



## 3N potentials in the Faddeev coordinate space approach to Nd scattering

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**Abstract.** For studying 3N bound states and Nd scattering, the Tucson-Melbourne (TM) and Urbana 3N forces have been derived from the chiral EFT in the momentum representation. The Faddeev equations in configuration space have attractive properties when applied for nd and pd scattering above the two-body threshold. For that reason, we derived components of the TM 3N potential in the coordinate representation.

**Keywords:** nucleon-nucleon interactions, Faddeev equations, three-nucleon force

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## 1. Introduction

Most compellingly the need for the 3N forces comes from the underbinding of light nuclei [1, 2]. Also certain discrepancies exist in Nd scattering observables: the notorious  $A_y$ -puzzle for the analyzing power. The differential cross-sections tensor-analyzing powers and spin-transfer coefficients are rather well described at low energies using solely 2N forces. However the results of these calculations start to deviate from the data as the energy increases [3].

Phenomenological 2N potential models include the CD-Bonn2000, Argonne V-18 (AV18) and Nijmegen I and II potentials [4]. The 3N forces are represented by the Tucson-Melbourne potential and its chirally-corrected version (TM99) [5], Brazilian potential [6], Urbana IX potential [7, 8] and and Illinois potentials [9]. All potentials contain the longest-range contribution due to the two-pion exchange. The TM and Brazilian potentials also include the shorter -range contribution due to  $\pi\rho$  and  $\rho\rho$  exchanges. In the Urbana potential this short range contribution is introduced phenomenologically. The Illinois models include parametrizations of three-pion exchange terms due to ring diagrams with one  $\Delta$  in the intermediate state.

One should note that the phenomenological 3N forces are parametrized in the context of a particular 2N-force model. It is to be noted that the Urbana 3N force taken together with AV14 2N force [10] has been adjusted to the triton and  ${}^4\text{He}$  binding energies [11] and has been used in the 3N scattering calculations below the breakup threshold [12].

A more consistent approach can be developed in the frame of chiral perturbation theory, where both 2N and 3N forces are derived from a given effective Lagrangian at different orders of perturbation expansion. A detailed discussion of the structure and application of chiral nuclear forces may be found in the review articles [13, 14, 15] and references therein.

In this first attempt to include 3N forces in our calculational scheme [16] based on the Faddeev equations in configuration space (FECS)[17]. The FECS have attractive properties for the studying Nd scattering above the two-body threshold due to the clear asymptotics of the wave function in correspondence to different channels and simple taking into account the Coulomb force. This property provides mathematically rigorous possibilities for practical applications [17, 18, 19]. To use the Tucson-Melbourne 3N potential for the study, we present our derivation for components of the TM 3N potential obtained in the coordinate space. We shall mostly consider the simplest contribution to TM potential which comes from the two-pion exchange. We apply the approach which was initiated by S. Merkuriev, C. Gignoux and A. Laverne (MGL) [20] who derived general formulae for nd breakup scattering in configuration space.

## 2. MGL basis

For partial wave analysis of the Faddeev equations in the coordinate space, we have chosen the basis proposed by Merkuriev et al. for nd case [20]. This basis without any changes may be applied for pd case too [21, 16, 22]. The basis is intermediate between LS and Jj coupling schemes. Let:  $\vec{\sigma}$ ,  $\vec{l}$  and  $\mathbf{J} = \vec{\sigma} + \vec{l}$  be the spin, orbital and total angular momenta of the pair 23,  $\mathbf{s} = \mathbf{1}/2 + \mathbf{J}$  the total "spin" of the system 123 considering the pair 23 as a particle with "spin"  $\mathbf{J}$ .  $\vec{\lambda}$  the orbital momentum conjugate to  $\mathbf{y}$ , that is of the relative motion of particle 1 with respect to the c.m. of pair 23.  $\mathbf{M} = \vec{\lambda} + \mathbf{s}$  the three-particle angular momentum with its  $z$ -projection  $M_z$ . The set of quantum numbers  $\{l\sigma J s \lambda\} \equiv \alpha$  defines a state on this basis.

## 3. TM- $\pi\pi$ potential in the coordinate space

The TM- $\pi\pi$  potential in the momentum space can be taken from [23]. It reads

$$\begin{aligned} & \langle p'_1, p'_2, p'_3 | W_{\pi\pi}(3) | p_1, p_2, p_3 \rangle = \\ & (2\pi)^3 \frac{\delta^3(\sum p'_i - \sum p_i)}{(q^2 + \mu^2)(q'^2 + \mu^2)} \frac{g^2}{4m^2} F_{\pi NN}^2(q) F_{\pi NN}^2(q') (\sigma_1 q) (\sigma_2 q') \left\{ (\tau_1 \tau_2) \left[ a + b(qq') \right] \right. \\ & \left. - d(\tau_3 \cdot \tau_1 \times \tau_2) (\sigma_3 \cdot q \times q') \right\} \quad (1) \end{aligned}$$

Here it is assumed that nucleon 3 exchanges a pion with each of the two rest nucleons 1 and 2.  $g^2 = 13.4$ ,  $q = p_1 - p'_1$  and  $q' = p'_2 - p_2$ . According to later studies [5] the so-called  $c$ -term with  $q^2 + q'^2$  in the square brackets, which is present in [23], is omitted as essentially equivalent to the first,  $a$ -term with a new value of  $a$ . The Fourier transform gives

$$\begin{aligned} & \langle r'_1, r'_2, r'_3 | W_{\pi\pi}(3) | r_1, r_2, r_3 \rangle = \\ & \int \prod_{i=1}^3 \frac{d^3 p'_i}{(2\pi)^3} \frac{d^3 p_i}{(2\pi)^3} \exp \left( \sum_{i=1}^3 i(p'_i r'_i - p_i r_i) \right) \langle p'_1, p'_2, p'_3 | W_{\pi\pi}(3) | p_1, p_2, p_3 \rangle \quad (2) \end{aligned}$$

Of the three final momenta  $p'_1, p'_2$  and  $p'_3$  the last can be fixed by the  $\delta$ -function in (1). The two others can be expressed via  $q$  and  $q'$  as  $p'_1 = p_1 - q$  and  $p'_2 = p_2 + q'$ . The exponent becomes

$$i \sum_{i=1}^3 (p'_i r'_i - p_i r_i) = i \sum_{i=1}^3 p_i (r'_i - r_i) - iq(r'_1 - r'_3) + iq'(r'_2 - r'_3)$$

Integration over  $p_i$ ,  $i = 1, 2, 3$  gives a factor

$$(2\pi)^9 \delta^3(r'_1 - r_1) \delta^3(r'_2 - r_2) \delta^3(r'_3 - r_3)$$

which makes the potential local in the coordinate space. So finally we obtain

$$\begin{aligned}
\langle r'_1, r'_2, r'_3 | W_{\pi\pi}(3) | r_1, r_2, r_3 \rangle &= \delta^3(r'_1 - r_1) \delta^3(r'_2 - r_2) \delta^3(r'_3 - r_3) \\
&\frac{g^2}{4m^2} \int \frac{d^3q}{(2\pi)^3} \frac{d^3q'}{(2\pi)^3} e^{-iqr_{13} + iq'r_{23}} \frac{F_{\pi NN}^2(q)}{q^2 + \mu^2} \frac{F_{\pi NN}^2(q')}{q'^2 + \mu^2} (\sigma_1 q) (\sigma_2 q') \\
&\left\{ (\tau_1 \tau_2) \left[ a + b(qq') \right] - d(\tau_3 \cdot \tau_1 \times \tau_2) (\sigma_3 \cdot q \times q') \right\} \quad (3)
\end{aligned}$$

where  $r_{13} = r_1 - r_3$  and  $r_{23} = r_2 - r_3$ . In the following, to simplify notations, we omit subindex 3 and write  $r_{13}$  just as  $r_1$  and  $r_{23}$  as  $r_2$  (as if the third nucleon is located at the origin). In terms linear or quadratic in momenta we substitute the latter by the derivatives. Introducing also a function

$$Z(r) = \frac{4\pi}{\mu} \int \frac{d^3q}{(2\pi)^3} \frac{F_{\pi NN}^2(q)}{q^2 + \mu^2} \quad (4)$$

we find the expression for the (local)  $W_{\pi\pi}(3)$  potential

$$\begin{aligned}
W_{\pi\pi}(3) &= \frac{g^2 \mu^2}{64\pi^2 m^2} (\sigma_1 \nabla_1) (\sigma_2 \nabla_2) \left\{ (\tau_1 \tau_2) \left[ a + b(\nabla_1 \nabla_2) \right] \right. \\
&\quad \left. - d(\tau_3 \cdot \tau_1 \times \tau_2) (\sigma_3 \cdot \nabla_1 \times \nabla_2) \right\} Z(r_1) Z(r_2) \quad (5)
\end{aligned}$$

As one knows, acting on a function of modulus, gradients become proportional to vectors:

$$\nabla f(r) = \mathbf{r} \frac{f'(r)}{r}, \quad \nabla_i \nabla_k f(r) = \delta_{ik} \frac{f'(r)}{r} + r_i r_k \frac{f''(r)}{r^2}$$

Using this and introducing derivatives

$$Z^{(1)} = \frac{1}{r} Z'(r), \quad Z^{(2)} = \frac{1}{r^2} Z''(r) \quad (6)$$

we rewrite the potential in its final form

$$W_{\pi\pi}(3) = \frac{g^2 \mu^2}{64\pi^2 m^2} \left( aW^{(a)} + bW^{(b)} + dW^{(d)} \right) \quad (7)$$

where

$$W^{(a)} = (\tau_1 \tau_2) (\sigma_1 r_1) (\sigma_2 r_2) Z^{(1)}(r_1) Z^{(1)}(r_2) \quad (8)$$

$$\begin{aligned}
W^{(b)} &= (\tau_1 \tau_2) \left[ (\sigma_1 \sigma_2) Z^{(1)}(r_1) Z^{(1)}(r_2) + (\sigma_1 r_1) (\sigma_2 r_1) Z^{(2)}(r_1) Z^{(1)}(r_2) \right. \\
&\quad \left. + (\sigma_1 r_2) (\sigma_2 r_2) Z^{(1)}(r_1) Z^{(2)}(r_2) + (\sigma_1 r_1) (\sigma_2 r_2) (r_1 r_2) Z^{(2)}(r_1) Z^{(2)}(r_2) \right] \quad (9)
\end{aligned}$$

$$\begin{aligned}
 W^{(d)} = & -(\tau_3 \cdot \tau_1 \times \tau_2) \left[ (\sigma_3 \cdot \sigma_1 \times \sigma_2) Z^{(1)}(r_1) Z^{(1)}(r_2) \right. \\
 & + (\sigma_3 \cdot \sigma_1 \times r_2)(\sigma_2 r_2) Z^{(1)}(r_1) Z^{(2)}(r_2) + (\sigma_3 \cdot r_1 \times \sigma_2)(\sigma_1 r_1) Z^{(2)}(r_1) Z^{(1)}(r_2) \\
 & \left. + (\sigma_3 \cdot r_1 \times r_2)(\sigma_1 r_1)(\sigma_2 r_2) Z^{(2)}(r_1) Z^{(2)}(r_2) \right] \quad (10)
 \end{aligned}$$

The latest set of parameters (TM99 [5]) is

$$\mu a = -1.12, \quad \mu^3 b = -2.80, \quad \mu^3 d = -0.75 \quad (11)$$

with the pion mass  $\mu = 138.0$  MeV and the form-factor squared

$$F_{\pi NN}^2(q) = \frac{(\Lambda^2 - \mu^2)^2}{(\Lambda^2 + q^2)^2} \quad (12)$$

with  $\Lambda = 5.8\mu$ .

## 4. Isospin operators in the MGL basis

We have to calculate 4 operators

$$(\tau_2 \tau_3), \quad (\tau_3 \tau_1), \quad (\tau_1 \tau_2), \quad (\tau_3 \cdot \tau_1 \times \tau_2)$$

in the MGL isospin basis formed by the three states  $\eta_{1/2,t}^{T,T_z}$  with given values of the total isospin  $T$  and isospin  $t$  of the pair 23:

$$\eta_{1/2,0}^{1/2,1/2} \equiv \eta_1, \quad \eta_{1/2,1}^{1/2,1/2} \equiv \eta_2, \quad \eta_{1/2,1}^{3/2,1/2} \equiv \eta_3. \quad (13)$$

The simplest operator is obviously  $(\tau_2 \tau_3)$  which is diagonal in this basis:

$$(\tau_2 \tau_3)_{ik} = \delta_{ik} a_i, \quad i = 1, 2, 3, \quad a_1 = -3, \quad a_{2,3} = 1 \quad (14)$$

To find matrix elements of  $(\tau_3 \tau_1)$  and  $(\tau_1 \tau_2)$  we recall that permutations of nucleons 123 $\rightarrow$ 231 and 123 $\rightarrow$ 312 are accomplished by operators  $P^+$  and  $P^-$  respectively [24]

$$P^{I\pm} = \begin{pmatrix} -1/2 & \mp\sqrt{3}/2 & 0 \\ \pm\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (15)$$

Note that  $P^\pm$  are unitary:

$$P^+ P^- = 1 \quad (16)$$

If we denote  $\eta_i^{(n)}$ ,  $i = 1, 2, 3$  the basis in which isospins of the two nucleons different from  $n$  are first summed and the isospin of nucleon  $n$  is added to form the final total isospin  $T$  then our basis is  $\eta_i^{(1)}$  and we have

$$\eta_i^{(2)} = \sum_k P_{ik}^+ \eta_k^{(1)}, \quad \eta_i^{(3)} = \sum_k P_{ik}^- \eta_k^{(1)}, \quad (17)$$

or simply

$$\eta^{(2)} = P^+ \eta^{(1)}, \quad \eta^{(3)} = P^- \eta^{(1)} \quad (18)$$

Applying  $P^-$  and  $P^+$  to the first and second relations (18) we get

$$\eta^{(1)} = P^- \eta^{(2)}, \quad \eta^{(1)} = P^+ \eta^{(3)} \quad (19)$$

Using these relations we find

$$\begin{aligned} (\tau_1 \tau_2)_{ik} &= \langle \eta_i^{(1)} | (\tau_1 \tau_2) | \eta_k^{(1)} \rangle = \sum_{i', k'} P_{ii'}^+ P_{kk'}^+ \langle \eta_{i'}^{(3)} | (\tau_1 \tau_2) | \eta_{k'}^{(3)} \rangle \\ &= \sum_{i', k'} P_{ii'}^+ P_{kk'}^+ a_{i'} \delta_{i' k'} = \sum_l P_{il}^+ a_l P_{lk}^- \end{aligned} \quad (20)$$

where  $a_i$  are defined in (14). So as a matrix

$$\begin{aligned} (\tau_1 \tau_2)_{ik} &= \\ &= \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & \sqrt{3} & 0 \\ \sqrt{3} & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{aligned} \quad (21)$$

To find  $\tau_3 \tau_1$  we have only to substitute  $P^+ \leftrightarrow P^-$ , which gives

$$(\tau_1 \tau_3)_{ik} = \begin{pmatrix} 0 & -\sqrt{3} & 0 \\ -\sqrt{3} & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (22)$$

Our last operator ( $\tau_3 \cdot \tau_1 \times \tau_2$ ) is symmetric in all the three nucleons. To find its matrix elements we use

$$(\tau_2 \tau_1)(\tau_2 \tau_3) = \tau_1 \tau_3 - i(\tau_3 \cdot \tau_1 \times \tau_2), \quad (\tau_2 \tau_3)(\tau_2 \tau_1) = \tau_1 \tau_3 + i(\tau_3 \cdot \tau_1 \times \tau_2) \quad (23)$$

wherefrom we conclude

$$2i(\tau_3 \cdot \tau_1 \times \tau_2) = (\tau_2 \tau_3)(\tau_2 \tau_1) - (\tau_2 \tau_1)(\tau_2 \tau_3) \quad (24)$$

For the matrix elements we find from this

$$i(\tau_3 \cdot \tau_1 \times \tau_2)_{ik} = \frac{1}{2}(a_i - a_k)(\tau_2 \tau_1)_{ik} \quad (25)$$

As a matrix

$$i(\tau_3 \cdot \tau_1 \times \tau_2) = \begin{pmatrix} 0 & -2\sqrt{3} & 0 \\ 2\sqrt{3} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (26)$$

## 5. Spin-coordinate operators in the MGL basis. Generalities

In the coordinate space our basic function is expanded in the MGL states  $|\alpha\rangle$

$$\sum_{\alpha} \frac{\phi_{\alpha}(x, y)}{xy} |\alpha\rangle \quad (27)$$

The spin-coordinate part of  $|\alpha\rangle$  is labelled as

$$|\alpha\rangle = |\lambda, s, l, \sigma, j\rangle \quad (28)$$

where we suppress the quantum numbers which are conserved: total angular momentum  $M$  its projection  $M_z$  and parity  $P$ . Our task is to expand in  $|\alpha\rangle$  the result of action of some operator  $O(\mathbf{x}, \mathbf{y})$  on our basic state

$$O(\mathbf{x}, \mathbf{y}) \sum_{\alpha} \frac{\phi_{\alpha}(x, y)}{xy} |\alpha\rangle = \sum_{\alpha} \frac{D_{\alpha}(x, y)}{xy} |\alpha\rangle \quad (29)$$

Orthogonality of states  $|\alpha\rangle$  allows to find

$$D_{\alpha}(x, y) = \sum_{\beta} O_{\alpha\beta} \phi_{\beta}(x, y) \quad (30)$$

where

$$O_{\alpha\beta} = \langle \alpha | O(\hat{\mathbf{x}}, \hat{\mathbf{y}}) | \beta \rangle \quad (31)$$

is the matrix element in the MGL states taken over spin and angular variables.

In the calculation of matrix elements of the 3N potential a much more convenient is the basis  $|a\rangle$  in which individual spin projections of the nucleons and orbital momenta of pair 23 and nucleon 1 respective this pair are given

$$|a\rangle = |\lambda, \lambda_z, l, l_z, p_1, p_2, p_3\rangle = Y_{\lambda, \lambda_z}(\hat{\mathbf{y}}) Y_{l, l_z}(\hat{\mathbf{x}}) \chi_{p_1}^{(1)} \chi_{p_2}^{(2)} \chi_{p_3}^{(3)} \quad (32)$$

Here  $\chi_{p_i}^{(i)}$  is a spinor describing the  $i$ -th nucleon spin state with its projection  $p_i = \pm 1/2$ . The relation between the two bases is direct:

$$|\alpha\rangle = \sum_a |a\rangle \langle a | \alpha \rangle \equiv \sum_a F_{\alpha}^a |a\rangle \quad (33)$$

Coefficients  $F_{\alpha}^a$  are expressed as a product of four Clebsh-Gordon coefficients:

$$F_{\alpha}^a = C_{ssz \lambda \lambda_z}^{MMz} C_{\frac{1}{2} p_1 J J_z}^{ssz} C_{\sigma \sigma_z l l_z}^{JJz} C_{\frac{1}{2} p_2 \frac{1}{2} p_3}^{\sigma \sigma_z} \quad (34)$$

and the sum over  $a$  is in fact the sum over projections of the momenta

$$\sum_a = \sum_{\lambda_z, l_z, p_1, p_2, p_3} \quad (35)$$

Calculation of matrix elements in the MGL basis then reduces to their calculation in the factorized  $a$ -basis. For any operator  $O$

$$\langle \alpha' | O | \alpha \rangle = \sum_{a, a'} F_{\alpha'}^{a'} F_a^a \langle a' | O | a \rangle \quad (36)$$

(here we use that  $F_a^a$  are real).

Taking matrix elements of spin operators in the  $a$ -basis is trivial, since it gives the standard Pauli matrices either in Cartesian or spherical coordinates. Just to remind: in the Cartesian coordinates

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (37)$$

whereas in the spherical contravariant coordinates

$$\sigma^{+1} = -\sqrt{2} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^{-1} = \sqrt{2} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (38)$$

Calculating the orbital part one encounters integrals of three spherical functions with possible weights  $\hat{\mathbf{x}}_\mu$ ,  $\hat{\mathbf{x}}_\mu \hat{\mathbf{x}}_\nu$  and  $\hat{\mathbf{x}}_\mu \hat{\mathbf{x}}_\nu \hat{\mathbf{x}}_\epsilon$ . Correspondingly we define

$$B(l'l_z \rho \tau | ll_z) \equiv \int d\hat{\mathbf{x}} Y_{l'l_z}^*(\hat{\mathbf{x}}) Y_{\rho\tau}^*(\hat{\mathbf{x}}) Y_{ll_z}(\hat{\mathbf{x}}) = \frac{1}{\sqrt{4\pi}} \frac{\prod_{l'\rho}}{\prod_l} C_{l'0\rho 0}^{l0} C_{l'l_z \rho \tau}^{ll_z} \quad (39)$$

where we denote  $\prod_{abc\dots} = [(2a+1)(2b+1)(2c+1)\dots]^{1/2}$ . Note that the right-hand side is real. So we also have

$$B(l'l_z \rho \tau | ll_z) = \int d\hat{\mathbf{x}} Y_{l'l_z}(\hat{\mathbf{x}}) Y_{\rho\tau}(\hat{\mathbf{x}}) Y_{ll_z}^*(\hat{\mathbf{x}}) \quad (40)$$

We use relations (see Ref. [25], Varshalovich 13.2.3.10, 13.2.3.11 and 13.2.3.17)

$$\hat{\mathbf{x}}_\mu Y_{ll_z}(\hat{\mathbf{x}}) = \sum_{l''l_z''} \sqrt{\frac{2l+1}{2l''+1}} C_{ll_z 1\mu}^{l''l_z''} Y_{l''l_z''}(\hat{\mathbf{x}}) \quad (41)$$

and

$$\hat{\mathbf{x}}_\mu \hat{\mathbf{x}}_\nu Y_{ll_z}(\hat{\mathbf{x}}) = \frac{1}{3} (-1)^\mu \delta_{\mu-\nu} Y_{ll_z}(\hat{\mathbf{x}}) + \sum_{l''l_z''} \sqrt{\frac{2(2l+1)}{3(2l''+1)}} C_{l020}^{l''0} C_{1\mu 1\nu}^{2\kappa} C_{ll_z 2\kappa}^{l''l_z''} Y_{l''l_z''}(\hat{\mathbf{x}}) \quad (42)$$

Multiplying (42) by  $\mathbf{x}_\epsilon$  and using (41) we get

$$\hat{\mathbf{x}}_\mu \hat{\mathbf{x}}_\nu \hat{\mathbf{x}}_\epsilon Y_{ll_z}(\hat{\mathbf{x}}) = \frac{(-1)^\mu}{3} \delta_{\mu\nu} \sum_{l''l_z''} \sqrt{\frac{2l+1}{2l''+1}} C_{ll_z 1\epsilon}^{l''l_z''} Y_{l''l_z''}(\hat{\mathbf{x}})$$



$$+ \sum_{l''l_z''\bar{l}''\bar{l}_z''} \sqrt{\frac{2(2l+1)}{3(2\bar{l}''+1)}} C_{l020}^{l''0} C_{1\mu1\nu}^{2\kappa} C_{l_z2\kappa}^{l''l_z''} C_{10l''0}^{\bar{l}''0} C_{1\epsilon l''l_z''}^{\bar{l}''\bar{l}_z''} Y_{\bar{l}''\bar{l}_z''} \quad (43)$$

Correspondingly we define

$$B_\mu(l'l_z\rho\tau|ll_z) \equiv \int d\hat{\mathbf{x}} \hat{\mathbf{x}}_\mu Y_{l'l_z}^*(\hat{\mathbf{x}}) Y_{\rho\tau}^*(\hat{\mathbf{x}}) Y_{ll_z}(\hat{\mathbf{x}}) \\ = \sum_{l''l_z''} \sqrt{\frac{2l+1}{2l''+1}} C_{l_z1\mu}^{l''l_z''} B(l'l_z\rho\tau|l''l_z'') \quad (44)$$

$$B_{\mu\nu}(l'l_z\rho\tau|ll_z) \equiv \int d\hat{\mathbf{x}} \hat{\mathbf{x}}_\mu \hat{\mathbf{x}}_\nu Y_{l'l_z}^*(\hat{\mathbf{x}}) Y_{\rho\tau}^*(\hat{\mathbf{x}}) Y_{ll_z}(\hat{\mathbf{x}}) \\ = \frac{1}{3} (-1)^\mu \delta_{\mu-\nu} B(l'l_z\rho\tau|ll_z) + \sum_{l''l_z''} \sqrt{\frac{2(2l+1)}{3(2l''+1)}} C_{l020}^{l''0} C_{1\mu1\nu}^{2\kappa} C_{l_z2\kappa}^{l''l_z''} B(l'l_z\rho\tau|l''l_z'') \quad (45)$$

and

$$B_{\mu\nu\epsilon}(l'l_z\rho\tau|ll_z) \equiv \frac{(-1)^\mu}{3} \delta_{\mu\nu} \sum_{l''l_z''} \sqrt{\frac{2l+1}{2l''+1}} C_{l_z1\epsilon}^{l''l_z''} B(l'l_z\rho\tau|l''l_z'') \\ + \sum_{l''l_z''\bar{l}''\bar{l}_z''} \sqrt{\frac{2(2l+1)}{3(2\bar{l}''+1)}} C_{l020}^{l''0} C_{1\mu1\nu}^{2\kappa} C_{l_z2\kappa}^{l''l_z''} C_{10l''0}^{\bar{l}''0} C_{1\epsilon l''l_z''}^{\bar{l}''\bar{l}_z''} B(l'l_z\rho\tau|\bar{l}''\bar{l}_z'') \quad (46)$$

Finally we recall that in our basis

$$\mathbf{r}_2 - \mathbf{r}_3 = \mathbf{x}, \quad \mathbf{r}_3 - \mathbf{r}_1 = -\frac{1}{2}\mathbf{x} - \frac{\sqrt{3}}{2}\mathbf{y}, \quad \mathbf{r}_1 - \mathbf{r}_2 = -\frac{1}{2}\mathbf{x} + \frac{\sqrt{3}}{2}\mathbf{y} \quad (47)$$

## 6. Operators to study

We rewrite our 3N potential  $W_{\pi\pi}(3)$  as

$$W_{\pi\pi}(3) = \frac{g^2\mu^2}{64\pi^2m^2} \left\{ (\tau_1\tau_2) \left[ aO_2(3) + b \left( O_1(3) + O_3(3) + O_4(3) + O_5(3) \right) \right] \right. \\ \left. - d(\tau_3 \cdot \tau_1 \times \tau_2) \left[ O_6(3) + O_7(3) + O_8(3) + O_9(3) \right] \right\} \quad (48)$$

We have 9 different operators. For  $W_{\pi\pi}(2)$  and  $W_{\pi\pi}(1)$  we have to study 18 operators more  $O_i(n)$   $i = 1, \dots, 9$ ,  $n = 1, 2$ . So in all we have 27 different operators. Below we present a list of them in terms of our vectors  $\mathbf{x}$  and  $\mathbf{y}$

$$O_1(3) = (\sigma_1\sigma_2) Z^{(1)}(r_{13}) Z^{(1)}(r_{23}) \quad (49)$$

$$O_1(2) = (\sigma_1\sigma_3) Z^{(1)}(r_{12}) Z^{(1)}(r_{32}) \quad (50)$$

$$O_1(1) = (\sigma_2\sigma_3)Z^{(1)}(r_{21})Z^{(1)}(r_{31}) \quad (51)$$

$$\begin{aligned} O_2(3) &= (\sigma_1r_{13})(\sigma_2r_{23})Z^{(1)}(r_{13})Z^{(1)}(r_{23}) \\ &= \left[ \frac{1}{2}(\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_2\mathbf{x}) + \frac{\sqrt{3}}{2}(\vec{\sigma}_1\mathbf{y})(\vec{\sigma}_2\mathbf{x}) \right] Z^{(1)}(r_{13})Z^{(1)}(r_{23}) \quad (52) \end{aligned}$$

$$\begin{aligned} O_2(2) &= (\sigma_3r_{32})(\sigma_1r_{12})Z^{(1)}(r_{12})Z^{(1)}(r_{32}) \\ &= \left[ \frac{1}{2}(\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_3\mathbf{x}) - \frac{\sqrt{3}}{2}(\vec{\sigma}_1\mathbf{y})(\vec{\sigma}_3\mathbf{x}) \right] Z^{(1)}(r_{12})Z^{(1)}(r_{23}) \quad (53) \end{aligned}$$

$$\begin{aligned} O_2(1) &= (\sigma_2r_{21})(\sigma_3r_{31})Z^{(1)}(r_{21})Z^{(1)}(r_{31}) \\ &= \left[ -\frac{1}{4}(\vec{\sigma}_2\mathbf{x})(\vec{\sigma}_3\mathbf{x}) - \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_2\mathbf{x})(\vec{\sigma}_3\mathbf{y}) - (\vec{\sigma}_3\mathbf{x})(\vec{\sigma}_2\mathbf{y}) \right) \right. \\ &\quad \left. + \frac{3}{4}(\vec{\sigma}_2\mathbf{y})(\vec{\sigma}_3\mathbf{y}) \right] Z^{(1)}(r_{21})Z^{(1)}(r_{31}) \quad (54) \end{aligned}$$

$$\begin{aligned} O_3(3) &= (\sigma_1r_{13})(\sigma_2r_{13})Z^{(2)}(r_{13})Z^{(1)}(r_{23}) \\ &= \left[ \frac{1}{4}(\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_2\mathbf{x}) + \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_2\mathbf{y}) + (\vec{\sigma}_2\mathbf{x})(\vec{\sigma}_1\mathbf{y}) \right) \right. \\ &\quad \left. + \frac{3}{4}(\vec{\sigma}_1\mathbf{y})(\vec{\sigma}_2\mathbf{y}) \right] Z^{(2)}(r_{13})Z^{(1)}(r_{23}) \quad (55) \end{aligned}$$

$$O_4(3) = (\sigma_1r_{23})(\sigma_2r_{23})Z^{(1)}(r_{13})Z^{(2)}(r_{23}) = (\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_2\mathbf{x})Z^{(1)}(r_{13})Z^{(2)}(r_{23}) \quad (56)$$

$$\begin{aligned} O_3(2) &= (\sigma_1r_{12})(\sigma_3r_{12})Z^{(2)}(r_{12})Z^{(1)}(r_{23}) \\ &= \left[ \frac{1}{4}(\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_3\mathbf{x}) - \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_3\mathbf{y}) + (\vec{\sigma}_3\mathbf{x})(\vec{\sigma}_1\mathbf{y}) \right) \right. \\ &\quad \left. + \frac{3}{4}(\vec{\sigma}_1\mathbf{y})(\vec{\sigma}_3\mathbf{y}) \right] Z^{(2)}(r_{12})Z^{(1)}(r_{23}) \quad (57) \end{aligned}$$

$$\begin{aligned} O_4(2) &= (\sigma_1r_{32})(\sigma_3r_{32})Z^{(1)}(r_{12})Z^{(2)}(r_{23}) \\ &= (\vec{\sigma}_1\mathbf{x})(\vec{\sigma}_3\mathbf{x})Z^{(1)}(r_{12})Z^{(2)}(r_{23}) \quad (58) \end{aligned}$$

$$\begin{aligned}
 O_3(1) &= (\sigma_2 r_{21})(\sigma_3 r_{21})Z^{(2)}(r_{21})Z^{(1)}(r_{31}) \\
 &= \left[ \frac{1}{4}(\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{x}) - \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{y}) + (\vec{\sigma}_3 \mathbf{x})(\vec{\sigma}_2 \mathbf{y}) \right) \right. \\
 &\quad \left. + \frac{3}{4}(\vec{\sigma}_2 \mathbf{y})(\vec{\sigma}_3 \mathbf{y}) \right] Z^{(2)}(r_{12})Z^{(1)}(r_{31}) \quad (59)
 \end{aligned}$$

$$\begin{aligned}
 O_4(1) &= (\sigma_2 r_{31})(\sigma_3 r_{31})Z^{(1)}(r_{21})Z^{(2)}(r_{31}) \\
 &= \left[ \frac{1}{4}(\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{x}) + \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{y}) + (\vec{\sigma}_3 \mathbf{x})(\vec{\sigma}_2 \mathbf{y}) \right) \right. \\
 &\quad \left. + \frac{3}{4}(\vec{\sigma}_2 \mathbf{y})(\vec{\sigma}_3 \mathbf{y}) \right] Z^{(1)}(r_{21})Z^{(2)}(r_{31}) \quad (60)
 \end{aligned}$$

$$\begin{aligned}
 O_5(3) &= (\sigma_1 r_{13})(\sigma_2 r_{23})(r_{13} r_{23})Z^{(2)}(r_{13})Z^{(2)}(r_{23}) \\
 &= \left[ \frac{1}{2}(\vec{\sigma}_1 \mathbf{x})(\vec{\sigma}_2 \mathbf{x}) + \frac{\sqrt{3}}{2}(\vec{\sigma}_1 \mathbf{y})(\vec{\sigma}_2 \mathbf{x}) \right] (r_{13} r_{23})Z^{(2)}(r_{13})Z^{(2)}(r_{23}) \quad (61)
 \end{aligned}$$

$$\begin{aligned}
 O_5(2) &= (\sigma_3 r_{32})(\sigma_1 r_{12})(r_{12} r_{32})Z^{(2)}(r_{12})Z^{(2)}(r_{32}) \\
 &= \left[ \frac{1}{2}(\vec{\sigma}_1 \mathbf{x})(\vec{\sigma}_3 \mathbf{x}) - \frac{\sqrt{3}}{2}(\vec{\sigma}_1 \mathbf{y})(\vec{\sigma}_3 \mathbf{x}) \right] (r_{12} r_{32})Z^{(2)}(r_{12})Z^{(2)}(r_{32}) \quad (62)
 \end{aligned}$$

$$\begin{aligned}
 O_5(1) &= (\sigma_2 r_{21})(\sigma_3 r_{31})(r_{21} r_{31})Z^{(2)}(r_{21})Z^{(2)}(r_{31}) \\
 &= \left[ -\frac{1}{4}(\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{x}) - \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{y}) - (\vec{\sigma}_3 \mathbf{x})(\vec{\sigma}_2 \mathbf{y}) \right) \right. \\
 &\quad \left. + \frac{3}{4}(\vec{\sigma}_2 \mathbf{y})(\vec{\sigma}_3 \mathbf{y}) \right] (r_{21} r_{31})Z^{(2)}(r_{21})Z^{(2)}(r_{31}) \quad (63)
 \end{aligned}$$

$$O_6(3) = (\sigma_3 \cdot \sigma_1 \times \sigma_2)Z^{(1)}(r_{13})Z^{(1)}(r_{23}) \quad (64)$$

$$O_6(2) = (\sigma_2 \cdot \sigma_3 \times \sigma_1)Z^{(1)}(r_{32})Z^{(1)}(r_{12}) \quad (65)$$

$$O_6(1) = (\sigma_1 \cdot \sigma_2 \times \sigma_3)Z^{(1)}(r_{21})Z^{(1)}(r_{31}) \quad (66)$$

$$\begin{aligned}
O_7(3) &= (\sigma_3 \cdot \sigma_1 \times r_{23})(\sigma_2 r_{23}) Z^{(1)}(r_{13}) Z^{(2)}(r_{23}) \\
&= (\vec{\sigma}_3 \cdot \vec{\sigma}_1 \times \mathbf{x})(\vec{\sigma}_2 \mathbf{x}) Z^{(1)}(r_{13}) Z^{(2)}(r_{23}) \quad (67)
\end{aligned}$$

$$\begin{aligned}
O_8(3) &= (\sigma_3 \cdot r_{13} \times \sigma_2)(\sigma_1 r_{13}) Z^{(2)}(r_{13}) Z^{(1)}(r_{23}) \\
&= \left[ \frac{1}{4} (\vec{\sigma}_3 \cdot \mathbf{x} \times \vec{\sigma}_2)(\vec{\sigma}_1 \mathbf{x}) + \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_3 \cdot \mathbf{x} \times \vec{\sigma}_2)(\vec{\sigma}_1 \mathbf{y}) + (\vec{\sigma}_3 \cdot \mathbf{y} \times \vec{\sigma}_2)(\vec{\sigma}_1 \mathbf{x}) \right) \right. \\
&\quad \left. + \frac{3}{4} (\vec{\sigma}_3 \cdot \mathbf{y} \times \vec{\sigma}_2)(\vec{\sigma}_1 \mathbf{y}) \right] Z^{(2)}(r_{13}) Z^{(1)}(r_{23}) \quad (68)
\end{aligned}$$

$$\begin{aligned}
O_7(2) &= (\sigma_2 \cdot \sigma_3 \times r_{12})(\sigma_1 r_{12}) Z^{(1)}(r_{23}) Z^{(2)}(r_{12}) \\
&= \left[ \frac{1}{4} (\vec{\sigma}_2 \cdot \vec{\sigma}_3 \times \mathbf{x})(\vec{\sigma}_1 \mathbf{x}) - \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_2 \cdot \vec{\sigma}_3 \times \mathbf{x})(\vec{\sigma}_1 \mathbf{y}) + (\vec{\sigma}_2 \cdot \vec{\sigma}_3 \times \mathbf{y})(\vec{\sigma}_1 \mathbf{x}) \right) \right. \\
&\quad \left. + \frac{3}{4} (\vec{\sigma}_3 \cdot \vec{\sigma}_3 \times \mathbf{y})(\vec{\sigma}_1 \mathbf{y}) \right] Z^{(1)}(r_{23}) Z^{(2)}(r_{12}) \quad (69)
\end{aligned}$$

$$\begin{aligned}
O_8(2) &= (\sigma_2 \cdot r_{32} \times \sigma_1)(\sigma_3 r_{32}) Z^{(2)}(r_{32}) Z^{(1)}(r_{12}) \\
&= (\vec{\sigma}_2 \cdot \mathbf{x} \times \vec{\sigma}_1)(\vec{\sigma}_3 \mathbf{x}) Z^{(2)}(r_{32}) Z^{(1)}(r_{12}) \quad (70)
\end{aligned}$$

$$\begin{aligned}
O_7(1) &= (\sigma_1 \cdot \sigma_2 \times r_{31})(\sigma_3 r_{31}) Z^{(1)}(r_{23}) Z^{(2)}(r_{31}) \\
&= \left[ \frac{1}{4} (\vec{\sigma}_1 \cdot \vec{\sigma}_2 \times \mathbf{x})(\vec{\sigma}_3 \mathbf{x}) + \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_1 \cdot \vec{\sigma}_2 \times \mathbf{x})(\vec{\sigma}_3 \mathbf{y}) + (\vec{\sigma}_1 \cdot \vec{\sigma}_2 \times \mathbf{y})(\vec{\sigma}_3 \mathbf{x}) \right) \right. \\
&\quad \left. + \frac{3}{4} (\vec{\sigma}_1 \cdot \vec{\sigma}_2 \times \mathbf{y})(\vec{\sigma}_3 \mathbf{y}) \right] Z^{(1)}(r_{23}) Z^{(2)}(r_{31}) \quad (71)
\end{aligned}$$

$$\begin{aligned}
O_8(1) &= (\sigma_1 \cdot r_{21} \times \sigma_3)(\sigma_2 r_{21}) Z^{(2)}(r_{21}) Z^{(1)}(r_{31}) \\
&= \left[ \frac{1}{4} (\vec{\sigma}_1 \cdot \mathbf{x} \times \vec{\sigma}_3)(\vec{\sigma}_2 \mathbf{x}) - \frac{\sqrt{3}}{4} \left( (\vec{\sigma}_1 \cdot \mathbf{x} \times \vec{\sigma}_3)(\vec{\sigma}_2 \mathbf{y}) + (\vec{\sigma}_1 \cdot \mathbf{y} \times \vec{\sigma}_3)(\vec{\sigma}_2 \mathbf{x}) \right) \right. \\
&\quad \left. + \frac{3}{4} (\vec{\sigma}_1 \cdot \mathbf{y} \times \vec{\sigma}_3)(\vec{\sigma}_2 \mathbf{y}) \right] Z^{(2)}(r_{21}) Z^{(1)}(r_{31}) \quad (72)
\end{aligned}$$

$$\begin{aligned}
 O_9(3) &= (\sigma_3 \cdot r_{13} \times r_{23})(\sigma_1 r_{13})(\sigma_2 r_{23})Z^{(2)}(r_{13})Z^{(2)}(r_{23}) \\
 &= (\vec{\sigma}_3 \cdot \mathbf{y} \times \mathbf{x}) \left[ \frac{\sqrt{3}}{4}(\vec{\sigma}_1 \mathbf{x})(\vec{\sigma}_2 \mathbf{x}) + \frac{3}{4}(\vec{\sigma}_1 \mathbf{y})(\vec{\sigma}_2 \mathbf{x}) \right] Z^{(2)}(r_{13})Z^{(2)}(r_{23}) \quad (73)
 \end{aligned}$$

$$\begin{aligned}
 O_9(2) &= (\sigma_2 \cdot r_{32} \times r_{12})(\sigma_3 r_{32})(\sigma_1 r_{12})Z^{(2)}(r_{32})Z^{(2)}(r_{12}) \\
 &= (\vec{\sigma}_2 \cdot \mathbf{y} \times \mathbf{x}) \left[ \frac{\sqrt{3}}{4}(\vec{\sigma}_3 \mathbf{x})(\vec{\sigma}_1 \mathbf{x}) - \frac{3}{4}(\vec{\sigma}_1 \mathbf{y})(\vec{\sigma}_3 \mathbf{x}) \right] Z^{(2)}(r_{32})Z^{(2)}(r_{12}) \quad (74)
 \end{aligned}$$

$$\begin{aligned}
 O_9(1) &= (\sigma_1 \cdot r_{21} \times r_{31})(\sigma_2 r_{21})(\sigma_3 r_{31})Z^{(2)}(r_{21})Z^{(2)}(r_{31}) \\
 &= (\vec{\sigma}_1 \cdot \mathbf{y} \times \mathbf{x}) \left[ -\frac{\sqrt{3}}{8}(\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{x}) + \frac{3}{8} \left( (\vec{\sigma}_3 \mathbf{x})(\vec{\sigma}_2 \mathbf{y}) - (\vec{\sigma}_2 \mathbf{x})(\vec{\sigma}_3 \mathbf{y}) \right) \right. \\
 &\quad \left. + \frac{3\sqrt{3}}{8}(\vec{\sigma}_2 \mathbf{y})(\vec{\sigma}_3 \mathbf{y}) \right] Z^{(2)}(r_{21})Z^{(2)}(r_{31}) \quad (75)
 \end{aligned}$$

Our idea is first to construct matrix elements of these operators in the  $a$ -basis, which is almost trivial and only needs a good bookkeeping. In principle the desired matrix elements in the MGL basis can then be obtained by Eq. (36). Written in terms of Clebsh-Gordon coefficients this includes multiple (though finite) summations over momentum projections. It is to be seen whether some of these summations can be done analytically (as for Coulomb matrix elements). This problem is to be treated at the next step.

## 7. Spin-coordinate operators in the $a$ -basis

### 7.1 Operators $O_1$

We illustrate our technique in the simplest case of operator  $O_1(3)$  As we mentioned, the spin part is trivial

$$\langle p'_1 p'_2 p'_3 | (\sigma_1 \sigma_2) | p_1 p_2 p_3 \rangle = \vec{\sigma}_{p'_1 p_1} \vec{\sigma}_{p'_2 p_2} \delta_{p'_3 p_3} \quad (76)$$

Now the spatial part

$$Z^{(1)} \left( \left| \frac{1}{2} \mathbf{x} + \frac{\sqrt{3}}{2} \mathbf{y} \right| \right) Z^{(1)}(x)$$

As with the Coulomb matrix elements we expand the first factor in Legendre polynomials in  $\cos \theta$  where  $\theta$  is the angle between  $\mathbf{x}$  and  $\mathbf{y}$  and then convert this

expansion into the one in bipolar harmonics. Having in mind permutations  $2 \leftrightarrow 3$  we expand

$$\begin{aligned} Z^{(1)}\left(\left|\frac{1}{2}\mathbf{x} \pm \frac{\sqrt{3}}{2}\mathbf{y}\right|\right) &= \sum_{\rho} (2l+1)P_{\rho}(\cos\theta)(\mp 1)^{\rho} Z_{\rho}^{(1)}(x, y) \\ &= 4\pi \sum_{\rho, \tau} Y^{*}(\hat{\mathbf{x}})_{\rho\tau} Y(\hat{\mathbf{y}})_{\rho\tau} (\mp 1)^{\rho} Z_{\rho}^{(1)}(x, y) \end{aligned} \quad (77)$$

Taking matrix elements will give two  $B$  coefficients

$$\begin{aligned} \langle \lambda' \lambda'_z l' l'_z | Z^{(1)}\left(\left|\frac{1}{2}\mathbf{x} \pm \frac{\sqrt{3}}{2}\mathbf{y}\right|\right) | \lambda \lambda_z l l_z \rangle \\ = 4\pi \sum_{\rho\tau} (\mp 1)^{\rho} Z_{\rho}^{(1)}(x, y) B(l' l'_z \rho \tau | l l_z) B(\lambda \lambda_z \rho \tau | \lambda' \lambda'_z) \end{aligned} \quad (78)$$

So finally we get

$$\begin{aligned} \langle a' | O_1(3) | a \rangle \\ = 4\pi \vec{\sigma}_{p'_1 p_1} \vec{\sigma}_{p'_2 p_2} \delta_{p'_3 p_3} Z^{(1)}(x) \sum_{\rho\tau} (-1)^{\rho} Z_{\rho}^{(1)}(x, y) B(l' l'_z \rho \tau | l l_z) B(\lambda \lambda_z \rho \tau | \lambda' \lambda'_z) \end{aligned} \quad (79)$$

This explicit expression is difficult to read and write. So in the following we use a convenient short-hand matrix notation. We shall not write out the components of the matrix element of Pauli matrices but leave them as they stand:

$$(\vec{\sigma}_1 \vec{\sigma}_2)$$

As to the spatial part, we introduce matrices

$$\langle l' l'_z | B^{\tau}(\rho) | l, l_z \rangle \equiv B(l' l'_z \rho \tau | l l_z), \quad \langle \lambda' \lambda'_z | D^{\tau}(\rho) | \lambda, \lambda_z \rangle \equiv B(\lambda \lambda_z \rho \tau | \lambda' \lambda'_z) \quad (80)$$

and their scalar product

$$B(\rho) D(\rho) \equiv \sum_{\tau} B^{\tau}(\rho) D^{\tau}(\rho) \equiv (BD)_{\rho} \quad (81)$$

In these notations

$$\langle a' | O_1(3) | a \rangle = \langle a' | 4\pi (\vec{\sigma}_1 \vec{\sigma}_2) Z^{(1)}(x) \sum_{\rho} (-1)^{\rho} Z_{\rho}^{(1)}(x, y) (BD)_{\rho} | a \rangle \quad (82)$$

or simply, omitting the states  $a$  and  $a'$

$$O_1(3) = 4\pi (\vec{\sigma}_1 \vec{\sigma}_2) Z^{(1)}(x) \sum_{\rho} (-1)^{\rho} Z_{\rho}^{(1)}(x, y) (BD)_{\rho} \quad (83)$$

Permutation 2 ↔ 3 will obviously give

$$O_1(2) = 4\pi(\vec{\sigma}_1\vec{\sigma}_3)Z^{(1)}(x)\sum_{\rho}Z_{\rho}^{(1)}(x,y)(BD)_{\rho} \quad (84)$$

In  $O_1(1)$  the spatial part is

$$Z^{(1)}\left(\left|\frac{1}{2}\mathbf{x} + \frac{\sqrt{3}}{2}\mathbf{y}\right|\right)Z^{(1)}\left(\left|\frac{1}{2}\mathbf{x} - \frac{\sqrt{3}}{2}\mathbf{y}\right|\right)$$

We expand it as a whole in Legendre polynomials

$$\begin{aligned} & Z^{(1)}\left(\left|\frac{1}{2}\mathbf{x} + \frac{\sqrt{3}}{2}\mathbf{y}\right|\right)Z^{(1)}\left(\left|\frac{1}{2}\mathbf{x} - \frac{\sqrt{3}}{2}\mathbf{y}\right|\right) \\ &= \sum_{\rho}(2l+1)P_{\rho}(\cos\theta)Z_{\rho}^{(11)}(x,y) = 4\pi\sum_{\rho,\tau}Y^{*}(\hat{\mathbf{x}})_{\rho\tau}Y(\hat{\mathbf{y}})_{\rho\tau}Z_{\rho}^{(11)}(x,y) \end{aligned} \quad (85)$$

Obviously only even value of  $\rho$  contribute. After that we find

$$O_1(1) = 4\pi(\vec{\sigma}_2\vec{\sigma}_3)\sum_{\rho}Z_{\rho}^{(11)}(x,y)(BD)_{\rho} \quad (86)$$

## 7.2 Operators $O_2 - O_5$

Operators  $O_2 - O_5$  can be written in a straightforward manner using our list of operators in terms of vectors  $\mathbf{x}$  and  $\mathbf{y}$  and attaching subindexes  $\mu$  and  $\nu$  to matrices  $B$  or  $D$ .

$$\begin{aligned} O_2(3) = & \\ & 4\pi\sum_{\mu\nu}\sigma_1^{\mu}\sigma_2^{\nu}xZ^{(1)}(x)\sum_{\rho}Z_{\rho}^{(1)}(x,y)(-1)^{\rho}\left[\frac{1}{2}x(B_{\mu\nu}D)_{\rho} + \frac{\sqrt{3}}{2}y(B_{\nu}D_{\mu})_{\rho}\right] \end{aligned} \quad (87)$$

$$O_2(2) = 4\pi\sum_{\mu\nu}\sigma_1^{\mu}\sigma_3^{\nu}xZ^{(1)}(x)\sum_{\rho}Z_{\rho}^{(1)}(x,y)\left[\frac{1}{2}x(B_{\mu\nu}D)_{\rho} - \frac{\sqrt{3}}{2}y(B_{\nu}D_{\mu})_{\rho}\right] \quad (88)$$

$$\begin{aligned} O_2(1) = 4\pi\sum_{\mu\nu}\sigma_2^{\mu}\sigma_3^{\nu}\sum_{\rho}Z_{\rho}^{(11)}(x,y)\left[-\frac{1}{4}x^2(B_{\mu\nu}D)_{\rho} \right. \\ \left. - \frac{\sqrt{3}}{4}xy(B_{\mu}D_{\nu})_{\rho} - B_{\nu}D_{\mu})_{\rho}\right] + \frac{3}{4}y^2(BD_{\mu\nu})_{\rho} \end{aligned} \quad (89)$$

$$O_3(3) = 4\pi\sum_{\mu\nu}\sigma_1^{\mu}\sigma_2^{\nu}Z^{(1)}(x)\sum_{\rho}Z_{\rho}^{(2)}(x,y)(-1)^{\rho}\left[\frac{1}{4}x^2(B_{\mu\nu}D)_{\rho}\right.$$

$$+ \frac{\sqrt{3}}{4}xy \left( B_\mu D_\nu \right)_\rho + B_\nu D_\mu \Big)_\rho + \frac{3}{4}y^2(BD_{\mu\nu})_\rho \Big] \quad (90)$$

$$O_3(2) = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_3^\nu Z^{(1)}(x) \sum_\rho Z_\rho^{(2)}(x, y) \left[ \frac{1}{4}x^2(B_{\mu\nu}D)_\rho \right. \\ \left. - \frac{\sqrt{3}}{4}xy \left( B_\mu D_\nu \right)_\rho + B_\nu D_\mu \Big)_\rho + \frac{3}{4}y^2(BD_{\mu\nu})_\rho \right] \quad (91)$$

$$O_3(1) = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu \sum_\rho Z_\rho^{(21)}(x, y) \left[ \frac{1}{4}x^2(B_{\mu\nu}D)_\rho \right. \\ \left. - \frac{\sqrt{3}}{4}xy \left( B_\mu D_\nu \right)_\rho + B_\nu D_\mu \Big)_\rho + \frac{3}{4}y^2(BD_{\mu\nu})_\rho \right] \quad (92)$$

$$O_4(3) = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu x^2 Z^{(2)}(x) \sum_\rho Z_\rho^{(1)}(x, y) (-1)^\rho (B_{\mu\nu}D)_\rho \quad (93)$$

$$O_4(2) = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_3^\nu x^2 Z^{(2)}(x) \sum_\rho Z_\rho^{(1)}(x, y) (B_{\mu\nu}D)_\rho \quad (94)$$

$$O_4(1) = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu \sum_\rho Z_\rho^{(12)}(x, y) \left[ \frac{1}{4}x^2(B_{\mu\nu}D)_\rho \right. \\ \left. + \frac{\sqrt{3}}{4}xy \left( B_\mu D_\nu \right)_\rho + B_\nu D_\mu \Big)_\rho + \frac{3}{4}y^2(BD_{\mu\nu})_\rho \right] \quad (95)$$

$$O_5(3) = \\ 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu x Z^{(2)}(x) \sum_\rho U_\rho^{(2)}(x, y) (-1)^\rho \left[ \frac{1}{2}x(B_{\mu\nu}D)_\rho + \frac{\sqrt{3}}{2}y(B_\nu D_\mu)_\rho \right] \quad (96)$$

$$O_5(2) = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu x Z^{(2)}(x) \sum_\rho U_\rho^{(2)}(x, y) \left[ \frac{1}{2}x(B_{\mu\nu}D)_\rho - \frac{\sqrt{3}}{2}y(B_\nu D_\mu)_\rho \right] \quad (97)$$

$$O_5(1) = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu x \sum_\rho U_\rho^{(22)}(x, y) \left[ -\frac{1}{4}x^2(B_{\mu\nu}D)_\rho \right. \\ \left. - \frac{\sqrt{3}}{4}xy \left( B_\mu D_\nu \right)_\rho - B_\nu D_\mu \Big)_\rho + \frac{3}{4}y^2(BD_{\mu\nu})_\rho \right] \quad (98)$$

In operators  $O_5$  we introduce functions of the angle ( $\mathbf{xy}$ )

$$U^{(1)} = (\mathbf{r}_{12}\mathbf{r}_{32})Z^{(2)}(r_{12}), \quad U^{(22)} = (\mathbf{r}_{21}\mathbf{r}_{31})Z^{(2)}(r_{21})Z^{(2)}(r_{31}) \quad (99)$$

Also  $Z_\rho^{(12)}$  and  $Z_\rho^{(21)}$  are the partial of functions  $Z^{(1)}(r_{12})Z^{(2)}(r_{13})$  and  $Z^{(2)}(r_{12})Z^{(1)}(r_{13})$  respectively. They differ by factor  $(-1)^\rho$ .



## 8. Operators $O_6 - O_9$

Operators  $O_6$  are simple

$$O_6(3) = 4\pi(\vec{\sigma}_3 \cdot \vec{\sigma}_1 \times \vec{\sigma}_2)Z^{(1)}(x) \sum_{\rho} (-1)^{\rho} Z_{\rho}^{(1)}(x, y)(BD)_{\rho} \quad (100)$$

$$O_6(2) = 4\pi(\vec{\sigma}_2 \cdot \vec{\sigma}_3 \times \vec{\sigma}_1)Z^{(1)}(x) \sum_{\rho} Z_{\rho}^{(1)}(x, y)(BD)_{\rho} \quad (101)$$

$$O_6(1) = 4\pi(\vec{\sigma}_1 \cdot \vec{\sigma}_2 \times \vec{\sigma}_3) \sum_{\rho} Z_{\rho}^{(11)}(x, y)(BD)_{\rho} \quad (102)$$

To write out other operators we use the form of the vector product in spherical coordinates:

$$[a \times b]^{\epsilon} = i\sqrt{2} \sum_{\mu\nu} C_{1\mu 1\nu}^{1\epsilon} a^{\mu} b^{\nu} \quad (103)$$

The we easily find

$$O_7(3) = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^{\epsilon} \sigma_1^{\mu} \sigma_2^{\phi} x^2 Z^{(2)}(x) \sum_{\rho} (-1)^{\rho} Z_{\rho}^{(1)}(x, y)(B_{\nu\phi}D)_{\rho} \quad (104)$$

$$O_7(2) = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^{\epsilon} \sigma_3^{\mu} \sigma_1^{\phi} Z^{(1)}(x) \sum_{\rho} Z_{\rho}^{(2)}(x, y) \left[ \frac{1}{4}x^2(B_{\nu\phi}D)_{\rho} - \frac{\sqrt{3}}{4}xy \left( (B_{\nu}D_{\phi})_{\rho} + (B_{\phi}D_{\nu})_{\rho} \right) + \frac{3}{4}y^2(BD_{\nu\phi})_{\rho} \right] \quad (105)$$

$$O_7(1) = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^{\epsilon} \sigma_2^{\mu} \sigma_3^{\phi} \sum_{\rho} Z_{\rho}^{(12)}(x, y) \left[ \frac{1}{4}x^2(B_{\nu\phi}D)_{\rho} + \frac{\sqrt{3}}{4}xy \left( (B_{\nu}D_{\phi})_{\rho} + (B_{\phi}D_{\nu})_{\rho} \right) + \frac{3}{4}y^2(BD_{\nu\phi})_{\rho} \right] \quad (106)$$

$$O_8(3) = -4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^{\epsilon} \sigma_2^{\mu} \sigma_1^{\phi} Z^{(1)}(x) \sum_{\rho} (-1)^{\rho} Z_{\rho}^{(2)}(x, y) \left[ \frac{1}{4}x^2(B_{\nu\phi}D)_{\rho} + \frac{\sqrt{3}}{4}xy \left( (B_{\nu}D_{\phi})_{\rho} + (B_{\phi}D_{\nu})_{\rho} \right) + \frac{3}{4}y^2(BD_{\nu\phi})_{\rho} \right] \quad (107)$$

$$O_8(2) = -4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^{\epsilon} \sigma_3^{\mu} \sigma_1^{\phi} x^2 Z^{(2)}(x) \sum_{\rho} Z_{\rho}^{(1)}(x, y)(B_{\nu\phi}D)_{\rho} \quad (108)$$

$$O_8(1) = -4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_3^\mu \sigma_2^\phi \sum_{\rho} Z_{\rho}^{(21)}(x, y) \left[ \frac{1}{4} x^2 (B_{\nu\phi} D)_{\rho} - \frac{\sqrt{3}}{4} xy \left( (B_{\nu} D_{\phi})_{\rho} + (B_{\phi} D_{\nu})_{\rho} \right) + \frac{3}{4} y^2 (B D_{\nu\phi})_{\rho} \right] \quad (109)$$

$$O_9(3) = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_1^\phi \sigma_2^\chi x^2 Z^{(2)}(x) \sum_{\rho} (-1)^{\rho} Z_{\rho}^{(2)}(x, y) \left( \frac{\sqrt{3}}{4} x (B_{\nu\phi\chi} D_{\mu})_{\rho} + \frac{3}{4} y (B_{\nu\chi} D_{\mu\phi})_{\rho} \right) \quad (110)$$

$$O_9(2) = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\phi \sigma_1^\chi x^2 Z^{(2)}(x) \sum_{\rho} Z_{\rho}^{(2)}(x, y) \left( \frac{\sqrt{3}}{4} x (B_{\nu\phi\chi} D_{\mu})_{\rho} - \frac{3}{4} y (B_{\nu\chi} D_{\mu\phi})_{\rho} \right) \quad (111)$$

$$O_9(1) = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\phi \sigma_3^\chi xy \sum_{\rho} Z_{\rho}^{(22)}(x, y) \left[ -\frac{\sqrt{3}}{8} x^2 (B_{\nu\phi\chi} D_{\mu})_{\rho} + \frac{3}{8} xy \left( (B_{\nu\chi} D_{\mu\phi})_{\rho} - (B_{\nu\phi} D_{\mu\chi})_{\rho} \right) + \frac{3\sqrt{3}}{8} y^2 (B_{\nu} D_{\mu\phi\chi})_{\rho} \right] \quad (112)$$

## 9. Functions to be expanded in partial waves

Our basic functions can be taken from [23] Take the form-factor as

$$F_{\pi\pi}(q) = \frac{\Lambda^2 - \mu^2}{\Lambda^2 - q^2} \quad (113)$$

Define

$$G(r) = \frac{e^{-r}}{r} \left( 1 + \frac{1}{r} \right), \quad F(r) = \frac{e^{-r}}{r} \left( 1 + \frac{3}{r} + \frac{3}{r^2} \right) \quad (114)$$

Then

$$Z^{(1)}(r) = -\mu \left[ G(\mu r) - \frac{\Lambda^2}{\mu^2} G(\Lambda r) - \frac{1}{2} \left( \frac{\Lambda^2}{\mu^2} - 1 \right) e^{-\Lambda r} \right] \quad (115)$$

and

$$Z^{(2)}(r) = \frac{1}{r} Z^{(1)}(r) + X_2(r) \quad (116)$$

where

$$X_2(r) = \mu^2 \left[ F(\mu r) - \frac{\Lambda^3}{\mu^3} F(\Lambda r) - \frac{1}{2} \frac{\Lambda^2 r}{\mu} \left( \frac{\Lambda^2}{\mu^2} - 1 \right) G(\Lambda r) \right] \quad (117)$$

The angular dependence comes from the expressions for  $r_{12}$  and  $r_{13}$ :

$$r_{12} = \sqrt{\frac{1}{4}x^2 + \frac{3}{4}y^2 - \frac{\sqrt{3}}{2}xy \cos \theta}, \quad r_{13} = \sqrt{\frac{1}{4}x^2 + \frac{3}{4}y^2 + \frac{\sqrt{3}}{2}xy \cos \theta} \quad (118)$$

For any function  $F$  partial waves of  $F(r_{12})$  and  $F(r_{13})$  will differ by a factor  $(-1)^\rho$ . We standardly define partial wave for  $F(r_{12})$ :

$$F_\rho(x, y) = \frac{1}{2} \int_{-1}^{+1} d \cos \theta P_\rho(\cos \theta) F(r_{12}) \quad (119)$$

For  $F(r_{13})$  partial waves will then be  $(-1)^\rho F_\rho(x, y)$ . The product of two identical functions  $F(r_{12})F(r_{13})$  is even in  $\cos \theta$  and its partial wave expansion will contain only even values of  $\rho$ . When a product of different functions is partial wave expanded, then partial waves  $Z^{(ik)}$  correspond to the product  $Z^{(i)}(r_{12})Z^{(k)}(r_{13})$

## 10 Dynamical and geometrical factors

Our next step is present our matrix elements in terms of dynamical factors, depending on  $x$  and  $y$  and geometrical ones, which depend only on the labels of the states between which the matrix elements are taken. Their role is different in the calculational procedure. Geometrical factors can be calculated once and for all before the actual computation, which is based on scanning the grid in  $x, y$  plane.

To simplify notations, from now on we denote

$$O_i(k) = O_{ik}, \quad i = 1, \dots, 9, \quad k = 1, 2, 3 \quad (120)$$

We present

$$O_{ik} = \sum_{l=1}^{l_{ik}} \sum_{\rho} O_{ik\rho}^{(l)}(x, y) q_{ik\rho}^{(l)} \quad (121)$$

where  $O_{ik\rho}^{(l)}(x, y)$  are dynamical factors and matrix elements of  $q_{ik\rho}^{(l)}$  give geometrical factors. The number of terms  $l_{ik}$  maybe 1, 2 or 3 for different  $ik$ .

Expansion (121) can be made in a straightforward manner on the inspection of expressions for the operators in Section 6 .

$$O_{13\rho} = Z^{(1)}(x)Z_\rho^{(1)}(x, y)(-1)^\rho, \quad q_{13\rho} = 4\pi(\vec{\sigma}_1\vec{\sigma}_2)(BD)_\rho \quad (122)$$

$$O_{12\rho} = Z^{(1)}(x)Z_\rho^{(1)}(x, y), \quad q_{12\rho} = 4\pi(\vec{\sigma}_1\vec{\sigma}_3)(BD)_\rho \quad (123)$$

$$O_{11\rho} = z_\rho^{(11)}(x, y), \quad q_{11\rho} = 4\pi(\vec{\sigma}_2\vec{\sigma}_3)(BD)_\rho \quad (124)$$

$$O_{23\rho}^{(1)} = \frac{1}{2}x^2 Z^{(1)}(x)Z_\rho^{(1)}(x,y)(-1)^\rho, \quad q_{23\rho}^{(1)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu (B_{\mu\nu}D)_\rho \quad (125)$$

$$O_{23\rho}^{(2)} = \frac{\sqrt{3}}{2}xy Z^{(1)}(x)Z_\rho^{(1)}(x,y)(-1)^\rho, \quad q_{23\rho}^{(2)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu (B_\nu D_\mu)_\rho \quad (126)$$

$$O_{22\rho}^{(1)} = (-1)^\rho O_{23\rho}^{(1)}, \quad q_{22\rho}^{(1)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_3^\nu (B_{\mu\nu}D)_\rho \quad (127)$$

$$O_{22\rho}^{(2)} = -(-1)^\rho O_{23\rho}^{(1)}, \quad q_{22\rho}^{(2)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_3^\nu (B_\nu D_\mu)_\rho \quad (128)$$

$$O_{21\rho}^{(1)} = -\frac{1}{4}x^2 Z_\rho^{(11)}(x,y), \quad q_{21\rho} = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu (B_{\mu\nu}D)_\rho \quad (129)$$

$$O_{21\rho}^{(2)} = -\frac{\sqrt{3}}{4}xy Z_\rho^{(11)}(x,y), \quad q_{21\rho}^{(2)} = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu (B_\mu D_\mu - B_\nu D_\mu)_\rho \quad (130)$$

$$O_{21\rho}^{(3)} = \frac{3}{4}y^2 Z_\rho^{(11)}(x,y), \quad q_{21\rho}^{(3)} = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu (BD_{\mu\nu})_\rho \quad (131)$$

$$O_{33\rho}^{(1)} = \frac{1}{4}x^2 Z^{(1)}(x)Z_\rho^{(2)}(x,y)(-1)^\rho, \quad q_{33\rho}^{(1)} = q_{23\rho}^{(1)} \quad (132)$$

$$O_{33\rho}^{(2)} = \frac{\sqrt{3}}{4}xy Z^{(1)}(x)Z_\rho^{(2)}(x,y)(-1)^\rho, \quad q_{33\rho}^{(2)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu (B_\mu D_\mu + B_\nu D_\mu)_\rho \quad (133)$$

$$O_{33\rho}^{(3)} = \frac{3}{4}y^2 Z^{(1)}(x)Z_\rho^{(2)}(x,y)(-1)^\rho, \quad q_{33\rho}^{(3)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_2^\nu (BD_{\mu\nu})_\rho \quad (134)$$

$$O_{32\rho}^{(1)} = \frac{1}{4}x^2 Z^{(1)}(x)Z_\rho^{(2)}(x,y), \quad q_{32\rho}^{(1)} = q_{22\rho}^{(1)} \quad (135)$$

$$O_{32\rho}^{(2)} = -\frac{\sqrt{3}}{4}xy Z^{(1)}(x)Z_\rho^{(2)}(x,y), \quad q_{32\rho}^{(2)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_3^\nu (B_\mu D_\mu + B_\nu D_\mu)_\rho \quad (136)$$

$$O_{32\rho}^{(3)} = \frac{3}{4}y^2 Z^{(1)}(x)Z_\rho^{(2)}(x,y), \quad q_{32\rho}^{(3)} = 4\pi \sum_{\mu\nu} \sigma_1^\mu \sigma_3^\nu (BD_{\mu\nu})_\rho \quad (137)$$

$$O_{31\rho}^{(1)} = \frac{1}{4}x^2 Z_\rho^{(21)}(x,y), \quad q_{31\rho}^{(1)} = q_{21\rho}^{(1)} \quad (138)$$

$$O_{31\rho}^{(2)} = -\frac{\sqrt{3}}{4}xy Z_\rho^{(21)}(x,y), \quad q_{31\rho}^{(2)} = 4\pi \sum_{\mu\nu} \sigma_2^\mu \sigma_3^\nu (B_\mu D_\mu + B_\nu D_\mu)_\rho \quad (139)$$

$$O_{31\rho}^{(3)} = \frac{3}{4}y^2 Z_\rho^{(21)}(x,y), \quad q_{31\rho}^{(3)} = q_{21\rho}^{(3)} \quad (140)$$

$$O_{43\rho} = x^2 Z^{(2)}(x)Z_\rho^{(1)}(x,y)(-1)^\rho, \quad q_{43\rho} = q_{23\rho}^{(1)} \quad (141)$$

$$O_{42\rho} = x^2 Z^{(2)}(x) Z_\rho^{(1)}(x, y), \quad q_{42\rho} = q_{22\rho}^{(1)} \quad (142)$$

$$O_{41\rho}^{(1)} = \frac{1}{4} x^2 Z_\rho^{(12)}(x, y), \quad q_{41\rho}^{(1)} = q_{21\rho}^{(1)} \quad (143)$$

$$O_{41\rho}^{(2)} = \frac{\sqrt{3}}{4} xy Z_\rho^{(12)}(x, y), \quad q_{41\rho}^{(2)} = q_{31\rho}^{(2)} \quad (144)$$

$$O_{41\rho}^{(3)} = \frac{3}{4} y^2 Z^{(12)}(x, y), \quad q_{41\rho}^{(3)} = q_{21\rho}^{(3)} \quad (145)$$

$$O_{53\rho}^{(1)} = \frac{1}{2} x^2 Z^{(2)}(x) U_\rho^{(2)}(x, y) (-1)^\rho, \quad q_{53\rho}^{(1)} = q_{23\rho}^{(1)} \quad (146)$$

$$O_{53\rho}^{(2)} = \frac{\sqrt{3}}{2} xy Z^{(2)}(x) U_\rho^{(2)}(x, y) (-1)^\rho, \quad q_{53\rho}^{(2)} = q_{23\rho}^{(2)} \quad (147)$$

$$O_{52\rho}^{(1)} = (-1)^\rho O_{53\rho}^{(1)}, \quad q_{52\rho}^{(1)} = q_{22\rho}^{(1)} \quad (148)$$

$$O_{52\rho}^{(2)} = -(-1)^\rho O_{53\rho}^{(2)}, \quad q_{52\rho}^{(2)} = q_{22\rho}^{(2)} \quad (149)$$

$$O_{51\rho}^{(1)} = -\frac{1}{4} x^2 U_\rho^{(22)}(x, y), \quad q_{51\rho}^{(1)} = q_{21\rho}^{(1)} \quad (150)$$

$$O_{51\rho}^{(2)} = -\frac{\sqrt{3}}{4} xy U_\rho^{(22)}(x, y), \quad q_{51\rho}^{(2)} = q_{21\rho}^{(2)} \quad (151)$$

$$O_{51\rho}^{(3)} = \frac{3}{4} y^2 U_\rho^{(22)}(x, y), \quad q_{51\rho}^{(3)} = q_{21\rho}^{(3)} \quad (152)$$

$$O_{63\rho} = O_{13\rho}, \quad q_{13\rho} = 4\pi(\vec{\sigma}_3 \cdot \vec{\sigma}_1 \times \vec{\sigma}_2)(BD)_\rho \quad (153)$$

$$O_{62\rho} = O_{12\rho}, \quad q_{12\rho} = 4\pi(\vec{\sigma}_2 \cdot \vec{\sigma}_3 \vec{\sigma}_1)(BD)_\rho \quad (154)$$

$$O_{61\rho} = O_{11\rho}, \quad q_{1\rho} = 4\pi(\vec{\sigma}_1 \cdot \vec{\sigma}_2 \times \vec{\sigma}_3)(BD)_\rho \quad (155)$$

$$O_{73\rho} = x^2 Z^{(2)} x Z_\rho^{(1)}(x, y) (-1)^\rho, \quad q_{73\rho} = 4\pi i \sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_1^\mu \sigma_2^\phi (B_\nu \phi D)_\rho \quad (156)$$

$$O_{72\rho}^{(1)} = \frac{1}{4} x^2 Z^{(1)} x Z_\rho^{(2)}(x, y), \quad q_{72\rho}^{(1)} = 4\pi i \sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\mu \sigma_1^\phi (B_\nu \phi D)_\rho \quad (157)$$

$$O_{72\rho}^{(2)} = -\frac{\sqrt{3}}{4} xy Z^{(1)}(x) Z_\rho^{(2)}(x, y),$$

$$q_{72\rho}^{(2)} = 4\pi i \sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\mu \sigma_1^\phi (B_\nu D_\phi + B_\phi D_\nu)_\rho \quad (158)$$

$$O_{72\rho}^{(3)} = \frac{3}{4}y^2 Z^{(1)}(x)Z_\rho^{(2)}(x, y), \quad q_{72\rho}^{(3)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\mu \sigma_1^\phi (BD_\nu\phi)_\rho \quad (159)$$

$$O_{71\rho}^{(1)} = \frac{1}{4}x^2 Z_\rho^{(12)}(x, y), \quad q_{71\rho}^{(1)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\mu \sigma_3^\phi (B_\nu\phi D)_\rho \quad (160)$$

$$O_{71\rho}^{(2)} = \frac{\sqrt{3}}{4}xy Z_\rho^{(12)}(x, y), \quad q_{71\rho}^{(2)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\mu \sigma_3^\phi (B_\nu D\phi + B_\phi D_\nu)_\rho \quad (161)$$

$$O_{71\rho}^{(3)} = \frac{3}{4}y^2 Z_\rho^{(12)}(x, y), \quad q_{72\rho}^{(3)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\mu \sigma_3^\phi (BD_\nu\phi)_\rho \quad (162)$$

$$O_{83\rho}^{(1)} = -\frac{1}{4}x^2 Z^{(1)}(x)Z_\rho^{(2)}(x, y)(-1)^\rho, \quad q_{83\rho}^{(1)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_2^\mu \sigma_1^\phi (B_\nu\phi D)_\rho \quad (163)$$

$$O_{83\rho}^{(2)} = -\frac{\sqrt{3}}{4}xy Z^{(1)}x Z_\rho^{(2)}(x, y)(-1)^\rho, \quad q_{83\rho}^{(2)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_2^\mu \sigma_1^\phi (B_\nu D\phi + B_\phi D_\nu)_\rho \quad (164)$$

$$O_{83\rho}^{(3)} = -\frac{3}{4}y^2 Z^{(1)}(x)Z_\rho^{(2)}(x, y)(-1)^\rho, \quad q_{83\rho}^{(3)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_2^\mu \sigma_1^\phi (BD_\nu\phi)_\rho \quad (165)$$

$$O_{82\rho} = -x^2 Z^{(2)}(x)Z_\rho^{(1)}(x, y), \quad q_{82\rho} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\mu \sigma_1^\phi (B_\nu\phi D)_\rho \quad (166)$$

$$O_{81\rho}^{(1)} = -\frac{1}{4}x^2 Z_\rho^{(21)}(x, y), \quad q_{71\rho}^{(1)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_3^\mu \sigma_2^\phi (B_\nu\phi D)_\rho \quad (167)$$

$$O_{81\rho}^{(2)} = \frac{\sqrt{3}}{4}xy Z_\rho^{(21)}(x, y), \quad q_{81\rho}^{(2)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_3^\mu \sigma_2^\phi (B_\nu D\phi + B_\phi D_\nu)_\rho \quad (168)$$

$$O_{71\rho}^{(3)} = -\frac{3}{4}y^2 Z_\rho^{(21)}(x, y), \quad q_{72\rho}^{(3)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_3^\mu \sigma_2^\phi (BD_{\nu\phi})_\rho \quad (169)$$

$$O_{93\rho}^{(1)} = \frac{\sqrt{3}}{4}x^3 Z^{(2)}(x) Z_\rho^{(2)}(x, y) (-1)^\rho, \quad q_{93\rho}^{(1)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_1^\phi \sigma_2^\chi (B_{\nu\phi\chi} D_\mu)_\rho \quad (170)$$

$$O_{93\rho}^{(2)} = \frac{3}{4}x^2 y Z^{(2)}(x) Z_\rho^{(2)}(x, y) (-1)^\rho, \quad q_{93\rho}^{(2)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_3^\epsilon \sigma_1^\phi \sigma_2^\chi (B_{\nu\chi} D_{\mu\phi})_\rho \quad (171)$$

$$O_{92\rho}^{(1)} = \frac{\sqrt{3}}{4}x^3 Z^{(2)}(x) Z_\rho^{(2)}(x, y), \quad q_{92\rho}^{(1)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\phi \sigma_1^\chi (B_{\nu\phi\chi} D_\mu)_\rho \quad (172)$$

$$O_{92\rho}^{(2)} = \frac{3}{4}x^2 y Z^{(2)}(x) Z_\rho^{(2)}(x, y), \quad q_{93\rho}^{(2)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_2^\epsilon \sigma_3^\phi \sigma_1^\chi (B_{\nu\chi} D_{\mu\phi})_\rho \quad (173)$$

$$O_{91\rho}^{(1)} = -\frac{\sqrt{3}}{8}x^3 y Z_\rho^{(22)}(x, y), \quad q_{91\rho}^{(1)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\phi \sigma_3^\chi (B_{\nu\phi\chi} D_\mu)_\rho \quad (174)$$

$$O_{91\rho}^{(2)} = \frac{3}{8}x^2 y^2 Z_\rho^{(22)}(x, y), \quad q_{91\rho}^{(2)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\phi \sigma_3^\chi (B_{\nu\chi} D_{\mu\phi} - B_{\nu\mu\phi} D_{\mu\chi})_\rho \quad (175)$$

$$O_{91\rho}^{(3)} = \frac{3\sqrt{3}}{8}xy^3 Z_\rho^{(22)}(x, y), \quad q_{91\rho}^{(3)} = 4\pi i\sqrt{2} \sum_{\mu\nu\epsilon\phi\chi} C_{1\mu 1\nu}^{1\epsilon} \sigma_1^\epsilon \sigma_2^\phi \sigma_3^\chi (B_\nu D_{\mu\phi\chi})_\rho \quad (176)$$

## 11 Geometrical factors in the MGL basis

To pass to the MGL basis we have only to transform matrix elements of operators  $q$  in the  $a$ -basis with the help of coefficient functions  $F$ :

$$\langle \alpha' | q_{ik\rho}^{(l)} | \alpha \rangle = \sum_{a', a} F_{\alpha'}^{a'} \langle a' | q_{ik\rho}^{(l)} | a \rangle F_\alpha^a \quad (177)$$

This expression involves many summations over projection of momenta. Possibly they can be done analytically, using the appropriate formulas from Ref. [25]. To this aim one should use representation of matrices Pauli in terms of Clebsh-Gordon coefficients:

$$\sigma_{p'p}^\mu = \sqrt{2}(-1)^{1/2+\mu-p} C_{\frac{1}{2}-p'\frac{1}{2}p}^{1\mu}, \quad [\sigma_\mu]_{p'p} = \sqrt{2}(-1)^{1/2-p} C_{\frac{1}{2}p'\frac{1}{2}-p}^{1\mu} \quad (178)$$

so that the whole expression (177) turns out to be a product of Clebsh-Gordon coefficients summed over momentum projections. Since there are many operators  $q_{ik\rho}^{(l)}$  to be processed in this way, probably it is more practical to do the sums numerically on the computer to calculate matrix elements (177) as a preliminary for dynamical calculations.

In the following, just for illustration, we shall try to do the sum over projections analytically for some simplest operators  $q$ .

### 11.1 Operators $O_1$

We are going to study the matrix element

$$\langle \alpha' | q_{13\rho} | \alpha \rangle = 4\pi \langle \alpha' | (\vec{\sigma}_1 \vec{\sigma}_2) (BD)_\rho | \alpha \rangle \quad (179)$$

First let us write out the relevant factors

$$F_{\alpha'}^a F_\alpha^a = C_{s's'_z \lambda' \lambda'_z}^{MM_z} C_{\frac{1}{2}p'_1 J' J'_z}^{s' s'_z} C_{\sigma' \sigma'_z l' l'_z}^{J' J'_z} C_{\frac{1}{2}p'_2 \frac{1}{2}p'_3}^{\sigma' \sigma'_z} C_{ss_z \lambda \lambda_z}^{MM_z} C_{\frac{1}{2}p_1 J J_z}^{ss_z} C_{\sigma \sigma_z l l_z}^{J J_z} C_{\frac{1}{2}p_2 \frac{1}{2}p_3}^{\sigma \sigma_z} \quad (180)$$

$$\langle \alpha' | q_{13\rho} | \alpha \rangle =$$

$$2(-1)^{1-p_1-p_2} \frac{\prod_{l'\rho} C_{l'0\rho 0}^{l0}}{\prod_l} \frac{\prod_{\lambda\rho} C_{\lambda 0\rho 0}^{\lambda' l 0}}{\prod_{\lambda'}} \delta_{p'_3 p_3} \sum_{\mu\tau} (-1)^\mu C_{\frac{1}{2}-p'_1 \frac{1}{2}p_1}^{1\mu} C_{\frac{1}{2}p'_2 \frac{1}{2}-p_2}^{1\mu} C_{l' l'_z \rho \tau}^{ll_z} C_{\lambda \lambda_z \rho \tau}^{\lambda' \lambda'_z} \quad (181)$$

Multiplying (180) and (181) we obtain an explicit expression for the matrix element (179)

$$\langle \alpha' | q_{13\rho} | \alpha \rangle = 2 \frac{\prod_{l'\rho} C_{l'0\rho 0}^{l0}}{\prod_l} \frac{\prod_{\lambda\rho} C_{\lambda 0\rho 0}^{\lambda' l 0}}{\prod_{\lambda'}} \sum_{\lambda'_z, l'_z, p'_1, p'_2} \sum_{\lambda_z, l_z, p_1, p_2} \sum_{\mu, \tau, p_3} (-1)^{1-p_1-p_2+\mu} C_{s's'_z \lambda' \lambda'_z}^{MM_z} C_{\frac{1}{2}p'_1 J' J'_z}^{s' s'_z} C_{\sigma' \sigma'_z l' l'_z}^{J' J'_z} C_{\frac{1}{2}p'_2 \frac{1}{2}p_3}^{\sigma' \sigma'_z} C_{ss_z \lambda \lambda_z}^{MM_z} C_{\frac{1}{2}p_1 J J_z}^{ss_z} C_{\sigma \sigma_z l l_z}^{J J_z} C_{\frac{1}{2}p_2 \frac{1}{2}-p_2}^{1\mu} C_{\frac{1}{2}-p'_1 \frac{1}{2}p_1}^{1\mu} C_{l' l'_z \rho \tau}^{ll_z} C_{\lambda \lambda_z \rho \tau}^{\lambda' \lambda'_z} \quad (182)$$



We can perform partial summation over  $p_2, p'_2, p_3$

$$\begin{aligned} S_1 &= \sum_{p_2, p'_2, p_3} (-1)^{1/2-p_2} C_{\frac{1}{2}p_2 \frac{1}{2}p_3}^{\sigma\sigma_z} C_{\frac{1}{2}p'_2 \frac{1}{2}p_3}^{\sigma'\sigma'_z} C_{\frac{1}{2}p'_2 \frac{1}{2}-p_2}^{1\mu} \\ &= (-1)^{\sigma+\sigma'} \sum_{p_2, p'_2, p_3} (-1)^{1/2-p_2} C_{\frac{1}{2}p_3 \frac{1}{2}p_2}^{\sigma\sigma_z} C_{\frac{1}{2}p_3 \frac{1}{2}p'_2}^{\sigma'\sigma'_z} C_{\frac{1}{2}p'_2 \frac{1}{2}-p_2}^{1\mu} \end{aligned} \quad (183)$$

We use Varshalovich 8.7.3.(17) [25] with

$$b\beta = \frac{1}{2}p_3, \quad a\alpha = \frac{1}{2}p_2, \quad c\gamma = \sigma\sigma_z, \quad d\delta = \frac{1}{2}p'_2, \quad e\epsilon = \sigma'\sigma'_z, \quad f\phi = 1, \mu$$

to obtain

$$S_1 = (-1)^{-\sigma} \prod_{\sigma 1} C_{\sigma\sigma_z 1\mu}^{\sigma'\sigma'_z} \left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & \sigma \\ \sigma' & 1 & \frac{1}{2} \end{array} \right\} \quad (184)$$

As a next step we may try to sum

$$S_2 = (-1)^{-\mu} \sum_{l_z, l'_z, \sigma_z, \sigma'_z} C_{\sigma'\sigma'_z l'_z}^{J'J'_z} C_{\sigma\sigma_z l_z}^{JJ_z} C_{l'_z \rho\tau}^{ll_z} C_{\sigma\sigma_z 1\mu}^{\sigma'\sigma'_z} \quad (185)$$

We note that

$$\mu = \sigma'_z = \sigma_z, \quad \sigma_z = J_z - l_z, \quad \text{so that } \mu = \sigma'_z + l_z - J_z$$

and (185) can be rewritten as

$$S_2 = (-1)^{-J_z - l - \sigma'} \sum_{l_z, l'_z, \sigma_z, \sigma'_z} (-1)^{l - l_z + \sigma' - \sigma'_z} C_{\sigma'\sigma'_z l'_z}^{J'J'_z} C_{\sigma\sigma_z l_z}^{JJ_z} C_{l'_z \rho\tau}^{ll_z} C_{\sigma\sigma_z 1\mu}^{\sigma'\sigma'_z} \quad (186)$$

This sum corresponds to Varshalovich 8.7.4(30) [25] with

$$a\alpha = \rho\tau, \quad b\beta = l'l'_z, \quad c\gamma = ll_z, \quad d\delta = 1\mu,$$

$$e\epsilon = \sigma'\sigma'_z, \quad f\phi = \sigma\sigma_z, \quad g\eta = J'J'_z, \quad j\mu = JJ_z$$

Taking into account factors arising due to replacements in lower arguments in Clebsh-Gordon coefficients we find

$$S_2 = (-1)^{l+l'-J-\mu-\tau-J_z} \prod_{l\sigma'JJ'} \sum_{k\kappa} C_{J'J'_z J-J_z}^{k\kappa} C_{1\mu\rho-\tau}^{k\kappa} \left\{ \begin{array}{ccc} l & l' & \rho \\ \sigma & \sigma' & 1 \\ J & J' & k \end{array} \right\} \quad (187)$$

Now we sum

$$S_3 = (-1)^{1/2-p_1-J_z} \sum_{J_z J'_z p_1 p'_1} C_{\frac{1}{2}p'_1 J'J'_z}^{\sigma'\sigma'_z} C_{\frac{1}{2}p_1 JJ_z}^{\sigma\sigma_z} C_{J'J'_z J-J_z}^{k\kappa} C_{\frac{1}{2}-p'_1 \frac{1}{2}p_1}^{1\mu} \quad (188)$$

We have  $p_1 + J_z = s_z$  and

$$C_{\frac{1}{2}-p'_1 \frac{1}{2} p_1}^{1\mu} = C_{\frac{1}{2} p'_1 \frac{1}{2} -p_1}^{1-\mu}$$

so that

$$S_3 = (-1)^{1/2-s_z} \sum_{J_z J'_z p_1 p'_1} C_{\frac{1}{2} p'_1 J'_z J'_z}^{s' s'_z} C_{\frac{1}{2} p_1 J J_z}^{s s_z} C_{J'_z J'_z J - J_z}^{k \kappa} C_{\frac{1}{2} p_1 \frac{1}{2} -p_1}^{1-\mu} \quad (189)$$

We use Varshalovich 8.7.4.(21) with

$$a\alpha = k\kappa, \quad b\beta = J'J'_z, \quad c\gamma = JJ_z, \quad d\delta = 1 - \mu,$$

$$e\epsilon = \frac{1}{2}p'_1, \quad f\phi = \frac{1}{2}p_1, \quad g\eta = s's'_z, \quad j\mu = ss_z$$

Taking into account factors due to interchanges of lower indexes we find

$$S_3 = (-1)^{J-2s'-s-s_z} \prod_{k_1 s'_1 s} \sum_{k_1 \kappa_1} C_{s'_1 s'_z s - s_z}^{k_1 \kappa_1} C_{1-\mu k \kappa}^{k_1 \kappa_1} \left\{ \begin{array}{ccc} J & J' & k \\ \frac{1}{2} & \frac{1}{2} & 1 \\ s & s' & k_1 \end{array} \right\} \quad (190)$$

Collecting our results, at this step we have

$$\begin{aligned} \langle \alpha' | q_{13\rho} | \alpha \rangle = & 6 \prod_{l' \rho \rho \lambda \sigma \sigma' J J' k s s'} \prod_{\lambda'}^{-1} C_{l' 0 \rho 0}^{l 0} C_{\lambda 0 \rho 0}^{\lambda' 0} \\ & \left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & \sigma \\ \sigma' & 1 & \frac{1}{2} \end{array} \right\} \left\{ \begin{array}{ccc} l & l' & \rho \\ \sigma & \sigma' & 1 \\ J & J' & k \end{array} \right\} \left\{ \begin{array}{ccc} J & J' & k \\ \frac{1}{2} & \frac{1}{2} & 1 \\ s & s' & k_1 \end{array} \right\} \sum_{\lambda'_z, s'_z, \lambda_z, s_z, \mu, \tau, \kappa \kappa_1} (-1)^{-\sigma+l+l'-2s'-s-\mu-\tau-s_z} \\ & C_{s'_z s'_z \lambda' \lambda'_z}^{M M_z} C_{s s_z \lambda \lambda_z}^{M M_z} C_{1\mu\rho-\tau}^{k \kappa} C_{\lambda \lambda_z \rho \tau}^{\lambda' \lambda'_z} C_{s'_z s'_z s - s_z}^{k_1 \kappa_1} C_{1-\mu k \kappa}^{k_1 \kappa_1} \quad (191) \end{aligned}$$

Now we sum

$$S_4 = \frac{1}{2M+1} \sum_{M_z, \lambda_z, \lambda'_z} C_{s'_z s'_z \lambda' \lambda'_z}^{M M_z} C_{s s_z \lambda \lambda_z}^{M M_z} C_{\lambda \lambda_z \rho \tau}^{\lambda' \lambda'_z} \quad (192)$$

We transform

$$C_{\lambda \lambda_z \rho \tau}^{\lambda' \lambda'_z} = (-1)^{\lambda-\lambda_z} \prod_{\lambda'} \prod_{\rho}^{-1} C_{\lambda \lambda_z \lambda' \lambda' - \lambda'_z}^{\rho - \tau} \quad (193)$$

to transform

$$S_4 = (-1)^{\lambda+\lambda'-\rho} \prod_{\lambda'} \prod_{\rho}^{-1} \frac{1}{2M+1} \sum_{M_z, \lambda_z, \lambda'_z} (-1)^{\lambda-\lambda_z} C_{s'_z s'_z \lambda' \lambda'_z}^{M M_z} C_{s s_z \lambda \lambda_z}^{M M_z} C_{\lambda-\lambda_z \lambda' \lambda'_z}^{\rho \tau} \quad (194)$$

We use Varshalovich 8.7.3.16 [25] with

$$a\alpha = \lambda' \lambda'_z, \quad b\beta = \lambda - \lambda_z, \quad c\gamma = \rho \tau, \quad d\delta = M M_z, \quad e\epsilon = s s_z, \quad f\phi = s' s'_z$$

to obtain

$$S_4 = (-1)^{\lambda'+M+s'} \prod_{\lambda'} \prod_s^{-1} C_{\rho\tau s' s'_z}^{ssz} \left\{ \begin{matrix} \lambda' & \lambda & \rho \\ s & s' & M \end{matrix} \right\} \quad (195)$$

Our next sum is

$$S_5 = \sum_{\tau, \kappa, \kappa_1, s_z} (-1)^{-\tau-s_z} C_{s' s'_z s-s_z}^{k_1 \kappa_1} C_{1-\mu k \kappa}^{k_1 \kappa_1} C_{\rho\tau s' s'_z}^{ssz} C_{1\mu\rho-\tau}^{k\kappa} \quad (196)$$

We have  $\tau + s'_z = s_z$  so that  $(-1)^{-\tau-s_z} = (-1)^{\tau-s_z} = (-1)^{-s'_z}$  and can be taken out of the sum. The rest corresponds to Varshalovich 8.7.4.(24) with

$$\begin{aligned} a\alpha &= 1\mu, & b\beta &= \rho\tau, & c\gamma &= k - \kappa, & d\delta &= s' - s'_z, \\ e\epsilon &= s - s_z, & f\phi &= k_1\kappa_1, & g\eta &= s' s'_z, & j\mu &= 1 - \mu \end{aligned}$$

We obtain

$$S_5 = (-1)^{-s'_z} (-1)^{\rho-k-s'-s'_z-\mu} \prod_{k s k_1 k_1} \sum_{k_2 \kappa_2} C_{s'-s'_z 1-\mu}^{k_2 \kappa_2} C_{s'-s'_z 1-\mu}^{k_2 \kappa_2} \left\{ \begin{matrix} k & \rho & 1 \\ k_1 & s & s' \\ 1 & s' & k_2 \end{matrix} \right\} \quad (197)$$

The last sum over  $s'_z$  and  $\mu$  cannot be done because of the factor  $(-1)^{-2s'_z}$  ( $(-1)^{-\mu}$  is cancelled by the same factor in (191)), which is strange.

To check we shall try to use an alternative formula Varshalovich 8.7.4.[25] (20) transforming the relevant Clebsh-Gordon coefficients to the form corresponding to this formula (putting all the projections to be summed down). We have

$$S_5 = (-1)^{-s'_z} \tilde{S}_5 \quad (198)$$

where

$$\tilde{S}_5 = \sum_{\tau, \kappa, \kappa_1, s_z} C_{s' s'_z s-s_z}^{k_1 \kappa_1} C_{1-\mu k \kappa}^{k_1 \kappa_1} C_{\rho\tau s' s'_z}^{ssz} C_{1\mu\rho-\tau}^{k\kappa} \quad (199)$$

Now

$$\begin{aligned} C_{s' s'_z s-s_z}^{k_1 \kappa_1} &= (-1)^{s'+s-k+s+s_z} \sqrt{\frac{2k_1+1}{2s'+1}} C_{s-s_z k_1-\kappa_1}^{s'-s'_z} \\ C_{1-\mu k \kappa}^{k_1 \kappa_1} &= (-1)^{1+k+k_1+k-\kappa} \sqrt{\frac{2k_1+1}{3}} C_{k\kappa k_1-\kappa_1}^{1\mu} \\ C_{\rho\tau s' s'_z}^{ssz} &= (-1)^{\rho-\tau} \sqrt{\frac{2s+1}{2s'+1}} C_{\rho\tau s-s_z}^{s'-s'_z} \\ C_{1\mu\rho-\tau}^{k\kappa} &= (-1)^{1+\rho-k+\rho+\tau} \sqrt{\frac{2k+1}{2\rho+1}} C_{\rho-\tau k-\kappa}^{1-\mu} = (-1)^{\rho+k-1} C_{\rho\tau k\kappa}^{1\mu} \end{aligned}$$

So we get

$$\tilde{S}_5 = (-1)^{s'+2s-k_1+\rho+k-1} \prod_{k_1 k_1 s k} \prod_{s' 1 s' \rho}^{-1} \sum_{\tau, \kappa, \kappa_1, s_z} (-1)^{-s_z - \kappa} C_{s-s_z k_1 - \kappa_1}^{s' - s'_z} C_{k \kappa k_1 - \kappa_1}^{1 \mu} C_{\rho \tau s - s_z}^{s' - s'_z} C_{\rho \tau k \kappa}^{1 \mu} \quad (200)$$

However we have

$$\kappa_1 = s'_z - s_z = \kappa - \mu, \quad \text{so that } \kappa = s'_z - s_z + \mu$$

and also obviously  $\kappa$  is an integer and

$$(-1)^{-s_z - \kappa} = (-1)^{-s_z + \kappa} = (-1)^{s'_z + \mu}$$

So we can take the sign factor out of the sum, where  $(-1)^{s_z}$  cancels with the sign factor in (198). The sum itself corresponds to Varshalovich. 8.7.4.(20) with

$$a\alpha = s' - s'_z, \quad b\beta = s s_z, \quad c\gamma = k_1 \kappa_1, \quad d\delta = 1\mu, \quad e\epsilon = \rho\tau, \quad f\phi = k\kappa, \quad g\eta = s' - s'_z, \quad j\mu = 1\mu$$

Summation gives

$$\tilde{S}_5 = (-1)^{s'+2s-k_1+k-1} (-1)^{s_z + \mu} \prod_{k_1 k_1 s k_1} \sum_{k_2 \kappa_2} C_{s' - s'_z 1 \mu}^{k_2 \kappa_2} C_{1 \mu s' - s'_z}^{k_2 \kappa_2} \begin{Bmatrix} k_1 & s & s' \\ k & \rho & 1 \\ 1 & s' & k_2 \end{Bmatrix} \quad (201)$$

Factor  $(-1)^{-\mu}$  cancels with the same factor in (191). and  $(-1)^{s'_z}$  with the inverse factor in (198), so that no sign factors depending on projections  $s_z$  and  $\mu$  remain. This allows to do the last summation over  $s_z$  and  $\mu$ :

$$S_6 = \sum_{s_z, \mu} C_{s' - s'_z 1 \mu}^{k_2 \kappa_2} C_{1 \mu s' - s'_z}^{k_2 \kappa_2} = 1 \quad (202)$$

Collecting all the factors, we get

$$\begin{aligned} < \alpha' | q_{13\rho} | \alpha > = \\ & -6\sqrt{3} \prod_{l' \rho \lambda \sigma \sigma' J J' s s'} C_{l' 0 \rho 0}^{l 0} (-1)^{l+l' - \sigma + \lambda' + \rho + M + s' + 2s} C_{\lambda 0 \rho 0}^{\lambda' l 0} \sum_{k, k_1, k_2} (-1)^{k-k_1} \\ & \prod_{k k k_1 k_1} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \sigma \\ \sigma' & 1 & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} l & l' & \rho \\ \sigma & \sigma' & 1 \\ J & J' & k \end{Bmatrix} \begin{Bmatrix} J & J' & k \\ \frac{1}{2} & \frac{1}{2} & 1 \\ s & s' & k_1 \end{Bmatrix} \begin{Bmatrix} \lambda' & \lambda & \rho \\ s & s' & M \end{Bmatrix} \begin{Bmatrix} k_1 & s & s' \\ k & \rho & 1 \\ 1 & s' & k_2 \end{Bmatrix} \quad (203) \end{aligned}$$

This expression should serve as a test for the numerical code to do the summation over projections numerically.

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