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SCATTERING OF PARTICLES WITH SPIN IN THE LATTICE QCD

Doctoral thesis

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Only the parts of the thesis related to the derivation of Luscher's relation are kept

Contents

notation:

in Lectures we used p for momenta of particles in CMF
E=sqrt(p^2+m1^2)+sqrt(p^2+m2^2)

in thesis this is called q (dimemsionfull momenta)
E=sqrt(q^2+m1^2)+sqrt(q^2+m2^2)

Chapter 1

Relation between scattering amplitude and eigen-energies on the lattice

This chapter addresses the relation between the scattering amplitude for two-hadron scattering and eigen-energies obtained from a lattice simulation. It is based on the Lüscher formalism for the scattering of particles [1, 2, 3]. Rigorous derivation for the scattering of two particles without spin can be found in [4], [5]. The scattering of particles with spin is considered in the paper by Briceno [6].

We derive how the scattering amplitude for two-hadron scattering is related to eigen-energies obtained from a lattice simulation. These eigen-energies are obtained using two-hadron operators derived in paper ([7]). The scattering amplitude $\mathcal{M}$ (1.17)

$$S(E) = e^{2i\delta_l(E)} \ , \quad \mathcal{M}(E) \propto e^{2i\delta_l(E)} - 1 \tag{1.1}$$

is related to the scattering phase shift $\delta_l(E)$ in the simplest case when a single partial wave l is present. The scattering amplitude is related to possible resonances or bound states that appear in a given channel. The energy-dependence of a phase shift is

$$\cot \delta_l(E) = \frac{M^2 - E^2}{E\ \Gamma(E)} \tag{1.2}$$

for a simple Breit-Wigner type resonance with mass M and with Γ in a given channel. The relation for determination of the scattering phase shift δ on the lattice will be derived in this chapter.

The relation between the scattering amplitude and eigen-energies E, which will be derived below, is given by

$$\det[\mathbb{1} + i\ const.\ \mathcal{M}(E)\ \mathcal{G}(E)] = 0, \tag{1.3}$$

where constant $const. = \frac{1}{2}$ for identical particles and $const. = 1$ otherwise. We are interested in the scattering of non-identical particles, therefore $const. = 1$ from this point forward. The infinite-volume scattering amplitude $\mathcal{M}$ (1.17) is a function of E. $\mathcal{G}$ is a known kinematical matrix, which is also a function of energy E and the lattice size L. The equation (1.3) is satisfied only for specific energies E, which correspond to eigen-energies obtained from a lattice simulation. This renders $\mathcal{M}(E)$ for discrete values of E since $\mathcal{G}(E)$ is a known function.

Expressions for the kinematical matrix $\mathcal{G}$ and scattering amplitude $\mathcal{M}$ can also be found in the literature ([4], [5],[8], [6],...). Kinematical functions $\mathcal{G}$, scattering amplitude $\mathcal{M}$ and relations between will be derived below.

1.1 Scattering of two hadron states without spin on the lattice

Operators O in correlation function $C(E)$ 1.4 should have a good overlap with states we are investigating. In further calculations, E and $\boldsymbol{P_{tot}}$ are total energy and momentum. We will focus on example with

$$\boldsymbol{P}_{tot} = 0, \quad P = (E, \boldsymbol{P}_{tot}) = (E, \boldsymbol{0})$$

as we are interested only in scatterings with zero total momentum and we also derived this kind of operators in the paper ([7])

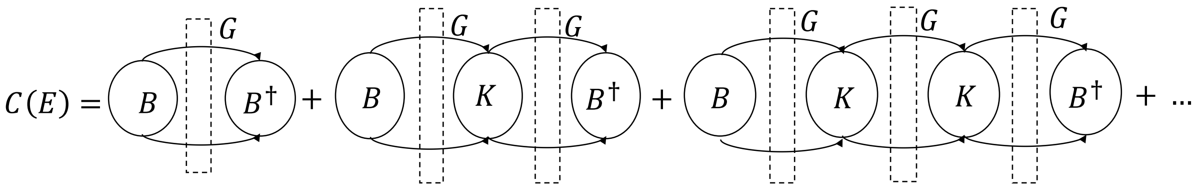

Figure 1.1: Diagram of expansion for correlation function C. Dashed boxes are integral over the momentum of fully dressed propagator G (eq. 1.6).

The correlator $C(E)$ can be expressed in terms of Bethe-Salpeter kernel K as indicated in Fig. 1.1

$$C(E) = \int d^4x e^{i(-\boldsymbol{P}_{tot}\boldsymbol{x}+Ex^0)} < 0|O(x)O^{\dagger}(0)|0 > \xrightarrow{\boldsymbol{P}=0} \tag{1.4}$$

$$C(E) = B\ G\ B^{\dagger} + B\ G\ K\ G\ B^{\dagger} + ... \tag{1.5}$$

K is a sum of all amputated two particle irreducible scattering diagrams in $s-$channel. The exact form of operators O is not essential for this discussion. G is an integral of a product of two fully dressed propagators over the momentum

$$G(E) = \frac{1}{L^3}\sum_{\boldsymbol{k}}\int \frac{dk_0}{2\pi}[z(k)\Delta(k)][z(k')\Delta(k')] \quad k' = P - k\ . \tag{1.6}$$

Here

$$[z(k)\Delta(k)] = \int d^4x e^{ikx}\left\langle \phi(x)\phi(0)\right\rangle, \qquad \Delta(k) = \frac{i}{k^2 - m^2 + i\epsilon} \tag{1.7}$$

and z is the dressing function, which is connected with the field-strenght renormalization constant Z as

$$z(k) = Z\ \text{(scalars)},\ z(k) = Z\sum_s u^s(k)\bar{u}^s(k)\ \text{(fermions)},$$
$$z(k) = Z\sum_r \epsilon^r(k)\epsilon^{*r}(k)\ \text{(vectors)}\ . \tag{1.8}$$

Field renormalization stregnth Z is a residue of the single particle pole in the two-point funcion.

Let us first discuss the renormalized scattering amplitude $\mathcal{M}$ and how it is affected by the field renormalization Z. The relation between the renormalized (Γ) and bare (Γ_B) n-point function is $\Gamma^{(n)} = (\sqrt{Z})^n \Gamma_B^{(n)}$. We consider $2 \to 2$ scattering, where the relation

$$\Gamma^4 = (\sqrt{Z})^4 \Gamma_B^4 \qquad \mathcal{M} \propto \Gamma^4 \tag{1.9}$$

directly follows from the LSZ reduction formula (chapter 7.2 of [9])

$$\prod_{i=1,2} \int d^4x_i e^{ip_i x_i} \prod_{j=1,2} \int d^4y_j e^{-ik_j y_j} \left\langle 0 | H_1(x_1) H_2(x_2) H_1^\dagger(y_1) H_2^\dagger(y_2) | 0 \right\rangle = \tag{1.10}$$
$$\underset{\substack{p_i^0 \to E_{p_i} \\ k_j^0 \to E_{k_j}}}{\sim} \left(\prod_{i=1,2} \frac{\sqrt{Z} i}{p_i^2 - m^2 + i\epsilon}\right)\left(\prod_{j=1,2} \frac{\sqrt{Z} i}{k_j^2 - m^2 + i\epsilon}\right) \langle p_1 p_2 | S | k_1 k_2 \rangle .$$

One can employ fully dressed fields in (1.9) which are renormalized or not. If one works with renormalized fields, then their $Z = 1$ in (1.6) and M in figure 1.2 already corresponds to the renomalized scattering amplitude. If one employs non-renormalized fields, then the renormalized $2 \to 2$ scattering amplitude is

$$\mathcal{M} = (\sqrt{Z})^4 \mathcal{M}_B = Z^2 \mathcal{M}_B = ZKZ + ...$$

in Fig. 1.2. Indeed, K in Fig. 1.2 is multipled by Z^2: one Z is present in G on the left and one Z in the G on the right. Therefore $Z-$factors present in G (1.6) are responsible for rendering the renormalized scattering amplitude M.

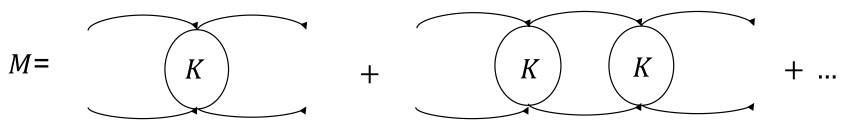

Figure 1.2: Any number of kernels K are packed into scattering amplitude M. Scattering amplitude is a function of angular momentum l. If particles carry spin than $\mathcal{M}$ is a function of total angular momentum J and spin S.

Now let us turn to the function G, which describes product of two propagators (1.7)

$$G(E) = \frac{1}{L^3} \sum_{\boldsymbol{k}} \int \frac{dk_0}{2\pi} z(k) \Delta(k) \Delta(k') z(k') \ , \quad k' = P - k, \ P = (E, \mathbf{0}). \tag{1.11}$$

Two hadron loop G is divided into the infinite volume contribution G^∞, while the reminder represents the finite volume correction G^{FV}

$$\begin{aligned} G(E) =& \frac{1}{L^3} \sum_{\boldsymbol{k}} \int \frac{dk_0}{2\pi} z(k) \frac{1}{(k^2 - m^2 + i\epsilon)(k'^2 - m^2 + i\epsilon)} z(k') = \\ =& \int \frac{d^4k}{(2\pi)^4} z(k) \Delta(k) \Delta(k') z(k') + \int d\Omega d\Omega' z(q) \mathcal{F}(q, q') z(q') = \\ =& G^\infty(E) + G^{FV}(E) \end{aligned} \tag{1.12}$$

Momenta q and q' are size of the on-shell momenta $q = |\boldsymbol{q}|$, $q' = |\boldsymbol{q}|'$, where $E = E_1 + E_2 = \sqrt{\boldsymbol{q}^2 + m_1^2} + \sqrt{\boldsymbol{q}^2 + m_2^2}$. Kinematical properties originating from the propagator Δ and

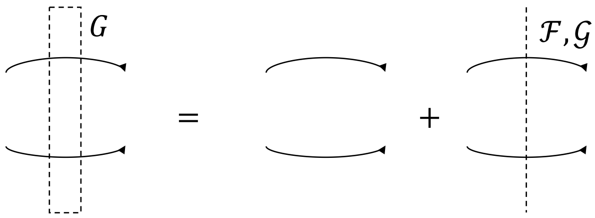

Figure 1.3: Division of two hadron loop G into the infinite volume contribution and finite volume effect in kinematical matrix $\mathcal{G}$.

finite volume dependence of G^{FV} are packed in the new function $\mathcal{F}$. $\mathcal{F}$ is a function of momentum q and q'[1], size of the lattice L and the particle masses. The identity 1.12 is shown in figure 1.3. $G^{FV}(E)$ containing finite volume corrections can be conveniently evaluated with the use of Cauchy residue theorem and Poisson summation formula as shown in appendix A.1 and later on in this section.

The correlator in Eq. (1.4) and Fig. 1.1 contains G, which is a sum of two terms in equation (1.12) and is graphically presented in Fig. 1.3. We will consider

$$C^{FV}(E) = C(E) - C^{\infty}(E) \tag{1.13}$$

where $C^{\infty}(E)$ contains no finite volume insertion $\mathcal{F}$ (Fig. 1.4).

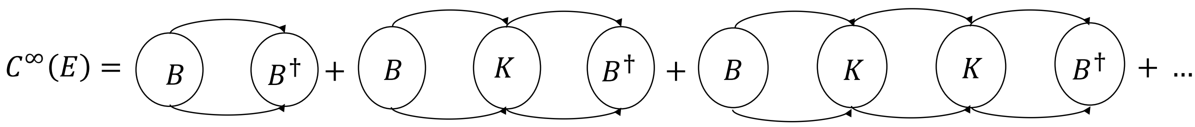

Figure 1.4: Graphical representation of $C^{\infty}(E)$, which is obtained by reorganization of terms after insertions of G in Fig. 1.1 are substituted by decomposition shown in Fig. 1.3.

One can show based on Figs. 1.1, 1.3 and 1.5 that C^{FV} can be expressed as a combination of new functions $\mathcal{A}, \mathcal{A}', \mathcal{M}$ and $\mathcal{G}$ (Fig.1.6). Fig. 1.5 defines these new variables A' and A, which are related to external operator and will not play essential role in the following.

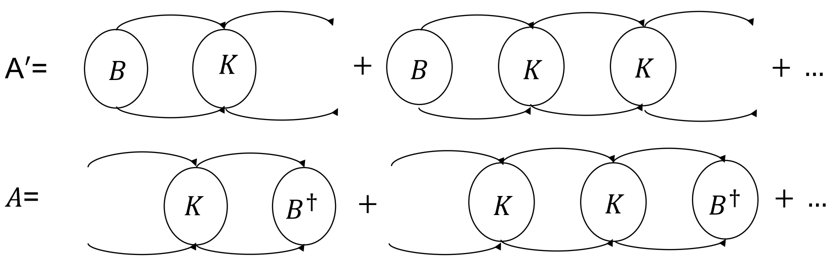

Figure 1.5: Decomposition presented in 1.3 is used in definition of new finite volume variables A' and A which are here graphically presented. Operators B or B' and all neighboring kernels K with infinite contributions are packed together into variables A and A'.

[1]Four vector k $\boldsymbol{k}^2 = \omega_k^2 - m^2$ can be either written in carthesian coordinates $k = (k_0, \boldsymbol{k}) = (k_0, (k_x, k_y, k_z))$ $k = (\omega_k, \boldsymbol{k})$ or in spherical coordinates $k = (k_0, (|\boldsymbol{k}|, \vartheta, \varphi)) = (k_0, (|\boldsymbol{k}|, \Omega))$.

It is convenient to expand new variables defined in Fig. 1.5, Fig. 1.2 and $\mathcal{F}$ in terms of spherical harmonics

$$\begin{aligned}
A(q) &\equiv \sqrt{4\pi}\sum_{l_2,m_{l_2}} \mathcal{A}_{l_2,m_{l_2}}(|\boldsymbol{q}|)Y_{l_2,m_{l_2}}(\Omega)\\
A'(q) &\equiv \sqrt{4\pi}\sum_{l_1,m_{l_1}} \mathcal{A}'_{l_1,m_{l_1}}(|\boldsymbol{q}|)Y^*_{l_1,m_{l_1}}(\Omega)\\
M(q,q') &= \sum_{l_1,m_1;l_2,m_2} 4\pi\mathcal{M}_{l_1,m_1;l_2,m_2}Y_{l_1,m_1}(|\boldsymbol{q}|)(\Omega)Y^*_{l_2,m_2}(\Omega')\\
\mathcal{F}(q,q') &= \sum_{l_1,m_1;l_2,m_2} -\frac{1}{4\pi}\mathcal{G}_{l_1,m_1;l_2,m_2}(|\boldsymbol{q}|)Y_{l_1,m_1}(\Omega)Y^*_{l_2,m_2}(\Omega'). \qquad (1.14)
\end{aligned}$$

C^{FV} for two partial waves l_1 and l_2 can be now rewritten in terms of geometrical series [2]

$$\begin{aligned}
C^{FV}(E) &= -\mathcal{A}'\mathcal{G}\mathcal{A} + \mathcal{A}'\mathcal{G}i\ \mathcal{M}\mathcal{G}\mathcal{A} + \ldots =\\
&= -\mathcal{A}'\mathcal{G}\frac{1}{1+i\ \mathcal{M}\mathcal{G}}\mathcal{A}. \qquad (1.15)
\end{aligned}$$

of kinematical factor $\mathcal{G}$, scattering amplitude $\mathcal{M}$ and operators $\mathcal{A}$ and $\mathcal{A}'$, which are all defined above in equation (1.14). Graphical representation of C^{FV} defined in (1.15) is shown on Figure 1.6. Each vertical line on figure 1.6 represents one insertion of kine-

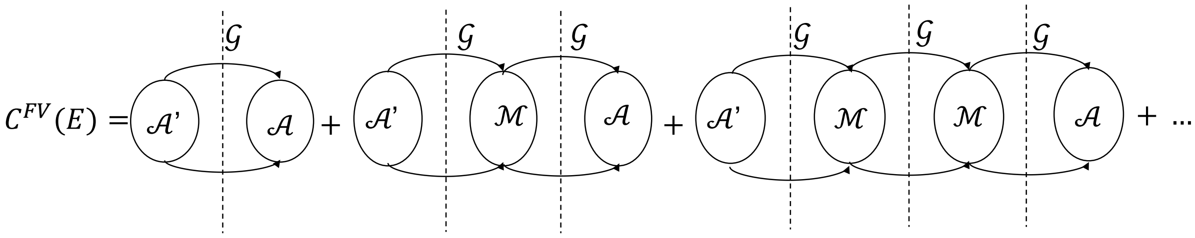

Figure 1.6: Diagramatical representation of finite volume contributions to corelation function C^{FV} with new variables $\mathcal{G}$,$\mathcal{M}$, $\mathcal{A}$ and $\mathcal{A}'$.

matical factor $\mathcal{F}$ which is connected with kinematical function $\mathcal{G}$ as written in equation (1.14). The same result would be obtained if variables A,A',M and $\mathcal{F}$ would be used instead of new ones because the identity

$$\sum_{l_1,m_1} Y_{l_1,m_1}(\Omega)Y^*_{l_1,m_1}(\Omega') = \delta\left(\Omega - \Omega'\right)$$

would occur between each pair of variables.

Poles of $C^{FV}(E)$ (1.15), originating from the insertions of the function $\mathcal{F}\mathcal{G}$ (Fig. 1.6), are equal to those of $C(E)$, because the infinite volume contribution C^∞

The poles in the finite volume corrections of correlation function $C^{FV}(E)$ (1.15) correspond to eigen-energies on the finite lattice. In order to find the poles of C^{FV} (1.15) one has to solve the following equation

$$\det\left[1 + i\mathcal{M}(E)\mathcal{G}(E)\right] = 0, \qquad (1.16)$$

[2] $(1\pm x)^{-m} = 1 \mp mx + \frac{m(m+1)}{2!}x^2 \mp \frac{m(m+1)(m+2)}{3!}x^3 + \ldots$

which represents one form of the Lüscher's equation. The solutions of the Lüscher's equation occur for certain discrete energies E, which correspond to eigenenergies on the finite lattice. They depend on the scattering amplitude $\mathcal{M}$ for partial wave l

$$\mathcal{M}_{l_1,m_1;l_2,m_2}(E) = \mathcal{M}_{l_1}(E)\ \delta_{l_1 l_2}\delta_{m_1 m_2}\ , \qquad \mathcal{M}_{l_1}(E) = \frac{8\pi E}{|\boldsymbol{q}|}\frac{e^{2i\delta_{l_1}(q)}-1}{2i}, \tag{1.17}$$

Here $q \equiv |\boldsymbol{q}|$ is the magnitude of the on-shell spatial hadron momentum in cmf-frame corresponding to the energy E

$$E = E_1 + E_2 = \sqrt{\boldsymbol{q}^2 + m_1^2} + \sqrt{\boldsymbol{q}^2 + m_2^2}\ , \quad q \equiv |\boldsymbol{q}|\ . \tag{1.18}$$

The quantization condition (1.16) depends also on the kinematical factor $\mathcal{G}$. $\mathcal{G}$ is obtained from G^{FV} (1.12). The later is equal to $G_1^{FV}(q^2)$, as shown in the Appendix A.2,

$$G^{FV}(E) = G_1^{FV}(q^2), \quad G_1^{FV}(q^2) \equiv -\left(\frac{q f_{00}(q)}{8\pi E} - \frac{i}{2E}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}(q) c_{lm}(q^2)\right) \tag{1.19}$$

where

$$f(\boldsymbol{k}) = z(\boldsymbol{k})\ z(\boldsymbol{k}) \tag{1.20}$$

is the product of dressing functions for both hadrons, q is an (dimensionfull) on-shell momentum (1.18) and c_{lm} is defined below (1.21). The above relation reduces G^{FV} to G_1^{FV}, where the later is more practical for actual numerical evaluation. The sum over four-momentum k in G^{FV} (1.12) is reduced to a function $G_1^{FV}(q^2)$ at an *on-shell* value of the momentum q that is related to the energy E as given in (1.18). The c_{lm} from (1.19) is defined in terms of the well-known Lüscher's zeta functions Z_{lm}

$$c_{lm}(|\boldsymbol{q}|^2) \equiv -\frac{\sqrt{4\pi}}{L^3}\left(\frac{2\pi}{L}\right)^{l-2} Z_{lm}\left[1; (\frac{|\boldsymbol{q}|L}{2\pi})^2\right]\ , \quad Z_{lm}\left[s, \tilde{q}^2\right] \equiv \sum_{\boldsymbol{n}\in N^3} \frac{|\boldsymbol{n}|^l\, Y_{lm}(\boldsymbol{n})}{(n^2 - \tilde{q}^2)^s} \tag{1.21}$$

Given the expression for the finite volume corrections to the loop function G^{FV} (1.19), it is straightforward to determine $\mathcal{G}$, which is related to G^{FV} via (1.12,1.14). In the Appendix A.2 we show that $\mathcal{G}$ that corresponds to G^{FV} above is

$$\begin{aligned}\mathcal{G}_{l_1 m_1; l_2 m_2}(q) &= \frac{q}{8\pi E}(\delta_{l_1,l_2}\delta_{m_1,m_2} + i\mathcal{G}^{FV}_{l_1 m_1; l_2 m_2})(q) \\ \mathcal{G}^{FV}_{l_1 m_1; l_2 m_2}(q) &= -\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(4\pi)^{\frac{3}{2}}}{q^{l+1}} c_{lm}(q^2)\int d\Omega Y^*_{l_1 m_2}(\Omega) Y^*_{lm}(\Omega) Y_{l_2 m_2}(\Omega)\end{aligned} \tag{1.22}$$

In practice, Appendix A.2 shows that when $\mathcal{G}$ (1.22) is inserted to the expression for G^{FV} (1.12,1.14) then one indeed gets (1.19).

In conclusion, the final relation between eigen-energies and scattering matrix is (1.16), where the scattering matrix $\mathcal{M}$ is defined in (1.17) and $\mathcal{G}$ is a know kinematical function given in (1.22). Examples of the Lüscher equation will be shown in section 1.2 for scattering without spin and in section 1.3 for scattering with spin.

1.2 Simplified Lüscher equation for spinless scattering

Poles of C^{FV} given in 1.15 are determined by $\det(1 + i\mathcal{M}\mathcal{G}) = 0$ ((1.16).

These poles correspond to the energy spectrum in the observed channel. $\mathcal{G}$ inherits its poles from function c_{lm} defined in equation 1.21. For simplicity of following derivation one can define new matrix $\mathcal{X}$

$$\mathcal{X} = 1 + i\mathcal{M}\mathcal{G}. \tag{1.23}$$

which equals

$$\begin{aligned}\mathcal{X}_{l_1,m_1;l_2,m_2} &= (1 + i\ \mathcal{M}\mathcal{G})_{l_1,m_1;l_2,m_2} = \\ &= \delta_{l_1,l_2}\delta_{m_1,m_2} + \frac{8\pi E}{|\boldsymbol{q}|}\mathcal{G}_{l_1,m_1;l_2,m_2}(e^{2i\delta_{l_1}(|\boldsymbol{q}|)} - 1),\end{aligned} \tag{1.24}$$

where $\delta_{l_1}(|\boldsymbol{q}|)$ is phase shift for partial wave l_1 and $\delta_{l_1,l_2}, \delta_{m_1,m_2}$ is Kronecker delta function for $l_{1,2}$ and $m_{1,2}$ respectively.

Let us consider scattering where one has contributions of two partial waves l_1 and l_2 present in channel under consideration [3]

$$\begin{aligned}\det \mathcal{X} &= 0\\ \mathcal{X}_{l_1l_1}\mathcal{X}_{l_2l_2} - \mathcal{X}_{l_1l_2}\mathcal{X}_{l_2l_1} &= 0\\ (\delta_{m_1,m_2} + \frac{8\pi E}{|\boldsymbol{q}|}\mathcal{G}_{l_1,m_1;l_1,m_2}(e^{2i\delta_{l_1}(|\boldsymbol{q}|)} - 1))(\delta_{m_1,m_2} + \frac{8\pi E}{|\boldsymbol{q}|}\mathcal{G}_{l_2,m_1;l_2,m_2}(e^{2i\delta_{l_2}(q)} - 1)) - &\\ - \left(\frac{8\pi E}{|\boldsymbol{q}|}\right)^2 \mathcal{G}^2_{l_1,m_1;l_2,m_2}(e^{2i\delta_{l_1}(q)} - 1)(e^{2i\delta_{l_2}(q)} - 1) &= 0.\end{aligned} \tag{1.25}$$

If both partial waves are non-negligible and if $\mathcal{G}_{l_1,m_1;l_2,m_2} \neq 0$, one has to employ the above Lüscher's equation 1.25. It represents one equation for two unknowns $\delta_{l_1}(E)$ and $\delta_{l_2}(E)$ at given energy E.

In the analysis of our results, we will employ a simplifying approximation, where only one partial wave l_1 is dominant in a given channel, while others are negligible. In this case $\delta_{l_2}(E) = 0$ and $e^{2i\delta_{l_2}(|\boldsymbol{q}|)} - 1 = 0$, so 1.25 simplifies to

$$\delta_{m_1,m_2} + \frac{8\pi E}{|\boldsymbol{q}|}\mathcal{G}_{l_1,m_1;l_1,m_1}(e^{2i\delta_{l_1}(|\boldsymbol{q}|)} - 1) = 0. \tag{1.26}$$

Scattering in partial wave with l_1 therefore gives the equation 1.26 and leads to

$$\begin{aligned}1 - e^{2i\delta_{l_1}(|\boldsymbol{q}|)} &= \left(\frac{8\pi E}{|\boldsymbol{q}|}\mathcal{G}_{l_1,m_1;l_1,m_1}\right)^{-1}\\ \frac{1 + i\cot\delta_{l_1}(|\boldsymbol{q}|)}{1 + \cot^2\delta_{l_1}(|\boldsymbol{q}|)} &= \frac{1 + i\frac{4\pi}{|\boldsymbol{q}|}c_{00}(|\boldsymbol{q}|^2)}{1 + \left(\frac{4\pi}{|\boldsymbol{q}|}c_{00}(|\boldsymbol{q}|^2)\right)^2}.\end{aligned} \tag{1.27}$$

One can read from equation 1.27 that Lüscher equation is now

$$\cot\left(\delta_{l_1}(|\boldsymbol{q}|)\right) = \frac{4\pi}{|\boldsymbol{q}|}c_{00}(|\boldsymbol{q}|^2) = \frac{2Z_{00}\left[1; \left(|\boldsymbol{q}|\frac{L}{2\pi}\right)^2\right]}{\sqrt{\pi}L|\boldsymbol{q}|}, \tag{1.28}$$

with $c_{00}(|\boldsymbol{q}|^2)$ and Z_{00} defined in 1.21.

[3] For example partial waves with $l_1 = 1$ and $l_2 = 3$, where $\mathcal{G}_{1,m_1;3,m_2}$ is indeed not zero.

1.3 Generalization for scattering with spin

Finally the generalization of equations derived above for scattering of particles with spin should be performed. The original derivation for scattering of particles with arbitrary spin can be found in [6]. This paper is a generalization of the previous work on finding a finite volume spectrum by several authors ([4], [10],[11], [12],[13],...). For scattering of two particles with total spin S more than one partial wave l can contribute at given total angular momentum J ($\boldsymbol{J} = \boldsymbol{l} \oplus \boldsymbol{S}$) even in continuum. For example in scattering of vector meson J/ψ with spin $S_1 = 1$ and proton with spin $S_2 = \frac{1}{2}$ in channel with total spin $S = \frac{3}{2}$ and total angular momentum $J^P = \frac{3}{2}^-$, dinamical mixing of partial waves with $l = 0$ and $l = 2$ occurs. The scattering matrix S for this example is equal to

$$S = \mathcal{M} + 1 = \begin{bmatrix} S\left[J/\psi N\left({}^4S_{\frac{3}{2}}\right)|J/\psi N\left({}^4S_{\frac{3}{2}}\right)\right] & S\left[J/\psi N\left({}^4S_{\frac{3}{2}}\right)|J/\psi N\left({}^4D_{\frac{3}{2}}\right)\right] \\ S\left[J/\psi N\left({}^4D_{\frac{3}{2}}\right)|J/\psi N\left({}^4S_{\frac{3}{2}}\right)\right] & S\left[J/\psi N\left({}^4D_{\frac{3}{2}}\right)|J/\psi N\left({}^4D_{\frac{3}{2}}\right)\right] \end{bmatrix}, \tag{1.29}$$

here states are noted in the form $H_1H_2\left({}^{2S+1}l_J\right)$ on the source and the sink.

As an example, we will predict the eigen-energies of NJ/ψ based on the experimental masses of P_c pentaquark resonances in one-channel approximation. We will take additional approximation where only one partial wave is dominant in each channel where pentakquark P_c was observed. So only one phase shift $\delta_{l,S}$ would be non zero and contribute to the Lüscher equation.

The relation between eigen-energies and scattering matrix, i.e. the quantization condition, (1.3)

$$\det\left[1 + i\mathcal{M}(E)\mathcal{G}(E)\right] = 0$$

is now a function of spin S, orbital angular momentum l and total angular momentum J

$$\det\left[(1 + i\mathcal{M}(E)\mathcal{G}(E))_{\substack{J_1,m_{J_1};l_1,S_1 \\ J_2,m_{J_2};l_2,S_2}}\right] = 0. \tag{1.30}$$

Scattering amplitude $\mathcal{M}$ is a function of orbital angular momentum l, total spin S, and angular momentum J. Matrix $\mathcal{M}$ is diagonal in angular momentum J, for different combinations of l and S is in general not diagonal(1.29).

As an example we will predict eigen-energies of NJ/ψ based on the experimental masses of P_c pentaquark in one channel approximation. We will take additional approximation where only one partial wave l is dominant in each channel (only one diagonal element of S 1.29) is non-zero) and only one phase shift δ_{l_1,S_1} would be non zero and contributes to the Lüscher equation

$$S_{\substack{Jm_Jl_1S_1 \\ Jm_Jl_2S_2}} = \delta_{S_1S_2}\delta_{l_1l_2}S\left[J/\psi N\left({}^{2S_1+1}(l_1)_J\right)|J/\psi N\left({}^{2S_2+1}(l_2)_J\right)\right] = e^{2i\delta_{(l_1,S_1)}} \tag{1.31}$$

$$S_{\substack{Jm_Jl_1S_1 \\ Jm_Jl_2S_2}} = \delta_{S_1S_2}\delta_{l_1l_2}\left(\mathcal{M}_{\substack{Jm_Jl_1S_1 \\ Jm_Jl_2S_2}} + 1\right).$$

Kinematical matrix $\mathcal{G}$ is similar to $\mathcal{M}$ a function of total angular momentum J, orbital angular momentum l and spin S. It is diagonal in spin S, but it is not diagonal in J. So, scattering amplitude $\mathcal{M}$ and kinematical function $\mathcal{G}$ in quantized condition (1.30) depend on total spin S and total angular momentum J in addition to the orbital angular momentum l, which is the only independent variable in calculation of Lüscher equation for scattering of partices without spin (Eq. 1.17 , 1.22 and 1.28).

1.3.1 Transformation from variables for scattering without spin to scattering with spin

Functions used in quantization condition in previous chapter $\mathcal{M}_{l_1,m_{l_1};l_2,m_{l_2}}$ and $\mathcal{G}_{l_1,m_{l_1};l_2,m_{l_2}}$ are dependent on $l_{1,2}$ and its third component $m_{l_{1,2}}$. No explicit dependence on spin S was explicitly written for $S=0$. Their dependence on spin origins from factor z (1.7) contained in the particle propagator. The scattering amplitude $\mathcal{M}$ (1.29) is diagonal for $S=0$ (in that case $l=J$ and scattering matrix is always diagonal in J). The kinematical function $\mathcal{G}$ is a function of orbital angular momentum $l_1, m_1; l_2, m_2$ for $S=0$ and we expand it in terms of total angular momentum J and spin S for $S \neq 0$.

There is a simple transformation for variables in scattering of particles without spin to those for scattering of particles with spin via Clebsch-Gordan coefficients

$$F_{\substack{J_1,m_{J_1};l_1,S_1\\ J_2,m_{J_2};l_2,S_2}}(|\boldsymbol{q}|) = \sum_{\substack{m_{l_1},m_{S_1}\\ m_{l_2},m_{S_2}}} C^{J_1,m_{J_1}}_{l_1,m_{l_1};S_1,m_{S_1}} C^{J_2,m_{J_2}}_{l_2,m_{l_2};S_2,m_{S_2}} \langle l_2 m_{l_2}; S_2 m_{S_2}|\, F(|\boldsymbol{q}|)\, |l_1 m_{l_1}; S_1 m_{S_1}\rangle\,,$$
$$\langle l_2 m_{l_2}; S_2 m_{S_2}|\, F(|\boldsymbol{q}|)\, |l_1 m_{l_1}; S_1 m_{S_1}\rangle = F_{\substack{l_1 m_{l_1};S_1 m_{S_1}\\ l_2 m_{l_2};S_2 m_{S_2}}}. \tag{1.32}$$

Mathematical derivation of 1.32 for some arbitrary function F which is a function of orbital angular momentum l and on shell momentum q to a function of total angular momentum J, orbital angular momentum l and spin S can be found in appendix A.3. Similar transition expression can be found for scattering of nucleon in pion in paper [14],[8],[10],....

We use previous relation 1.32 (or more explicitly A.30) in (A.29)) and after short calculation one gets kinematical function $\mathcal{G}$ as a function of the on shell momentum $|\boldsymbol{q}|$ (1.18)

$$\mathcal{G}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|) = \frac{|\boldsymbol{q}|}{8\pi E}\delta_{S_1,S_2}\left[\delta_{l_1 l_2}\delta_{J_1,J_2}\delta_{m_{J_1},m_{J_2}} + i\mathcal{G}^{FV}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|)\right], \tag{1.33}$$

where finite volume correction are

$$\mathcal{G}^{FV}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|) = \sum_{\substack{m_{l_1},m_S\\ m_{l_2}}} C^{J_1 m_{J_1}}_{l_1 m_{l_1},S_1 m_S} C^{J_2 m_{J_2}}_{l_2 m_{l_2},S_2 m_S} \mathcal{G}^{FV}_{\substack{l_1 m_{l_1}\\ l_2 m_{l_2}}}(|\boldsymbol{q}|)$$
$$\mathcal{G}^{FV}_{\substack{l_1,S_1,J_1,m_{J_1}\\ l_2,S_2,J_2,m_{J_2}}}(|\boldsymbol{q}|) = -\sum_{\substack{m_{l_1},m_S\\ m_{l_2}}} C^{J_1 m_{J_1}}_{l_1 m_{l_1},S_1 m_S} C^{J_2 m_{J_2}}_{l_2 m_{l_2},S_2 m_S}$$
$$\sum_{l,m} \frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}} c_{lm}(|\boldsymbol{q}|^2) \int d\Omega Y^*_{l_1,m_{l_1}}(\Omega) Y^*_{l,m}(\Omega) Y_{l_2,m_{l_2}}(\Omega).$$

Kinematical function $\mathcal{G}$ is diagonal only in spin S_1. In Lüscher equation (1.3,1.30) kinematical function $\mathcal{G}$ and scattering amplitude $\mathcal{M}$ (1.29) are used.

Lüscher equation in case when one channel (l, S) dominates

The previous subsection treated scattering scattering of particles with spin in complete generality. Here we consider an aproximation where only one partial wave l and one spin S contributes to the scattering amplitude $\mathcal{M}$ and therefore all off-diagonal elements in scattering matrix (1.29) are equal to 0

$$\mathcal{M}_{\substack{J,m_J;l_1,S_1\\J,m_J;l_2,S_2}}(|\boldsymbol{q}|) = \delta_{l_1,l_2}\ \delta_{S_1,S_2}\ \mathcal{M}_{\substack{J,m_J,l_1,S_1\\J,m_J,l_1,S_1}}(|\boldsymbol{q}|), \qquad \mathcal{M}_{\substack{J,m_J,l_1,S_1\\J,m_J,l_1,S_1}}(|\boldsymbol{q}|) = \frac{16\pi E}{|\boldsymbol{q}|}\frac{e^{2i\delta_{(l_1,S_1)}}-1}{2i}. \tag{1.34}$$

where $l_1 = l_2$, $S_1 = S_2$ and $J_1 = J_2$. Phase shift $\delta_{(l,S)}$ then depends on the orbital angular momentum l and on the spin S. Dependence on spin was not explicitly written because for $S = 0$ scattering matrix is diagonal in orbital angular momentum l. For $S = 0$ angular momentum J is equal to orbital angular momentum l. Generalization for scattering with spin ($S \neq 0$) is made in (1.29).

We insert this simplified scattering matrix $\mathcal{M}$ (1.34) into the general quantization condition (1.30). For derivation of the Lüscher equation one needs also kinematical function $\mathcal{G}$ (A.29), which in general remains off-diagonal in J. For simplicity, new variable $\mathcal{X}$ is introduced in the quantization condition (1.30) [4]

$$\mathcal{X}(|\boldsymbol{q}|) = 1 + i\mathcal{M}(|\boldsymbol{q}|)\mathcal{G}(|\boldsymbol{q}|), \qquad \mathcal{X}_{\substack{J_1,m_{J_1},l_1,S_1\\J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|) = (1 + i\mathcal{M}(|\boldsymbol{q}|)\mathcal{G})_{\substack{J_1,m_{J_1},l_1,S_1\\J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|). \tag{1.35}$$

With use of previously derived quantities $\mathcal{M}$ and $\mathcal{G}$ (Eq. 1.34 and 1.33) one gets general matrix element for new already simplified function $\mathcal{X}$

$$\mathcal{X}_{\substack{J_1,m_{J_1},l_1,S_1\\J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|) = \delta_{J_1J_2}\delta_{m_{J_1}m_{J_2}}\delta_{l_1l_2}\delta_{S_1S_2} + i\delta_{S_1S_2}\mathcal{M}_{l_1,S_1}(|\boldsymbol{q}|)\mathcal{G}_{\substack{J_1,m_{J_1},l_1,S_1\\J_2,m_{J_2},l_2,S_2}}(|\boldsymbol{q}|). \tag{1.36}$$

When only partial wave (l_1, S_1) dominates and other are negligible, then $\mathcal{M}_{l_1,S_1}$ is the only non-zero aplitude. The quantization condition $\det(\mathcal{X}) = 0$ translates to

$$\left(e^{2i\delta_{l_1,S_1}} + i\left(e^{2i\delta_{l_1,S_1}} - 1\right)\mathcal{G}^{FV}_{\substack{J_1,m_{J_1},l_1,S_1\\J_1,m_{J_1},l_1,S_1}}(|\boldsymbol{q}|)\right) = 0. \tag{1.37}$$

Simplified quantization condition (1.37) gives Lüscher equation for scattering of two particles with spin

$$\cot\delta_{(l=l_1,S=S_1)} = \frac{2Z_{0,0}\left(1;\left(|\boldsymbol{q}|\frac{L}{2\pi}\right)^2\right)}{\sqrt{\pi}L|\boldsymbol{q}|}. \tag{1.38}$$

Expression for phase shift (1.38) for scattering with spin is of same form as the one for scattering with $S = 0$ (1.28).

1.4 Predictions of eigen-energies in charmed pentaquark P_c^+ channel

In 2015, two peaks in proton-J/ψ invariant mass with minimal flavor structure of $uudc\bar{c}$ were observed by LHCb ([15],[16]). In 2019 same collaboration anounced ([17]) that upper

[4] Similar proceedure was performed for spinless case in section 1.2

Bibliography

[1] M. Lüscher, *Volume dependence of the energy spectrum in massive quantum field theories*, Communications in Mathematical Physics **105**, 153 (1986).

[2] M. Lüscher and U. Wolff, *How to calculate the elastic scattering matrix in two-dimensional quantum field theories by numerical simulation*, Nuclear Physics B **339**, 222 (1990).

[3] M. Lüscher, *Two-particle states on a torus and their relation to the scattering matrix*, Nuclear Physics B **354**, 531 (1991).

[4] C. h. Kim, C. T. Sachrajda and S. R. Sharpe, *Finite-Volume Effects for Two-Hadron States in Moving Frames*, Nuclear Physics B **727**, 218 (2005).

[5] M. T. Hansen and S. R. Sharpe, *Multiple-channel generalization of Lellouch-Luscher formula*, Physical Review D **86**, 10.1103/PhysRevD.86.016007 (2012).

[6] R. A. Briceño, *Two-particle multichannel systems in a finite volume with arbitrary spin*, Physical Review D **89**, 10.1103/physrevd.89.074507 (2014).

[7] S. Prelovsek, U. Skerbis and C. B. Lang, *Lattice operators for scattering of particles with spin*, Journal of High Energy Physics **2017**, 10.1007/jhep01(2017)129 (2017).

[8] N. Li and C. Liu, *Generalized Lüscher formula in multichannel baryon-meson scattering*, Physical Review D **87**, 10.1103/physrevd.87.014502 (2013).

[9] M. E. Peskin and D. V. Schroeder, *Introduction To Quantum Field Theory* (Westview Press, 1995).

[10] R. A. Briceño and Z. Davoudi, *Moving multichannel systems in a finite volume with application to proton-proton fusion*, Physical Review D **88**, 10.1103/physrevd.88.094507 (2013).

[11] P. F. Bedaque, *Aharonov–Bohm effect and nucleon–nucleon phase shifts on the lattice*, Physics Letters B **593**, 82 (2004).

[12] P. F. Bedaque and J.-W. Chen, *Twisted valence quarks and hadron interactions on the lattice*, Physics Letters B **616**, 208 (2005).

[13] V. Bernard, M. Lage, U.-G. Meißner and A. Rusetsky, *Scalar mesons in a finite volume*, Journal of High Energy Physics **2011**, 10.1007/jhep01(2011)019 (2011).

[14] V. Bernard, M. Lage, U.-G. Meißner and A. Rusetsky, *Resonance properties from the finite-volume energy spectrum*, Journal of High Energy Physics **2008**, 024 (2008).

[15] L. Collaboration (LHCb Collaboration), *Observation of $J/\psi p$ Resonances Consistent with Pentaquark States in $\Lambda_b^0 \to J/\psi K^- p$ Decays*, Physical Review Letters **115**, 072001 (2015).

[16] L. Collaboration (LHCb Collaboration), *Model-Independent Evidence for $J/\psi p$ Contributions to $\Lambda_b^0 \to J/\psi p K^-$ Decays*, Physical Review Letters **117**, 082002 (2016).

[17] L. collaboration, *Observation of a Narrow Pentaquark State, $P_c(4312)^+$, and of the Two-Peak Structure of the $P_c(4450)^+$*, Physical Review Letters **122**, 10.1103/physrevlett.122.222001 (2019).

[18] D. Collaboration, *Inclusive production of the P_c^+ resonances in $p\bar{p}$ collisions*, (2019).

[19] F.-K. Guo, H.-J. Jing, U.-G. Meißner and S. Sakai, *Isospin breaking decays as a diagnosis of the hadronic molecular structure of the $P_c(4457)$*, Physical Review D **99**, 10.1103/PhysRevD.99.091501 (2019).

[20] H.-X. Chen, W. Chen and S.-L. Zhu, *Possible interpretations of the $P_c(4312)$, $P_c(4440)$, and $P_c(4457)$*, Physical Review D **100**, 10.1103/PhysRevD.100.051501 (2019).

[21] M.-L. Du, V. Baru, F.-K. Guo, C. Hanhart, U.-G. Meißner, J. A. Oller and Q. Wang, *Interpretation of the LHCb P_c States as Hadronic Molecules and Hints of a Narrow $P_c(4380)$*, Physical Review Letters **124**, 10.1103/PhysRevLett.124.072001 (2020).

[22] T. Gutsche and V. E. Lyubovitskij, *Structure and decays of hidden heavy pentaquarks*, Physical Review D **100**, 10.1103/PhysRevD.100.094031 (2019).

[23] J. He and D.-Y. Chen, *Molecular states from $\Sigma_c^{(*)}\bar{D}^{(*)} - \Lambda_c\bar{D}^{(*)}$* interaction 10.1140/epjc/s10052-019-7419-7 (2019).

[24] Y.-W. Pan, M.-Z. Liu, F.-Z. Peng, M. S. Sánchez, L.-S. Geng and M. P. Valderrama, *Model independent determination of the spins of the $P_c(4440)$ and $P_c(4457)$ from the spectroscopy of the triply charmed dibaryons*, Physical Review D **102**, 10.1103/PhysRevD.102.011504 (2020).

[25] F.-Z. Peng, M.-Z. Liu, Y.-W. Pan, M. S. Sánchez and M. P. Valderrama, *Five-flavor pentaquarks and other light- and heavy-flavor symmetry partners of the LHCb hidden-charm pentaquark*, (2019).

[26] A. Ramos, A. Feijoo, Q. Llorens and G. Montaña, *The molecular nature of some exotic hadrons*, (2020).

[27] S. Sakai, H.-J. Jing and F.-K. Guo, *Decays of P_c into $J/\psi Nand\eta_c N$ with heavy quark spin symmetry*, Physical Review D **100**, 10.1103/PhysRevD.100.074007 (2019).

[28] Y. Shimizu, Y. Yamaguchi and M. Harada, *Heavy quark spin multiplet structure of $P_c(4312)$, $P_c(4440)$, and $P_c(4457)$*, (2019).

[29] M. B. Voloshin, *Hidden-charm pentaquark formation in antiproton - deuterium collisions*, Physical Review D **99**, 10.1103/PhysRevD.99.093003 (2019).

[30] F.-L. Wang, R. Chen, Z.-W. Liu and X. Liu, *Possible triple-charm molecular pentaquarks from $\Xi_{cc}D_1/\Xi_{cc}D_2^*$ interactions*, Physical Review D **99**, 054021 (2019).

[31] Z.-G. Wang, H.-J. Wang and Q. Xin, *The hadronic coupling constants of the lowest hidden-charm pentaquark state with the QCD sum rules in solid quark-hadron duality*, (2020).

[32] C. W. Xiao, J. Nieves and E. Oset, *Prediction of hidden charm strange molecular baryon states with heavy quark spin symmetry*, Physics Letters B **799**, 135051 (2019).

[33] Y. Yamaguchi, H. Garcia-Tecocoatzi, A. Giachino, A. Hosaka, E. Santopinto, S. Takeuchi and M. Takizawa, *P_c pentaquarks with chiral tensor and quark dynamics*, Physical Review D **101**, 10.1103/PhysRevD.101.091502 (2020).

[34] G. Yang, J. Ping and J. Segovia, *Doubly Charmed Pentaquarks*, Physical Review D **101**, 10.1103/PhysRevD.101.074030 (2020).

[35] L. Leskovec and S. Prelovsek, *Scattering phase shifts for two particles of different mass and nonzero total momentum in lattice QCD*, Physical Review D **85**, 10.1103/physrevd.85.114507 (2012).

Appendix A

Derivations related to the Lüscher equation

A.1 Division of two hadron loop into the infinite and finite volume contribution

In general loop summation is of the form

$$G(E) = \frac{1}{L^3} \sum_{\boldsymbol{k}} \int \frac{dk_0}{2\pi} \frac{-f(k)}{(k^2 - m^2 + i\epsilon)((P-k)^2 - m^2 + i\epsilon)}, \qquad k = (k_0, \boldsymbol{k}) \tag{A.1}$$

where P is four-vector. Function $f(k_0, \boldsymbol{k})$ is defined as $f(k) = z(k)z(k') = z(k)z(P-k)$, where dressing function $z(k)$ is listed in main text (1.8). For us $\boldsymbol{P}_{tot} = 0$ ($P = (E, 0)$), $k = (k_0, \boldsymbol{k})$ and we have particles with different masses m_1, m_2 therefore G is rewritten

$$\begin{aligned} G(E) &= \frac{1}{L^3} \sum_{\boldsymbol{k}} \int \frac{dk_0}{2\pi} \frac{-f(k)}{(k^2 - m_1^2 + i\epsilon)((P-k)^2 - m_2^2 + i\epsilon)} = \\ &= \frac{1}{L^3} \sum_{\boldsymbol{k}} \int \frac{dk_0}{2\pi} \frac{-f(k_0, \boldsymbol{k})}{(k_0^2 - \boldsymbol{k}^2 - m_1^2)((E-k_0)^2 - \boldsymbol{k}^2 - m_2^2)}. \end{aligned} \tag{A.2}$$

One uses Cauchy residue theorem and gets decomposition of G to

$$G(E) = -\frac{i}{L^3} \sum_{\boldsymbol{k}} \left(\frac{f(\omega_1, \boldsymbol{k})}{2\omega_1((E-\omega_1)^2 - \omega_2^2)} + \frac{f(\omega_2, \boldsymbol{k})}{2\omega_2((E+\omega_2)^2 - \omega_1^2)} \right), \tag{A.3}$$

with new variables $\omega_1^2 = \boldsymbol{k}^2 + m_1^2$ and $\omega_2^2 = \boldsymbol{k}^2 + m_2^2$. One is interested in the singularities which carry informations on finite volume corrections and can be found in the first term of decomposition given in A.3.

$$G_1(E) = -\frac{i}{L^3} \sum_{\boldsymbol{k}} \frac{f(\boldsymbol{k})}{2\omega_1((E-\omega_1)^2 - \omega_2^2)} \tag{A.4}$$

In term of interest G_1 one uses definition of $E = E_1 + E_2$ with $E_i = \sqrt{\boldsymbol{q}^2 + m_i^2}$, $\omega_1^2 = \boldsymbol{k}^2 + m_1^2$ and $\omega_2^2 = \boldsymbol{k}^2 + m_2^2$. Function f is from here forward written as $f(\boldsymbol{k})$ instead of $f(\omega_i, \boldsymbol{k})$ as technically ω is a function of $\boldsymbol{k}$ and therefore only independent variable in f is $\boldsymbol{k}$. With use of definitions for energy E, ω_1 and ω_2 one can rewrite G_1 in following form

$$G_1(q^2) = -\frac{1}{L^3}\frac{i}{2E}\sum_{\boldsymbol{k}}\frac{f(\boldsymbol{k})}{q^2-k^2}\frac{E_1+\omega_1}{2\omega_1}. \tag{A.5}$$

For simplicity we define new function

$$h(\boldsymbol{k}) = -\frac{i}{2E}f(\boldsymbol{k})\frac{E_1+\omega_1}{2\omega_1}, \tag{A.6}$$

$$h(\boldsymbol{q}) = -\frac{i}{2E}f(\boldsymbol{q}), \qquad \text{because} \quad \left.\frac{E_1+\omega_1}{2\omega_1}\right|_{k=q} = 1$$

with non singular fourier transform $\tilde{h}(\boldsymbol{k})$. Function $h(\boldsymbol{k})$ can be expanded in terms of spherical harmonics

$$h(\boldsymbol{k}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} h_{lm}(\boldsymbol{k})k^l\sqrt{4\pi}Y_{lm}(\vartheta,\varphi), \qquad \boldsymbol{k} = (k = |\boldsymbol{k}|, \vartheta, \varphi). \tag{A.7}$$

With this definition, the function G_1 (equation A.5) can be written as

$$G_1(q^2) = \frac{1}{L^3}\sum_{\boldsymbol{k}}\frac{h(\boldsymbol{k})}{q^2-k^2}, \tag{A.8}$$

and it can be expanded in lm terms as

$$G_1(q^2) = \sum_{l,m}\frac{1}{L^3}\sum_{\boldsymbol{k}}\frac{h_{lm}(\boldsymbol{k})}{q^2-k^2}k^l\sqrt{4\pi}Y_{lm}(\vartheta,\varphi). \tag{A.9}$$

Poisson summation formula will be used for the evaluation of $G_1(q)$.

Poisson summation formula for an arbitrary function $g(\boldsymbol{k})$ reads

$$\frac{1}{L^3}\sum_{\boldsymbol{k}} g(\boldsymbol{k}) = \int\frac{d^3k}{(2\pi)^3}g(\boldsymbol{k}) + \sum_{\boldsymbol{l}\neq 0}\int\frac{d^3k}{(2\pi)^3}\, e^{iL\,\boldsymbol{l}\cdot\boldsymbol{k}}\, g(\boldsymbol{k}), \tag{A.10}$$

where $\boldsymbol{k} = \frac{2\pi}{L}\boldsymbol{n}$ with $\boldsymbol{n} = (n_1, n_2, n_3)$, $\boldsymbol{l} = (l_1, l_2, l_3)$ and $n_i, l_i \in \mathbb{N}$. In the following, we consider functions g whose Fourier transforms, $\tilde{g}(r)$, are non-singular, and are either contained in a finite spatial region or decrease exponentially as $|\boldsymbol{r}| \to \infty$. If we apply the Poisson summation formula to such functions, the terms with $l \neq 0$ on the right-hand-side decrease at least exponentially as the box size is sent to infinity, so that

$$\frac{1}{L^3}\sum_{\boldsymbol{k}} g(\boldsymbol{k}) = \int\frac{d^3k}{(2\pi)^3}g(\boldsymbol{k}), \tag{A.11}$$

up to corrections that are at most exponentially small.

Eq. (A.11) should be applied to (A.9), where $g(\boldsymbol{k})$ is substituted with $\frac{h_{lm}(\boldsymbol{k})}{q^2-k^2}k^lY_{lm}(\vartheta,\varphi)$. The singularity at $k^2 = q^2$ forbides one to use equation A.11 directly on $G_{1,lm}$ (A.9). Kim et.al [4] apply a trick where they subtract a function, $h(q)e^{\alpha(q^2-k^2)}$, which cancels that pole from summand in equation A.11. With this trick one can interchange sum with integral over $\boldsymbol{k}$. Exponential factor $e^{\alpha(q^2-k^2)}$ with $\alpha > 0$ takes care that the subtraction does not introduce ultraviolet singularities. G_1 now reads

$$
\begin{aligned}
G_1(q^2) =& \sum_{l,m} \frac{1}{L^3} \sum_{\boldsymbol{k}} \frac{h_{lm}(\boldsymbol{k}) - h_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) + \\
&+ \sum_{l,m} \frac{1}{L^3} \sum_{\boldsymbol{k}} \frac{h_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) = \\
=& \sum_{l,m} \int \frac{d^3k}{(2\pi)^3} \frac{h_{lm}(\boldsymbol{k}) - h_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) + \\
&+ \sum_{l,m} \frac{1}{L^3} \sum_{\boldsymbol{k}} \frac{h_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) = \\
=& \sum_{l,m} \int \frac{d^3k}{(2\pi)^3} \frac{h_{lm}(\boldsymbol{k})}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) - \int \frac{d^3k}{(2\pi)^3} \frac{h_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) + \\
&+ \sum_{l,m} \frac{1}{L^3} \sum_{\boldsymbol{k}} \frac{h_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi).
\end{aligned}
\tag{A.12}
$$

New function $c_{lm}(\boldsymbol{q}^2)$, defined as

$$
\begin{aligned}
c_{lm}(q^2) =& \frac{1}{L^3} \sum_{\boldsymbol{k}} \frac{e^{\alpha(q^2-k^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\phi) \\
c_{00}(q^2) =& \frac{1}{L^3} \sum_{\boldsymbol{k}} \frac{e^{\alpha(q^2-k^2)}}{q^2-k^2} \qquad - \mathcal{P} \int \frac{d^3k}{(2\pi)^3} \frac{e^{\alpha(q^2-k^2)}}{q^2-k^2}.
\end{aligned}
\tag{A.13}
$$

Contributions of the infinite volume

$$
G_1^{\infty}(q^2) = -\frac{i}{2E} \int \frac{d^3k}{(2\pi)^3} \frac{f(\boldsymbol{k})}{q^2-k^2+i\epsilon} \frac{E_1+\omega_1}{2\omega_1}
\tag{A.14}
$$

With use of new functions A.13, A.14 and definitions for h, E_i and ω_i (A.6) G_1 is rewritten into two parts

$$
\begin{aligned}
G_1(q^2) = G_1^{\infty}(q^2) - \Bigg(& \frac{i}{2E} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int \frac{d^3k}{(2\pi)^3} \frac{f_{lm}(\boldsymbol{q}) e^{\alpha(\boldsymbol{q}^2-\boldsymbol{k}^2)}}{q^2-k^2} k^l \sqrt{4\pi} Y_{lm}(\vartheta,\varphi) \\
& - \frac{i}{2E} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm}(q) c_{lm}(q^2) \Bigg) = \\
= G_1^{\infty}(q^2) - \Bigg(& \frac{q\ f_{00}(q)}{8\pi E} - \frac{i}{2E} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} f_{lm}(q) c_{lm}(q^2) \Bigg) = \\
= G_1^{\infty}(q^2) + & G_1^{FV}(q^2).
\end{aligned}
\tag{A.15}
$$

Finite volume effects are packed in the function G_1^{FV}

$$G_1^{FV}(q^2) = -\left(\frac{qf_{00}(q)}{8\pi E} - \frac{i}{2E}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}(q)c_{lm}(q^2)\right). \tag{A.16}$$

It is independent of particle masses and is equal to G^{FV} derived in equation 1.12. From equality of functions in 1.12 and A.16 one can determine kinematical function $\mathcal{G}$ needed for determination of Lüscher equation.

In literature different form than one given in A.13 of function $c_{lm}(q)$ is more commonly used

$$c_{lm}(q^2) = -\frac{\sqrt{4\pi}}{L^3}\left(\frac{2\pi}{L}\right)^{l-2} Z_{lm}\left(1;\left(\frac{qL}{2\pi}\right)^2\right) \quad \text{with}$$
$$Z_{lm}\left(s;\tilde{q}^2\right) = \sum_{\boldsymbol{n}} \frac{\tilde{\boldsymbol{n}}^l}{(\tilde{\boldsymbol{n}}^2 - \tilde{\boldsymbol{q}}^2)^s} Y_{lm}(\tilde{\boldsymbol{n}}), \qquad \tilde{\boldsymbol{q}} = \frac{\boldsymbol{q}L}{2\pi}, \tag{A.17}$$

corrections to equation above, indicate $\tilde{q} = \frac{qL}{2\pi}$ is dimensionless.

Definition for c_{lm} in A.17 is equal to one in A.13 to term which vanish exponentially with lattice size L. In our approximation these two expressions A.17 and A.13 are equivalent and can be interchange freely. We note that Z_{lm} is finite for $s = 1$ when $(l, m) \neq (0, 0)$ but it is infinite for $(l, m) = (0, 0)$. This can be easily seen if the sum is rewritten in terms of the integral for large $\boldsymbol{n}$ and this integral is zero for $l > 0$ due to rotational symmetry. One has to use $Z_{00}(s, \tilde{q}^2)$, which is analytically continued from $s > 3/2$ to $s = 1$ and is then finite ([35]). This is then analogous to c_{00} in A.17 where infinite part gets subtracted.

A.2 Derivation of kinematical function $\mathcal{G}$ for spinless scattering

This appendix shows that when $\mathcal{G}$ defined in (1.22) is inserted to the expression for G^{FV} (1.12,1.14) then one indeed gets desired G_1^{FV} (1.19, A.16). We begin with relations between G^{FV} and $\mathcal{G}$ through $\mathcal{F}$ (eq. 1.12,1.14,1.22)

$$G^{FV}(|\boldsymbol{q}|) = \int d\Omega d\Omega' z(q)\mathcal{F}(q,q')z(q'), \qquad q = (|\boldsymbol{q}|, \Omega),\ q' = (|\boldsymbol{q}|, \Omega')$$
$$\mathcal{F}(q,q') = -\frac{1}{4\pi}\sum_{\substack{l_1,m_1\\ l_2,m_2}} \mathcal{G}_{l_1,m_1;l_2,m_2}(|\boldsymbol{q}|)\, Y_{l_1,m_1}(\Omega)\, Y^*_{l_2,m_2}(\Omega') \tag{A.18}$$
$$\mathcal{G}_{l_1,m_1;l_2,m_2}(|\boldsymbol{q}|) = \frac{|\boldsymbol{q}|}{8\pi E}\left(\delta_{l_1,l_2}\delta_{m_1,m_2} - i\sum_{l,m}\frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}} c_{lm}\left(|\boldsymbol{q}|^2\right)\int d\Omega'' Y^*_{l_1,m_1}(\Omega'')\, Y^*_{l,m}(\Omega'')\, Y_{l_2,m_2}(\Omega'')\right).$$

A.2. Derivation of kinematical function $\mathcal{G}$ for spinless scattering

After plugging this $\mathcal{G}$ to G^{FV} one gets

$$G^{FV}(|\boldsymbol{q}|) = \int d\Omega d\Omega' z(q) z(q') \left(-\frac{1}{4\pi}\right)\frac{|\boldsymbol{q}|}{8\pi E}\sum_{\substack{l_1,m_1\\ l_2,m_2}}\Big(\delta_{l_1,l_2}\delta_{m_1,m_2}Y_{l_1,m_1}(\Omega)\,Y^*_{l_2,m_2}(\Omega') - \tag{A.19}$$
$$- i\sum_{l,m}\frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}}c_{lm}\left(|\boldsymbol{q}|^2\right)\int d\Omega'' Y^*_{l_1,m_1}(\Omega'')\,Y^*_{l,m}(\Omega'')\,Y_{l_2,m_2}(\Omega'')\,Y_{l_1,m_1}(\Omega)\,Y^*_{l_2,m_2}(\Omega')\Big).$$

We use δ functions under sum in the first term of G^{FV} and expression simplifies

$$G^{FV}(|\boldsymbol{q}|) = \int d\Omega d\Omega' z(q) z(q')\left(-\frac{1}{4\pi}\right)\frac{|\boldsymbol{q}|}{8\pi E}\Big(\sum_{l_1,m_1}Y_{l_1,m_1}(\Omega)\,Y^*_{l_1,m_1}(\Omega') - \tag{A.20}$$
$$-i\sum_{l,m}\frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}}c_{lm}\left(|\boldsymbol{q}|^2\right)\int d\Omega''\sum_{l_1,m_1}Y^*_{l_1,m_1}(\Omega'')\,Y_{l_1,m_1}(\Omega)\,Y^*_{l,m}(\Omega'')\sum_{l_2,m_2}Y_{l_2,m_2}(\Omega'')\,Y^*_{l_2,m_2}(\Omega')\Big).$$

Next we calculate sum over l_1, m_{l_1} and l_2, m_{l_2} using $\sum_{l,m}Y_{l,m}(\Omega)Y^*_{l,m}(\Omega') = \delta(\Omega-\Omega')$

$$G^{FV}(|\boldsymbol{q}|) = \int d\Omega d\Omega' z(q) z(q')\left(-\frac{1}{4\pi}\right)\frac{|\boldsymbol{q}|}{8\pi E}\Big(\delta(\Omega-\Omega') - \tag{A.21}$$
$$-i\sum_{l,m}\frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}}c_{lm}\left(|\boldsymbol{q}|^2\right)\int d\Omega''\delta(\Omega''-\Omega)\,Y^*_{l,m}(\Omega'')\,\delta(\Omega''-\Omega')\Big).$$

Product of two z functions was already defined as f in the main text (1.20)

$$z(q)z(q')\delta(\Omega-\Omega') = z(q)z(q) = f(q).$$

We use f in definition of G^{FV}

$$G^{FV}(|\boldsymbol{q}|) = \int d\Omega f(q)\left(-\frac{1}{4\pi}\right)\frac{|\boldsymbol{q}|}{8\pi E}\left(1 - i\sum_{l,m}\frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}}c_{lm}\left(|\boldsymbol{q}|^2\right)\int d\Omega''\delta(\Omega''-\Omega)\,Y^*_{l,m}(\Omega'')\right).$$

Now we expand new function $f(q)$ in terms of spherical harmonics

$$f(q) = \sum_{l'm'}f_{l'm'}(|\boldsymbol{q}|)\,|\boldsymbol{q}|^l\sqrt{4\pi}Y_{l'm'}(\Omega). \tag{A.22}$$

With some reorganization G is rewriten in following form

$$G^{FV}(|\boldsymbol{q}|) = -\frac{|\boldsymbol{q}|}{8\pi E}\Big(\sum_{l'm'}f_{l'm'}(|\boldsymbol{q}|)\,|\boldsymbol{q}|^{l'}\frac{1}{\sqrt{4\pi}}\int d\Omega Y_{l'm'}(\Omega) \tag{A.23}$$
$$- i\frac{4\pi}{|q|}\sum_{l'm'}f_{l'm'}(|\boldsymbol{q}|)\,|\boldsymbol{q}|^{l'}\sum_{l,m}\frac{1}{|\boldsymbol{q}|^l}c_{lm}\left(|\boldsymbol{q}|^2\right)\int d\Omega Y_{l'm'}(\Omega)\,Y^*_{l,m}(\Omega)\Big),$$

which is after taking properties of spherical harmonics Y_{lm} into the account equal to

$$G^{FV}(|\boldsymbol{q}|) = -\frac{|\boldsymbol{q}|}{8\pi E}\left(\sum_{l'm'} f_{l'm'}(|\boldsymbol{q}|)\,|\boldsymbol{q}|^{l'}\frac{1}{\sqrt{4\pi}}\sqrt{4\pi}\delta_{l',0}\delta_{m',0}\right. \\ \left. - i\frac{4\pi}{|q|}\sum_{l'm'} f_{l'm'}(|\boldsymbol{q}|)\,|\boldsymbol{q}|^{l'}\sum_{l,m}\frac{1}{|\boldsymbol{q}|^{l}}c_{lm}\left(|\boldsymbol{q}|^2\right)\delta_{l',l}\delta_{m',m}\right). \tag{A.24}$$

G^{FV} (A.24 can now be written in form

$$G^{FV}(|\boldsymbol{q}|) = -\frac{|\boldsymbol{q}|}{8\pi E}\left(f_{00}(|\boldsymbol{q}|) - i\frac{4\pi}{|\boldsymbol{q}|}\sum_{lm} f_{lm}(|\boldsymbol{q}|)\,c_{lm}\left(|\boldsymbol{q}|^2\right)\right),$$

which can be compared to G_1^{FV} in (A.16)

$$G_1^{FV}(|\boldsymbol{q}|) = -\left(\frac{|\boldsymbol{q}|\,f_{00}(|\boldsymbol{q}|)}{8\pi E} - \frac{i}{2E}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}(|\boldsymbol{q}|)c_{lm}(|\boldsymbol{q}|^2)\right).$$

We prooved that with chosen definition of $\mathcal{G}$ indeed leads to G_1^{FV} (A.16).

A.3 Transition from $l_1, m_{l_1}, l_2, m_{l_2}$ basis to J, m_J basis for $S! = 0$

Every function F of angular momentum l_1, l_2 and spin S can be expanded in terms of angular momentum l_1, l_2 and spin S

$$F = \sum_{\substack{m_{l_1}, m_{S_1}\\ m_{l_2}, m_{S_2}}} |l_2, m_{l_2}; S_2, m_{S_2}\rangle \langle l_2, m_{l_2}; S_2, m_{S_2}| F |l_1 m_{l_1}; S_1, m_{S_1}\rangle \langle l_1 m_{l_1}; S_1, m_{S_1}|. \tag{A.25}$$

One can always add full set of states $|J, m_J\rangle$ to any expansion. We add only one set because we are interested in one channel approximation in which $J_f = J_i$ and same for its third component. After insertion of full set equation A.25 reads

$$F = \sum_{J,m_J} |J, m_J\rangle \langle J, m_J| \sum_{\substack{m_{l_1}, m_{S_1}\\ m_{l_2}, m_{S_2}}} |l_2, m_{l_2}; S_2, m_{S_2}\rangle \langle l_2, m_{l_2}; S_2, m_{S_2}| F |l_1, m_{l_1}; S_1, m_{S_1}\rangle \langle l_1, m_{l_1}; S_1, m_{S_1}|. \tag{A.26}$$

States $|J, m_J\rangle$ and $|l_i, m_{l_i}\rangle$ comute so one can rewrite expansion A.26 in following form

$$F_{J,m_J} = \sum_{\substack{m_{l_1}, m_{S_1}\\ m_{l_2}, m_{S_2}}} \langle J m_J | l_2, m_{l_2}; S_2, m_{S_2}\rangle \langle l_2, m_{l_2}; S_2, m_{S_2}| F |l_1, m_{l_1}; S_1, m_{S_1}\rangle \langle l_1, m_{l_1}; S_1, m_{S_1} | J m_J\rangle. \tag{A.27}$$

One uses definition of Clebsch-Coeficient

$$\langle l_1, m_{l_1}; S_1, m_{S_1} | J m_J\rangle = C^{J,m_J}_{l_1,m_{l_1};S_1,m_{S_1}}$$

and that coeficients are real

$$C^{J,m_J}_{l_1,m_{l_1};S_1,m_{S_1}} = \left(C^{J,m_J}_{l_1,m_{l_1};S_1,m_{S_1}}\right)^*$$

and

$$F_{l_1,l_2,S_1,S_2} = \langle l_2, m_{l_2}; S_2, m_{S_2}| \, F \, |l_1, m_{l_1}; S_1, m_{S_1}\rangle$$

in equation A.27. One can write final transitional expression

$$F_{J,m_J} = \sum_{\substack{m_{l_1},m_{S_1}\\ m_{l_2},m_{S_2}}} C^{J,m_J}_{l_1,m_{l_1};S_1,m_{S_1}} C^{J,m_J}_{l_2,m_{l_2};S_2,m_{S_2}} F_{l_1,l_2,S_1,S_2}, \tag{A.28}$$

where function F, previously written in basis l, m_l (F_{l_1,l_2,S_1,S_2}) is now written in basis of total angular momentum J and its third component m_J (F_{J,m_J}) .

A.4 Transition to J, m_J, l, S basis for scattering amplitude and kinematical function

Here longer calculation for transition from one basis l, m_l to another J, m_J, l, S for both quantities in quntization condition ($\mathcal{M}$ and $\mathcal{G}$) are given. In transition rotation using CG coeficients (1.32) is used.

A.4.1 Kinematical function $\mathcal{G}$

In generalization of kinematical function $\mathcal{G}$ for scattering of particles with spin one should find dependence of $\mathcal{G}$ (equation 1.3) which was previously $l_1, m_1 \to l_2, m_2$ to dependence on $J_1, m_{J_1}, S_1, l_1 \to J_2, m_{J_2}, S_2, l_2$. With transition (1.32) one expand kinematical function previously in basis of angular momentum l to new basis depending on total angular momentum J, angular momentum l and spin S. Calculation is similar to the one for scattering amplitude $\mathcal{M}$. We perform transformation (1.32) on kinematical function $\mathcal{G}$

$$\mathcal{G}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}} = \sum_{\substack{m_{l_1},m_{S_1}\\ m_{l_2},m_{S_2}}} C^{J_1,m_{J_1}}_{l_1,m_{l_1};S_1,m_{S_1}} C^{J_2,m_{J_2}}_{l_2,m_{l_2};S_2,m_{S_2}} \langle l_2 m_{l_2}; S_2 m_{S_2}| \, \mathcal{G}(q) \, |l_1 m_{l_1}; S_1 m_{S_1}\rangle \, . \tag{A.29}$$

The kinematical function $\mathcal{G}$ was previously dependent only on angular momentum l and therefore had matrix element $\mathcal{G}_{\substack{l_1 m_{l_1}\\ l_2 m_{l_2}}}(q)$ (1.22)

$$\langle l_2 m_{l_2}; S_2 m_{S_2}| \, \mathcal{G}(q) \, |l_1 m_{l_1}; S_1 m_{S_1}\rangle = \delta_{S_1,S_2} \delta_{m_{S_1},m_{S_2}} \mathcal{G}_{\substack{l_1 m_{l_1}\\ l_2 m_{l_2}}}(q). \tag{A.30}$$

Final result for kinematical function is

$$\mathcal{G}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}}(q) = \frac{|\boldsymbol{q}|}{8\pi E} \delta_{S_1,S_2} \left[\delta_{l_1 l_2} \delta_{J_1,J_2} \delta_{m_{J_1},m_{J_2}} + i \mathcal{G}^{FV}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}}(q) \right], \tag{A.31}$$

where finite volume correction are in

$$\mathcal{G}^{FV}_{\substack{J_1,m_{J_1},l_1,S_1\\ J_2,m_{J_2},l_2,S_2}}(q) = \sum_{\substack{m_{l_1},m_S\\ m_{l_2}}} C^{J_1 m_{J_1}}_{l_1 m_{l_1},S_1 m_S} C^{J_2 m_{J_2}}_{l_2 m_{l_2},S_2 m_S} \mathcal{G}^{FV}_{\substack{l_1 m_{l_1}\\ l_2 m_{l_2}}}(q)$$

$$\mathcal{G}^{FV}_{\substack{l_1,S_1,J_1,m_{J_1}\\ l_2,S_2,J_2,m_{J_2}}}(q) = -\sum_{\substack{m_{l_1},m_S\\ m_{l_2}}} C^{J_1 m_{J_1}}_{l_1 m_{l_1},S_1 m_S} C^{J_2 m_{J_2}}_{l_2 m_{l_2},S_2 m_S} \sum_{l,m} \frac{(4\pi)^{\frac{3}{2}}}{|\boldsymbol{q}|^{l+1}} c_{lm}(|\boldsymbol{q}|^2) \int d\Omega Y^*_{l_1,m_{l_1}}(\Omega) Y^*_{l,m}(\Omega) Y_{l_2,m_{l_2}}(\Omega).$$