,n)	$\frac{1}{2}(P_{ijk}^{(3)}(\vec{S}_1)P_{lmn}^{(3)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2)P_{lmn}^{(3)}(\vec{S}_1))$	$V_{C_6}(r)\delta_{ij}\delta_{kl}\delta_{mn}$
		$V_{T_6}(r)P_{ij}^{(2)}(\vec{r})\delta_{kl}\delta_{mn}$
		$V_{Q_6}(r)P_{ijkl}^{(4)}(\vec{r})\delta_{mn}$
		$V_H(r)P_{ijklmn}^{(6)}(\vec{r})$

where upper index is spin-order and lower index is spacial index.

- Specific system for 0th order is

$$\frac{1}{2}(P^{(0)}(\vec{S}_1) + P^{(0)}(\vec{S}_2))V_C(r) = V_C(r). \quad (4.36)$$

- In 2nd order, 1st one is

$$\begin{aligned} & \frac{1}{2}\{\delta_{ij}\}\{P_i^{(1)}(\vec{S}_1)P_j^{(1)}(\vec{S}_2) + P_i^{(1)}(\vec{S}_2)P_j^{(1)}(\vec{S}_1)\}V_{C_2}(r) \\ & = S_1 \cdot S_2 V_{C_2}(r). \end{aligned} \quad (4.37)$$

- In 2nd order, 2nd one is

$$\begin{aligned} & \frac{1}{2}P_{ij}^{(2)}(\vec{r})(P_i^{(1)}(\vec{S}_1)P_j^{(1)}(\vec{S}_2) + P_i^{(1)}(\vec{S}_2)P_j^{(1)}(\vec{S}_1))V_T(r) \\ & = \frac{1}{2}(r_i r_j - \frac{r^2}{3}\delta_{ij})(S_1^i S_2^j + S_2^i S_1^j)V_T(r) \\ & = ((S_1 \cdot r)(S_2 \cdot r) - \frac{r^2}{3}S_1 \cdot S_2)V_T(r). \end{aligned} \quad (4.38)$$

- In 2nd order, 3rd one is

$$\frac{1}{2}P_{ij}^{(2)}(\vec{r})(P_{ij}^{(2)}(\vec{S}_1) + P_{ij}^{(2)}(\vec{S}_2))V_T(r)$$

$$\begin{aligned}
&= (r_i r_j - \frac{r^2}{3} \delta_{ij}) (\frac{1}{2} \{S_1^i, S_1^j\} - \frac{\delta_{ij}}{3} \vec{S}_1^2 + \frac{1}{2} \{S_2^i, S_2^j\} - \frac{\delta_{ij}}{3} \vec{S}_2^2) V_T(r) \\
&= (r_i r_j - \frac{r^2}{3} \delta_{ij}) (\frac{1}{2} \{S_1^i, S_1^j\} - \frac{\delta_{ij}}{3} \vec{S}_1^2 + \frac{1}{2} \{S_2^i, S_2^j\} - \frac{\delta_{ij}}{3} \vec{S}_2^2) V_T(r) \\
&= ((\vec{r} \cdot \vec{S}_1)^2 - \frac{\vec{r}^2}{3} \vec{S}_1^2 + (\vec{r} \cdot \vec{S}_2)^2 - \frac{\vec{r}^2}{3} \vec{S}_2^2) V_T(r).
\end{aligned} \tag{4.39}$$

Since the traceless, another one is vanish as

$$\frac{1}{2} \{ \delta_{ij} \} \{ P_{ij}^{(2)}(\vec{S}_1) + P_{ij}^{(2)}(\vec{S}_2) \} V_{C_2}(r) = 0. \tag{4.40}$$

- In 4th order, 1st one is

$$\begin{aligned}
&\frac{1}{2} (P_{ij}^{(2)}(\vec{S}_1) P_{kl}^{(2)}(\vec{S}_2) + P_{ij}^{(2)}(\vec{S}_2) P_{kl}^{(2)}(\vec{S}_1)) \delta_{ik} \delta_{jl} V_{C_4}(r) \\
&= P_{ij}^{(2)}(\vec{S}_1) P_{ij}^{(2)}(\vec{S}_2) V_{C_4}(r) \\
&= (\frac{1}{2} \{S_1^i, S_1^j\} - \frac{1}{3} \vec{S}_1^2 \delta_{ij}) (\frac{1}{2} \{S_2^i, S_2^j\} - \frac{1}{3} \vec{S}_2^2 \delta_{ij}) V_{C_4}(r) \\
&= (\frac{1}{4} \{S_1^i, S_1^j\} \{S_2^i, S_2^j\} - \frac{1}{6} \{ \vec{S}_1^i, \vec{S}_1^j \} \vec{S}_2^2 \delta_{ij}) V_{C_4}(r) \\
&= (\frac{1}{2} S_1^i S_1^j \{S_2^i, S_2^j\} + S_2^j S_2^i - \frac{1}{3} \vec{S}_1^2 \vec{S}_2^2) V_{C_4}(r) \\
&= (\frac{1}{2} (\vec{S}_1 \cdot \vec{S}_2)^2 + \sum_{i=1}^3 S_1^i (\vec{S}_1 \cdot \vec{S}_2) S_2^i - \frac{1}{3} \vec{S}_1^2 \vec{S}_2^2) V_{C_4}(r).
\end{aligned} \tag{4.41}$$

- In 4th order, 2nd one is

$$\begin{aligned}
&\frac{1}{2} (P_{ij}^{(2)}(\vec{S}_1) P_{kl}^{(2)}(\vec{S}_2) + P_{ij}^{(2)}(\vec{S}_2) P_{kl}^{(2)}(\vec{S}_1)) P_{ik}^{(2)}(\vec{r}) \delta_{jl} V_{T_4}(r) \\
&= P_{ij}^{(2)}(\vec{S}_1) P_{kj}^{(2)}(\vec{S}_2) P_{ik}^{(2)}(\vec{r}) V_{T_4}(r) \\
&= (\frac{1}{2} \{S_1^i, S_1^j\} - \frac{1}{3} S_1^2 \delta_{ij}) (\frac{1}{2} \{S_2^k, S_2^j\} - \frac{1}{3} \vec{S}_2^2 \delta_{kj}) (r_i r_k - \frac{1}{3} \vec{r}^2 \delta_{ik}) V_{T_4}(r) \\
&= (\frac{1}{4} \{S_1^i, S_1^j\} \{S_2^k, S_2^j\} - \frac{1}{6} S_1^2 \{S_2^k, S_2^j\} - \frac{1}{6} \{S_1^i, S_1^k\} \vec{S}_2^2 + \frac{1}{9} S_1^2 \delta_{ik} \vec{S}_2^2) (r_i r_k - \frac{1}{3} \vec{r}^2 \delta_{ik}) V_{T_4}(r).
\end{aligned} \tag{4.42}$$

Using follow relation

$$\begin{aligned}
\{S_1^i, S_1^j\} \{S_2^k, S_2^j\} &= (S_1^i S_1^j + S_1^j S_1^i) (S_2^k S_2^j + S_2^j S_2^k) \\
&= (S_1^i S_2^k (\vec{S}_1 \cdot \vec{S}_2) + S_1^j S_1^i S_2^k S_2^j + S_1^i (\vec{S}_1 \cdot \vec{S}_2) S_2^k + (\vec{S}_1 \cdot \vec{S}_2) S_1^i S_2^k),
\end{aligned} \tag{4.43}$$

we derive the



$$\begin{aligned}
& \left( \frac{1}{4} \{S_1^i, S_1^j\} \{S_2^k, S_2^l\} - \frac{1}{6} S_1^2 \{S_2^k, S_2^l\} - \frac{1}{6} \{S_1^i, S_1^k\} \vec{S}_2^2 + \frac{1}{9} S_1^2 \delta_{ik} \vec{S}_2^2 \right) (r_i r_k - \frac{1}{3} \vec{r}^2 \delta_{ik}) V_{T_4}(r) \\
&= \left( \frac{1}{4} (S_1^i S_2^k (\vec{S}_1 \cdot \vec{S}_2) + S_1^j S_1^k S_2^l S_2^j + S_1^i (\vec{S}_1 \cdot \vec{S}_2) S_2^k + (\vec{S}_1 \cdot \vec{S}_2) S_1^i S_2^k) \right. \\
&\quad \left. - \frac{1}{3} S_1^2 S_2^k S_2^l - \frac{1}{3} S_1^i S_1^k \vec{S}_2^2 + \frac{1}{9} S_1^2 \delta_{ik} \vec{S}_2^2 \right) (r_i r_k - \frac{1}{3} \vec{r}^2 \delta_{ik}) V_{T_4}(r) \\
&= \left( \frac{1}{4} ((\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2) (\vec{S}_1 \cdot \vec{S}_2) + S_1^j (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2) S_2^j \right. \\
&\quad \left. + (\vec{r} \cdot \vec{S}_1) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2) \right) - \frac{1}{3} S_1^2 (\vec{r} \cdot \vec{S}_2)^2 \\
&\quad - \frac{1}{3} (\vec{r} \cdot \vec{S}_1)^2 \vec{S}_2^2 + \frac{1}{9} S_1^2 \vec{r}^2 \vec{S}_2^2 - \frac{1}{3} \vec{r}^2 \left( \frac{1}{2} (S_1^j (\vec{S}_1 \cdot \vec{S}_2) S_2^j + (\vec{S}_1 \cdot \vec{S}_2)^2) - \frac{1}{3} S_1^2 \vec{S}_2^2 \right) V_{T_4}(r) \\
&= \left( \frac{1}{4} ((\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2) (\vec{S}_1 \cdot \vec{S}_2) + S_1^j (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2) S_2^j + (\vec{r} \cdot \vec{S}_1) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2) \right. \\
&\quad \left. + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2) \right) - \frac{1}{3} S_1^2 (\vec{r} \cdot \vec{S}_2)^2 - \frac{1}{3} (\vec{r} \cdot \vec{S}_1)^2 \vec{S}_2^2 + \frac{2}{9} \vec{r}^2 \vec{S}_1^2 \vec{S}_2^2 \\
&\quad - \frac{1}{6} \vec{r}^2 (S_1^j (\vec{S}_1 \cdot \vec{S}_2) S_2^j + (\vec{S}_1 \cdot \vec{S}_2)^2) V_{T_4}(r). \tag{4.44}
\end{aligned}$$

- In 4th order, 3rd one is

$$\begin{aligned}
& \frac{1}{2} (P_{ijk}^{(3)}(\vec{S}_1) P_l^{(1)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2) P_l^{(1)}(\vec{S}_1)) P_{ij}^{(2)}(\vec{r}) \delta_{kl} V_{T_4}(r) \\
&= (P_{ijk}^{(3)}(\vec{S}_1) P_k^{(1)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2) P_k^{(1)}(\vec{S}_1)) P_{ij}^{(2)}(\vec{r}) V_{T_4}(r) \\
&= (P_{ijk}^{(3)}(\vec{S}_1) P_k^{(1)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2) P_k^{(1)}(\vec{S}_1)) (r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij}) V_{T_4}(r) \\
&= \left( (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15} (\delta^{ij} S_1^k + \delta_1^{ik} S_1^j + \delta^{jk} S_1^l)) S_2^k + (A_2^{ijk} + \frac{1-3\vec{S}_2^2}{15} (\delta^{ij} S_2^k + \delta^{ik} S_2^j + \delta^{jk} S_2^l)) S_1^k \right) r_i r_j V_{T_4}(r) \\
&= \left( (A_1^{ijk} r_i r_j S_2^k + \frac{1-3\vec{S}_1^2}{15} (\vec{r}^2 (\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2))) + (S_1 \iff S_2) \right) V_{T_4}(r). \tag{4.45}
\end{aligned}$$

Using follow relation as

$$\begin{aligned}
A_1^{ijk} r_i r_j S_2^k &= \frac{1}{3!} (S^i S^j S^k + S^i S^k S^j + S^j S^i S^k + S^j S^k S^i + S^k S^i S^j + S^k S^j S^i) r_i r_j S_2^k \\
&= \frac{1}{3} ((\vec{r} \cdot \vec{S}_1)^2 (\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_1) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1)^2). \tag{4.46}
\end{aligned}$$

Therefore in 4th order 3rd one is

$$\begin{aligned}
& ((A_1^{ijk} r_i r_j S_2^k + \frac{1-3\vec{S}_1^2}{15}(\vec{r}^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1)(\vec{r} \cdot \vec{S}_2))) + (S_1 \iff S_2))V_{T_4}(r) \\
&= (\frac{1}{3}((\vec{r} \cdot \vec{S}_1)^2(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_1)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_1) + (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_1)^2) \\
&+ \frac{1-3\vec{S}_1^2}{15}(\vec{r}^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1)(\vec{r} \cdot \vec{S}_2)) \\
&+ \frac{1}{3}((\vec{r} \cdot \vec{S}_2)^2(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)^2) \\
&+ \frac{1-3\vec{S}_2^2}{15}(\vec{r}^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1)(\vec{r} \cdot \vec{S}_2)))V_{T_4}(r). \tag{4.47}
\end{aligned}$$

- In 4th order, 4th one is

$$\begin{aligned}
& \frac{1}{2}(P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2) + P_{ij}^{(2)}(\vec{S}_2)P_{kl}^{(2)}(\vec{S}_1))P_{ijkl}^{(4)}(\vec{r})V_Q(r) \\
&= \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)P_{ijkl}^{(4)}(\vec{r})V_Q(r) \\
&= \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(r_i r_j r_k r_l - \frac{\vec{r}^2}{7}(r_i r_j \delta_{kl} + r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik} + r_k r_l \delta_{ij}) \\
&+ \frac{\vec{r}^4}{35}(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}))V_Q(r) \\
&= [\frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(r_i r_j r_k r_l) \\
&+ \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(-\frac{\vec{r}^2}{7}(r_i r_j \delta_{kl} + r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik} + r_k r_l \delta_{ij})) \\
&+ \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(\frac{\vec{r}^4}{35}(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}))]V_Q(r) \\
&= [\frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(r_i r_j r_k r_l) \\
&+ \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(-\frac{\vec{r}^2}{7}(r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik})) \\
&+ \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(\frac{\vec{r}^4}{35}(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}))]V_Q(r) \\
&= [\frac{1}{2}(\frac{1}{2}\{\vec{S}_1 \cdot \vec{r}, \vec{S}_1 \cdot \vec{r}\} - \frac{1}{3}\vec{S}_1^2 \vec{r}^2)(\frac{1}{2}\{\vec{S}_2 \cdot \vec{r}, \vec{S}_2 \cdot \vec{r}\} - \frac{1}{3}\vec{S}_2^2 \vec{r}^2) \\
&+ \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(-\frac{\vec{r}^2}{7}(r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik})) \\
&+ \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)(\frac{\vec{r}^4}{35}(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}))]V_Q(r). \tag{4.48}
\end{aligned}$$

Since complicated, is calculated by dividing each term.

1st term is

$$\begin{aligned}
& \frac{1}{2}(\frac{1}{2}\{\vec{S}_1 \cdot \vec{r}, \vec{S}_1 \cdot \vec{r}\} - \frac{1}{3}\vec{S}_1^2 \vec{r}^2)(\frac{1}{2}\{\vec{S}_2 \cdot \vec{r}, \vec{S}_2 \cdot \vec{r}\} - \frac{1}{3}\vec{S}_2^2 \vec{r}^2) \\
&= \frac{1}{2}(\frac{1}{2}\{\vec{S}_1 \cdot \vec{r}, \vec{S}_1 \cdot \vec{r}\})(\frac{1}{2}\{\vec{S}_2 \cdot \vec{r}, \vec{S}_2 \cdot \vec{r}\} - \frac{1}{3}\vec{S}_2^2 \vec{r}^2) - \frac{1}{3}\vec{S}_1^2 \vec{r}^2(\frac{1}{2}\{\vec{S}_2 \cdot \vec{r}, \vec{S}_2 \cdot \vec{r}\} - \frac{1}{3}\vec{S}_2^2 \vec{r}^2) \\
&= \frac{1}{144}((18(\vec{S}_1 \cdot \vec{r})^2(\vec{S}_2 \cdot \vec{r})^2 - 12(\vec{S}_1 \cdot \vec{r})^2\vec{S}_2^2 \vec{r}^2) - 12\vec{S}_1^2 \vec{r}^2(\vec{S}_2 \cdot \vec{r})^2 + 8\vec{S}_1^2 \vec{S}_2^2 \vec{r}^4). \tag{4.49}
\end{aligned}$$

2nd term is

$$\begin{aligned}
& \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)\left(-\frac{\vec{r}^2}{7}(r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik})\right) \\
&= \frac{1}{2}\left(-\frac{\vec{r}^2}{7}(P_{ij}^{(2)}(\vec{S}_1)P_{kj}^{(2)}(\vec{S}_2)r_i r_k + P_{ij}^{(2)}(\vec{S}_1)P_{jl}^{(2)}(\vec{S}_2)r_i r_l + P_{ij}^{(2)}(\vec{S}_1)P_{ki}^{(2)}(\vec{S}_2)r_j r_k + P_{ij}^{(2)}(\vec{S}_1)P_{il}^{(2)}(\vec{S}_2)r_j r_l)\right) \\
&= \frac{1}{2}\left(-\frac{\vec{r}^2}{7}(P_{ji}^{(2)}(\vec{S}_1)P_{jk}^{(2)}(\vec{S}_2)r_i r_k + P_{ji}^{(2)}(\vec{S}_1)P_{jl}^{(2)}(\vec{S}_2)r_i r_l + P_{ij}^{(2)}(\vec{S}_1)P_{ik}^{(2)}(\vec{S}_2)r_j r_k + P_{ij}^{(2)}(\vec{S}_1)P_{il}^{(2)}(\vec{S}_2)r_j r_l)\right) \\
&= -\frac{2}{7}\vec{r}^2(P_{ji}^{(2)}(\vec{S}_1)P_{jk}^{(2)}(\vec{S}_2)r_i r_k) \\
&= -\frac{2}{7}\vec{r}^2\left(\left(\frac{1}{2}\{S_1^j, S_1^i\} - \frac{1}{3}S_1^2\delta_{ij}\right)\left(\frac{1}{2}\{S_2^j, S_2^k\} - \frac{1}{3}S_2^2\delta_{jk}\right)r_i r_k\right) \\
&= -\frac{2}{7}\vec{r}^2\left(\left(\frac{1}{2}\{S_1^j S_1^i + S_1^i S_1^j\} - \frac{1}{3}S_1^2\delta_{ij}\right)\left(\frac{1}{2}\{S_2^j S_2^k + S_2^k S_2^j\} - \frac{1}{3}S_2^2\delta_{jk}\right)r_i r_k\right) \\
&= -\frac{2}{7}\vec{r}^2\left(\left(\frac{1}{4}\{S_1^j S_1^i S_2^j S_2^k + S_1^i S_1^j S_2^j S_2^k + S_1^j S_1^i S_2^k S_2^j + S_1^i S_1^j S_2^k S_2^j\}\right.\right. \\
&\quad \left.\left.- \frac{1}{6}\{S_1^j S_1^i + S_1^i S_1^j\}S_2^2\delta_{jk} - \frac{1}{6}S_1^2\delta_{ij}\{S_2^j S_2^k + S_2^k S_2^j\} + \frac{1}{9}S_1^2 S_2^2\delta_{ik}\right)r_i r_k\right) \\
&= -\frac{2}{7}\vec{r}^2\left(\left(\frac{1}{4}\{(\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) + (\vec{S}_1 \cdot \vec{r})(\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_2 \cdot \vec{r})\right.\right. \\
&\quad \left.\left.+ S_1^j(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})S_2^j + (\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})(\vec{S}_1 \cdot \vec{S}_2)\right\}\right. \\
&\quad \left.- \frac{1}{3}(\vec{S}_1 \cdot \vec{r})^2 S_2^2 - \frac{1}{3}S_1^2(\vec{S}_2 \cdot \vec{r})^2 + \frac{1}{9}S_1^2 S_2^2 \vec{r}^2\right) \\
&= -\frac{1}{126}\vec{r}^2\left(\left(9\{(\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) + (\vec{S}_1 \cdot \vec{r})(\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_2 \cdot \vec{r})\right.\right. \\
&\quad \left.\left.+ \sum_{j=1}^3 S_1^j(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})S_2^j + (\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})(\vec{S}_1 \cdot \vec{S}_2)\right\}\right. \\
&\quad \left.- 12(\vec{S}_1 \cdot \vec{r})^2 S_2^2 - 12S_1^2(\vec{S}_2 \cdot \vec{r})^2 + 4S_1^2 S_2^2 \vec{r}^2\right). \tag{4.50}
\end{aligned}$$

last term is

$$\begin{aligned}
& \frac{1}{2}P_{ij}^{(2)}(\vec{S}_1)P_{kl}^{(2)}(\vec{S}_2)\left(\frac{\vec{r}^4}{35}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\right) \\
&= \frac{\vec{r}^4}{35}(P_{ij}^{(2)}(\vec{S}_1)P_{ij}^{(2)}(\vec{S}_2)) \\
&= \frac{\vec{r}^4}{35}\left(\frac{1}{2}(\vec{S}_1 \cdot \vec{S}_2)^2 + \sum_{i=1}^3 S_1^i(\vec{S}_1 \cdot \vec{S}_2)S_2^i - \frac{1}{3}\vec{S}_1^2 \vec{S}_2^2\right). \tag{4.51}
\end{aligned}$$

Therefore Eq. (4.48) is given as

$$\begin{aligned}
& \left[ \frac{1}{2} \left( \frac{1}{2} \{ \vec{S}_1 \cdot \vec{r}, \vec{S}_1 \cdot \vec{r} \} - \frac{1}{3} \vec{S}_1^2 \vec{r}^2 \right) \left( \frac{1}{2} \{ \vec{S}_2 \cdot \vec{r}, \vec{S}_2 \cdot \vec{r} \} - \frac{1}{3} \vec{S}_2^2 \vec{r}^2 \right) \right. \\
& + \frac{1}{2} P_{ij}^{(2)}(\vec{S}_1) P_{kl}^{(2)}(\vec{S}_2) \left( -\frac{\vec{r}^2}{7} (r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik}) \right) \\
& + \frac{1}{2} P_{ij}^{(2)}(\vec{S}_1) P_{kl}^{(2)}(\vec{S}_2) \left( \frac{\vec{r}^4}{35} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right) \Big] V_Q(r) \\
& = \left[ \frac{1}{144} \left( (18(\vec{S}_1 \cdot \vec{r})^2 (\vec{S}_2 \cdot \vec{r})^2 - 12(\vec{S}_1 \cdot \vec{r})^2 \vec{S}_2^2 \vec{r}^2) - 12\vec{S}_1^2 \vec{r}^2 (\vec{S}_2 \cdot \vec{r})^2 + 8\vec{S}_1^2 \vec{S}_2^2 \vec{r}^4 \right) \right. \\
& - \frac{1}{126} \vec{r}^2 \left( (9\{(\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) + (\vec{S}_1 \cdot \vec{r})(\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_2 \cdot \vec{r}) \right. \\
& + \sum_{j=1}^3 S_1^j (\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) S_2^j + (\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})(\vec{S}_1 \cdot \vec{S}_2) \} \\
& - 12(\vec{S}_1 \cdot \vec{r})^2 S_2^2 - 12S_1^2 (\vec{S}_2 \cdot \vec{r})^2 + 4S_1^2 S_2^2 \vec{r}^2) \\
& \left. + \frac{\vec{r}^4}{35} \left( \frac{1}{2} (\vec{S}_1 \cdot \vec{S}_2)^2 + \sum_{i=1}^3 S_1^i (\vec{S}_1 \cdot \vec{S}_2) S_2^i - \frac{1}{3} \vec{S}_1^2 \vec{S}_2^2 \right) \right] V_Q(r). \tag{4.52}
\end{aligned}$$

- In 4th order, 5th one is

$$\frac{1}{2} (P_{ijk}^{(3)}(\vec{S}_1) P_l^{(1)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2) P_l^{(1)}(\vec{S}_1)) P_{ijkl}^{(4)}(\vec{r}) V_Q(r) \tag{4.53}$$

Using follow relation

$$\begin{aligned}
P_{ijkl}^{(4)}(\vec{r}) P_{ijk}^{(3)}(\vec{S}_1) P_l^{(1)}(\vec{S}_2) &= (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2)^3 - \frac{\vec{r}^2}{7} ((\vec{r} \cdot \vec{S}_2)^2 (\vec{S}_1 \cdot \vec{S}_2) \\
& + (\vec{r} \cdot \vec{S}_2) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2)^2) \\
& - \frac{1 - 3\vec{S}_2^2}{5 \cdot 7} \{ \vec{r}^4 (\vec{S}_1 \cdot \vec{S}_2) - 5\vec{r}^2 (r \cdot S_1) (r \cdot S_2) \}. \tag{4.54}
\end{aligned}$$

Therefore Eq. (4.53) is given as

$$\begin{aligned}
& \frac{1}{2} (P_{ijk}^{(3)}(\vec{S}_1) P_l^{(1)}(\vec{S}_2) + P_{ijk}^{(3)}(\vec{S}_2) P_l^{(1)}(\vec{S}_1)) P_{ijkl}^{(4)}(\vec{r}) V_Q(r) \\
& = \frac{1}{2} \left[ (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2)^3 - \frac{\vec{r}^2}{7} ((\vec{r} \cdot \vec{S}_2)^2 (\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2)^2) \right. \\
& - \frac{1 - 3\vec{S}_2^2}{5 \cdot 7} \{ \vec{r}^4 (\vec{S}_1 \cdot \vec{S}_2) - 5\vec{r}^2 (r \cdot S_1) (r \cdot S_2) \} \\
& + (\vec{r} \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1)^3 - \frac{\vec{r}^2}{7} ((\vec{r} \cdot \vec{S}_1)^2 (\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_1) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1)^2) \\
& \left. - \frac{1 - 3\vec{S}_1^2}{5 \cdot 7} \{ \vec{r}^4 (\vec{S}_1 \cdot \vec{S}_2) - 5\vec{r}^2 (r \cdot S_1) (r \cdot S_2) \} \right] V_Q(r). \tag{4.55}
\end{aligned}$$

Since  $P_{ij}^{(2)}$  is traceless, another is vanish as

$$\frac{1}{2} (P_{ij}^{(2)}(\vec{S}_1) P_{kl}^{(2)}(\vec{S}_2) + P_{ij}^{(2)}(\vec{S}_2) P_{kl}^{(2)}(\vec{S}_1)) \delta_{ij} \delta_{kl} V_{C_4}(r) = 0. \tag{4.56}$$

- In 6th order, 1st one is

$$\begin{aligned}
P_{ijk}^{(3)}(\vec{S}_1)P_{ijk}^{(3)}(\vec{S}_2) &= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i))(A_2^{ijk} + \frac{1-3\vec{S}_2^2}{15}(\delta^{ij}S_2^k + \delta^{ik}S_2^j + \delta^{jk}S_2^i)) \\
&= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i))A_2^{ijk} \\
&= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{5}(\delta^{ij}S_1^k))A_2^{ijk} \tag{4.57}
\end{aligned}$$

Since complicated, is calculated by dividing each term.

In first term is

$$\begin{aligned}
A_1^{ijk}A_2^{ijk} &= \frac{1}{3!3!}(S_1^iS_1^jS_1^k + S_1^iS_1^kS_1^j + S_1^jS_1^iS_1^k + S_1^jS_1^kS_1^i + S_1^kS_1^iS_1^j + S_1^kS_1^jS_1^i) \\
&\quad \times (S_2^iS_2^jS_2^k + S_2^iS_2^kS_2^j + S_2^jS_2^iS_2^k + S_2^jS_2^kS_2^i + S_2^kS_2^iS_2^j + S_2^kS_2^jS_2^i) \\
&= \frac{1}{6}((\vec{S}_1 \cdot \vec{S}_2)^3 + (\vec{S}_1 \cdot \vec{S}_2)S_2^j(\vec{S}_1 \cdot \vec{S}_2)S_1^j + S_1^j(\vec{S}_1 \cdot \vec{S}_2)S_2^j(\vec{S}_1 \cdot \vec{S}_2) \\
&\quad + S_2^i(\vec{S}_1 \cdot \vec{S}_2)^2S_1^i + S_1^k(\vec{S}_1 \cdot \vec{S}_2)^2S_2^k + S_1^kS_1^j(\vec{S}_1 \cdot \vec{S}_2)S_2^jS_2^k) \tag{4.58}
\end{aligned}$$

In second term is

$$\begin{aligned}
(\delta^{ij}S_1^k)A_2^{ijk} &= \frac{1}{3!}S_1^k(S_2^iS_2^iS_2^k + S_2^iS_2^kS_2^i + S_2^iS_2^iS_2^k + S_2^iS_2^kS_2^i + S_2^kS_2^iS_2^i + S_2^kS_2^iS_2^i) \\
&= \frac{1}{3!}(4\vec{S}_2^2(\vec{S}_1 \cdot \vec{S}_2) + 2S_2^i(\vec{S}_1 \cdot \vec{S}_2)S_2^i) \\
&= \frac{1}{3!}(4\vec{S}_2^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{S}_2^2 - 1)(\vec{S}_1 \cdot \vec{S}_2)) \\
&= \frac{1}{3!}(6\vec{S}_2^2(\vec{S}_1 \cdot \vec{S}_2) - (\vec{S}_1 \cdot \vec{S}_2)) \tag{4.59}
\end{aligned}$$

Therefore Eq. (4.57) is given as

$$\begin{aligned}
P_{ijk}^{(3)}(\vec{S}_1)P_{ijk}^{(3)}(\vec{S}_2) &= \frac{1}{6}((\vec{S}_1 \cdot \vec{S}_2)^3 + (\vec{S}_1 \cdot \vec{S}_2)S_2^j(\vec{S}_1 \cdot \vec{S}_2)S_1^j + S_1^j(\vec{S}_1 \cdot \vec{S}_2)S_2^j(\vec{S}_1 \cdot \vec{S}_2) \\
&\quad + S_2^i(\vec{S}_1 \cdot \vec{S}_2)^2S_1^i + S_1^k(\vec{S}_1 \cdot \vec{S}_2)^2S_2^k \\
&\quad + S_1^kS_1^j(\vec{S}_1 \cdot \vec{S}_2)S_2^jS_2^k) + \frac{1-3\vec{S}_1^2}{30}(6\vec{S}_2^2(\vec{S}_1 \cdot \vec{S}_2) - (\vec{S}_1 \cdot \vec{S}_2)). \tag{4.60}
\end{aligned}$$

- In 6th order, 2nd one is

$$P_{ijk}^{(3)}(\vec{S}_1)P_{ljk}^{(3)}(\vec{S}_2)P_{il}^{(2)}(\vec{r})$$

$$\begin{aligned}
&= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i))(A_2^{ljk} + \frac{1-3\vec{S}_2^2}{15}(\delta^{lj}S_2^k + \delta^{lk}S_2^j + \delta^{jk}S_2^l))(r^i r^l - \frac{1}{3}\vec{r}^2\delta_{il}) \\
&= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i))(A_2^{ljk} + \frac{1-3\vec{S}_2^2}{15}(\delta^{lj}S_2^k + \delta^{lk}S_2^j))r^i r^l - \frac{1}{3}\vec{r}^2\delta_{il} \\
&= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i))(A_2^{ljk} r^i r^l + \frac{1-3\vec{S}_2^2}{15}(\delta^{lj}S_2^k + \delta^{lk}S_2^j)r^i r^l \\
&\quad - \frac{1}{3}\vec{r}^2 A_2^{ijk} - \frac{1}{3}\vec{r}^2 \frac{1-3\vec{S}_2^2}{15}(\delta^{ij}S_2^k + \delta^{ik}S_2^j)) \\
&= (A_1^{ijk} + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i))(A_2^{ljk} r^i r^l + \frac{1-3\vec{S}_2^2}{15}(\delta^{lj}S_2^k + \delta^{lk}S_2^j)r^i r^l - \frac{1}{3}\vec{r}^2 A_2^{ijk}) \\
&= A_1^{ijk} A_2^{ljk} r^i r^l + \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i)A_2^{ljk} r^i r^l \\
&\quad + (2\frac{1-3\vec{S}_2^2}{15})A_1^{ijk} S_2^k r^i r^j + \frac{1-3\vec{S}_1^2}{15}(2\frac{1-3\vec{S}_2^2}{15})(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i)S_2^k r^i r^j \\
&\quad - \frac{1}{3}\vec{r}^2 A_1^{ijk} A_2^{ijk} - \frac{1}{3}\vec{r}^2 \frac{1-3\vec{S}_1^2}{15}(\delta^{ij}S_1^k + \delta^{ik}S_1^j + \delta^{jk}S_1^i)A_2^{ijk}. \tag{4.61}
\end{aligned}$$

In 6th order, 3rd one and 4th one, it is too complex to calculate, we can't calculate in this paper.

### 4.3 Octet-Decuplet baryon

This section we consider octet-decuplet baryon system such as  $N - \Omega$ . Now that we are ready, we start to decompose a potential between decuplet baryon and decuplet baryon.

- Polynominal-degrees of spin matrices = 0, 2, 4, because of T-symmetry.

$$x \rightarrow -x, \quad p \rightarrow -p \quad S \rightarrow -S \quad i \rightarrow -i \tag{4.62}$$

- Possible forms of potentials can be expressed as products of spin-matrix structure and coordinate function structure, because a potential have rotational symmetry.

$$V_{\alpha'\beta':\alpha\beta}(\vec{r}, \vec{v}, \vec{S}_1, \vec{S}_2) = \sum_{n,m=0} V_{i_1, \dots, i_n; j_1, \dots, j_m}^{(n,m)}(\vec{r}, \vec{v}) \cdot (P_{i_1, \dots, i_n}^{(n)}(\vec{S}_1))(P_{j_1, \dots, j_m}^{(m)}(\vec{S}_2)) \tag{4.63}$$

order(index)	spin-matrix	coordinate function
0	$P^{(0)}(\vec{S}_1)$	$V_C(r)$
2(i,j)	$P_i^{(1)}(\vec{S}_1)P_j^{(1)}(\vec{S}_2)$	$V_{C_2}(r)\delta_{ij}$
	$P_{ij}^{(2)}(\vec{S}_2)$	$V_T(r)P_{ij}^{(2)}(\vec{r})$
4(i,j,k,l)	$P_{ijk}^{(3)}(\vec{S}_2)P_l^{(1)}(\vec{S}_1)$	$V_{C_4}(r)\delta_{ij}\delta_{kl}$
		$V_{T_4}(r)P_{ij}^{(2)}(\vec{r})\delta_{kl}$
		$V_Q(r)P_{ijkl}^{(4)}(\vec{r})$

where upper index is spin-order, lower index is spacial index,  $\vec{S}_1$  is spin of octet baryon and  $\vec{S}_2$  is spin of decuplet baryon. Specific system for 0th order is trivial.

$$V_C(r) \tag{4.64}$$

- In 2nd order, 1st one is

$$\delta_{ij}P_i^{(1)}(\vec{S}_1)P_j^{(1)}(\vec{S}_2)V_{C_2}(r) = \vec{S}_1 \cdot \vec{S}_2 V_{C_2}(r) \quad (4.65)$$

- In 2nd order, 2nd one is

$$P_{ij}^{(2)}(\vec{r})P_{ij}^{(2)}(\vec{S}_2)V_T(r) = ((\vec{r} \cdot \vec{S}_2)^2 - \frac{\vec{r}^2 \vec{S}_2^2}{3})V_T(r) \quad (4.66)$$

- In 2nd order, 3rd one is

$$P_{ij}^{(2)}(\vec{r})P_i^{(1)}(\vec{S}_1)P_j^{(1)}(\vec{S}_2)V_T(r) = ((\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) - \frac{r^2 \vec{S}_1 \cdot \vec{S}_2}{3})V_T(r) \quad (4.67)$$

Since  $P_{ij}^{(2)}$  is traceless, another one is vanish as

$$\delta_{ij}P_{ij}^{(2)}(\vec{S}_2) = 0. \quad (4.68)$$

- In 4th order, 1st one is

$$\begin{aligned} & P_{ij}^{(2)}(\vec{r})P_{ijk}^{(3)}(\vec{S}_2)P_k^{(1)}(\vec{S}_1)V_{T_4}(r) \\ &= (r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij})(A_{ijk} + \frac{1 - 3\vec{S}_2^2}{15}(\delta_{ij}S_2^k + \delta_{ik}S_2^j + \delta_{jk}S_2^i))S_1^k V_{T_4}(r) \\ &= (r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij})(A_{ijk}S_1^k + \frac{1 - 3\vec{S}_2^2}{15}(\delta_{ij}\vec{S}_1 \cdot \vec{S}_2 + S_1^i S_2^j + S_1^j S_2^i))V_{T_4}(r) \\ &= A_{ijk}S_1^k(r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij}) + (r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij})(\frac{1 - 3\vec{S}_2^2}{15}(\delta_{ij}\vec{S}_1 \cdot \vec{S}_2 + S_1^i S_2^j + S_1^j S_2^i))V_{T_4}(r) \\ &= A_{ijk}S_1^k(r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij}) + (\frac{1 - 3\vec{S}_2^2}{15}(2(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) - \frac{2}{3} \vec{r}^2 \vec{S}_1 \cdot \vec{S}_2))V_{T_4}(r), \end{aligned} \quad (4.69)$$

where  $A_{ijk}S_1^k(r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij})$  is given as

$$\begin{aligned} A_{ijk}S_1^k(r_i r_j - \frac{1}{3} \vec{r}^2 \delta_{ij}) &= \frac{1}{3!}((\vec{r} \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) \\ &+ (\vec{r} \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) \\ &+ (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) \\ &- \frac{1}{3} \vec{r}^2 (2\vec{S}_2^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{S}_2^2 - 1)(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{S}_1 \cdot \vec{S}_2)\vec{S}_2^2)) \\ &= \frac{1}{3}((\vec{r} \cdot \vec{S}_2)^2(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) \\ &+ (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)^2) - \frac{(3\vec{S}_2^2 - 1)5}{15} \frac{\vec{r}^2}{3} (\vec{S}_1 \cdot \vec{S}_2). \end{aligned} \quad (4.70)$$

Therefore we obtain

$$P_{ij}^{(2)}(\vec{r})P_{ijk}^{(3)}(\vec{S}_2)P_k^{(1)}(\vec{S}_1)V_{T_4}(r)$$

$$\begin{aligned}
&= \left(\frac{1}{3}((\vec{r} \cdot \vec{S}_2)^2(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)^2)\right. \\
&\quad \left. - \frac{(3\vec{S}_2^2 - 1)}{15}(\frac{5}{3}\vec{r}^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) - \frac{2}{3}\vec{r}^2\vec{S}_1 \cdot \vec{S}_2))\right)V_{T_4}(r) \\
&= \left[\frac{1}{3}((\vec{r} \cdot \vec{S}_2)^2(\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)^2)\right. \\
&\quad \left. - \frac{(3\vec{S}_2^2 - 1)}{15}(\vec{r}^2(\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}))\right]V_{T_4}(r). \tag{4.71}
\end{aligned}$$

- In 4th order, 2nd one is

$$P_{ijkl}^{(4)}(\vec{r})P_{ijk}^{(3)}(\vec{S}_2)P_l^{(1)}(\vec{S}_1)V_Q(r) \tag{4.72}$$

$$\begin{aligned}
&= (r_i r_j r_k r_l - \frac{\vec{r}^2}{7}(r_i r_j \delta_{kl} + r_i r_k \delta_{jl} + r_i r_l \delta_{jk} + r_j r_k \delta_{il} + r_j r_l \delta_{ik} + r_k r_l \delta_{ij})) \\
&\quad \times (A_{ijk} + \frac{1 - 3\vec{S}_2^2}{15}(\delta_{ij}S_2^k + \delta_{ik}S_2^j + \delta_{jk}S_2^i))S_1^l V_Q(r). \tag{4.73}
\end{aligned}$$

We use a property of traceless tensor. Eq. (4.72) is

$$\begin{aligned}
&P_{ijkl}^{(4)}(\vec{r})P_{ijk}^{(3)}(\vec{S}_2)P_l^{(1)}(\vec{S}_1)V_Q(r) \\
&= (r_i r_j r_k r_l - \frac{\vec{r}^2}{7}(r_i r_j \delta_{kl} + r_i r_k \delta_{jl} + r_j r_k \delta_{il})) \\
&\quad \times (A_{ijk} + \frac{1 - 3\vec{S}_2^2}{15}(\delta_{ij}S_2^k + \delta_{ik}S_2^j + \delta_{jk}S_2^i))S_1^l V_Q(r) \\
&= \{[r_i r_j r_k (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7}(r_i r_j S_1^k + r_i r_k S_1^j + r_j r_k S_1^i)]A_{ijk} \\
&\quad + [r_i r_j r_k (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7}(r_i r_j S_1^k + r_i r_k S_1^j + r_j r_k S_1^i)] \\
&\quad \times \frac{1 - 3\vec{S}_2^2}{15}(\delta_{ij}S_2^k + \delta_{ik}S_2^j + \delta_{jk}S_2^i)\}V_Q(r), \tag{4.75}
\end{aligned}$$

where the first term and second term are reduced as

$$\begin{aligned}
&\{r_i r_j r_k (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7}(r_i r_j S_1^k + r_i r_k S_1^j + r_j r_k S_1^i)\}A_{ijk} \\
&= \{r_i r_j r_k (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7}(r_i r_j S_1^k + r_i r_k S_1^j + r_j r_k S_1^i)\} \\
&\quad \times \frac{1}{3!}(S_2^i S_2^j S_2^k + S_2^i S_2^k S_2^j + S_2^j S_2^i S_2^k + S_2^j S_2^k S_2^i + S_2^k S_2^i S_2^j + S_2^k S_2^j S_2^i) \\
&= (\vec{r} \cdot \vec{S}_1)(\vec{r} \cdot \vec{S}_2)^3 - \frac{\vec{r}^2}{7}((\vec{r} \cdot \vec{S}_2)^2(\vec{S}_1 \cdot \vec{S}_2) \\
&\quad + (\vec{r} \cdot \vec{S}_2)(\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2)(\vec{r} \cdot \vec{S}_2)^2), \tag{4.76}
\end{aligned}$$



$$\begin{aligned}
& \{r_i r_j r_k (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7} (r_i r_j S_1^k + r_i r_k S_1^j + r_j r_k S_1^i) \\
& \times \frac{1 - 3\vec{S}_2^2}{15} (\delta_{ij} S_2^k + \delta_{ik} S_2^j + \delta_{jk} S_2^i) \\
& = \frac{1 - 3\vec{S}_2^2}{15} \{3\vec{r}^2 (\vec{r} \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) - \frac{3\vec{r}^2}{7} (\vec{r}^2 (\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2))\} \\
& = \frac{1 - 3\vec{S}_2^2}{5} \{\vec{r}^2 (\vec{r} \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7} (\vec{r}^2 (\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2))\}. \tag{4.77}
\end{aligned}$$

Therefore Eq. (4.72) is

$$\begin{aligned}
& P_{ijkl}^{(4)}(\vec{r}) P_{ijk}^{(3)}(\vec{S}_2) P_l^{(1)}(\vec{S}_1) V_Q(r) \\
& = [(\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2)^3 - \frac{\vec{r}^2}{7} ((\vec{r} \cdot \vec{S}_2)^2 (\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2)^2) \\
& + \frac{1 - 3\vec{S}_2^2}{5} \{\vec{r}^2 (\vec{r} \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_1) - \frac{\vec{r}^2}{7} (\vec{r}^2 (\vec{S}_1 \cdot \vec{S}_2) + 2(\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2))\}] V_Q(r) \\
& = [(\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2)^3 - \frac{\vec{r}^2}{7} ((\vec{r} \cdot \vec{S}_2)^2 (\vec{S}_1 \cdot \vec{S}_2) + (\vec{r} \cdot \vec{S}_2) (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2) + (\vec{S}_1 \cdot \vec{S}_2) (\vec{r} \cdot \vec{S}_2)^2) \\
& - \frac{1 - 3\vec{S}_2^2}{5 \cdot 7} \{\vec{r}^4 (\vec{S}_1 \cdot \vec{S}_2) - 5\vec{r}^2 (\vec{r} \cdot \vec{S}_1) (\vec{r} \cdot \vec{S}_2)\}] V_Q(r). \tag{4.78}
\end{aligned}$$

We have performed Okubo-marshark decomposition for Decuplet-Decuplet system except 6th order 3rd and 4th term and Octet-Decuplet system.

# Chapter 5

## Numerical results

### 5.1 Simulation set up

In this study, we have employed two ensembles of gauge configurations called Set 1 and Set 2, both of which were generated by 2+1 flavor QCD with the renormalization group improved gauge action and non-perturbatively  $\mathcal{O}(a)$  improved Wilson quark action. The Set 2 is larger volume than the Set 1. Our calculation were performed in on renormalization group improved gauge action and non-perturbatively  $\mathcal{O}(a)$  improved Wilson quark action [30]. In Set 1, we used 700 gauge configurations generated by CP-PACS and JLQCD Collaborations [33]. It's  $\beta = 1.83$  ( $a \simeq 0.12$  fm) on the  $16^3 \times 32$  lattice, whose physical extension becomes  $L = 1.92$  fm. The hopping parameters of Set 1 is  $\kappa_{ud} = 0.13760$ ,  $\kappa_s = 0.13710$  corresponding to  $m_\pi = 875(1)$  MeV and  $m_\Omega = 2104(8)$  MeV. In Set 2, we used 399 gauge configuration generated by PCAS-CS Collaborations [34]. It's  $\beta = 1.90$  ( $a \simeq 0.09$  fm) on the  $32^3 \times 64$  lattice, whose physical extension becomes  $L = 2.9$  fm. The hopping parameters of Set 1 is  $\kappa_{ud} = 0.13700$ ,  $\kappa_s = 0.13640$  corresponding to  $m_\pi = 701(5)$  MeV and  $m_\Omega = 1966(6)$  MeV. To improve statics we used full source (Set 1 is 32, Set 2 is 64) on different time slices per configuration and rotational symmetry Appendix E.

	Set 1	Set 2
Lattice volume	1.950(30) fm	2.902(42) fm
Hopping parameters of ud quarks	0.13760	0.13700
Hopping parameters of s quarks	0.13710	0.13640
$\beta$	1.83	1.90
Lattice spacing	0.1219(19) fm	0.0907(13) fm

Table 5.1: Lattice simulation set up of the Set 1 and Set 2.

### 5.2 Effective mass

For measurements the effective mass of the Omega baryon in full QCD, we use the sea quark mass corresponding to the hopping parameter  $\kappa_{ud} = 0.13760$ ,  $\kappa_s = 0.13710$   $\kappa_{ud} = 0.13700$ ,  $\kappa_s = 0.13640$  and We measure the effective mass from 2pt-correlator Eq. (2.28). The effective masses are carried out using 700 configuration in Set 1 and using 300 configuration in Set 2. Their errors are estimated by Jackknife method. In this study we use the dirichlet boundary is always separated from the source by  $T/2$ . So we defined the effective mass

$$m(t) = \log \frac{G(t)}{G(t+1)}, \quad (5.1)$$

which shown in Fig. 5.1 and Fig. 5.2 with CP-PACS/JLQCD collaboration result and PACS-CS collaboration result [33, 34]. Our results is calculated by using the wall source, on the other hand, PACS-CS collaboration results is used point and smeared sources.

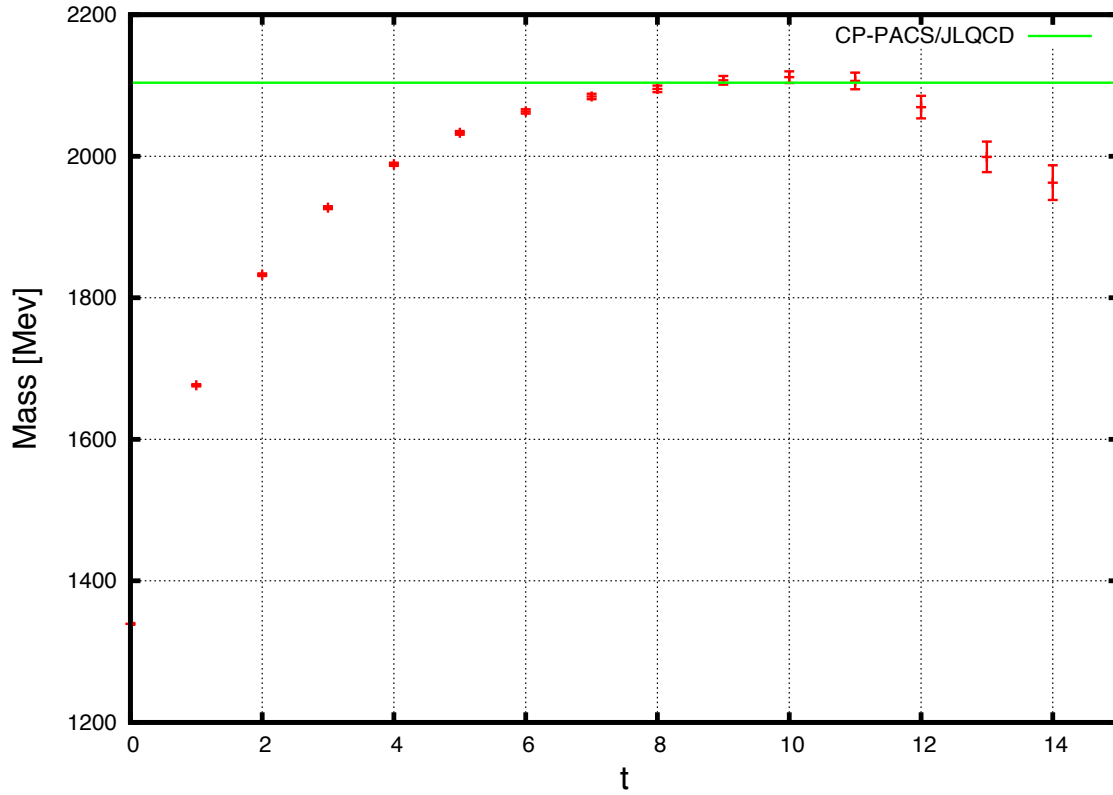


Figure 5.1: Effective mass at bin size = 1 in Set 1 with CP-PACS/JLQCD collaboration result.

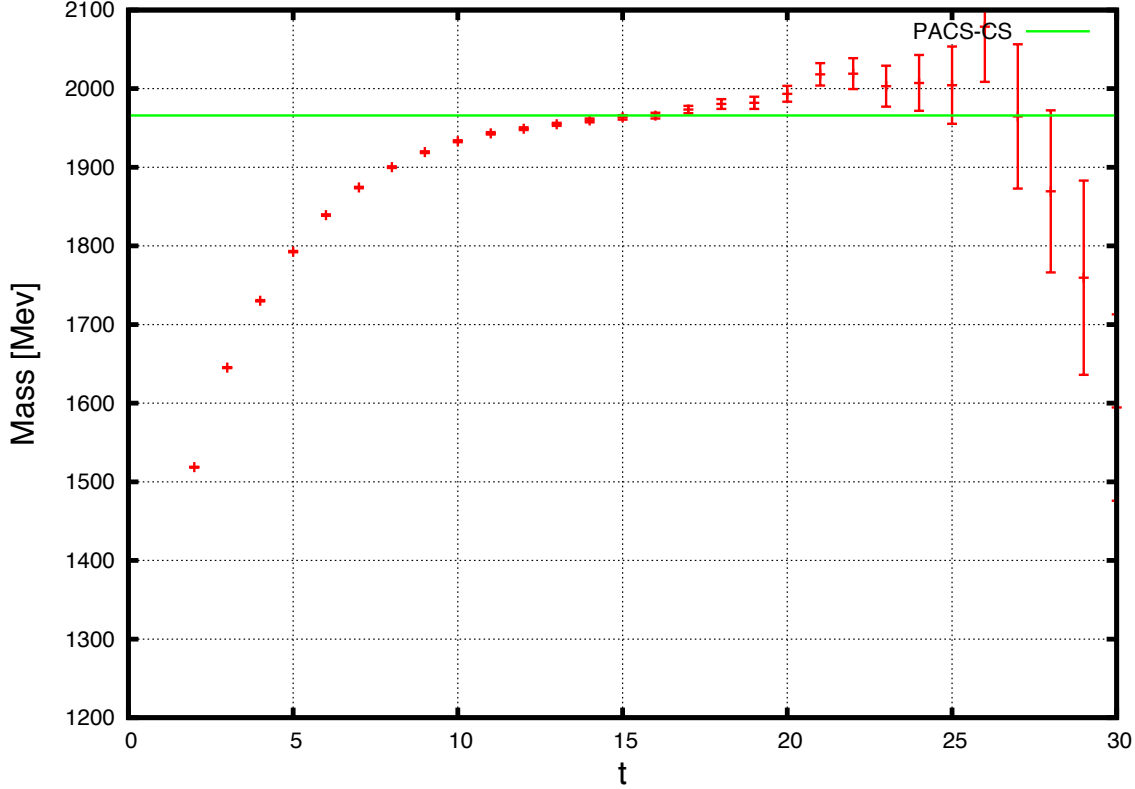


Figure 5.2: Effective mass at bin size = 1 in Set 2 with PACS-CS collaboration result.

### 5.3 NBS wave function

Let us show the  $\Omega - \Omega$  NBS wave function in Fig. 5.3 in the  $^1S_0$  channel at  $t - t_0 = 7, 8, 9$  in Set 1 and at  $t - t_0 = 11, 12, 13$  in Set 2. The wave function is normalized to 1 at the maximum distance by multiplying an overall factor, so normalization factors are different for each times. The normalization does not affect the potential because the potential is defined a ratio of the NBS wave functions. This error is plotted using the jackknife method of bin size 1. At the short range, the amplitude of the NBS wave function is small which is corresponding the repulsive core of the effective central potential. The form of the R-correlator is same as NBS wave functions, because R-correlator are NBS wave functions normalized by  $e^{-2m_\Omega t}$

$$R(t, r) \equiv \sum_n \frac{C_n(r, t)}{e^{-2mt}} = \sum_n A_n(\psi_n(r) e^{-E_n t}) \frac{1}{e^{-2mt}}. \quad (5.2)$$

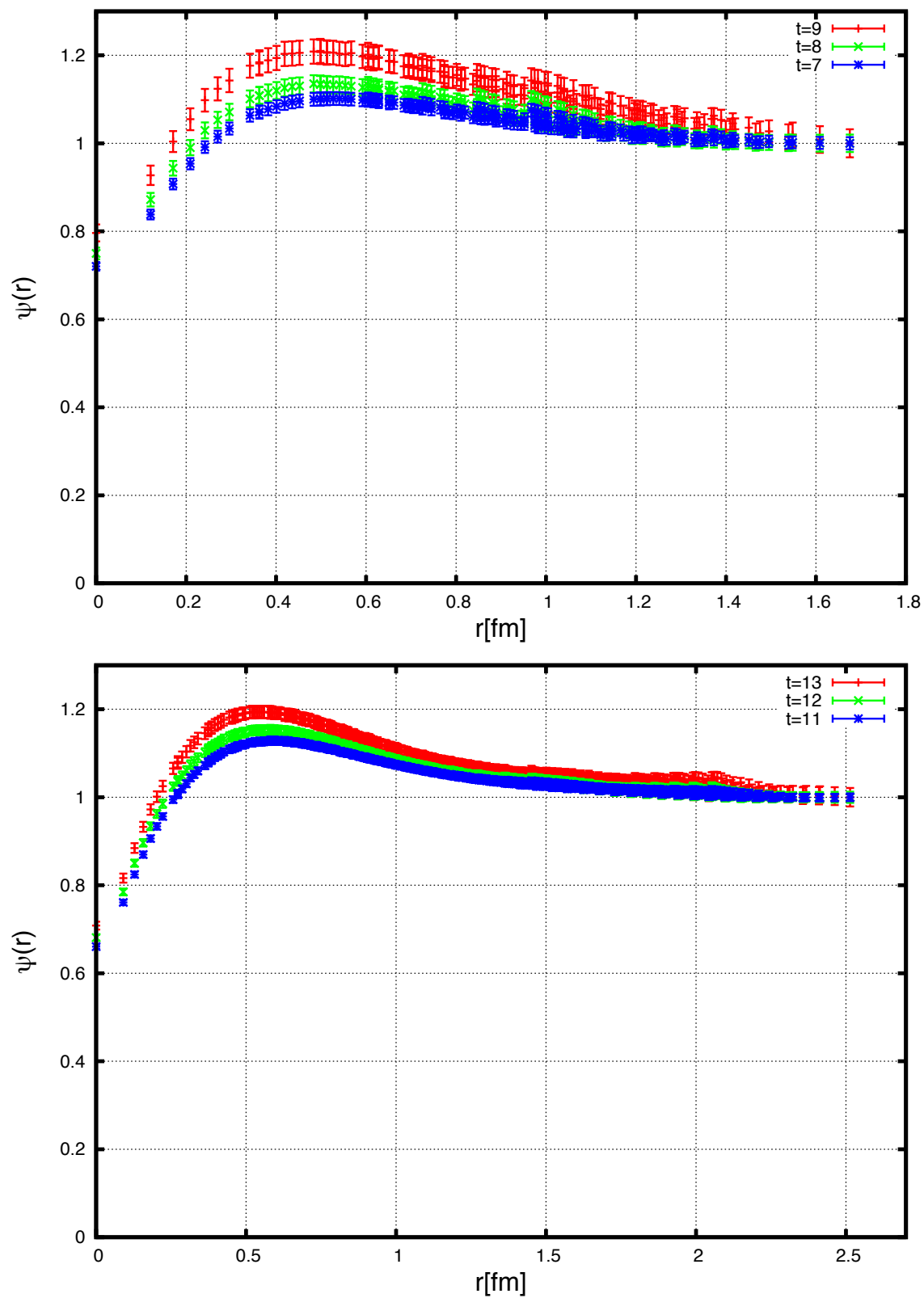


Figure 5.3: Top; NBS wave function at bin size = 1 in Set 1 at  $t - t_0 = 7, 8, 9$ . Bottom; NBS wave function at bin size = 1 in Set 2 at  $t - t_0 = 11, 12, 13$ .

## 5.4 Potential of the $\Omega - \Omega$

Shown in Fig. 5.4 are a part of the effective central potential with jackknife error at  $^1S_0$  channel in Set 1. We show the potential is derived as

$$\left(\frac{1}{m_N}\nabla^2 - \frac{\partial}{\partial t} + \frac{1}{4m_N}\frac{\partial^2}{\partial t^2}\right)R(t, t_0, r) = \int dr' U(r, r')R(t, t_0, r')dr'. \quad (5.3)$$

in section 2.7. We plot the laplacian part  $(\frac{1}{R}\frac{1}{m_N}\nabla^2 R)$ , time derivative part  $(\frac{1}{R}(-\frac{\partial}{\partial t} + \frac{1}{4m_N}\frac{\partial^2}{\partial t^2})R)$  and the total which is the effective central potential. The repulsive core is given by laplacian part and attractive pocket is caused both laplacian part and time derivative part. From this figure we find that the error of the time derivative part is larger than the error of the laplacian part because the time derivative part is used higher time slice as

$$\frac{\partial}{\partial t}f(t) \sim \frac{f(t+1) - f(t-1)}{2}. \quad (5.4)$$

Fig 5.5 represents the effective central potential at  $t = 7, 8, 9$  on Set 1, while Fig. 5.6 show the potential at  $t = 11, 12, 13$  on Set 2. Overall structures of potentials are similar to those of NN potentials previously obtained in the lattice QCD [10, 11, 12]. The effective central potential of the  $\Omega - \Omega$  has the repulsive core at short range and strong attractive pocket at medium range. We observe that  $t$  dependence is negligible for the potential on the Set 2 but the potential at  $t = 9$  on the Set 1 differs a litter from others, in particular at long distance. This  $t$  dependence of the potential on the Set 1 might be caused by the finite size effect due to the smaller volume of the Set 1 ( $L/2 = 0.96$  fm).

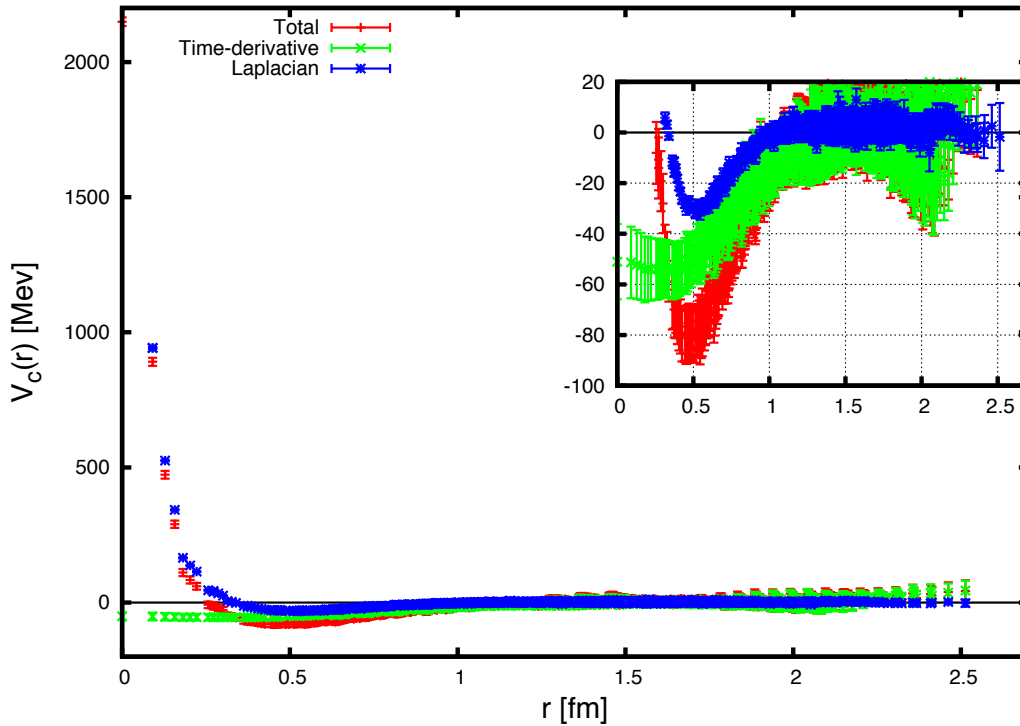


Figure 5.4: The effective central potential for Omega-Omega at  $t - t_0 = 12$  in Set 2, we separately plot Laplacian term(red), time derivative term(green) and total(blue).

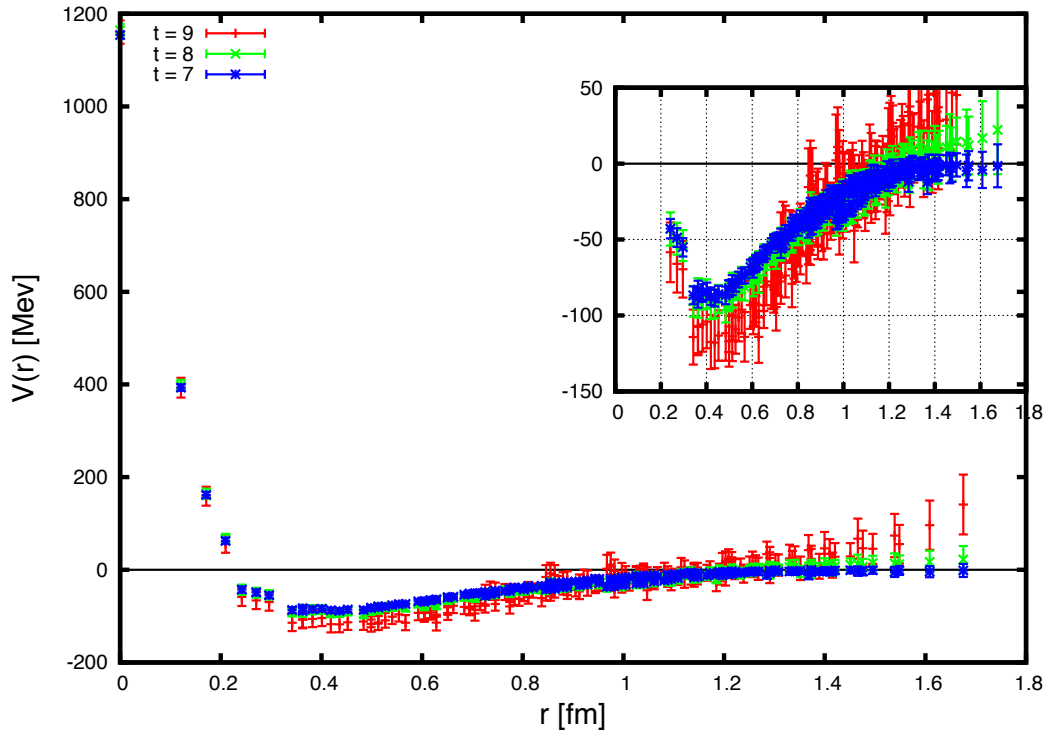


Figure 5.5: In Set 1, the Omega-Omega effective central potential in  $^1S_0$  channel at  $t - t_0 = 7, 8, 9$ .

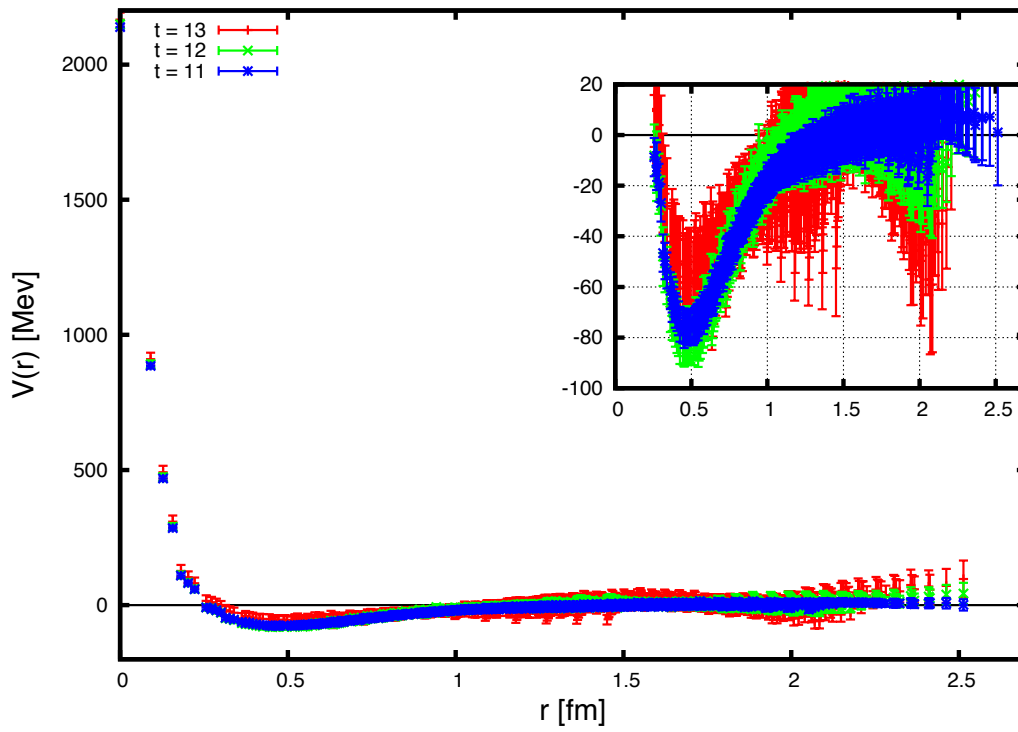


Figure 5.6: In Set 2, the Omega-Omega effective central potential in  $^1S_0$  at  $t - t_0 = 11, 12, 13$ .

## 5.5 Fitting of the potential

To calculate the phase shift, the binding energy and the scattering length, we fit the potential in Fig. 5.5 and Fig. 5.6 using the several different functional forms. The Gauss + (Yukawa) function given by

$$V(r) = a_1 e^{-a_2 r^2} + a_3 (1 - e^{-a_4 r^2}) \left( \frac{e^{-a_5 r}}{r} \right), \quad \lim_{r \rightarrow 0} V(r) = a_1, \quad (5.5)$$

the Gauss + (Yukawa)<sup>2</sup> function given by

$$V(r) = a_1 e^{-a_2 r^2} + a_3 (1 - e^{-a_4 r^2})^2 \left( \frac{e^{-a_5 r}}{r} \right)^2, \quad \lim_{r \rightarrow 0} V(r) = a_1, \quad (5.6)$$

the 2Gauss + (Yukawa)<sup>2</sup> function given by

$$V(r) = a_1 e^{-a_2 r^2} + a_3 e^{-a_4 r^2} + a_5 (1 - e^{-a_6 r^2})^2 \left( \frac{e^{-a_7 r}}{r} \right)^2, \quad \lim_{r \rightarrow 0} V(r) = a_1 + a_3. \quad (5.7)$$

Table 5.2 show the results of the fitting in Set 1. Because of chisq/dof, Gauss + (Yukawa)<sup>2</sup> function is better than Gauss + (Yukawa) function. In these functions, the long range part is mainly Yukawa and (Yukawa)<sup>2</sup> functions. The fit gives  $a_1 = 1.14(1) \times 10^3 \text{MeV}$ ,  $a_2 = 6.29(18) \times 10 \text{fm}^{-2}$ ,  $a_3 = -4.90(3.77) \times 10^2 \text{MeV}$ ,  $a_4 = 2.26(71) \text{fm}^{-2}$ ,  $a_5 = 1.47(33) \text{fm}^{-1}$  with  $\chi^2/\text{d.o.f} = 0.31(0.16)$  at  $t = 8$ , where errors are estimated by the Jack-Knife method with the bin size of 1 configurations.

Gauss + (Yukawa)

	$a_1 [\text{MeV}]$	$a_2 [\text{fm}^{-2}]$	$a_3 [\text{MeV}]$	$a_4 [\text{fm}^{-2}]$	$a_5 [\text{fm}^{-1}]$	chisq/dof
$t = 7$	$1.10(0.01) \times 10^3$	$5.41(0.12) \times 10$	$-3.15(0.33) \times 10^2$	$2.39(0.13)$	$2.60(0.20)$	$1.50(0.54)$
$t = 8$	$1.11(0.01) \times 10^3$	$5.34(0.21) \times 10$	$-3.26(0.53) \times 10^2$	$2.32(0.23)$	$2.52(0.32)$	$0.57(0.32)$
$t = 9$	$1.08(0.03) \times 10^3$	$4.78(0.44) \times 10$	$-4.46(0.90) \times 10^2$	$2.39(0.34)$	$2.69(0.49)$	$0.62(0.33)$

Gauss + (Yukawa)<sup>2</sup>

	$a_1 [\text{MeV}]$	$a_2 [\text{fm}^{-2}]$	$a_3 [\text{MeV}]$	$a_4 [\text{fm}^{-2}]$	$a_5 [\text{fm}^{-1}]$	chisq/dof
$t = 7$	$1.13(0.01) \times 10^3$	$6.33(0.13) \times 10$	$-3.84(3.41) \times 10^2$	$2.51(0.87)$	$1.42(0.41)$	$0.84(0.30)$
$t = 8$	$1.14(0.01) \times 10^3$	$6.26(0.18) \times 10$	$-4.90(3.77) \times 10^2$	$2.26(0.71)$	$1.47(0.33)$	$0.31(0.16)$
$t = 9$	$1.22(0.02) \times 10^3$	$6.04(0.35) \times 10$	$-6.00(2.93) \times 10^2$	$2.40(0.36)$	$1.51(0.33)$	$0.43(0.26)$

Table 5.2: Fitting parameters and chisq/dof at binsize = 1 in Set 1 .

For Set 2, we use the 2Gauss+(Yukawa)<sup>2</sup> type function whose chisq/dof is the smallest with chisq/dof = 0.50(0.35) at  $t - t_0 = 12$ . Table 5.3 show the results of the fitting in Set 2. We have adopted the 2Gauss + (Yukawa)<sup>2</sup> function, which gives  $a_1 = 1.69(6)10^3 \text{MeV}$ ,  $a_2 = 1.24(3)10^2 \text{fm}^{-2}$ ,  $a_3 = 4.44(68)10^2 \text{MeV}$ ,  $a_4 = 5.68(131) \text{fm}^{-2}$ ,  $a_5 = -7.06(1464)10^4 \text{MeV}$ ,  $a_6 = 6.25(577)10^{-1} \text{MeV}$ ,  $a_7 = 3.43(30) \text{MeV}$  at  $t - t_0 = 12$ . Using these function, we calculate the phase shift, binding energy and scattering length in next chapter.

2Gauss + (Yukawa)<sup>2</sup>

	$a_1 [\text{MeV}]$	$a_2 [\text{fm}^{-2}]$	$a_3 [\text{MeV}]$	$a_4 [\text{fm}^{-2}]$	$a_5 [\text{MeV}]$	$a_6 [\text{fm}^{-2}]$	$a_7 [\text{fm}^{-1}]$	chisq/dof
$t = 11$	$1.86(0.11) \times 10^3$	$1.16(0.11) \times 10^2$	$2.53(1.19) \times 10^2$	$1.73(1.24) \times 10$	$-2.88(3.00) \times 10^3$	$1.11(0.29)$	$2.12(0.50)$	$0.55(0.32)$
$t = 12$	$1.69(0.06) \times 10^3$	$1.24(0.03) \times 10^2$	$4.44(0.68) \times 10^2$	$5.68(1.31)$	$-7.06(14.64) \times 10^4$	$6.25(5.77) \times 10^{-1}$	$3.43(0.30)$	$0.50(0.35)$
$t = 13$	$1.63(0.29) \times 10^3$	$1.27(0.14) \times 10^2$	$5.23(3.13) \times 10^2$	$5.26(2.02)$	$-4.94(38.32) \times 10^5$	$2.79(8.45) \times 10^{-1}$	$3.72(1.01)$	$0.64(0.46)$

Table 5.3: Fitting parameters and chisq/dof at binsize = 1 in Set 2.



## 5.6 Phase shift, Binding energy and Scattering length

To calculate the phase shift and binding energy of the OmegaOmega system, we solve the Schrödinger equation in the infinite volume using the fitted potential in  $J^P = 0^+$  channel. From Eq. (B.11) we write the Schrödinger equation

$$\frac{\partial^2}{\partial r^2}\phi + \left(k^2 - \frac{l(l+1)}{r^2} - mV(r)\right)\phi(r) = 0, \quad (5.8)$$

where  $\phi(r) = r\psi(r)$ . Initial conditions are  $\phi(0) = 0$ ,  $\frac{\partial}{\partial r}\phi(r)|_{r=0} = 1$ . Let's derive these initial conditions. We assume  $\lim_{r \rightarrow 0}(V - E) = 0$  and  $\phi = Cr^\alpha$ . Eq. (5.8) is

$$(\alpha(\alpha - 1) - l(l + 1))Cr^{\alpha-2} = 0. \quad (5.9)$$

So  $\alpha = l + 1, -l$ . The regular solution at  $r = 0$  is  $\phi \propto r^{l+1}$ .

In Eq. (5.8), a radial wave function at asymptotic form as

$$\phi(r) = \frac{i}{2}(F_l(+k)\hat{h}_l^{(-)}(kr) - F_l(-k)\hat{h}_l^{(+)}(kr)), \quad S_l(k) \equiv \frac{F_l(-k)}{F_l(+k)} = e^{2i\delta_l}, \quad (5.10)$$

where  $\hat{h}_l^{(\pm)}$  is Hankel function,  $F_l(\pm k)$  is Jost function and  $\delta_l$  is the phase shift. To obtain the  $S_l(k)$  from  $F_l(\pm k)$ , we calculate  $\phi(r)$  and  $\frac{\partial}{\partial r}\phi(r)$  numerically, and solve the follow equation at large  $r$ .

$$\begin{pmatrix} \phi_l(r) \\ \frac{\partial}{\partial r}\phi_l(r) \end{pmatrix} = \begin{pmatrix} \hat{h}_l^{(-)}(kr) & -\hat{h}_l^{(+)}(kr) \\ \frac{\partial}{\partial r}\hat{h}_l^{(-)}(kr) & -\frac{\partial}{\partial r}\hat{h}_l^{(+)}(kr) \end{pmatrix} \begin{pmatrix} F_l(+k) \\ F_l(-k) \end{pmatrix}. \quad (5.11)$$

Since the S-matrix diverges at some  $k$ , corresponding to the binding energy, we can determine an existence of the bound state and its energy. Therefore we can estimate the phase shift and the binding energy.

As already explained, the phase shift and the binding energy can be extracted from lattice QCD by solving the Schrödinger equation involving the present potential in an infinite volume. Fig. 5.7 and Fig. 5.8 show the phase shift in the center of mass energy  $E$  at  $t = 7, 8, 9$  in Set 1 and  $t = 11, 12, 13$  in Set 2. The behavior of the phase shift in Set 1 (Fig. 5.7) suggests that the  $\Omega\Omega$  system has a bound state. On the other hand, the phase shift in Set 2 (Fig. 5.8) indicates that the  $\Omega\Omega$  system has strong attraction at low energy but bound state seems to exist only at  $t-t_0 = 12$ . At  $t-t_0 = 11$  and 13, the attraction is not strong enough to form a bound state.

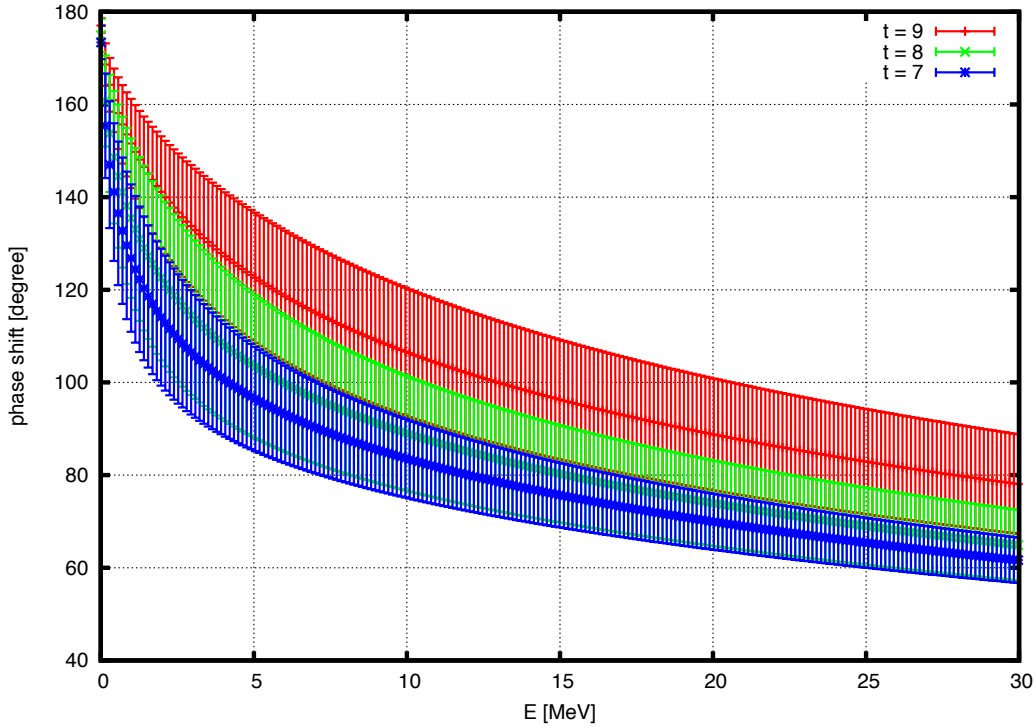


Figure 5.7: Phases-shifts of  $\Omega\Omega$  scattering as a function of energy in the center of mass frame, obtained from non-relativistic limit of lattice QCD in Set 1 in  $^1S_0$  channel at  $t - t_0 = 7, 8, 9$ .

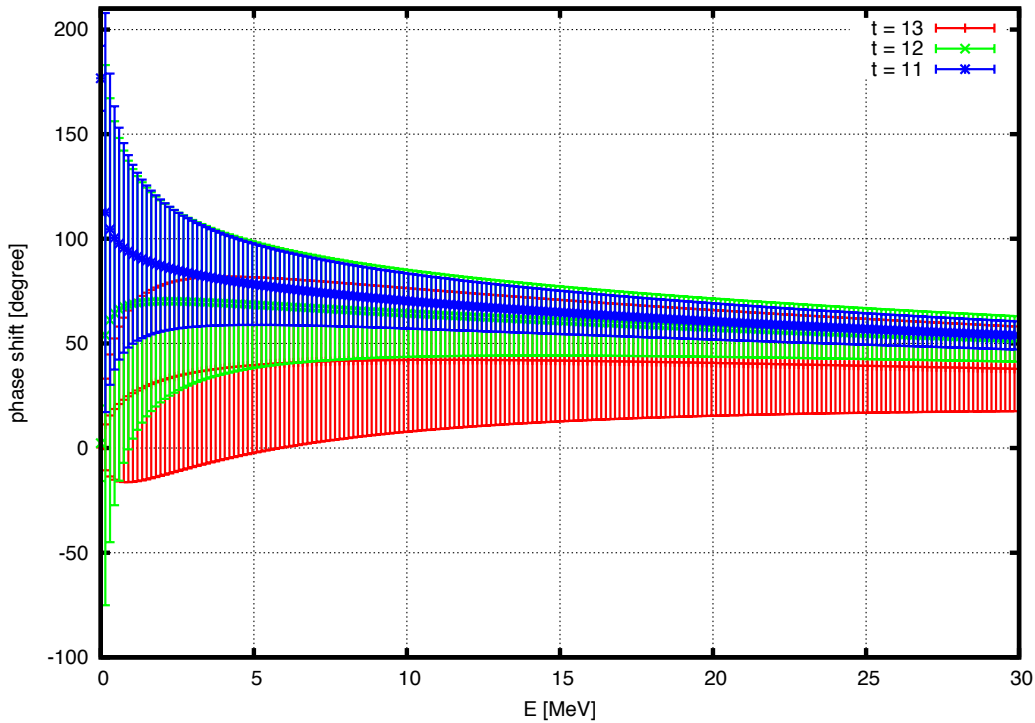


Figure 5.8: Phases-shifts of  $\Omega\Omega$  scattering as a function of energy in the center of mass, obtained from non-relativistic limit of lattice QCD in Set 2 in  $^1S_0$  channel at  $t - t_0 = 11, 12, 13$ .

We calculate the scattering length  $a$  and the effective range  $r_e$  using the asymptotic form of the wave function as

$$k \cot \delta(k) = \frac{1}{a} + \frac{1}{2}r_e k^2 + \mathcal{O}(k^4), \quad (5.12)$$

where  $k$  is related to the momentum. Table 5.4 show the scattering length  $a$  and the effective range  $r_e$  in Set 1. The Set 2 can't estimate the scattering length and the effective range due to large error bar.

Gauss + (Yukawa)<sup>2</sup>

	$a^{-1}$ [1/fm]	$r_e$ [fm]
$t = 7$	$-1.3(0.6) \times 10^{-4}$	1.0(0.1)
$t = 8$	$-9.8(5.3) \times 10^{-5}$	1.0(0.1)
$t = 9$	$-5.7(2.2) \times 10^{-5}$	$8.5(4.8) \times 10^{-1}$

Table 5.4: The scattering length and the effective range in Set 1 .

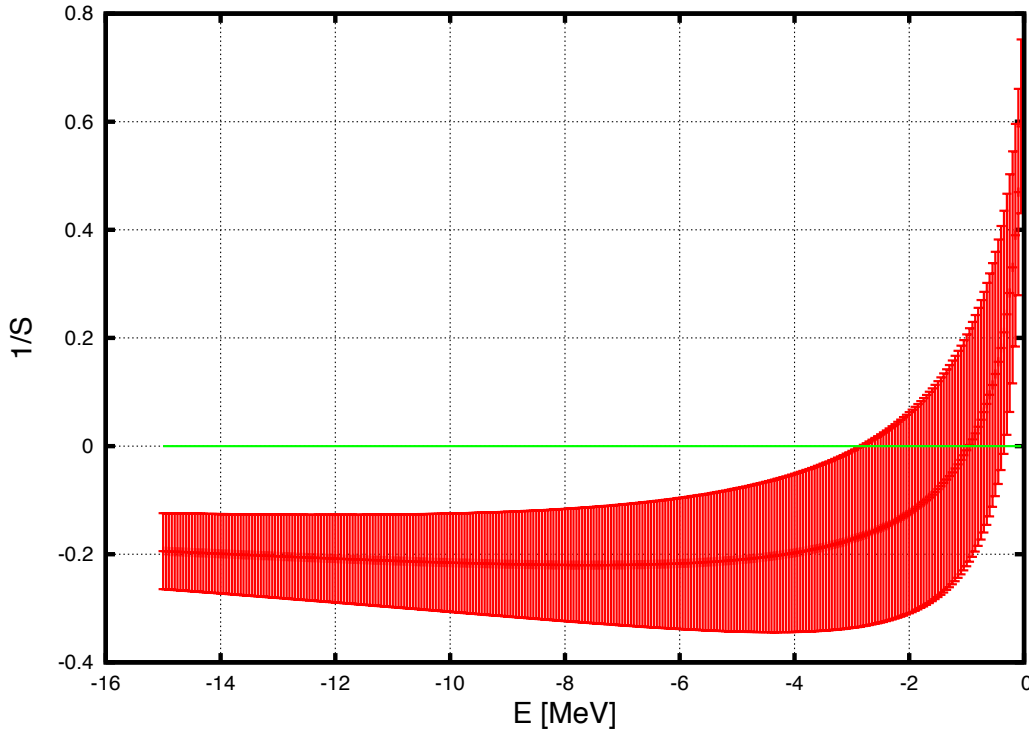


Figure 5.9: the energy dependence of the  $1/S$  in Set 1 at  $t - t_0 = 7$ .

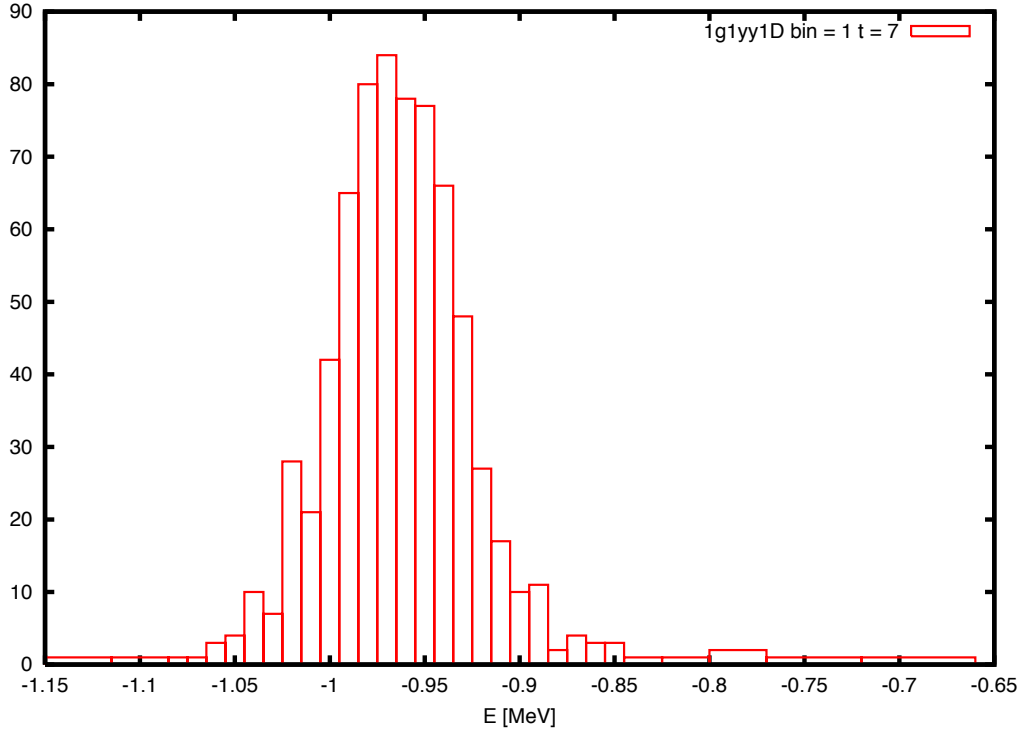


Figure 5.10: the histogram of the binding energy in Set 1 at  $t - t_0 = 7$ .

To estimate the binding energy, we search the divergence point of the S-matrix which is generated from bin sample of the fitted potential. Fig. 5.9 show the  $1/S$  at the energy in  $t = 7$  which is the shallowest binding energy. We find the divergence point at all bin sample in Set 1, it suggest  $^1S_0$  state of the  $\Omega\Omega$  has the bound state in Set 1 but, it's have a large error bars. We show the histogram of the binding energy at bin-sample in Fig 5.10. We show the binding energy in Table 5.5. These binding energies are very shallow.

Gauss + (Yukawa)<sup>2</sup>

	$E[\text{MeV}]$ with symmetric error
$t = 7$	$-0.96(1.06)$
$t = 8$	$-1.77(2.23)$
$t = 9$	$-6.69(6.81)$

Table 5.5: The binding energy with jackknife error using the Jack knife error at binsize = 1 in Set 1.

## 5.7 Effect of the periodic boundary in small volume

Because Set 1 is a small volume, we tried to fit the potential using effect of the periodic boundary as

$$\tilde{V}(\vec{r}) = \sum_{\vec{n} \in \mathbb{Z}^3} V(\vec{r} + L\vec{n}). \quad (5.13)$$

We fit data by using  $\tilde{V}(r)$  and  $\chi^2/\text{d.o.f}$  is reasonable. We compared in the potential, the effects of boundary conditions are on the middle distance Fig. 5.11. The difference between the short distance, it can not be determined whether the difference in the mass or the difference in cut-off. Finally, we show the periodic boundary effect of the phase shift Fig. 5.11. We estimate binding energy  $E = 0.15(0.31)$  MeV,

$E = 0.44(1.01)$  MeV,  $E = 3.91(4.75)$  MeV at  $t - t_0 = 7, 8, 9$  in bin size 1 analysis. There is still bound state and, the binding energy is smaller than when it does not take into account the boundary conditions.

Gauss + (Yukawa) with periodic boundary condition

	$a_1$ [MeV]	$a_2$ [fm $^{-2}$ ]	$a_3$ [MeV]	$a_4$ [fm $^{-2}$ ]	$a_5$ [fm $^{-1}$ ]	chisq/dof
$t = 7$	$1.09(0.01) \times 10^3$	$5.06(0.11) \times 10$	$-3.71(0.59) \times 10^2$	$2.59(0.35)$	$3.16(0.17)$	$2.23(0.70)$
$t = 8$	$1.10(0.02) \times 10^3$	$4.98(0.20) \times 10$	$-3.80(0.46) \times 10^2$	$2.53(0.33)$	$3.10(0.22)$	$0.93(0.44)$
$t = 9$	$1.05(0.04) \times 10^3$	$4.28(0.44) \times 10$	$-5.16(0.94) \times 10^2$	$2.65(0.54)$	$3.24(0.37)$	$0.91(0.38)$

Gauss + (Yukawa) $^2$  with periodic boundary condition

	$a_1$ [MeV]	$a_2$ [fm $^{-2}$ ]	$a_3$ [MeV]	$a_4$ [fm $^{-2}$ ]	$a_5$ [fm $^{-1}$ ]	chisq/dof
$t = 7$	$1.12(0.01) \times 10^3$	$6.13(0.10) \times 10$	$-8.81(2.02) \times 10^2$	$1.92(0.17)$	$1.88(0.11)$	$0.83(0.38)$
$t = 8$	$1.13(0.01) \times 10^3$	$6.06(0.17) \times 10$	$-8.72(3.15) \times 10^2$	$1.93(0.26)$	$1.83(0.18)$	$0.40(0.24)$
$t = 9$	$1.11(0.03) \times 10^3$	$5.79(0.35) \times 10$	$-9.10(4.60) \times 10^2$	$2.19(0.32)$	$1.82(0.32)$	$0.62(0.31)$

Table 5.6: Fitting parameters and chisq/dof at binsize = 1 in Set 1 considering the periodic boundary condition.

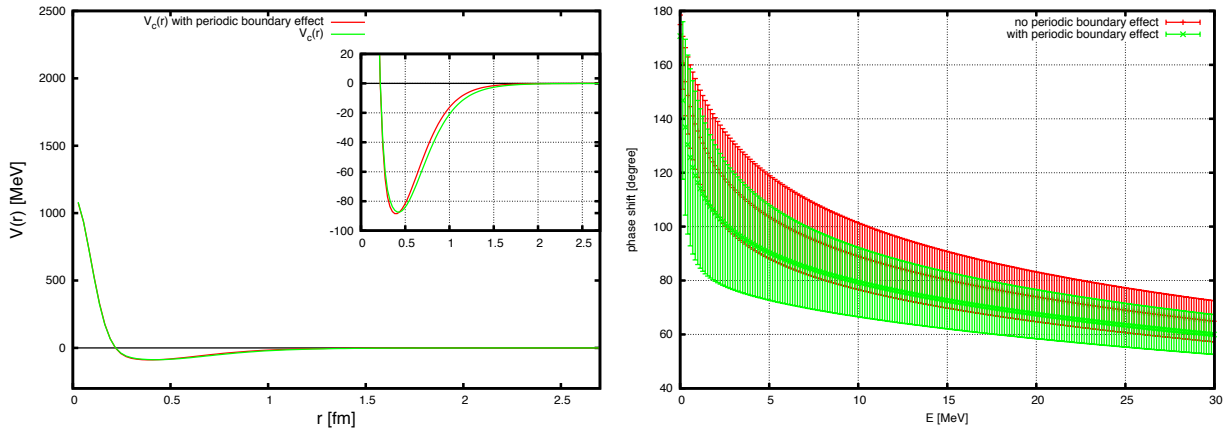


Figure 5.11: Left: Gauss + (Yukawa) $^2 V_c(r)$  and Gauss + (Yukawa) $^2$  include the periodic boundary effect  $\tilde{V}_c(r)$  in Set 1 at  $t = 8$ . Right: We plot phase shift  $\delta(k)$  from  $V_c(r)$  and  $\tilde{V}_c(r)$  in Set 1 at  $t = 8$ .

## Chapter 6

# Conclusion

In this paper, we have investigated the Omega-Omega interaction in  $J^P = 0^+$  channel with  $2 + 1$  flavor dynamical QCD by using the HAL QCD potential method which derive the QCD potential from lattice QCD. We used 2 simulation set up(Set 1 and Set 2). The effective central potential between Omega-Omega has a repulsive core at short range and deep attractive pocket at middle range. We estimate the binding energy and the phase shift by using the fitted potential, and we found the binding energy in Set 1(small volume) with large error bar. On the other hands, In Set 2(large volume), the Omega-Omega interaction is strong attraction but we can't estimate the bound state due to large error bar. Consequently, Omega-Omega system is strong attractive and it's in "unitary region" at low energy in these quark mass regions.

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## Appendix A

# Effective mass with periodic boundary condition

We explain that how to measure effective mass with periodic boundary condition. The periodic boundary condition is defined as

$$\langle \mathcal{O} \rangle_{pbc} = \sum_n \langle n | \mathcal{O} e^{iHT} | n \rangle \quad (\text{A.1})$$

The 2pt-correlator is defined by

$$\begin{aligned} \langle \phi(x)\phi(y) \rangle_{pbc} &= \sum_n \langle n | \phi(x)\phi(y) e^{iHT} | n \rangle \\ &= \langle 0 | \phi(x)\phi(y) e^{iHT} | 0 \rangle + \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x)\phi(y) e^{iHT} | E_n(p) \rangle. \end{aligned} \quad (\text{A.2})$$

Using completeness relation  $1 = |0\rangle \langle 0| + \sum_{k=0} \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_k} |E_k(p)\rangle \langle E_k(p)|$

$$\begin{aligned} \langle \phi(x)\phi(0) \rangle_{pbc} &= \sum_n \langle n | \phi(x)\phi(0) e^{iHT} | n \rangle = \langle 0 | \phi(x)\phi(0) e^{iHT} | 0 \rangle \\ &\quad + \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x)\phi(0) e^{iHT} | E_n(p) \rangle \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} \sum_x \langle 0 | \phi(x)\phi(y) | 0 \rangle_{pbc} &= \sum_x \langle 0 | \phi(x) | 0 \rangle \langle 0 | \phi(0) e^{iHT} | 0 \rangle \\ &\quad + \sum_x \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x) | 0 \rangle \langle 0 | \phi(0) e^{iHT} | E_n(p) \rangle \\ &\quad + \sum_x \sum_k \int \frac{d^3p'}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(x) | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | 0 \rangle \\ &\quad + \sum_x \sum_n \sum_k \int \frac{d^3p'}{(2\pi)^3} \frac{1}{2E_k} \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x) | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | E_n(p) \rangle \end{aligned} \quad (\text{A.4})$$

Removing the disconnect term  $\langle n | \mathcal{O} \mathcal{O} | n \rangle_{connect} = \langle n | \mathcal{O} \mathcal{O} | n \rangle - \langle n | \mathcal{O} | 0 \rangle \langle 0 | \mathcal{O} | n \rangle$



$$\begin{aligned}
\langle n | \mathcal{O} \mathcal{O} | n \rangle_{connect} &= \langle n | \mathcal{O} \mathcal{O} | n \rangle - \langle n | \mathcal{O} | 0 \rangle \langle 0 | \mathcal{O} | n \rangle \\
&= \sum_x \sum_n \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x) | 0 \rangle \langle 0 | \phi(0) e^{iHT} | E_n(p) \rangle \\
&\quad + \sum_x \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(x) | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | 0 \rangle \\
&\quad + \sum_x \sum_n \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x) | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | E_n(p) \rangle.
\end{aligned} \tag{A.5}$$

We show last term is vanish at large  $T$  because  $\mathcal{O}(e^{-E_n T})$

$$\begin{aligned}
&\sum_x \sum_n \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x) | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | E_n(p) \rangle \\
&= \sum_x \sum_n \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | e^{-i\hat{p}x} \phi(0) e^{i\hat{p}x} | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | E_n(p) \rangle \\
&= \sum_x \sum_n \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(0) | E_k(p') \rangle \langle E_k(p') | \phi(0) | E_n(p) \rangle e^{-ip_n x} e^{ip'_k x} e^{iE_n T}.
\end{aligned}$$

Using wick rotation

$$= \sum_x \sum_n \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(0) | E_k(p') \rangle \langle E_k(p') | \phi(0) | E_n(p) \rangle e^{p_n x} e^{-p'_k x} e^{-E_n T} \tag{A.6}$$

Due to this this term is  $\mathcal{O}(e^{-E_n T})$ . (another term is  $\mathcal{O}(e^{-\frac{1}{2}E_n T})$ ).

$$\begin{aligned}
&\sim \sum_x \sum_n \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(x) | 0 \rangle \langle 0 | \phi(0) e^{iHT} | E_n(p) \rangle \\
&\quad + \sum_x \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(x) | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | 0 \rangle \\
&= \sum_x \sum_n \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | e^{-i\hat{p}x} \phi(0) e^{i\hat{p}x} | 0 \rangle \langle 0 | \phi(0) e^{iHT} | E_n(p) \rangle \\
&\quad + \sum_x \sum_k \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | e^{-i\hat{p}x} \phi(0) e^{i\hat{p}x} | E_k(p') \rangle \langle E_k(p') | \phi(0) e^{iHT} | 0 \rangle \\
&= \sum_x \sum_n \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(0) | 0 \rangle \langle 0 | \phi(0) | E_n(p) \rangle e^{-ip'_n x} e^{iE_n T} \\
&\quad + \sum_x \sum_{k=0} \int \frac{d^3 p'}{(2\pi)^3} \frac{1}{2E_k} \langle 0 | \phi(0) | E_k(p') \rangle \langle E_k(p') | \phi(0) | 0 \rangle e^{ip'_k x} \\
&= \sum_x \sum_n \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(0) | 0 \rangle \langle 0 | \phi(0) | E_n(p) \rangle (e^{ip'_n x} + e^{-ip_n x} e^{iH_n T}).
\end{aligned}$$

Using wick rotation

$$\begin{aligned}
&= \sum_x \sum_n \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E_n} \langle E_n(p) | \phi(0) | 0 \rangle \langle 0 | \phi(0) | E_n(p) \rangle (e^{-p_n x} + e^{p_n x} e^{-E_n T}) \\
&= \sum_n \int d^3 p \frac{1}{2E_n} \langle E_n(p) | \phi(0) | 0 \rangle \langle 0 | \phi(0) | E_n(p) \rangle (e^{-E_n t} + e^{E_n t} e^{-E_n T}) \delta^3(p) \\
&= \sum_n \frac{1}{2E_n} \langle E_n(0) | \phi(0) | 0 \rangle \langle 0 | \phi(0) | E_n(0) \rangle (e^{-E_n t} e^{E_n \frac{T}{2}} + e^{E_n t} e^{E_n \frac{T}{2}}) e^{-E_n \frac{T}{2}}.
\end{aligned} \tag{A.7}$$

Remain only  $n = 0$  at large  $T$

$$\begin{aligned}
&\sim \frac{1}{2m_0} |\langle 0 | \phi(0) | m_0(0) \rangle|^2 (e^{-m_0 t} e^{m_0 \frac{T}{2}} + e^{m_0 t} e^{-m_0 \frac{T}{2}}) e^{-m_0 \frac{T}{2}} \\
&= \frac{1}{m_0} |\langle 0 | \phi(0) | m_0(0) \rangle|^2 \cosh(m_0(t - \frac{T}{2})) e^{-m_0 \frac{T}{2}}.
\end{aligned} \tag{A.8}$$

Finally we measure effective mass using  $\cosh(m_0(t - \frac{T}{2}))$  in periodic boundary condition.

# Appendix B

## NBS wave function and phase shift

In this appendix we derive the behavior of the NBS wave function which contain the information of the phase shift at asymptotic region. First we introduce the phase shift in Quantum mechanics, Second we introduce how to define the phase shift in Quantum field theory, Finally we show asymptotic form of the NBS wave function.

### B.1 Phase shift in Quantum mechanics

In this chapter, we study how to define the phase shift in quantum mechanics. Considering the central potential  $V(r)$  where  $r = |\vec{r}|$ . Let's start from Schrödinger equation

$$(\nabla^2 + k^2)\psi(x) = \Delta(r)\psi(x), \quad (\text{B.1})$$

where

$$\Delta(r) \equiv \frac{\hbar^2}{2m}V(r), \quad E \equiv \frac{\hbar^2}{2m}k^2. \quad (\text{B.2})$$

We consider this equation in polar coordinates

$$\Delta = \left(\frac{d}{dr}\right)^2 + \frac{2}{r}\frac{d}{dr} - \frac{L^2}{r^2} = \frac{1}{r}\left(\frac{d}{dr}\right)^2 r - \frac{L^2}{r^2}, \quad (\text{B.3})$$

where angular momentum operator is

$$L \equiv -i\vec{r} \times \frac{\partial}{\partial \vec{r}}. \quad (\text{B.4})$$

Eigenvalue problem on angular momentum operator

$$L^2 Y_{lm}(\theta, \phi) = l(l+1)Y_{lm}(\theta, \phi), \quad (\text{B.5})$$

$$L_z Y_{lm}(\theta, \phi) = mY_{lm}(\theta, \phi), \quad (\text{B.6})$$

where spherical harmonics  $Y_{lm}(\theta, \phi)$  is

$$Y_{lm}(\theta, \phi) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos \theta) \frac{1}{\sqrt{2\pi}} e^{im\phi}. \quad (\text{B.7})$$

The potential  $V(r)$  does not dependent on  $(\theta, \phi)$

$$[L, V(r)] = 0. \quad (\text{B.8})$$

Therefore angular momentum is conserved value. Additionally we take the input axis on the z-direction. We assume the solution which is symmetric around z-axis

$$\psi(\vec{r}) = \sum_{l=0}^{\infty} C_l R_l(r) Y_{l0}(\theta, \phi). \quad (\text{B.9})$$

The partial wave satisfy

$$\left[ \left( \frac{d}{dr} \right)^2 + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} - \Delta(r) + k^2 \right] R_l(r) = 0. \quad (\text{B.10})$$

We can rewrite this equation using  $R_l(r) \equiv \frac{\psi_l(r)}{r}$

$$\left[ \left( \frac{d}{dr} \right)^2 - \frac{l(l+1)}{r^2} - \Delta(r) + k^2 \right] \psi_l(r) = 0. \quad (\text{B.11})$$

First we assume the free system  $V(r) = 0$  for considering the plane wave which is not affected by the potential.

$$\left[ \left( \frac{d}{d\rho} \right)^2 - \frac{l(l+1)}{\rho^2} + 1 \right] \psi_l(\rho) = 0, \quad (\text{B.12})$$

where we define  $\rho \equiv kr$ . We know two Linearly independent solutions of this equation

$$j_l(\rho) = (-1)^l \rho^l \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^l \frac{\sin \rho}{\rho}, \quad (\text{B.13})$$

$$n_l(\rho) = (-1)^{l+1} \rho^l \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^l \frac{\cos \rho}{\rho}, \quad (\text{B.14})$$

where  $j_l(\rho)$  is called Bessel function and  $n_l(\rho)$  is called Neumann function. Properties of these functions are

$$j_l(\rho \rightarrow \infty) \sim \frac{1}{\rho} \sin\left(\rho - \frac{\pi}{2}l\right), \quad (\text{B.15})$$

$$n_l(\rho \rightarrow \infty) \sim -\frac{1}{\rho} \cos\left(\rho - \frac{\pi}{2}l\right), \quad (\text{B.16})$$

$$j_l(\rho \rightarrow 0) \sim \frac{\rho^l}{(2l+1)!!}, \quad (\text{B.17})$$

$$n_l(\rho \rightarrow 0) \sim -\frac{(2l-1)!!}{\rho^{l+1}}, \quad (\text{B.18})$$

where  $(2l-1)!! = \frac{(2l+1)!!}{2l+1}$  and  $1!! = 1$ . The solution in Eq. (B.12)

$$e^{ik \cdot z} = e^{ikr \cos \theta} = \sum_{l=0}^{\infty} C_l j_l(kr) P_l(\cos \theta). \quad (\text{B.19})$$

$e^{ik \cdot z}$  is the solution which is symmetric around z-axis and it is regular at  $\rho = 0$ , due to this we can perform the partial wave expansion. We note that  $n_l(\rho)$  is not regular at  $\rho = 0$ . To decide the value of  $C_l$ , we consider the orthogonality of the Legendre polynomial

$$\int_{-1}^1 d(\cos \theta) P_l(\cos \theta) P_{l'}(\cos \theta) = \delta_{l,l'} \frac{2}{2l+1}. \quad (\text{B.20})$$

Using the Eq. (B.19), we leads to the following relation

$$C_l j_l(\rho) = \frac{2l+1}{2} \int_{-1}^1 d(\cos \theta) e^{i\rho \cos \theta} P_l(\cos \theta). \quad (\text{B.21})$$

We perform the integration by parts to the right-hand side using  $x = \cos \theta$  at  $\rho \rightarrow \infty$

$$\int_{-1}^1 dx e^{i\rho x} P_l(x) = \frac{1}{i\rho} e^{i\rho x} P_l(x) \Big|_{-1}^1 - \frac{1}{i\rho} \int_{-1}^1 dx e^{i\rho x} P_l'(x). \quad (\text{B.22})$$

The second term is  $\mathcal{O}(\frac{1}{\rho^2})$  at left hand side. Comparing the first term and Eq. (B.15), we can decide the value of the  $C_l$  is

$$C_l = (2l+1)i^l. \quad (\text{B.23})$$

As a results, it is possible to determine the asymptotic form of the wave function at  $\rho \rightarrow \infty$ . Next let's consider Spherical potential  $V(r) \neq 0$ . Similarly the  $V(r) = 0$  case, we perform the partial wave expansion.

$$\psi(\vec{r}) = \sum_{l=0}^{\infty} A_l R_l(r) P_l(\cos \theta) \quad (\text{B.24})$$

Asymptotic form of the  $R_l(r)$  at  $r \rightarrow \infty$  is linear combination

$$j_l(\rho \rightarrow \infty) \sim \frac{1}{\rho} \sin(\rho - \frac{\pi}{2}l), \quad (\text{B.25})$$

$$n_l(\rho \rightarrow \infty) \sim -\frac{1}{\rho} \cos(\rho - \frac{\pi}{2}l). \quad (\text{B.26})$$

The regular solution at  $r \rightarrow 0$  is linear combination  $\sin(\rho - \frac{\pi}{2}l)$  and  $\cos(\rho - \frac{\pi}{2}l)$

$$R_l(r) \sim \frac{1}{kr} \sin(kr - \frac{\pi}{2}l + \delta_l). \quad (\text{B.27})$$

where  $\delta_l$  is phase shift. For  $\delta_l = 0$  at  $\Delta(r) = 0$ , we add  $-\frac{l}{2}$ . In other words  $R_l(r) = j_l(kr)$  at  $\Delta(r) = 0$ . Finally we check the role of the phase shift  $\delta_l$  in scattering theory. For Eq. (B.24)

$$\psi(\vec{r}) \sim \sum_{l=0}^{\infty} (2l+1) A_l P_l(\cos \theta) \frac{1}{kr} \sin(kr - \frac{\pi}{2}l + \delta_l) \quad (\text{B.28})$$

$$= \sum_{l=0}^{\infty} (2l+1) A_l P_l(\cos \theta) \frac{i}{2kr} [e^{-i(kr - \frac{\pi}{2}l + \delta_l)} - e^{i(kr - \frac{\pi}{2}l + \delta_l)}]. \quad (\text{B.29})$$

The plane wave coming incident is

$$e^{ik \cdot z} = \sum_{l=0}^{\infty} (2l+1) i^l P_l(\cos \theta) \frac{i}{2kr} [e^{-i(kr - \frac{\pi}{2}l)} - e^{i(kr - \frac{\pi}{2}l)}]. \quad (\text{B.30})$$

The scattering wave which is spherical wave is a difference between the plane wave and the wave that has passed through the potential. Asymptotic form of the scattering wave at  $r \rightarrow \infty$  is

$$\psi(r) - e^{ik \cdot z} = f(\theta) \frac{e^{ikr}}{r}. \quad (\text{B.31})$$

Using Eq. (B.29) and Eq. (B.30), we can decide  $A_l e^{-i\delta_l} = i^l$ . The wave that has passed through the potential at asymptotic state is

$$\begin{aligned}\psi(\vec{r}) &\sim \sum_{l=0}^{\infty} (2l+1) i^l P_l(\cos\theta) \frac{i}{2kr} [e^{-i(kr-\frac{\pi}{2}l)} - e^{2i\delta_l} e^{i(kr-\frac{\pi}{2}l)}] \\ &= \frac{i}{2kr} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) [(-1)^l e^{-ikr} - S_l e^{ikr}],\end{aligned}\quad (\text{B.32})$$

where  $S_l \equiv e^{2i\delta_l}$  called S-matrix. We derive the  $f(\theta)$  in Eq. (B.31).

$$\begin{aligned}\psi(r) - e^{ik \cdot z} &\sim \frac{i}{2kr} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) (1 - S_l) e^{ikr} \\ &= \sum_{l=0}^{\infty} (2l+1) \frac{S_l - 1}{2ik} P_l(\cos\theta) (1 - S_l) \frac{e^{ikr}}{r} \\ &\equiv f(\theta) \frac{e^{ikr}}{r},\end{aligned}\quad (\text{B.33})$$

where

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos\theta) \quad (\text{B.34})$$

$$f_l \equiv \frac{S_l - 1}{2ik} = e^{i\delta_l} \frac{1}{k} \sin \delta_l. \quad (\text{B.35})$$

The  $f(\theta)$  is corresponding to T-matrix and  $f_l$  is partial wave of the  $f(\theta)$

$$f_l = \frac{1}{2} \int_{-1}^1 d(\cos\theta) f(\theta) P_l(\cos\theta). \quad (\text{B.36})$$

The total scattering cross-section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \left| \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos\theta) \right|^2 \quad (\text{B.37})$$

$$\begin{aligned}\sigma &= \int \frac{d\sigma}{d\Omega} d\Omega \\ &= 4\pi \sum_{l=0}^{\infty} (2l+1) |f_l|^2 \\ &= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |S_l - 1|^2 \\ &= \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) (\sin \delta_l)^2.\end{aligned}\quad (\text{B.38})$$

## B.2 T-matrix and Phase shift in Quantum field theory

In this chapter we define the phase shift in quantum field theory by using the unitarity of the S-matrix. The S-matrix and T-matrix are

$$S = 1 + iT. \quad (\text{B.39})$$

The unitarity of the S-matrix is

$$S^\dagger S = 1. \quad (\text{B.40})$$

Using Eq. (B.39) and Eq. (B.40), we can derive

$$T - T^\dagger = iT^\dagger T. \quad (\text{B.41})$$

Sandwiching the both sides in the final state and the initial state

$$\langle f|T|i\rangle - \langle f|T^\dagger|i\rangle = i\langle f|T^\dagger T|i\rangle. \quad (\text{B.42})$$

Using the completeness relation as

$$\langle f|T|i\rangle - \langle f|T^\dagger|i\rangle = i\sum_n \langle f|T^\dagger|n\rangle \langle n|T|i\rangle. \quad (\text{B.43})$$

For simplicity we consider the scattering system of the scalars for calculate the T-matrix Fig. B.1.

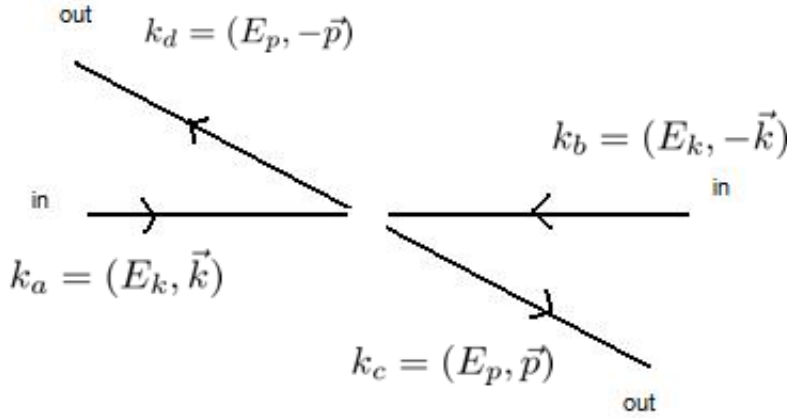


Figure B.1: The scattering system of the 2 scalar fields in center of mass system. The initial states are  $k_a = (E_k, \vec{k})$  and  $k_b = (E_k, -\vec{k})$ , the final states are  $k_c = (E_p, \vec{p})$  and  $k_d = (E_p, -\vec{p})$ . Mass of the all scalar fields are  $m$ .

The initial states are  $k_a = (E_k, \vec{k})$  and  $k_b = (E_k, -\vec{k})$ , the final states are  $k_c = (E_p, \vec{p})$  and  $k_d = (E_p, -\vec{p})$ . The  $k_a, k_b, k_c, k_d$  are satisfied the on-shell. We define the  $T(p, q)$

$$\langle k_c k_d | T | k_a k_b \rangle = (2\pi)^4 \delta^4(k_a + k_b - k_c - k_d) T(p, q) \quad (\text{B.44})$$

Using

$$\langle f| = \langle k_c, k_d| \quad , |i\rangle = |k_a k_b\rangle, \quad (\text{B.45})$$

$$\sum_n |n\rangle \langle n| = \int \frac{d^3 q_1 d^3 q_2}{(2\pi)^3 2E_{q_1} (2\pi)^3 2E_{q_2}} |q_1 q_2\rangle \langle q_1 q_2|. \quad (\text{B.46})$$

We can derive

$$\text{LHS} = (2\pi)^4 \delta^4(k_a + k_b - k_c - k_d) (T(\vec{p}, \vec{k}) - T^\dagger(\vec{p}, \vec{k})), \quad (\text{B.47})$$

$$\begin{aligned} \text{RHS} &= i \int \frac{d^3 q_1 d^3 q_2}{(2\pi)^3 2E_{q_1} (2\pi)^3 2E_{q_2}} \langle k_c k_d | T^\dagger | q_1 q_2 \rangle \langle q_1 q_2 | T | k_a k_b \rangle . \\ &= i \int \frac{d^3 q_1 d^3 q_2}{4E_{q_1} E_{q_2}} (2\pi)^2 \delta^3(\vec{k}_c + \vec{k}_d - \vec{q}_1 - \vec{q}_2) \delta^3(\vec{q}_1 + \vec{q}_2 - \vec{k}_a - \vec{k}_b) \\ &\quad \delta(E_p + E_p - E_{q_1} - E_{q_2}) \delta(E_k + E_k - E_{q_1} - E_{q_2}) T^\dagger(\vec{p}, \vec{q}) T(\vec{q}, \vec{k}) \\ &= i \int \frac{d^3 q_1}{4E_q^2} (2\pi)^2 \delta^3(\vec{k}_c + \vec{k}_d - \vec{k}_a - \vec{k}_b) \delta(2E_k - 2E_q) \delta(E_k + E_k - E_{q_1} - E_{q_2}) T^\dagger(\vec{p}, \vec{q}) T(\vec{q}, \vec{k}) \\ &= i \int \frac{dk d\Omega_q k^2}{4E_q^2} (2\pi)^2 \delta^3(\vec{k}_c + \vec{k}_d - \vec{k}_a - \vec{k}_b) \delta(2E_k - 2E_q) \delta(E_k + E_k - E_{q_1} - E_{q_2}) T^\dagger(\vec{p}, \vec{q}) T(\vec{q}, \vec{k}) \\ &= (2\pi)^4 \delta^4(k_a + k_b - k_c - k_d) \frac{ik}{32\pi^2 E_k} \int d\Omega_q T^\dagger(\vec{p}, \vec{q}) T(\vec{q}, \vec{k}). \end{aligned} \quad (\text{B.48})$$

We use the definition of the  $T(p, q)$  at the 2nd line and using the polar coordinates at 4th line. Comparing the both sides we derive

$$T(\vec{p}, \vec{k}) - T^\dagger(\vec{p}, \vec{k}) = \frac{ik}{32\pi^2 E_k} \int d\Omega_q T^\dagger(\vec{p}, \vec{q}) T(\vec{q}, \vec{k}). \quad (\text{B.49})$$

We divide the radial and angular direction using Spherical harmonics  $Y_{lm}(\Omega_p)$  and complex representation  $\overline{Y_{lm}(\Omega_k)}$ .

$$T(\vec{p}, \vec{q}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l T_l(k) Y_{lm}(\Omega_p) \overline{Y_{lm}(\Omega_k)} \quad (\text{B.50})$$

Spherical harmonics  $Y_{lm}(\Omega_p)$  satisfy the orthonormal relationship

$$\int d\Omega_q \overline{Y_{lm}(\Omega_q)} Y_{l'm'}(\Omega_q) = \delta_{l,l'} \delta_{m,m'}. \quad (\text{B.51})$$

Eq. (B.49) is

$$\text{LHS} = T(\vec{p}, \vec{q}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l [Y_{lm}(\Omega_p) \overline{Y_{lm}(\Omega_k)} T_l(k) - Y_{lm}(\Omega_p) \overline{Y_{lm}(\Omega_k)} T_l(k)], \quad (\text{B.52})$$

where  $T^\dagger(\vec{p}, \vec{k}) = \overline{T(\vec{k}, \vec{p})}$ .

$$\text{RHS} = (4\pi)^2 \sum_{l'} \sum_{m'} \frac{ik}{32\pi^2 E_k} \int d\Omega_q [\overline{T_l(k)} T_{l'}(k) \overline{Y_{lm}(\Omega_q)} Y_{lm}(\Omega_p) Y_{l'm'}(\Omega_q) \overline{Y_{l'm'}(\Omega_k)}] \quad (\text{B.53})$$

Comparing these equations, we can derive.

$$T_l(k) - \overline{T_l(k)} = i \frac{k}{8\pi E_k} \overline{T_l(k)} T_l(k) \quad (\text{B.54})$$

It is possible to derive the  $T_l(k)$  which satisfy Eq. (B.54)

$$T_l(k) = \frac{16\pi E_k}{k} e^{i\delta_l(k)} \sin \delta_l(k). \quad (\text{B.55})$$

It is the definition of the phase shift  $\delta_l(k)$ . In this section we can define the phase shift  $\delta_l(k)$  by using only unitarity of the S-matrix.



### B.3 Asymptotic form of the NBS wave function

In this chapter, we derive the behavior of the NBS wave function at large  $r$ . NBS wave has the same asymptotic form of the scattering wave in quantum mechanics, because NBS wave function has T-matrix at asymptotic state, and the phase shift  $\delta_l$  is the defined by T-matrix.

$$\psi(r \rightarrow \infty) \sim Z_\pi \frac{e^{i\delta_l}}{kl} \sin(kr - \frac{\pi l}{2} + \delta_l(k)) \quad (\text{B.56})$$

For simplicity we consider the scalar field, let us consider NBS wave function amplitude, defined by

$$\Psi_{\alpha\beta}(r, t) = \langle 0 | \pi_\alpha(x+r, t) \pi_\beta(x, t) | k_a, a, k_b, b; in \rangle \quad (\text{B.57})$$

Using completeness relation

$$1 = \sum_c \int \frac{d^3p}{(2\pi)^3 2p_0} |\vec{p}, c; out\rangle \langle \vec{p}, c; out| + \sum_X \frac{|X; out\rangle \langle X; out|}{2E_X}, \quad (\text{B.58})$$

we can divide the elastic wave function  $\psi^{elastic}$  and the inelastic wave function  $\psi^{inelastic}$

$$\psi(r) = \psi^{elastic} + \psi^{inelastic}, \quad (\text{B.59})$$

where

$$\psi^{elastic} = \sum_b \int \frac{d^3p}{(2\pi)^3 2p_0} \langle 0 | \pi_\alpha(x+r, t) | \vec{p}, b; out \rangle \langle \vec{p}, b; out | \pi_\beta(x, t) | \vec{k}, a, -\vec{k}, b; in \rangle, \quad (\text{B.60})$$

$$\psi^{inelastic} = \sum_X \langle 0 | \pi_\alpha(x+r, t) | X; out \rangle \frac{1}{2E_X} \langle X; out | \pi_\beta(x, t) | k_a, a, k_b, b; in \rangle \quad (\text{B.61})$$

and  $|X\rangle$  is not 1 particle state. The  $\langle 0 | \pi_\alpha(x+r, t) | \vec{p}, b; out \rangle$  is

$$\begin{aligned} \langle 0 | \pi_\alpha(x+r, t) | \vec{p}, b; out \rangle &= \langle 0 | e^{i\hat{p}\cdot x} \pi_\alpha(0) e^{-i\hat{p}\cdot(x+r)} | \vec{p}, b; out \rangle \\ &= \langle 0 | \pi_\alpha(0) | \vec{p}, b; out \rangle e^{-i\hat{p}\cdot(x+r)} \\ &= \langle 0 | U^{-1} U \pi_\alpha(0) U^{-1} U | \vec{p}, b; out \rangle e^{-i\hat{p}\cdot(x+r)} \\ &= \sqrt{Z_\pi} \delta_{ab} e^{i\vec{p}\cdot(\vec{x}+\vec{r})} e^{-ip_0 t}, \end{aligned} \quad (\text{B.62})$$

where  $Z_\pi$  is renormalized factor and we use Lorentz transformation  $U \in SO(3+1)$  in 3rd line

$$\langle 0 | U^{-1} = \langle 0 |, \quad (\text{B.63})$$

$$U \pi(0) U^{-1} = \pi(0). \quad (\text{B.64})$$

Elastic part of the NBS wave function can rewrite

$$\psi^{elastic}(\vec{r}) = \sqrt{Z_\pi} \int \frac{d^3p}{(2\pi)^3 2p_0} e^{i\vec{p}\cdot(\vec{x}+\vec{r})} e^{-ip_0 t} \langle p, a; out | \pi_b(x, t) | \vec{k}, a, -\vec{k}, b; in \rangle. \quad (\text{B.65})$$

Using NZH reduction formula Appendix G, we rewrite from the n-pt correlator to T-matrix.

$$\langle p, a; out | \pi_b(x, t) | \vec{k}, a, -\vec{k}, b; in \rangle = \langle 0 | a_{out}(\vec{p}) \pi_b(x, t) | \vec{k}, a, -\vec{k}, b; in \rangle$$

$$+i \int d^4x_1 f_p^*(x_1) (\square + m_\pi^2) < 0 | T(\pi_a(x_1) \pi_b(x, t)) | \vec{k}, a, -\vec{k}, b; in >. \quad (\text{B.66})$$

The 1st term in Eq. (B.66) is free part. We use NZH reduction formula again.

$$\begin{aligned} < 0 | T(\pi_a(x_1) \pi_b(x, t)) | \vec{k}, a, -\vec{k}, b; in > &= < 0 | T(\pi_a(x_1) \pi_b(x, t)) a_{in}^\dagger(\vec{k}_a) | -\vec{k}, b; in > \\ &= < 0 | a_{out}^\dagger(\vec{k}_a) T(\pi_a(x_1) \pi_b(x, t)) | -\vec{k}, b; in > \\ &- i \int d^4x_2 f_{k_a}(x_2) (\square + m_\pi^2) < 0 | T(\pi_a(x_1) \pi_b(x, t) \pi_a^\dagger(x_2)) | -\vec{k}, b; in > \end{aligned} \quad (\text{B.67})$$

Similarly this, we rewrite the 2nd term in Eq. (B.66)

$$\begin{aligned} < p, a; out | \pi_b(x, t) | \vec{k}, a, -\vec{k}, b; in > &= -i \int d^4x_1 d^4x_2 d^4x_3 f_p^*(x_1) f_{k_a}(x_2) f_{k_b}(x_3) \\ &\times (\square_1 + m_\pi^2) (\square_2 + m_\pi^2) (\square_3 + m_\pi^2) < 0 | T(\pi_a(x_1) \pi_b(x, t) \pi_a^\dagger(x_2) \pi_b^\dagger(x_3)) | 0 >, \end{aligned} \quad (\text{B.68})$$

where  $\square_1$  act only  $x_1$ .

$$\begin{aligned} < p, a; out | \pi_b(x, t) | \vec{k}, a, -\vec{k}, b; in > &= -i(-p^2 + m_\pi^2) \\ &< 0 | T(\pi_a(p) \pi_b(x) \pi_a^\dagger(k_a) \pi_b^\dagger(k_b)) | 0 > (-k_a^2 + m_\pi^2) (-k_b^2 + m_\pi^2) \\ &= \sqrt{Z_\pi} \frac{e^{-iq \cdot x}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}(p, q, k_a, k_b). \end{aligned} \quad (\text{B.69})$$

We note that  $\hat{T}(p, q, k_a, k_b)$  is half-shell ( $q$  is off-shell). Next we calculate the 1st term in Eq. (B.66)

$$< 0 | a_{out}(\vec{p}) \pi_b(x, t) | \vec{k}, a, -\vec{k}, b; in > = \sqrt{Z_\pi} 2k^0 (2\pi)^3 \delta^3(\vec{p} - \vec{k}) e^{-ik \cdot x}. \quad (\text{B.70})$$

We substitute Eq. (B.69) and Eq. (B.70) for Eq. (B.65)

$$\psi^{elastic}(\vec{r}) = Z_\pi e^{i\vec{k} \cdot (\vec{x} + \vec{r}) - ik^0 t} e^{-ik \cdot x} + Z_\pi \int \frac{d^3p}{(3\pi)^3 2p^0} \frac{e^{ip \cdot x} e^{-i\vec{p} \cdot \vec{r}} e^{-iq \cdot x}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}(p, q, k_a, k_b), \quad (\text{B.71})$$

where  $p = (p_0, \vec{p}), k_a = (k_0, \vec{k}), k_b = (k_0, -\vec{k})$  are on-shell, but  $q = ((2k - q)_0, -\vec{p})$  is off-shell. As a results elastic part of the NBS wave function is

$$\psi^{elastic}(\vec{r}) = Z_\pi e^{-2ik_0 t} (e^{i\vec{k} \cdot \vec{r}} + \int \frac{d^3p}{(2\pi)^3 2p_0} \frac{e^{i\vec{p} \cdot \vec{r}}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}(p, q, k_a, k_b)), \quad (\text{B.72})$$

and inelastic part of the NBS wave function is

$$\psi^{inelastic}(r) = e^{-2k_0 t} \sum_X \frac{\sqrt{Z_\pi Z_X}}{2E_X} \frac{e^{i\vec{p}_X \cdot \vec{r}}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}_X(p_x, q, k_a, k_b), \quad (\text{B.73})$$

where  $q = ((2k - q_X)_0, -\vec{p}_X)$ . We assume  $t = 0$  and using  $q = ((2k - q)_0, -\vec{p})$ , the total NBS wave function is

$$\begin{aligned}
\psi(r) &= \psi^{elastic} + \psi^{inelastic} \\
&= Z_\pi e^{-2ik_0 t} (e^{i\vec{k}\cdot\vec{r}} + \int \frac{d^3p}{(2\pi)^3 2p_0} \frac{e^{i\vec{p}\cdot\vec{r}}}{m_\pi^2 - q^2 - i\varepsilon} \hat{T}(p, q, k_a, k_b)) + \psi^{inelastic} \\
&= Z_\pi (e^{i\vec{k}\cdot\vec{r}} + \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\vec{p}\cdot\vec{r}}}{p^2 - k^2 - i\varepsilon} H(\vec{p}, \vec{k})) + \psi^{inelastic},
\end{aligned} \tag{B.74}$$

where  $H(\vec{p}, \vec{k})$  is

$$H(\vec{p}, \vec{k}) \equiv \frac{p_0 + k_0}{8p_0 k_0} \hat{T}(p, q, k_a, k_b). \tag{B.75}$$

We can ignore the inelastic part below threshold, and divide the angle direction and the radial direction using spherical harmonics  $Y_{lm}(\Omega_r)$

$$\psi^{elastic} = 4\pi \sum_{l,m} i^l \psi_l^{elastic}(r, k) Y_{lm}(\Omega_r) \overline{Y_{lm}(\Omega_k)}, \tag{B.76}$$

where we define  $\psi_l^{elastic}$  for expand coefficient. Using

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr \cos \theta} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}(\Omega_r) \overline{Y_{lm}(\Omega_k)}, \tag{B.77}$$

we can derive

$$\psi_l^{elastic}(\vec{k}, \vec{r}) = j_l(k, r) + \int \frac{dp p^2}{(2\pi)^3} 4\pi \frac{1}{p^2 - k^2 - i\varepsilon} H_l(p, k) j_l(pr). \tag{B.78}$$

The 1st term is a free part and the 2nd term is interaction part. We define the  $H(\vec{p}, \vec{k})$  for radius direction of the  $H(\vec{p}, \vec{k})$

$$H(\vec{p}, \vec{k}) = 4\pi \sum_{lm} H_l(p, k) Y_{lm}(\Omega_r) \overline{Y_{lm}(\Omega_k)}. \tag{B.79}$$

Using spherical Bessel function.

$$\begin{aligned}
&\int_0^\infty \frac{dp p^2}{4\pi^2} \frac{1}{p^2 - k^2 - i\varepsilon} H_l(p, k) j_l(pr) \\
&= -(kr)^l \left( \frac{1}{kr} \frac{d}{dkr} \right)^l \int_{-\infty}^\infty \frac{dp e^{ipr}}{4\pi^2 i pr} \left( \frac{1}{p-k} - \frac{1}{p+k} \right) \frac{H_l(p, k)}{2k}
\end{aligned} \tag{B.80}$$

The  $H_l(k, -k)$  is

$$H_l(k, -k) = (-1)^l H_l(k, k), \tag{B.81}$$

because

$$\begin{aligned}
H(\vec{p}, \vec{k}) &= 4\pi \sum_{lm} H_l(p, k) Y_{lm}(\Omega_p) \overline{Y_{lm}(\Omega_k)} \\
&= 4\pi \sum_{lm} H_l(-p, k) Y_{lm}(\Omega_{-p}) \overline{Y_{lm}(\Omega_k)} \\
&= 4\pi \sum_{lm} (-1)^l H_l(-p, k) Y_{lm}(\Omega_p) \overline{Y_{lm}(\Omega_k)},
\end{aligned} \tag{B.82}$$

where  $\Omega_{-p}$  is the  $\Omega p$  at  $\theta \rightarrow \pi - \theta$ ,  $\phi \rightarrow \phi + \pi$ . Using this relation, we can derive

$$\int_0^\infty \frac{dp p^2}{4\pi^2} \frac{1}{p^2 - k^2 - i\varepsilon} H_l(p, k) j_l(pr) = \frac{k}{4\pi} [n_l(kr) + i j_l(kr)] H_l(k, k). \quad (\text{B.83})$$

Considering the radius direction of the NBS wave function at  $r \rightarrow \infty$  using  $H_l(k, k) = \frac{4\pi}{k} e^{i\delta_l} \sin \delta_l(k)$

$$\begin{aligned} \psi_l(r, k) &= Z_\pi [j_l(kr) + \frac{k}{4\pi} H_l(k, k) \{n_l(kr) + i j_l(kr)\}] \\ &\sim Z_\pi \frac{e^{i\delta_l}}{kr} \sin(kr - \frac{l\pi}{2} + \delta_l(k)). \end{aligned} \quad (\text{B.84})$$

## Appendix C

# Omega operator in wall source at non-relativistic limit

This section shows that omega operator vanish exception of the spin 0 state with wall source at non-relativistic limit. The following examples are not applicable to other types of source. First we define omega operator in wall source as

$$\bar{\Omega} = \varepsilon^{abc} \sum_x \bar{s}^a(x) C\gamma_k \sum_{x'} \bar{s}^b(x') \sum_{x''} \bar{s}^c(x''), \quad (\text{C.1})$$

where  $a, b, c$  are color indices. For simply, we ignore  $C\gamma_k$  which is not important.

The two-Omega wall source operator is then given by

$$\bar{\Omega}\bar{\Omega} \equiv \varepsilon^{abc} \varepsilon^{a'b'c'} \left( \sum_x \bar{s}^a(x) \right) \left( \sum_{x'} \bar{s}^b(x') \right) \left( \sum_{x''} \bar{s}^c(x'') \right) \left( \sum_y \bar{s}^{a'}(y) \right) \left( \sum_{y'} \bar{s}^{b'}(y') \right) \left( \sum_{y''} \bar{s}^{c'}(y'') \right) \quad (\text{C.2})$$

The  $S = 3$  and  $S_z = 3$  operator vanish as

$$\begin{aligned} (\Omega\Omega)_{3,3} &\equiv \varepsilon^{abc} \varepsilon^{a'b'c'} \left( \sum_x \bar{s}_{\frac{1}{2}}^a(x) \right) \left( \sum_{x'} \bar{s}_{\frac{1}{2}}^b(x') \right) \left( \sum_{x''} \bar{s}_{\frac{1}{2}}^c(x'') \right) \left( \sum_y \bar{s}_{\frac{1}{2}}^{a'}(y) \right) \left( \sum_{y'} \bar{s}_{\frac{1}{2}}^{b'}(y') \right) \left( \sum_{y''} \bar{s}_{\frac{1}{2}}^{c'}(y'') \right) \\ &= -\varepsilon^{abc} \varepsilon^{a'b'c'} \left( \sum_y \bar{s}_{\frac{1}{2}}^{a'}(y) \right) \left( \sum_{y'} \bar{s}_{\frac{1}{2}}^{b'}(y') \right) \left( \sum_{y''} \bar{s}_{\frac{1}{2}}^{c'}(y'') \right) \left( \sum_x \bar{s}_{\frac{1}{2}}^a(x) \right) \left( \sum_{x'} \bar{s}_{\frac{1}{2}}^b(x') \right) \left( \sum_{x''} \bar{s}_{\frac{1}{2}}^c(x'') \right) \\ &= -\varepsilon^{abc} \varepsilon^{a'b'c'} \left( \sum_x \bar{s}_{\frac{1}{2}}^{a'}(x) \right) \left( \sum_{x'} \bar{s}_{\frac{1}{2}}^{b'}(x') \right) \left( \sum_{x''} \bar{s}_{\frac{1}{2}}^{c'}(x'') \right) \left( \sum_y \bar{s}_{\frac{1}{2}}^a(y) \right) \left( \sum_{y'} \bar{s}_{\frac{1}{2}}^b(y') \right) \left( \sum_{y''} \bar{s}_{\frac{1}{2}}^c(y'') \right) \quad (\text{C.3}) \\ &= -(\Omega\Omega)_{3,3} = 0. \end{aligned}$$

In second line, we use fermionic condition in exchanging two-Omega operators. In final line, we replace spatial indices, because these indices are inner indices in wall source. Since operators with  $S = 2$  and smaller  $S_z$  are obtained by applying the lowering operator  $\hat{S}_-$  to this operator, such operators also vanish. So the same conclusion is also indicated for different z-components. We thus conclude  $(\Omega\Omega)_{3,S_z} = 0$  for  $S_z = \pm 3, \pm 2, \pm 1, 0$ . We can proof  $S = 2$   $S_z = \pm 2, \pm 1, 0$  and  $S = 1$   $S_z = \pm 1, 0$ .

The  $S = 2$  and  $S_z = 2$  case is a little difficult for color. For simply we ignore  $x$  because of wall source. Spin0 will not disappear because we can not replace operator as

$$\begin{aligned}
(\Omega\Omega)_{2,2} &\equiv \frac{1}{\sqrt{2}}(\bar{\Omega}_{\frac{3}{2},\frac{3}{2}}\bar{\Omega}_{\frac{3}{2},\frac{1}{2}} - \bar{\Omega}_{\frac{3}{2},\frac{1}{2}}\bar{\Omega}_{\frac{3}{2},\frac{3}{2}}) \\
&= \varepsilon^{abc}\varepsilon^{def} \frac{1}{\sqrt{2}}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c(\sqrt{\frac{2}{3}}\frac{1}{\sqrt{2}}(\bar{s}_{\frac{1}{2}}^d\bar{s}_{-\frac{1}{2}}^e + \bar{s}_{-\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e)\bar{s}_{\frac{1}{2}}^f + \sqrt{\frac{1}{3}}\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f) \\
&\quad - (\sqrt{\frac{2}{3}}\frac{1}{\sqrt{2}}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^b + \bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b)\bar{s}_{\frac{1}{2}}^c + \sqrt{\frac{1}{3}}\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c)\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f) \\
&= \varepsilon^{abc}\varepsilon^{def} \frac{1}{\sqrt{2}}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c(\sqrt{\frac{1}{3}}(\bar{s}_{\frac{1}{2}}^d\bar{s}_{-\frac{1}{2}}^e + \bar{s}_{-\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e)\bar{s}_{\frac{1}{2}}^f + \sqrt{\frac{1}{3}}\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f) \\
&\quad - (\sqrt{\frac{1}{3}}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^b + \bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b)\bar{s}_{\frac{1}{2}}^c + \sqrt{\frac{1}{3}}\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c)\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f) \\
&= \varepsilon^{abc}\varepsilon^{def} \frac{1}{\sqrt{6}}((\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c((\bar{s}_{\frac{1}{2}}^d\bar{s}_{-\frac{1}{2}}^e + \bar{s}_{-\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e)\bar{s}_{\frac{1}{2}}^f + \bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f) - ((\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^b + \bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b)\bar{s}_{\frac{1}{2}}^c + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c)\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f)) \\
&= \varepsilon^{abc}\varepsilon^{def} \frac{1}{\sqrt{6}}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c(\bar{s}_{\frac{1}{2}}^d\bar{s}_{-\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f + \bar{s}_{-\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f + \bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f) + (-\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c - \bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c - \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c)\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f) \\
&= \varepsilon^{abc}\varepsilon^{def} \frac{1}{\sqrt{6}}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c(\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f\bar{s}_{\frac{1}{2}}^d + \bar{s}_{-\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f\bar{s}_{\frac{1}{2}}^d + \bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f\bar{s}_{-\frac{1}{2}}^d) + (-\bar{s}_{\frac{1}{2}}^c\bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b - \bar{s}_{-\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b - \bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^b)\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{\frac{1}{2}}^f) \\
&= \sqrt{6}\varepsilon^{abc}\varepsilon^{def}\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f \tag{C.4}
\end{aligned}$$

Using

$$\begin{aligned}
\varepsilon^{abc}\varepsilon^{def} &= \begin{vmatrix} \delta^{ad} & \delta^{ae} & \delta^{af} \\ \delta^{bd} & \delta^{be} & \delta^{bf} \\ \delta^{cd} & \delta^{ce} & \delta^{cf} \end{vmatrix} \\
&= \delta^{ad}(\delta^{be}\delta^{cf} - \delta^{bf}\delta^{ce}) + \delta^{ae}(\delta^{bf}\delta^{cd} - \delta^{bd}\delta^{cf}) + \delta^{af}(\delta^{bd}\delta^{ce} - \delta^{be}\delta^{cd}). \tag{C.5}
\end{aligned}$$

$$\begin{aligned}
(\Omega\Omega)_{2,2} &= \sqrt{6}(\delta^{ad}(\delta^{be}\delta^{cf} - \delta^{bf}\delta^{ce}) + \delta^{ae}(\delta^{bf}\delta^{cd} - \delta^{bd}\delta^{cf}) + \delta^{af}(\delta^{bd}\delta^{ce} - \delta^{be}\delta^{cd}))\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^d\bar{s}_{\frac{1}{2}}^e\bar{s}_{-\frac{1}{2}}^f \\
&= \sqrt{6}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c - \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^c\bar{s}_{-\frac{1}{2}}^b + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^b \\
&\quad - \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^a\bar{s}_{-\frac{1}{2}}^c + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{-\frac{1}{2}}^a - \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^a) \\
&= 2\sqrt{6}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^c\bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c) \\
&= -2\sqrt{6}(\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{-\frac{1}{2}}^c + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^c\bar{s}_{-\frac{1}{2}}^b + \bar{s}_{\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c\bar{s}_{\frac{1}{2}}^c\bar{s}_{-\frac{1}{2}}^a\bar{s}_{\frac{1}{2}}^b\bar{s}_{\frac{1}{2}}^c) \\
&= -(\Omega\Omega)_{2,2} = 0 \tag{C.6}
\end{aligned}$$

In the final line, we exchanged two quarks at same color and spin as  $\bar{s}_{\frac{1}{2}}^1\bar{s}_{\frac{1}{2}}^1 = -\bar{s}_{\frac{1}{2}}^1\bar{s}_{\frac{1}{2}}^1$ . We can proof  $S = 1$  case.

This proof does not hold for the  $S = 0$  and  $S_z = 0$  case, since the operator in this case is given by

$$\begin{aligned}
(\Omega\Omega)_{0,0} &\equiv \frac{1}{2}(\bar{\Omega}_{\frac{3}{2},\frac{3}{2}}\bar{\Omega}_{\frac{3}{2},-\frac{3}{2}} - \bar{\Omega}_{\frac{3}{2},\frac{1}{2}}\bar{\Omega}_{\frac{3}{2},-\frac{1}{2}} + \bar{\Omega}_{\frac{3}{2},-\frac{1}{2}}\bar{\Omega}_{\frac{3}{2},\frac{1}{2}} - \bar{\Omega}_{\frac{3}{2},-\frac{3}{2}}\bar{\Omega}_{\frac{3}{2},\frac{3}{2}}) \\
&= \frac{1}{6}\epsilon^{abc}\epsilon^{def}(3s_{\frac{1}{2}}^a s_{\frac{1}{2}}^b s_{\frac{1}{2}}^c s_{-\frac{1}{2}}^d s_{-\frac{1}{2}}^e s_{-\frac{1}{2}}^f - \sqrt{2}\frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^a s_{-\frac{1}{2}}^b + s_{-\frac{1}{2}}^a s_{\frac{1}{2}}^b)s_{\frac{1}{2}}^c s_{-\frac{1}{2}}^d s_{-\frac{1}{2}}^e s_{\frac{1}{2}}^f - s_{\frac{1}{2}}^a s_{\frac{1}{2}}^b s_{-\frac{1}{2}}^c s_{-\frac{1}{2}}^d s_{-\frac{1}{2}}^e s_{\frac{1}{2}}^f \\
&\quad - 2\frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^a s_{-\frac{1}{2}}^b + s_{-\frac{1}{2}}^a s_{\frac{1}{2}}^b)s_{\frac{1}{2}}^c \frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^d s_{-\frac{1}{2}}^e + s_{-\frac{1}{2}}^d s_{\frac{1}{2}}^e)s_{-\frac{1}{2}}^f - \sqrt{2}s_{\frac{1}{2}}^a s_{\frac{1}{2}}^b s_{-\frac{1}{2}}^c \frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^d s_{-\frac{1}{2}}^e + s_{-\frac{1}{2}}^d s_{\frac{1}{2}}^e)s_{-\frac{1}{2}}^f \\
&\quad + \sqrt{2}s_{-\frac{1}{2}}^a s_{-\frac{1}{2}}^b s_{\frac{1}{2}}^c \frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^d s_{-\frac{1}{2}}^e + s_{-\frac{1}{2}}^d s_{\frac{1}{2}}^e)s_{\frac{1}{2}}^f + 2\frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^a s_{-\frac{1}{2}}^b + s_{-\frac{1}{2}}^a s_{\frac{1}{2}}^b)s_{-\frac{1}{2}}^c \frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^d s_{-\frac{1}{2}}^e + s_{-\frac{1}{2}}^d s_{\frac{1}{2}}^e)s_{\frac{1}{2}}^f \\
&\quad + s_{-\frac{1}{2}}^a s_{-\frac{1}{2}}^b s_{\frac{1}{2}}^c s_{\frac{1}{2}}^d s_{\frac{1}{2}}^e s_{-\frac{1}{2}}^f + \sqrt{2}\frac{1}{\sqrt{2}}(s_{\frac{1}{2}}^a s_{-\frac{1}{2}}^b + s_{-\frac{1}{2}}^a s_{\frac{1}{2}}^b)s_{-\frac{1}{2}}^c s_{\frac{1}{2}}^d s_{\frac{1}{2}}^e s_{-\frac{1}{2}}^f \\
&\quad - 3s_{-\frac{1}{2}}^a s_{-\frac{1}{2}}^b s_{-\frac{1}{2}}^c s_{\frac{1}{2}}^d s_{\frac{1}{2}}^e s_{\frac{1}{2}}^f) \\
&= -9s_{\frac{1}{2}}^a s_{-\frac{1}{2}}^a s_{\frac{1}{2}}^b s_{-\frac{1}{2}}^b s_{\frac{1}{2}}^c s_{-\frac{1}{2}}^c
\end{aligned} \tag{C.7}$$

We can't exchange two quarks at same spin and color. Consequently, we can calculate only spin 0 state of Omega-Omega system in wall source.

## Appendix D

# Spin projection to spin $\frac{3}{2}$ operator

In the section we show spin projection, and we show summarized results at end of this section. For spin projection from  $\text{spin}1 \otimes \text{spin}\frac{1}{2}$  to  $\text{spin}\frac{3}{2}$ , we construct di-vector operator in non-relativistic limit. In non-relativistic limit, upper components of the quark correspond to  $\text{spin}\frac{1}{2}$ .

$$\psi = \begin{pmatrix} \uparrow \\ \downarrow \\ 0 \\ 0 \end{pmatrix} \quad (\text{D.1})$$

We use dirac-matrix in dirac representation, To project  $\bar{\Omega} = -\varepsilon^{c_3 c_2 c_1} \delta_{g'_3 g} \bar{s}_{g_3}^{c_3} (\bar{s}_{g_2}^{c_2} \gamma_{k_1} C (\bar{s}_{g_1}^{c_1})^T)$  in source part.

$$C\gamma^i = \begin{pmatrix} 0 & -i\sigma^2 \\ -i\sigma^2 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix} \quad (\text{D.2})$$

$$C\gamma^0 = \begin{pmatrix} & & 1 \\ & -1 & \\ 1 & & \end{pmatrix} \quad C\gamma^1 = \begin{pmatrix} -i & & \\ & i & \\ & & i \\ & & & -i \end{pmatrix} \quad (\text{D.3})$$

$$C\gamma^2 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \quad C\gamma^3 = \begin{pmatrix} & i & & \\ i & & & \\ & & & -i \\ & & -i & \end{pmatrix} \quad (\text{D.4})$$

So we can make spin1 operator

$$\text{spin}1, z + 1 \quad \frac{1}{2} \psi (iC\gamma^1 + C\gamma^2) \psi \quad (\text{D.5})$$

$$\text{spin}1, z0 \quad -\frac{i}{\sqrt{2}} \psi C\gamma^3 \psi \quad (\text{D.6})$$

$$\text{spin}1, z - 1 \quad \frac{1}{2} \psi (-iC\gamma^1 + C\gamma^2) \psi \quad (\text{D.7})$$

On the other hands, To project in sink part, we use follow matrix

$$\gamma^0 C = \begin{pmatrix} & & -1 \\ & 1 & \\ -1 & & \end{pmatrix} \quad \gamma^1 C = \begin{pmatrix} -i & & \\ & i & \\ & & i \\ & & & -i \end{pmatrix} \quad (\text{D.8})$$



$$\gamma^2 C = \begin{pmatrix} -1 & & & \\ & -1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \quad \gamma^3 C = \begin{pmatrix} & i & & \\ i & & & \\ & & & -i \\ & & -i & \end{pmatrix} \quad (\text{D.9})$$

So we can make spin1 operator

$$\text{spin1, } z+1 \quad \frac{1}{2}\psi(i\gamma^1 C - \gamma^2 C)\psi \quad (\text{D.10})$$

$$\text{spin1, } z0 \quad -\frac{i}{\sqrt{2}}\psi\gamma^3 C\psi \quad (\text{D.11})$$

$$\text{spin1, } z-1 \quad \frac{1}{2}\psi(-i\gamma^1 C - \gamma^2 C)\psi \quad (\text{D.12})$$

Now we have  $\text{spin1} \otimes \text{spin}\frac{1}{2} = \text{spin}\frac{1}{2} \oplus \text{spin}\frac{3}{2}$  state. Next we perform projection to  $\text{spin}\frac{3}{2}$  state using highest weight method. First we define the highest weight

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle = |1, 1\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle, \quad (\text{D.13})$$

where  $|S, S_z\rangle$  is  $\text{spin}S$ , spin  $z$ -component  $S_z$  state. Lowering operator is

$$l_- |j, m\rangle = \sqrt{(j+m)(j-m+1)\hbar} |j, m-1\rangle. \quad (\text{D.14})$$

We can easy make  $\text{spin}\frac{3}{2}$  states and  $\text{spin}\frac{1}{2}$  states.

$\text{spin}\frac{3}{2}$  states

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle = |1, 1\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle \quad (\text{D.15})$$

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} |1, 0\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} |1, 1\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{D.16})$$

$$\left| \frac{3}{2}, -\frac{1}{2} \right\rangle = \sqrt{\frac{1}{3}} |1, -1\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} |1, 0\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{D.17})$$

$$\left| \frac{3}{2}, -\frac{3}{2} \right\rangle = |1, -1\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{D.18})$$

$\text{spin}\frac{1}{2}$  states

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = -\sqrt{\frac{1}{3}} |1, 0\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} |1, 1\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{D.19})$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle = -\sqrt{\frac{2}{3}} |1, -1\rangle \left| \frac{1}{2}, \frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} |1, 0\rangle \left| \frac{1}{2}, -\frac{1}{2} \right\rangle \quad (\text{D.20})$$

Finally we make  $\text{spin}3$ ,  $\text{spin}2$ ,  $\text{spin}1$ ,  $\text{spin}0$  states. The  $\text{spin}3$  for  $S_z = \pm 3, \pm 2, \pm 1, 0$ .

$$l_- |3, 3\rangle = \sqrt{6} |3, 2\rangle = \sqrt{3} \left( \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle \right) \\ |3, 2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle + \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle \right) \quad (\text{D.21})$$

$$\begin{aligned}
l_- |3, 2\rangle &= \sqrt{10} |3, 1\rangle \\
&= \frac{1}{\sqrt{2}} (2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle) \\
&\quad + \frac{1}{\sqrt{2}} (\sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 2 \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle)
\end{aligned} \tag{D.22}$$

$$|3, 1\rangle = \frac{1}{\sqrt{5}} \left( \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \right) \tag{D.23}$$

$$\begin{aligned}
l_- |3, 1\rangle &= \sqrt{12} |3, 0\rangle \\
&= \frac{1}{\sqrt{5}} (\sqrt{3} \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle) \\
&\quad + \sqrt{3} (2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 2 \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle) \\
&\quad + \sqrt{3} \left( \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \right)
\end{aligned} \tag{D.24}$$

$$|3, 0\rangle = \frac{1}{\sqrt{20}} \left( \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle + 3 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 3 \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \right) \tag{D.25}$$

$$\begin{aligned}
l_- |3, 0\rangle &= \sqrt{12} |3, -1\rangle \\
&= \frac{1}{\sqrt{20}} (\sqrt{3} \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 3 (\sqrt{3} \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle)) \\
&\quad + 3 (2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle) + \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle
\end{aligned} \tag{D.26}$$

$$|3, -1\rangle = \frac{1}{\sqrt{5}} \left( \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \right) \tag{D.27}$$

$$\begin{aligned}
l_- |3, -1\rangle &= \sqrt{10} |3, -2\rangle \\
&= \frac{1}{\sqrt{5}} (2 \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + 3 \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle) \\
&\quad + 3 \left( \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle + 2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \right)
\end{aligned} \tag{D.28}$$

$$|3, -2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \right) \tag{D.29}$$

$$\begin{aligned}
l_- |3, -2\rangle &= \sqrt{6} |3, -3\rangle \\
&= \frac{1}{\sqrt{2}} (\sqrt{3} \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle)
\end{aligned} \tag{D.30}$$

$$|3, -3\rangle = \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle$$

The spin2 for  $S_z = \pm 2, \pm 1, 0$ .

$$|2, 2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle - \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.31})$$

$$\begin{aligned} l_- |2, 2\rangle &= 2 |2, 1\rangle \\ &= \frac{1}{\sqrt{2}} \left( \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 2 \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - 2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle - \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle \right) \end{aligned} \quad (\text{D.32})$$

$$|2, 1\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.33})$$

The spin1 for  $S_z = \pm 1, 0$ .

$$|1, 1\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.34})$$

The spin0 for  $S_z = 0$ .

$$|0, 0\rangle = \frac{1}{2} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle - \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.35})$$

Finally, we summarize the above results.

spin3 states

$$|3, 3\rangle = \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \quad (\text{D.36})$$

$$|3, 2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.37})$$

$$|3, 1\rangle = \frac{1}{\sqrt{5}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.38})$$

$$|3, 0\rangle = \frac{1}{\sqrt{20}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle + 3 \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + 3 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.39})$$

$$|3, -1\rangle = \frac{1}{\sqrt{5}} \left( \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle \right) \quad (\text{D.40})$$

$$|3, -2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle + \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \right) \quad (\text{D.41})$$

$$|3, -3\rangle = \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \quad (\text{D.42})$$

spin2 states

$$|2, 2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle - \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.43})$$

$$|2, 1\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.44})$$

$$|2, 0\rangle = \frac{1}{2} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle + \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.45})$$

$$|2, -1\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle - \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle \right) \quad (\text{D.46})$$

$$|2, -2\rangle = \frac{1}{\sqrt{2}} \left( \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle - \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \right) \quad (\text{D.47})$$

spin1 states

$$|1, 1\rangle = \frac{1}{\sqrt{10}} \left( \sqrt{3} \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - 2 \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.48})$$

$$|1, 0\rangle = \frac{1}{\sqrt{20}} \left( 3 \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle - \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle + 3 \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.49})$$

$$|1, -1\rangle = \frac{1}{\sqrt{10}} \left( \sqrt{3} \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle - 2 \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \sqrt{3} \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle \right) \quad (\text{D.50})$$

spin0 state

$$|0, 0\rangle = \frac{1}{2} \left( \left| \frac{3}{2}, \frac{3}{2} \right\rangle \left| \frac{3}{2}, -\frac{3}{2} \right\rangle - \left| \frac{3}{2}, \frac{1}{2} \right\rangle \left| \frac{3}{2}, -\frac{1}{2} \right\rangle + \left| \frac{3}{2}, -\frac{1}{2} \right\rangle \left| \frac{3}{2}, \frac{1}{2} \right\rangle - \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \left| \frac{3}{2}, \frac{3}{2} \right\rangle \right) \quad (\text{D.51})$$

# Appendix E

## Cubic group

For improve statical errors, we increase the statics using cubic group symmetry. In this section, we explain the cubic group  $O_h$  which corresponding to the  $SO(3)$ . First we define the projection operator. Second, we show the representation matrix of the group  $SO(3)$  which is rotation in continuous space and  $O_h$  which is rotation in lattice space, because the projection operator include the representation matrix. We start a orthogonality of the irreducible representation

$$\sum_i^g D_{\mu\nu}^a(R_i)^* D_{\mu'\nu'}^b(R_i) = \frac{g}{d_a} \delta_{ab} \delta_{\mu\mu'} \delta_{\nu\nu'}, \quad (\text{E.1})$$

where  $a, b$  are irreducible representation indices,  $i$  is label of the element,  $\mu, \nu$  are indices of the representation matrix,  $R$  is elements,  $D_{\mu\nu}(R)$  is a representation matrix,  $g$  is the number of elements and  $d$  is a dimension of the irreducible representation. We define a character  $\chi$  as

$$\chi(R_i) \equiv \text{Tr}\{D(R_i)\}. \quad (\text{E.2})$$

The character has a orthogonality from the orthogonality of the irreducible representation.

$$\begin{aligned} \sum_i^g \chi^a(R_i)^* \chi^b(R_i) &= \sum_i^g \sum_{\mu} D_{\mu\mu}^a(R_i)^* \sum_{\nu} D_{\nu\nu}^b(R_i) \\ &= \frac{g}{d_a} \sum_{\nu\mu} \delta_{ab} \delta_{\mu\nu} \delta_{\nu\mu} \\ &= g \delta_{ab} \end{aligned} \quad (\text{E.3})$$

Using it, we define the projection operator  $P_{\nu}^a$

$$P_{\nu}^a = \frac{d_a}{g} \sum_i D_{\nu\nu}^a(R_i)^* R_i. \quad (\text{E.4})$$

Let us check the projection to

$$\phi_{\mu} = c^a \phi_{\mu_a}^a + c^b \phi_{\mu_b}^b + c^c \phi_{\mu_c}^c + \dots = \sum_{a'} c^{a'} \phi_{\mu_{a'}}^{a'}, \quad (\text{E.5})$$

where  $\phi_{\mu_{a'}}^{a'}$  is base of the irreducible representation and  $c^a$  is coefficient.

$$\begin{aligned}
P_{\nu_a}^a \phi &= \sum_{a'} c^{a'} \frac{d_a}{g} \sum_i D_{\nu_a \nu_a}^a(R_i) {}^* R_i^{a'} \phi_{\mu_{a'}}^{a'} \\
&= \sum_{a'} c^{a'} \frac{d_a}{g} \sum_i \sum_{\nu'} D_{\mu_a \mu_a}^a(R_i) {}^* D_{\mu_{a'} \nu_{a'}}^{a'}(R_i) \phi_{\nu_{a'}}^{a'} \\
&= \sum_{a'} \sum_{\nu'} c^{a'} \frac{d_a}{g} \frac{g}{d_a} \delta_{aa'} \delta_{\mu_a \mu_{a'}} \delta_{\mu_a \nu_{a'}} \phi_{\nu_{a'}}^{a'} \\
&= c^a \phi_{\mu_a}^a
\end{aligned} \tag{E.6}$$

In 2nd line, we use  $R_i^{a'} \phi_{\mu}^{a'} = \sum_{\nu'} D_{\mu_{a'} \nu_{a'}}^{a'} \phi_{\nu_{a'}}^{a'}$ . So  $P_{\nu_a}^a$  is a projection operator.

We discuss about a character of the  $SO(3)$  in continuous space. Considering the similarity transformation of the spherical harmonic

$$R(\alpha, \beta, \gamma) Y_m^l = \sum_{m'=-l}^l D^l(\alpha, \beta, \gamma)_{mm'} Y_{m'}^l(\theta, \phi). \tag{E.7}$$

We perform the rotation to the spherical harmonics

$$R(\alpha, 0, 0) Y_m^l(\theta, \phi) = \sum_{m'=-l}^l \delta_{mm'} e^{im'\alpha} Y_{m'}^l(\theta, \phi), \tag{E.8}$$

Representation matrix is

$$D^l(\alpha, 0, 0) = \begin{pmatrix} e^{-il\alpha} & & & & \\ & e^{-i(l-1)\alpha} & & & \\ & & \ddots & & \\ & & & e^{i(l-1)\alpha} & \\ & & & & e^{il\alpha} \end{pmatrix}. \tag{E.9}$$

We can calculate the character

$$\chi^l(\alpha) = \text{Tr} D^l(\alpha, 0, 0) = e^{-il\alpha} \frac{1 - e^{i(2l+1)\alpha}}{1 - e^{i\alpha}} = \frac{\sin[(l + \frac{1}{2})\alpha]}{\sin(\frac{\alpha}{2})}. \tag{E.10}$$

We show the character of the  $SO(3)$  at each orbital angular momentum  $l$  in Table E.1. Meaning of symbols  $C_n$  are described later in cubic group.

	E	$6C_4$	$3C_2$	$8C_3$	$6C_2$
a	0	$\frac{\pi}{2}$	$\pi$	$\frac{2\pi}{3}$	$\pi$
$l=\frac{1}{2}$	2	$\sqrt{2}$	0	1	0
$l=\frac{3}{2}$	4	0	0	-1	0
$l=\frac{5}{2}$	6	$-\sqrt{2}$	0	0	0
$l=\frac{7}{2}$	8	0	0	1	0
$l=\frac{9}{2}$	10	$\sqrt{2}$	0	-1	0
$l=\frac{11}{2}$	12	0	0	0	0
$l=\frac{13}{2}$	14	$-\sqrt{2}$	0	1	0
$l=\frac{15}{2}$	16	0	0	-1	0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table E.1: Character of a spatial rotation at angular momentum  $l$  for  $O_h$  group.

Next we explain the  $O_h$  which is rotation in lattice space.  $O_h$  has 48 elements (24 rotation and parity). In Fig. E.1, we show  $O_h$  group elements which is corresponding to a kind of rotation. Symbol of  $mC_n$  show that  $n$  is rotation of  $\frac{2\pi}{n}$  and  $m$  is the number of rotation axes. For example, given the rotation around axis A, there are 6 rotating  $\frac{\pi}{2}$  is called  $6C_4$  which is corresponding to the number of vertexes. To summarize below

- around A axis  $(\frac{\pi}{2}, \pi)$

In rotation  $\frac{\pi}{2}$ , there are the number of vertexes  $6C_4$ . In rotation  $\pi$ , there are the number of half vertexes  $3C_4^2$ .

- around B axis  $(\frac{2\pi}{3})$

In rotation  $\frac{2\pi}{3}$ , there are the number of planes  $8C_3$ .

- around C axis  $(\pi)$

In rotation  $\pi$ , there are the number of sides  $6C_2$ .

The total of elements are  $1 + 6 + 3 + 8 + 6 = 24$  in  $O$  group (include identity element).  $O \otimes I = O_h$ , therefore  $O_h$  has 48 elements, where  $I$  is parity. We show the character of the  $O_h$  at each dimensional representations in Table E.2 and Table E.3 show the correspondence table of  $l$  and  $O_h$  group elements.

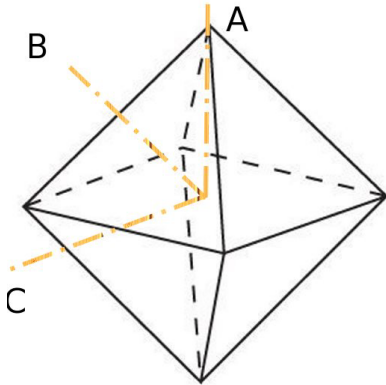


Figure E.1: Rotation in the lattice space. Around axis A:  $6C_4, 3C_4^2$ . Around axis B:  $8C_3$ . Around axis C:  $6C_2$ .

irreducible\elements	$E$	$6C_4$		$3C_4^2$	$6C_2'$	$8C_3$		
$A_{1g}$	1	1		1	1	1		
$A_{2g}$	1	-1		1	-1	1		
$E_g$	2	0		2	0	-1		
$T_{1g}$	3	1		-1	-1	0		
$T_{2g}$	3	-1		-1	1	0		
$A_{1u}$	1	1		1	1	1		
$A_{2u}$	1	-1		1	-1	1		
$E_u$	2	0		2	0	-1		
$T_{1u}$	3	1		-1	-1	0		
$T_{2u}$	3	-1		-1	1	0		
$E_{\frac{1}{2}g}$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	1	-1
$E_{\frac{5}{2}g}$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	1	-1
$G_{\frac{3}{2}g}$	4	-4	0	0	0	0	-1	1
$E_{\frac{1}{2}u}$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	1	-1
$E_{\frac{5}{2}u}$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	1	-1
$G_{\frac{3}{2}u}$	4	-4	0	0	0	0	-1	1
irreducible\elements	$I$	$6IC_4$		$3\sigma_h = 3IC_4^2$	$6\sigma_d = 6IC_2'$	$8IC_3$		
$A_{1g}$	1	1		1	1	1		
$A_{2g}$	1	-1		1	-1	1		
$E_g$	2	0		2	0	-1		
$T_{1g}$	3	1		-1	-1	0		
$T_{2g}$	3	-1		-1	1	0		
$A_{1u}$	-1	-1		-1	-1	-1		
$A_{2u}$	-1	1		-1	1	-1		
$E_u$	-2	0		-2	0	1		
$T_{1u}$	-3	-1		1	1	0		
$T_{2u}$	-3	1		1	-1	0		
$E_{\frac{1}{2}g}$	2	-2	$\sqrt{2}$	$-\sqrt{2}$	0	0	1	-1
$E_{\frac{5}{2}g}$	2	-2	$-\sqrt{2}$	$\sqrt{2}$	0	0	1	-1
$G_{\frac{3}{2}g}$	4	-4	0	0	0	0	-1	1
$E_{\frac{1}{2}u}$	-2	2	$-\sqrt{2}$	$\sqrt{2}$	0	0	-1	1
$E_{\frac{5}{2}u}$	-2	2	$\sqrt{2}$	$-\sqrt{2}$	0	0	-1	1
$G_{\frac{3}{2}u}$	-4	4	0	0	0	0	1	-1

Table E.2: Character of  $O_h$  group.  $g$  is parity even,  $u$  is parity odd,  $A$  is 1 dimension representation,  $E$  is 2 dimension representation,  $T$  is 3 dimension representation,  $G$  is 4 dimension representation and  $I$  is parity transformation.



$l=0$	$A_1$	$l=\frac{1}{2}$	$E_{\frac{1}{2}}$
$l=1$	$T_1$	$l=\frac{3}{2}$	$G_{\frac{3}{2}}$
$l=2$	$E \oplus T_2$	$l=\frac{5}{2}$	$E_{\frac{5}{2}} \oplus G_{\frac{3}{2}}$
$l=3$	$A_2 \oplus T_1 \oplus T_2$	$l=\frac{7}{2}$	$E_{\frac{1}{2}} \oplus E_{\frac{5}{2}} \oplus G_{\frac{3}{2}}$
$l=4$	$A_1 \oplus E \oplus T_1 \oplus T_2$	$l=\frac{9}{2}$	$E_{\frac{1}{2}} \oplus 2G_{\frac{3}{2}}$
$\vdots$	$\vdots$	$l=\frac{11}{2}$	$E_{\frac{1}{2}} \oplus E_{\frac{5}{2}} \oplus 2G_{\frac{3}{2}}$
		$l=\frac{13}{2}$	$E_{\frac{1}{2}} \oplus 2E_{\frac{5}{2}} \oplus 2G_{\frac{3}{2}}$
		$l=\frac{15}{2}$	$E_{\frac{1}{2}} \oplus E_{\frac{5}{2}} \oplus 3G_{\frac{3}{2}}$
		$\vdots$	

Table E.3: Correspondence table of  $l$  and  $O_h$  group elements.

Finally, we show the representation matrixes.

$E$	$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	(E.11)
-----	---	--------

$6C_4$	$C_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad C_{4y} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad C_{4z} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	(E.12)
	$C_x^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \quad C_{4y}^{-1} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad C_{4z}^{-1} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	(E.13)

$8C_3$	$C_x C_y = C_y C_z = C_z C_x = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	(E.14)
	$(C_x C_y)^2 = (C_y C_z)^2 = (C_z C_x)^2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	(E.15)
	$C_y C_x = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix} \quad C_z C_y = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} \quad C_x C_z = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$	(E.16)
	$(C_y C_x)^2 = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad (C_z C_y)^2 = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad (C_x C_z)^2 = \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$	(E.17)

$9C_2$ 

$$C_x^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad C_y^2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad C_z^2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{E.18})$$

$$C_x C_y C_z = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad C_y C_z C_x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad C_z C_x C_y = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (\text{E.19})$$

$$C_x^{-1} C_y^{-1} C_z = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad C_y^{-1} C_z^{-1} C_x = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (\text{E.20})$$

$$C_z^{-1} C_x^{-1} C_y = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \quad (\text{E.21})$$

We show representation matrixes for spinor.

$$\begin{aligned} S(C_{nj}) &= \exp\left(\frac{i}{4}\omega_{\mu\nu}[\gamma_\mu, \gamma_\nu]\right) \quad \omega_{kl} \equiv -\frac{2\pi}{n}\epsilon_{jkl} \\ &= \exp\left(-i\frac{\pi}{2n}\epsilon_{jkl}[\gamma_k, \gamma_l]\right) \\ &= \exp\left(-i\frac{\pi}{2n}([\gamma_2, \gamma_3], [\gamma_3, \gamma_1], [\gamma_1, \gamma_2])\right) \end{aligned} \quad (\text{E.22})$$

We consider the rotation around the Z-axis

$$\begin{aligned} &= \exp\left(-i\frac{\pi}{2n}\left[\begin{pmatrix} & -i\sigma_1 \\ i\sigma_1 & \end{pmatrix}, \begin{pmatrix} & -i\sigma_2 \\ i\sigma_2 & \end{pmatrix}\right]\right) \\ &= \exp\left(-i\frac{\pi}{n}\begin{pmatrix} \sigma_3 & \\ & \sigma_3 \end{pmatrix}\right) \\ &= \sum_k \frac{1}{k!} \left(-\frac{\pi}{n}\begin{pmatrix} \sigma_3 & \\ & \sigma_3 \end{pmatrix}\right)^k \\ &= \begin{pmatrix} e^{-i\frac{\pi}{n}\sigma_3} & \\ & e^{-i\frac{\pi}{n}\sigma_3} \end{pmatrix} \end{aligned} \quad (\text{E.23})$$

All representation matrixes can be made from  $C_{4y}$  and  $C_{4z}$ .

$$S(C_{4y}) = \begin{pmatrix} e^{-i\sigma_2\frac{\pi}{4}} & 0 \\ 0 & e^{-i\sigma_2\frac{\pi}{4}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.24})$$

$$S(C_{4z}) = \begin{pmatrix} e^{-i\sigma_3\frac{\pi}{4}} & 0 \\ 0 & e^{-i\sigma_3\frac{\pi}{4}} \end{pmatrix} = \begin{pmatrix} \frac{1-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1-i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1+i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.25})$$

$$S(C_{4x}) = S(C_y)S(C_z)S(C_y^{-1}) = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.26})$$

For considering monovalent representation, we deal with  $\frac{1}{2}\pi$  and  $\frac{1}{2}\pi + 2\pi$  as a different. For example

$$C_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \quad C_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad C_z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1-i & 0 \\ 0 & 1+i \end{pmatrix}, \quad (\text{E.27})$$

$$(C_x)^5 = \overline{C_x} = \frac{-1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \quad (C_y)^5 = \overline{C_y} = \frac{-1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad (C_z)^5 = \overline{C_z} = \frac{-1}{\sqrt{2}} \begin{pmatrix} 1-i & 0 \\ 0 & 1+i \end{pmatrix}. \quad (\text{E.28})$$

Parity transformation is

$$S(I) = \gamma_4.$$

We show the all representation matrixes for spinor.

$E \times 2$

$$E = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \quad \overline{E} = - \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \quad (\text{E.29})$$

$6C_4 \times 2$

$$C_{4x} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad C_{4y} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.30})$$

$$C_{4z} = \begin{pmatrix} \frac{1-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1-i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1+i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.31})$$

$$(C_x)^7 = C_x^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (C_y)^7 = C_y^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.32})$$

$$(C_z)^7 = C_z^{-1} = \begin{pmatrix} \frac{1+i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1-i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1+i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1-i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.33})$$

$$\overline{C_{4x}} = - \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad \overline{C_{4y}} = - \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.34})$$

$$\overline{C_{4z}} = - \begin{pmatrix} \frac{1-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1-i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1+i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.35})$$

$$(C_x)^3 = \overline{C_x}^{-1} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.36})$$

$$(C_y)^3 = \overline{C_y}^{-1} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (\text{E.37})$$

$$(C_z)^3 = \overline{C_z}^{-1} = \begin{pmatrix} -\frac{1+i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & -\frac{1-i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{1+i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -\frac{1-i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.38})$$

$8C_3 \times 2$

$$C_x C_y = C_y C_z = C_z C_x = \begin{pmatrix} \frac{1-i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{1-i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} \quad (\text{E.39})$$

$$\overline{C_x C_y} = \overline{C_y C_z} = \overline{C_z C_x} = \begin{pmatrix} \frac{1-i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{1-i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} \quad (\text{E.40})$$

$$(C_x C_y)^2 = (C_y C_z)^2 = (C_z C_x)^2 = \begin{pmatrix} \frac{-1-i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1-i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{-1+i}{2} \end{pmatrix} \quad (\text{E.41})$$

$$(\overline{C_x C_y})^2 = (\overline{C_y C_z})^2 = (\overline{C_z C_x})^2 = \begin{pmatrix} \frac{-1-i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1-i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{-1+i}{2} \end{pmatrix} \quad (\text{E.42})$$

$$C_y C_x = \begin{pmatrix} \frac{1+i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{1-i}{2} & 0 & 0 \\ 0 & 0 & \frac{1+i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{1-i}{2} \end{pmatrix} \quad C_z C_y = \begin{pmatrix} \frac{1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ \frac{1+i}{2} & \frac{1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{1-i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1+i}{2} & \frac{1-i}{2} \end{pmatrix} \quad (\text{E.43})$$

$$C_x C_z = \begin{pmatrix} \frac{1-i}{2} & \frac{1-i}{2} & 0 & 0 \\ \frac{-1-i}{2} & \frac{1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{1-i}{2} & \frac{1-i}{2} \\ 0 & 0 & \frac{-1-i}{2} & \frac{1+i}{2} \end{pmatrix} \quad (\text{E.44})$$

$$\overline{C_y C_x} = \begin{pmatrix} \frac{1+i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{1-i}{2} & 0 & 0 \\ 0 & 0 & \frac{1+i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{1-i}{2} \end{pmatrix} \quad \overline{C_z C_y} = \begin{pmatrix} \frac{1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ \frac{1+i}{2} & \frac{1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{1-i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1+i}{2} & \frac{1-i}{2} \end{pmatrix} \quad (\text{E.45})$$

$$\overline{C_x C_z} = \begin{pmatrix} \frac{1-i}{2} & \frac{1-i}{2} & 0 & 0 \\ \frac{-1-i}{2} & \frac{1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{1-i}{2} & \frac{1-i}{2} \\ 0 & 0 & \frac{-1-i}{2} & \frac{1+i}{2} \end{pmatrix} \quad (\text{E.46})$$

$$(C_y C_x)^2 = \begin{pmatrix} \frac{-1+i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{-1-i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1+i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{-1-i}{2} \end{pmatrix} \quad (C_z C_y)^2 = \begin{pmatrix} \frac{-1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ \frac{1+i}{2} & \frac{-1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1-i}{2} & \frac{-1+i}{2} \\ 0 & 0 & \frac{1+i}{2} & \frac{-1+i}{2} \end{pmatrix} \quad (\text{E.47})$$

$$(C_x C_z)^2 = \begin{pmatrix} \frac{-1-i}{2} & \frac{1-i}{2} & 0 & 0 \\ \frac{-1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1-i}{2} & \frac{1-i}{2} \\ 0 & 0 & \frac{-1-i}{2} & \frac{-1+i}{2} \end{pmatrix} \quad (\text{E.48})$$

$$(\overline{C_y C_x})^2 = \begin{pmatrix} \frac{-1+i}{2} & \frac{-1-i}{2} & 0 & 0 \\ \frac{1-i}{2} & \frac{-1-i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1+i}{2} & \frac{-1-i}{2} \\ 0 & 0 & \frac{1-i}{2} & \frac{-1-i}{2} \end{pmatrix} \quad (\overline{C_z C_y})^2 = \begin{pmatrix} \frac{-1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ \frac{1+i}{2} & \frac{-1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1-i}{2} & \frac{-1+i}{2} \\ 0 & 0 & \frac{1+i}{2} & \frac{-1+i}{2} \end{pmatrix} \quad (\text{E.49})$$

$$(\overline{C_x C_z})^2 = \begin{pmatrix} \frac{-1-i}{2} & \frac{1-i}{2} & 0 & 0 \\ \frac{-1-i}{2} & \frac{-1+i}{2} & 0 & 0 \\ 0 & 0 & \frac{-1-i}{2} & \frac{1-i}{2} \\ 0 & 0 & \frac{-1-i}{2} & \frac{-1+i}{2} \end{pmatrix} \quad (\text{E.50})$$

$9C_2$

$$C_x^2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \end{pmatrix} \quad C_y^2 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad C_z^2 = \begin{pmatrix} -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix} \quad (\text{E.51})$$

$$C_x^6 = (\overline{C_x^{-1}})^2 = - \begin{pmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \end{pmatrix} \quad C_y^6 = (\overline{C_y^{-1}})^2 = - \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (\text{E.52})$$

$$C_z^6 = (\overline{C_z^{-1}})^2 = - \begin{pmatrix} -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix} \quad (\text{E.53})$$

$$C_x C_y C_z = \begin{pmatrix} -\frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \quad C_y C_z C_x = \begin{pmatrix} 0 & -\frac{1+i}{\sqrt{2}} & 0 & 0 \\ \frac{1-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1+i}{\sqrt{2}} \\ 0 & 0 & \frac{1-i}{\sqrt{2}} & 0 \end{pmatrix} \quad (\text{E.54})$$

$$C_z C_x C_y = \begin{pmatrix} -\frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.55})$$

$$\overline{C_x C_y C_z} = - \begin{pmatrix} -\frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \quad \overline{C_y C_z C_x} = - \begin{pmatrix} 0 & -\frac{1+i}{\sqrt{2}} & 0 & 0 \\ \frac{1-i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1+i}{\sqrt{2}} \\ 0 & 0 & \frac{1-i}{\sqrt{2}} & 0 \end{pmatrix} \quad (\text{E.56})$$

$$\overline{C_z C_x C_y} = - \begin{pmatrix} -\frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.57})$$

$$C_x^{-1} C_y^{-1} C_z = (C_x)^3 (C_y)^3 C_z = \begin{pmatrix} -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.58})$$

$$C_y^{-1} C_z^{-1} C_x = (C_y)^3 (C_z)^3 C_x = \begin{pmatrix} 0 & \frac{1-i}{\sqrt{2}} & 0 & 0 \\ -\frac{1+i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-i}{\sqrt{2}} \\ 0 & 0 & -\frac{1+i}{\sqrt{2}} & 0 \end{pmatrix} \quad (\text{E.59})$$

$$C_z^{-1} C_x^{-1} C_y = (C_z)^3 (C_x)^3 C_y = \begin{pmatrix} \frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.60})$$

$$(\overline{C_x})^{-1}(\overline{C_y})^{-1}C_z = (C_x)^7(C_y)^7C_z = - \begin{pmatrix} -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{i}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.61})$$

$$(\overline{C_y})^{-1}(\overline{C_z})^{-1}C_x = (C_y)^7(C_z)^7C_x = - \begin{pmatrix} 0 & \frac{1-i}{\sqrt{2}} & 0 & 0 \\ -\frac{1+i}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-i}{\sqrt{2}} \\ 0 & 0 & -\frac{1+i}{\sqrt{2}} & 0 \end{pmatrix} \quad (\text{E.62})$$

$$(\overline{C_z})^{-1}(\overline{C_x})^{-1}C_y = (C_z)^7(C_x)^7C_y = - \begin{pmatrix} \frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{i}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} \quad (\text{E.63})$$

# Appendix F

## Traceless symmetric tensor

We show that traceless symmetric tensors are base of the spherical harmonics. First we define the spherical harmonics. In spherical coordinates, Laplace's equation can be written as

$$\nabla^2 \Psi(r, \theta, \phi) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r} \Psi(r, \theta, \phi)) + \frac{1}{r^2} \nabla_\theta^2 \Psi(r, \theta, \phi) = 0, \quad (\text{F.1})$$

where  $\nabla_\theta^2$  is the Laplacian at  $\theta, \phi$  direction. To use the method of separation of variables, we can seek a solution of the form

$$\Psi(r, \theta, \phi) \equiv R(r)F(\theta, \phi), \quad (\text{F.2})$$

where  $F(\theta, \phi)$  is spherical harmonics. Laplace's equation is written as

$$\frac{1}{R} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r} R(r)) + \frac{1}{F} \nabla_\theta^2 F(\theta, \phi) = 0. \quad (\text{F.3})$$

First term is only depend on  $r$  and second term is only depend on  $\theta, \phi$ , Thus we can write

$$\nabla_\theta^2 F = C_\theta F, \quad (\text{F.4})$$

$$\frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r} R(r)) = -C_\theta R. \quad (\text{F.5})$$

The unit vector in spherical harmonics is

$$\hat{n} \equiv \sin \theta \cos \phi e_x + \sin \theta \sin \phi e_y + \cos \theta e_z. \quad (\text{F.6})$$

Let's show that we can construct the traceless symmetric tensor. Such a power series can be written as

$$F(\hat{n}) = C_0^{(0)} + C_i^{(1)} \hat{n}_i + C_{ij}^{(2)} \hat{n}_i \hat{n}_j + \dots + C_{i_1 i_2 \dots i_l}^{(l)} \hat{n}_{i_1} \hat{n}_{i_2} \dots \hat{n}_{i_l} + \dots, \quad (\text{F.7})$$

where repeated indices are summed from 1 to 3 (as Cartesian coordinates).  $F(\hat{n})$  is satisfied Eq. (F.4). The symmetric mean that the tensors  $C_{i_1 i_2 \dots i_l}^{(l)}$  are symmetric under any reordering of the indices

$$C_{i_1 i_2 \dots i_l}^{(l)} = C_{j_1 j_2 \dots j_l}^{(l)}, \quad (\text{F.8})$$

where  $\{j_1, j_2, \dots, j_l\}$  is any permutation of  $\{i_1, i_2, \dots, i_l\}$ . The traceless mean that if any two indices are set equal to each other and summed, the result is equal to zero (except  $C^{(0)}$  and  $C_i^{(1)}$ ). Firstly we check  $C_{i_1 i_2 \dots i_l}^{(l)}$  can be constructed the traceless symmetric tensor, secondly we show  $F(\hat{n})$  is a spherical harmonics.



The symmetric can check easily as

$$F_l = C_{ij}^{(2)} \hat{n}_i \hat{n}_j = C_{ji}^{(2)} \hat{n}_j \hat{n}_i = C_{ji}^{(2)} \hat{n}_i \hat{n}_j, \quad (\text{F.9})$$

thus  $C_{ij}^{(2)}$  is symmetric. Now we show  $l = 2$  case, but we can apply to all  $l$ . We show  $C_{ij}^{(2)}$  can be constructed traceless. If  $C_{ij}^{(2)}$  is not traceless

$$\delta_{ij} C_{ij}^{(2)} = \lambda \neq 0. \quad (\text{F.10})$$

We can be constructed the traceless to redefine the  $C^{(0)}$  and  $C_{ij}^{(2)}$  as

$$\hat{C}_{ij}^{(2)} \equiv C_{ij}^{(2)} - \frac{1}{3} \delta_{ij} \lambda, \quad (\text{F.11})$$

$$\hat{C}^{(0)} \equiv C^{(0)} + \frac{1}{3} \lambda. \quad (\text{F.12})$$

It follow that  $\hat{C}_{ij}^{(2)}$  is traceless

$$\delta_{ij} \hat{C}_{ij}^{(2)} = C_{ii}^{(2)} - \frac{1}{3} \delta_{ii} \lambda = 0. \quad (\text{F.13})$$

Finally, we can write

$$C^{(0)} + C_i^{(1)} + C_{ij}^{(2)} \hat{n}_i \hat{n}_j = \hat{C}^{(0)} + C_i^{(1)} + \hat{C}_{ij}^{(2)} \hat{n}_i \hat{n}_j, \quad (\text{F.14})$$

so we can make the traceless symmetric tensor with no restriction on what functions can be expressed in this form.

We show  $F(\hat{n})$  is a spherical harmonics. We define

$$F_l(\hat{n}) \equiv C_{i_1 i_2 \dots i_l}^{(l)} \hat{n}_{i_1} \hat{n}_{i_2} \dots \hat{n}_{i_l}. \quad (\text{F.15})$$

Using a radial variable  $r$  we can represent coordinate vectors

$$\vec{r} \equiv r \hat{n} = \sum_{i=1}^3 x_i \hat{e}^i, \quad (\text{F.16})$$

where  $\hat{e}_i$  is unit vector. So we can define  $\hat{F}_l(\vec{r})$  by

$$\hat{F}_l(\vec{r}) \equiv C_{i_1 i_2 \dots i_l}^{(l)} x_{i_1} x_{i_2} \dots x_{i_l} = r^l C_{i_1 i_2 \dots i_l}^{(l)} \hat{n}_{i_1} \hat{n}_{i_2} \dots \hat{n}_{i_l} = r^l F_l(\hat{n}). \quad (\text{F.17})$$

Let's show

$$\nabla^2 \hat{F}_l(\vec{r}) = 0 \quad (\text{F.18})$$

for all  $l$ . We check  $l = 0, 1, 2, 3$  case.  $l = 0, 1$  is a trivial

$$\nabla^2 \hat{F}_0(\vec{r}) = \nabla^2 C^{(0)} = 0, \quad (\text{F.19})$$

$$\nabla^2 \hat{F}_1(\vec{r}) = C_i^{(1)} \nabla^2 x_i = 0. \quad (\text{F.20})$$

In  $l = 2$  case,

$$\begin{aligned}
\nabla^2 \hat{F}_2(\vec{r}) &= C_{ij}^{(2)} \nabla^2 x_i x_j \\
&= C_{ij}^{(2)} \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_k} x_i x_j \\
&= C_{ij}^{(2)} \frac{\partial}{\partial x_k} (\delta_{ik} x_j + x_i \delta_{jk}) \\
&= C_{ij}^{(2)} \frac{\partial}{\partial x_k} (\delta_{ik} \delta_{kj} + \delta_{ik} \delta_{jk}) \\
&= 2C_{ij}^{(2)} \delta_{ij} = 0
\end{aligned} \tag{F.21}$$

because  $C_{ij}$  is traceless. In  $l = 3$  case.

$$\begin{aligned}
\nabla^2 \hat{F}_3(\vec{r}) &= C_{ijk}^{(3)} \nabla^2 x_i x_j x_k \\
&= C_{ijk}^{(3)} \frac{\partial}{\partial x_m} \frac{\partial}{\partial x_m} x_i x_j x_k \\
&= C_{ijk}^{(3)} \frac{\partial}{\partial x_m} (\delta_{im} x_j x_k + x_i \delta_{jm} x_k + x_i x_j \delta_{km}) \\
&= C_{ijk}^{(3)} (\delta_{im} \delta_{jm} x_k + \delta_{im} x_j \delta_{km} + \delta_{im} \delta_{jm} x_k + x_i \delta_{jm} \delta_{km} + \delta_{im} x_j \delta_{km} + x_i \delta_{jm} \delta_{km}) \\
&= 2C_{ijk}^{(3)} (\delta_{ij} x_k + \delta_{ik} x_j + \delta_{jk} x_i) = 0
\end{aligned} \tag{F.22}$$

From Eq. (F.17) and Eq. (F.18)

$$\begin{aligned}
0 &= \nabla^2 \hat{F}_l(\vec{r}) \\
&= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r} \hat{F}_l(\vec{r})) + \frac{1}{r^2} \nabla_\theta^2 \hat{F}_l(\vec{r}) \\
&= \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r} (r^l F_l(\hat{n}))) + \frac{1}{r^2} \nabla_\theta^2 r^l F_l(\hat{n}) \\
&= \frac{1}{r^2} \frac{\partial}{\partial r} (l r^{l+1}) F_l(\hat{n}) + r^{l-2} \nabla_\theta^2 F_l(\hat{n}) \\
&= l(l+1) r^{l-2} F_l(\hat{n}) + r^{l-2} \nabla_\theta^2 F_l(\hat{n})
\end{aligned} \tag{F.23}$$

$$-l(l+1) F_l(\hat{n}) = \nabla_\theta^2 F_l(\hat{n}). \tag{F.24}$$

Therefore, we have found the eigenfunctions  $F_l(\hat{n})$  and eigenvalues  $-l(l+1)$  of the  $\nabla_\theta^2$ . So we show that traceless symmetric tensors are base of the spherical harmonics.

# Appendix G

## NZH reduction formula

We derive the NZH reduction formula. NZH reduction formula is

$$a_{out}(\vec{p})T(\mathcal{O}) - T(\mathcal{O})a_{in}(\vec{p}) = (-p^2 + m^2)T(\phi'(p)\mathcal{O}), \quad (\text{G.1})$$

$$T(\mathcal{O})a_{in}^\dagger(\vec{p}) - a_{out}^\dagger(\vec{p})T(\mathcal{O}) = (-p^2 + m^2)T(\mathcal{O}\phi'^\dagger(p)), \quad (\text{G.2})$$

where  $T$  is time order product and  $\mathcal{O}$  is Heisenberg field. For asymptotic field, we define Heisenberg field which is renormalized as

$$\phi'(x) \equiv \frac{1}{\sqrt{Z}}\phi(x). \quad (\text{G.3})$$

We define asymptotic field as

$$\phi'(x^0 \rightarrow \pm\infty) = \phi^{as}(x). \quad (\text{G.4})$$

Time order product of the Heisenberg field is

$$T[\phi'(x_1)\phi'(x_2)\cdots\phi'(x_n)] \equiv \phi'(x_1)\phi'(x_2)\cdots\phi'(x_n), \quad (\text{G.5})$$

where  $x_1^0 > x_2^0 > \cdots > x_n^0$ . We define the annihilation operator as

$$a_{as}(\vec{k}) = i \int d^3x (f_k^*(x)\partial_0\phi^{as}(x) - (\partial_0 f_k^*(x))\phi^{as}(x)), \quad (\text{G.6})$$

$$f_k(x) \equiv \frac{e^{-ik\cdot x}}{\sqrt{(2\pi)^3 2k_0}}. \quad (\text{G.7})$$

Let's start time order product of the fields

$$T[a_{as}(\vec{k})\phi'(x_2)\cdots\phi'(x_n)]_{x_1^0=-\infty}^{x_1^0=\infty}. \quad (\text{G.8})$$

It is possible to rewrite Eq. (G.8) to 2 patterns. First we consider asymptotic form

$$T[a_{as}(\vec{k})\phi'(x_2)\cdots\phi'(x_n)]_{x_1^0=-\infty}^{x_1^0=\infty} = a_{out}(\vec{k})[\phi'(x_2)\phi'(x_3)\cdots\phi'(x_n)] - T[\phi'(x_2)\phi'(x_3)\cdots\phi'(x_n)]a_{in}(\vec{k}). \quad (\text{G.9})$$

On the other hand, Eq. (G.8) can rewrite as

$$\begin{aligned}
T[a_{as}(\vec{k})\phi'(x_2)\cdots\phi'(x_n)]_{x_1^0=-\infty}^{x_1^0=\infty} &= \int_{-\infty}^{\infty} dx_1^0 \partial_0 [i \int d^3x (f_k^*(x_1) \\
&\quad \partial_0 T[\phi'(x_1)\cdots\phi'(x_n)] - (\partial_0 f_k^*(x))T[\phi'(x_1)\cdots\phi'(x_n)]] \\
&= i \int d^4x_1 [f_k^*(x_1)\partial_0^2 T[\phi'(x_1)\cdots\phi'(x_n)] - (\partial_0^2 f_k^*(x_1))T[\phi'(x_1)\cdots\phi'(x_n)]].
\end{aligned} \tag{G.10}$$

In the second line,  $\partial_0$  is act only  $x_1^0$ . Using Klein-Gordon equation

$$\partial_0^2 f_k^*(x_1) = (\nabla^2 - m^2)f_k^*(x_1), \tag{G.11}$$

and perform the integration by parts, we can rewrite Eq. (G.10)

$$T[a_{as}(\vec{k})\phi'(x_2)\cdots\phi'(x_n)]_{x_1^0=-\infty}^{x_1^0=\infty} = i \int d^4x_1 f_k^*(x_1)(\square + m_\pi^2)T[\phi'(x_1)\cdots\phi'(x_n)]. \tag{G.12}$$

Comparison of Eq. (G.9) and Eq. (G.12), we can derive the NZH reduction formula

$$a_{out}(\vec{p})T(\mathcal{O}) - T(\mathcal{O})a_{in}(\vec{p}) = (-p^2 + m^2)T(\phi'(p)\mathcal{O}). \tag{G.13}$$

Next we lead a similarly Eq. (G.2). We define  $a_{as}^\dagger$

$$a_{as}^\dagger(\vec{k}) = -i \int d^3x (f_k(x)\partial_0\phi^{as}(x) - (\partial_0 f_k(x))\phi^{as}(x)) \tag{G.14}$$

$$f_k(x) \equiv \frac{e^{-ik\cdot x}}{\sqrt{(2\pi)^3 2k_0}} \tag{G.15}$$

and time order product of the Heisenberg field is

$$T[a_{as}(\vec{k})\phi'(x_2)\cdots\phi'(x_n)]_{x_n^0=-\infty}^{x_n^0=\infty} = T[\phi'(x_1)\phi'(x_2)\cdots\phi(x_{n-1})]a_{in}^\dagger(\vec{k}) - a_{out}^\dagger(\vec{k})T[\phi'(x_1)\phi'(x_2)\cdots\phi'(x_{n-1})]. \tag{G.16}$$

Performing the same process, we can derive the NZH reduction formula as

$$a_{out}(\vec{p})T(\mathcal{O}) - T(\mathcal{O})a_{in}(\vec{p}) = (-p^2 + m^2)T(\phi'(p)\mathcal{O}), \tag{G.17}$$

$$T(\mathcal{O})a_{in}^\dagger(\vec{p}) - a_{out}^\dagger(\vec{p})T(\mathcal{O}) = (-p^2 + m^2)T(\mathcal{O}\phi^\dagger(p)). \tag{G.18}$$

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