

# 1 Momentum distributions

## 2 Second quantization

This section will be somewhat over-elaborated. But it can serve as a recapitulation of second quantization.

The one body momentum distribution operator is defined as,

$$\hat{n}(p) = \frac{1}{(2\pi)^3} \int d^2\Omega_{\mathbf{p}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \quad (1)$$

It's action on a multi particle ground state  $|\Phi\rangle$ ,

$$\langle\Phi|\hat{n}(p)|\Phi\rangle = \frac{1}{(2\pi)^3} \int d^2\Omega_{\mathbf{p}} \langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle \quad (2)$$

The creation and annihilation operators  $a_{\mathbf{p},\mathbf{p}}^\dagger, a_{\mathbf{p}}$  have only meaning working on particles with definite momentum or the vacuum state  $|0\rangle$ .

$$\langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \int d^3\mathbf{p}_1 \dots d^3\mathbf{p}_A \langle\Phi|\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}_A\rangle \langle\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}_A|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle \quad (3)$$

$$= \int d^A\mathbf{p}_1 \dots d^3\mathbf{p}_A \langle\Phi|\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}_A\rangle \langle 0|a_{\mathbf{p}_1} a_{\mathbf{p}_2} \dots a_{\mathbf{p}_A} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle \quad (4)$$

Using the anticommutation relation  $\{a_{\mathbf{p}}, a_{\mathbf{q}}^\dagger\} = \delta(\mathbf{p} - \mathbf{q})$ , we get

$$\langle 0|a_{\mathbf{p}_1} a_{\mathbf{p}_2} \dots a_{\mathbf{p}_A} a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \langle 0|a_{\mathbf{p}_1} a_{\mathbf{p}_2} \dots \delta(\mathbf{p} - \mathbf{p}_A) a_{\mathbf{p}}|\Phi\rangle - \langle 0|a_{\mathbf{p}_1} a_{\mathbf{p}_2} \dots a_{\mathbf{p}_{A-1}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}_A} a_{\mathbf{p}}|\Phi\rangle \quad (5)$$

$$= \delta(\mathbf{p} - \mathbf{p}_A) \langle\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}|\Phi\rangle - \delta(\mathbf{p} - \mathbf{p}_{A-1}) \langle 0|a_{\mathbf{p}_1} \dots a_{\mathbf{p}_{A-2}} a_{\mathbf{p}_A} a_{\mathbf{p}}|\Phi\rangle \quad (6)$$

$$+ \langle 0|a_{\mathbf{p}_1} \dots a_{\mathbf{p}_{A-2}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}_{A-1}} a_{\mathbf{p}_A} a_{\mathbf{p}}|\Phi\rangle \quad (7)$$

$$= \delta(\mathbf{p} - \mathbf{p}_A) \langle\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}_A|\Phi\rangle + \delta(\mathbf{p} - \mathbf{p}_{A-1}) \langle\mathbf{p}_1 \dots \mathbf{p}_{A-2} \mathbf{p}_{A-1} \mathbf{p}_A|\Phi\rangle \quad (8)$$

$$+ \langle 0|a_{\mathbf{p}_1} \dots a_{\mathbf{p}_{A-2}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}_{A-1}} a_{\mathbf{p}_A} a_{\mathbf{p}}|\Phi\rangle = \dots \quad (9)$$

$$= \sum_{i=1}^A \delta(\mathbf{p} - \mathbf{p}_i) \langle\mathbf{p}_1 \dots \mathbf{p}_A|\Phi\rangle + (-1)^A \underbrace{\langle 0|a_{\mathbf{p}}^\dagger a_{\mathbf{p}_1} \dots a_{\mathbf{p}_A} a_{\mathbf{p}}|\Phi\rangle}_{=0} \quad (10)$$

Hence,

$$\langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \int d^3\mathbf{p}_1 \dots d^3\mathbf{p}_A \langle\Phi|\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}_A\rangle \sum_{i=1}^A \delta(\mathbf{p} - \mathbf{p}_i) \langle\mathbf{p}_1\mathbf{p}_2 \dots \mathbf{p}_A|\Phi\rangle \quad (11)$$

If  $|\Phi\rangle$  is a slater determinant of orthonormal single particle wave functions  $|\phi_{\alpha_i}\rangle$  we get,

$$\langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \sum_{i=1}^A |\langle\mathbf{p}|\phi_{\alpha_i}\rangle|^2 = \sum_{i=1}^A \phi_{\alpha_i}^\dagger(\mathbf{p}) \phi_{\alpha_i}(\mathbf{p}) \quad (12)$$

Note that we also could have derived this result by instead of inserting the unit  $\prod_{i=1}^A d^3\mathbf{p}_i |\mathbf{p}_i\rangle \langle\mathbf{p}_i|$  we expand  $|\Phi\rangle$  in terms of single particle creation operators,

$$a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\alpha_1\alpha_2 \dots \alpha_A\rangle = a_{\mathbf{p}}^\dagger a_{\mathbf{p}} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_A}^\dagger|0\rangle \quad (13)$$

The commutation relations between  $a_{\mathbf{p}}$  and  $a_{\alpha_i}$  are easily derived by expanding  $a_{\alpha_i}$  in momentum creation operators,

$$a_{\alpha_i}^\dagger = \int d^3\mathbf{k} \phi_{\alpha_i}(\mathbf{k}) a_{\mathbf{k}}^\dagger \quad (14)$$

$$\Rightarrow a_{\mathbf{p}} a_{\alpha_i}^\dagger = \int d^3\mathbf{k} \phi_{\alpha_i}(\mathbf{k}) a_{\mathbf{p}} a_{\mathbf{k}}^\dagger = \phi_{\alpha_i}(\mathbf{p}) - a_{\alpha_i}^\dagger a_{\mathbf{p}} \quad (15)$$

So,

$$a_{\mathbf{p}} |\Phi\rangle = a_{\mathbf{p}} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_A}^\dagger |0\rangle = (\phi_{\alpha_1}(\mathbf{p}) - a_{\alpha_1}^\dagger a_{\mathbf{p}}) a_{\alpha_2}^\dagger \dots a_{\alpha_A}^\dagger |0\rangle \quad (16)$$

$$= \sum_{i=1}^A (-1)^{i-1} \phi_{\alpha_i}(\mathbf{p}) |\alpha_1 \dots \alpha_{i-1} \alpha_{i+1} \dots \alpha_A\rangle \quad (17)$$

The conjugate gives,

$$\langle \Phi | a_{\mathbf{p}}^\dagger = \sum_{j=1}^A (-1)^{j-1} \langle \alpha_1 \dots \alpha_{j-1} \alpha_{j+1} \dots \alpha_A | \phi_{\alpha_j}^\dagger(\mathbf{p}) \quad (18)$$

Hence,

$$\langle \Phi | a_{\mathbf{p}}^\dagger a_{\mathbf{p}} | \Phi \rangle = \sum_{i,j=1}^A (-1)^{i+j} \phi_{\alpha_j}^\dagger(\mathbf{p}) \phi_{\alpha_i}(\mathbf{p}) \underbrace{\langle \alpha_1 \dots \alpha_{j-1} \alpha_{j+1} \dots \alpha_A | \alpha_1 \dots \alpha_{i-1} \alpha_{i+1} \dots \alpha_A \rangle}_{=\delta_{ij}} \quad (19)$$

$$= \sum_i \phi_{\alpha_i}^\dagger(\mathbf{p}) \phi_{\alpha_i}(\mathbf{p}) \quad (20)$$

Which is exactly the same result as before.

So the one body momentum distribution is given by,

$$\langle \Phi | \hat{n}(p) | \Phi \rangle = \sum_{i=1}^A \frac{1}{(2\pi)^3} \int d^2\Omega_{\mathbf{p}} \phi_{\alpha_i}^\dagger(\mathbf{p}) \phi_{\alpha_i}(\mathbf{p}) \quad (21)$$

Note that this distribution is normed to the number of particles  $A$ . To get the momentum distribution normed to unity we have to divide by  $A$ ,

$$\langle \Phi | \hat{n}(p) | \Phi \rangle = \frac{1}{A} \sum_{i=1}^A \frac{1}{(2\pi)^3} \int d^2\Omega_{\mathbf{p}} \phi_{\alpha_i}^\dagger(\mathbf{p}) \phi_{\alpha_i}(\mathbf{p}) \quad (22)$$

## 3 Nucleus

### 3.1 shell.h

This class contains the quantum number of a shell  $nlj$ . It has two (proton & neutron) static arrays containing all the shells.

```
shellsN = [ Shell(n1,l1,j1), Shell(n2,l2,j2), ... ]
shellsP = [ Shell(n1,l1,j1), Shell(n2,l2,j2), ... ]
```

These two arrays are initialised and deleted by the static methods `Shell::initialiseShells`, `Shell::deleteShells`.

### 3.2 nucleus.h

First important method here is `Nucleus::makePairs`. Note that this relies on overloaded virtual functions to function. It iterates over the quantum numbers,  $n_1 l_1 j_1 m_{j_1}, n_2 l_2 j_2 m_{j_2}$  and makes a pair for each of these combinations: `Pair::Pair(mosh, n1, l1, j1, mj1, t1, n2, l2, j2, mj2, t2)`. `mosh` is the return value of `RecMosh::createRecMosh(n1, l1, n2, l2, inputdir, outputdir)`, being a `RecMosh` object. The moshinsky brackets  $\langle n_1 l_1 n_2 l_2; \Lambda | nlNL; \Lambda \rangle$  can be accessed by calling `RecMosh::getCoefficient(n, l, N, L, Lambda)`. Open shells are taken care of by calculating a open shell correction factor and applying it to the pair via `Pair::setfnorm(factor)`.

Once the pairs (`Pair::Pair`) are generated we can generate a

## 4 Pair coupling

### 4.1 pair.h

This class represents the state

$$|\alpha_1, \alpha_2\rangle_{\text{nas}}, |\alpha\rangle \equiv |nljm_j tm_t\rangle \quad (23)$$

The class calculates all the coefficients,

$$C_{\alpha_1 \alpha_2}^A = \langle A \equiv \{nSjm_j, NLM_L TM_T\} | \alpha_1 \alpha_2 \rangle \quad (24)$$

The main method here is `Pair::makecoeflist()`. It loops over all possible values of  $A \equiv \{S, T, n, l, N, M_L, j, m_j\}$ . Where in the summation over  $\{n, l, N, L\}$  the energy conservation  $2n_1 + l_1 + 2n_2 + l_2 = 2n + l + 2N + L$  is taken into account to eliminate one of the summation loops,  $L = 2n_1 + l_1 + 2n_2 + l_2 - 2n - l - 2N$ . Note that  $M_T$  is also fixed by  $M_T = m_{t_1} + m_{t_2}$  and no summation over this is performed, as we want to keep the contribution from different pairs separated. For each  $A$  a new object `Newcoef` is generated and stored in the member `std::vector<NewCoef*> coeflist`.

### 4.2 newcoef.h

This class takes the parameters  $n_1 l_1 j_1 m_{j_1} m_{t_1} n_2 l_2 j_2 m_{j_2} m_{t_2} NLM_L nlSjm_j TM_T$ , and calculates the coefficient given in Eq. (24). It takes also a pointer to a `RecMosh` object that holds the Moshinsky brackets. The only function in this class is to calculate  $C_{\alpha_1 \alpha_2}^A$  using the formula,

$$\begin{aligned} & \sum_{JM_J} \sum_{\Lambda} [1 - (-1)^{L+S+T}] \langle t_1 m_{t_1} t_2 m_{t_2} | TM_T \rangle \langle j_1 m_{j_1} j_2 m_{j_2} | JM_J \rangle \langle j m_j LM_L | JM_J \rangle \\ & \langle nlNL; \Lambda | n_1 l_1 n_2 l_2; \Lambda \rangle_{\text{SMB}} \sqrt{2\Lambda + 1} \sqrt{2j + 1} \left\{ \begin{matrix} j & L & J \\ \Lambda & S & l \end{matrix} \right\} \\ & \sqrt{2j_1 + 1} \sqrt{2j_2 + 1} \sqrt{2S + 1} \sqrt{2\Lambda + 1} \left\{ \begin{matrix} l_1 & s_1 & j_1 \\ l_2 & s_2 & j_2 \\ \Lambda & S & J \end{matrix} \right\} \quad (25) \end{aligned}$$

It is easy to check that the result indeed depends on  $\alpha_1, \alpha_2, A$ . Note that it is always assumed that  $s_i, t_i \equiv \frac{1}{2}$  as we are dealing with protons and neutrons. This class also defines a “key” to be able to index the coefficients, `key = ‘‘nlSjm-j.NLM.L.TM.T’’`.

### 4.3 paircoef.h

This is a very thin class designed to do some bookkeeping. As outlined in Maartens thesis pg 156, different  $|\alpha_1 \alpha_2\rangle$  combinations will sometimes map to the same “rcm” states  $A = |nlSjm_j NLM_L TM_T\rangle$ . In matrix element calculations,

$$\langle \alpha_1 \alpha_2 | \hat{O} | \alpha_1 \alpha_2 \rangle = \sum_{AB} C_{\alpha_1 \alpha_2}^{A\dagger} C_{\alpha_1 \alpha_2}^B \langle A | \hat{O} | B \rangle \quad (26)$$

We want to calculate matrix elements as  $\langle A|\hat{O}|B\rangle$  only once.  $|\alpha_1\alpha_2\rangle$  that map to the same  $A, B$  states should lookup the earlier calculated values for  $\langle A|\hat{O}|B\rangle$ . In general the matrix element  $\langle A|\hat{O}|B\rangle$  is not diagonal. A `Paircoef` object has all the quantum numbers in a rcm state  $A$ . In addition it holds a value and a map `std::map<Paircoef*, double>`. The map is used to link a rcm state  $|A\rangle$  to all other rcm states  $|B\rangle$  which yield a non zero contribution for  $\langle A|\hat{O}|B\rangle$ . The value for the transformation coefficients  $C_{\alpha_1, \alpha_2}^{A, \dagger} C_{\alpha_1, \alpha_2}^B$  is stored in the second field of the map (`double`). So that the the summation over  $B$  (Eq. 26) is replaced by,

$$\langle \alpha_1 \alpha_2 | \hat{O} | \alpha_1 \alpha_2 \rangle = \sum_A \sum_{\text{Paircoef}(A).links} \text{link.strength} \langle A | \hat{O} | B \rangle \quad (27)$$

`Paircoef::add(double val)` adds `val` to private member `value` but as far as I can see this private member `value` is NEVER used!

## 5 Matrix Elements

First some theory on the matrix elements. In the calculation of the norm we only have the correlation operator  $\hat{\imath}$  between the bras and kets.

$$\langle \alpha \beta | \hat{\imath}(\vec{x}_1, \vec{x}_2) + \hat{\imath}^\dagger(\vec{x}_1, \vec{x}_2) + \hat{\imath}^\dagger(\vec{x}_1, \vec{x}_2) \hat{\imath}(\vec{x}_1, \vec{x}_2) | \alpha \beta \rangle$$

$\hat{\imath}$  contains a central, tensor and spin-isospin part,

$$\hat{\imath}(\vec{x}_1, \vec{x}_2) = -f_c(r_{12}) + f_{t\tau}(r_{12}) \hat{S}_{12} \hat{\tau}_1 \cdot \hat{\tau}_2 + f_{\sigma\tau}(r_{12}) \hat{\sigma}_1 \cdot \hat{\sigma}_2 \hat{\tau}_1 \cdot \hat{\tau}_2.$$

Transforming to the c.m. and relative coordinates a general matrix-element term can be written as,

$$\langle n(lS)jm_j N L M_L T M_T | \hat{O}^{p\dagger} f_p^\dagger f_q \hat{O}^q | n'(l'S')j'm'_j N' L' M'_L T' M'_T \rangle$$

With  $f_{p,q} \in \{1, f_c, f_{t\tau}, f_{\sigma\tau}\}$  and  $\hat{O}^{p,q}$  the corresponding operator  $\in \{\mathbb{1}, \hat{S}_{12} \hat{\tau}_1 \cdot \hat{\tau}_2, \hat{\sigma}_1 \cdot \hat{\sigma}_2 \hat{\tau}_1 \cdot \hat{\tau}_2\}$ . As no operators act on the c.m. part  $|N L M_L\rangle$  here we have,

$$\delta_{NN'} \delta_{LL'} \delta_{M_L M'_L} \langle n(lS)jm_j T M_T | \hat{O}^{p\dagger} f_p^\dagger f_q \hat{O}^q | n'(l'S')j'm'_j T' M'_T \rangle$$

Let us now take a look at the separate cases for  $\delta_{NN'} \delta_{LL'} \delta_{M_L M'_L} \langle n(lS)jm_j T M_T | \hat{O}^{p\dagger} f_p^\dagger f_q \hat{O}^q | n'(l'S')j'm'_j T' M'_T \rangle$ ,

- $\hat{O}^p = \mathbb{1}$ ,  $f_p = 1$ ,  $\hat{O}^q = \mathbb{1}$ ,  $f_q = f_c(r_{12})$

$$\begin{aligned} \delta_{NN'} \delta_{LL'} \delta_{M_L M'_L} \langle n(lS)jm_j T M_T | f_c(r_{12}) | n'(l'S')j'm'_j T' M'_T \rangle \\ = \delta_{NN'} \delta_{LL'} \delta_{M_L M'_L} \delta_{SS'} \delta_{jj'} \delta_{m_j m'_j} \delta_{TT'} \delta_{M_T M'_T} \delta_{ll'} \langle nl | f_c(r_{12}) | n'l' \rangle \end{aligned}$$

$$\langle nl | f_c(r_{12}) | n'l' \rangle = \int dr_{12} r_{12}^2 R_{nl}(r_{12}) f_c(r_{12}) R_{n'l'}(r_{12})$$

With  $R_{nl}(r) = \left[ \frac{2n!}{\Gamma(n+l+3/2)} \nu^{l+3/2} \right]^{\frac{1}{2}} r^l e^{-\nu r^2/2} L_n^{l+1/2}(\nu r^2) = N_{nl} \nu^{\frac{l+3/2}{2}} r^l e^{-\nu r^2/2} L_n^{l+1/2}(\nu r^2)$  and  $\nu = M_N \omega / \hbar$ .

$$\langle nl | f_c(r_{12}) | n'l' \rangle = N_{nl} N_{n'l'} \nu^{\frac{l+l'+3}{2}} \int dr_{12} r_{12}^2 r_{12}^l e^{-\nu r_{12}^2/2} L_n^{l+1/2}(\nu r_{12}^2) f_c(r_{12}) r_{12}^{l'} e^{-\nu r_{12}^2/2} L_{n'}^{l'+1/2}(\nu r_{12}^2)$$

The correlation functions  $f_p(r)$  are expanded as  $\sum_{\lambda} b_{\lambda} r^{\lambda} e^{-br^2}$ , expanding the generalized laguerre polynomials as well,  $L_n^l(r) = \sum_k a_{nl,k} r^k$ ,

$$\langle nl|f_c(r_{12})|n'l'\rangle = N_{nl}N_{n'l'}\nu^{\frac{l+l'+3}{2}} \sum_{kk'\lambda} a_{nl,k}a_{n'l',k'}b_{\lambda} \int dr_{12} r_{12}^{2+l+l'} e^{-\nu r_{12}^2} (\nu r_{12}^2)^k r_{12}^{\lambda} e^{-br_{12}^2} (\nu r_{12}^2)^{k'}$$

With the substitution  $r = \sqrt{\nu} r_{12}$ ,  $B = b/\nu$  (units are  $[\nu] = \text{m}^{-2}$ ,  $[b] = \text{m}^{-2}$ ,  $[r] = 1$ ,  $[B] = 1$ ) we get,

Maarten says  $B = b/\sqrt{\nu}$  (D.19), I think this is incorrect (units do not match),  $Bx^2$  of (D.19) is NOT dimensionless while it should be... (appears to be correct in the code however...)

$$\begin{aligned} \langle nl|f_c(r_{12})|n'l'\rangle &= N_{nl}N_{n'l'}\nu^{\frac{l+l'+3}{2}} \sum_{kk'\lambda} a_{nl,k}a_{n'l',k'}b_{\lambda} \nu^{-\frac{3+l+l'+\lambda}{2}} \int dr r^{2+l+l'} e^{-r^2} r^{2k} r^{\lambda} e^{-Br^2} r^{2k'} \\ &= N_{nl}N_{n'l'} \sum_{kk'\lambda} \nu^{-\frac{\lambda}{2}} a_{nl,k}a_{n'l',k'}b_{\lambda} \int dr r^{2+l+l'+\lambda+2k+2k'} e^{-(B+1)r^2} \\ &= N_{nl}N_{n'l'} \sum_{kk'\lambda} \nu^{-\frac{\lambda}{2}} a_{nl,k}a_{n'l',k'}b_{\lambda} \frac{1}{2} \Gamma\left(\frac{K+1}{2}\right) (1+B)^{-\frac{K+1}{2}} \\ &= \frac{N_{nl}N_{n'l'}}{2} \sum_{kk'\lambda} \nu^{-\frac{\lambda}{2}} a_{nl,k}a_{n'l',k'}b_{\lambda} \Gamma\left(\frac{K+1}{2}\right) (1+B)^{-\frac{K+1}{2}} \quad (28) \end{aligned}$$

$K = 2 + l + l' + \lambda + 2k + 2k'$ . To recapitulate,  $a_{nl,k}$  is the  $k$ 'th expansion coefficient of the Laguerre polynomials. The sum over  $k$  ( $k'$ ) ranges from 0 to  $n$  ( $n'$ ).  $b_{\lambda}$  is the  $\lambda$ 'th expansion coefficient of the correlation function, runs from 0 to a finite value (10 or 11 for Maartens' fits).  $\nu = M_N\omega/\hbar$  is the H.O.-potential parameter and is nucleus dependent.  $N_{nl} = \left[\frac{2n!}{\Gamma(n+l+3/2)}\right]^{\frac{1}{2}} = \left[\frac{2\Gamma(n+1)}{\Gamma(n+l+3/2)}\right]^{\frac{1}{2}}$  are the normalisation factors of the orbital wave functions, these factors are nucleus independent (only  $n, l$  dependencies).

Orthonormality using this expansion (Eq. 28) can easily be checked,  $\langle nl|1|n'l\rangle$  ( $l = l'$  because of the orthonormality of the spherical harmonics), if we set  $b_{\lambda} = \delta_{\lambda,0}$ ,  $b = 0$ .

$$\langle nl|1|n'l\rangle = \frac{N_{nl}N_{n'l}}{2} \sum_{kk'=0}^{nn'} a_{nl,k}a_{n'l,k'}\Gamma\left(\frac{3+2l+2k+2k'}{2}\right) \quad (29)$$

- $\hat{\mathcal{O}}^p = 1$ ,  $f_p = f_c(r_{12})$ ,  $\hat{\mathcal{O}}^q = 1$ ,  $f_q = f_c(r_{12})$ , the non trivial part of the matrix element now comes down to calculating,

$$\begin{aligned} \langle nl|f_c^2(r_{12})|n'l'\rangle &= \int dr_{12} r_{12}^2 R_{nl}(r_{12}) f_c^2(r_{12}) R_{n'l'}(r_{12}) \\ &= N_{nl}N_{n'l'}\nu^{\frac{l+l'+3}{2}} \sum_{kk'\lambda\lambda'} a_{nl,k}a_{n'l',k'}b_{\lambda}b_{\lambda'} \int dr_{12} r_{12}^{2+l+l'} e^{-\nu r_{12}^2} (\nu r_{12}^2)^k r_{12}^{\lambda+\lambda'} e^{-2br_{12}^2} (\nu r_{12}^2)^{k'} \\ &= N_{nl}N_{n'l'}\nu^{\frac{l+l'+3}{2}} \sum_{kk'\lambda\lambda'} a_{nl,k}a_{n'l',k'}b_{\lambda}b_{\lambda'} \nu^{-\frac{3+l+l'+\lambda+\lambda'}{2}} \int dr r^{2+l+l'+2k+2k'+\lambda+\lambda'} e^{-(2B+1)r^2} \\ &= \frac{N_{nl}N_{n'l'}}{2} \sum_{kk'\lambda\lambda'} \nu^{-\frac{\lambda+\lambda'}{2}} a_{nl,k}a_{n'l',k'}b_{\lambda}b_{\lambda'} \Gamma\left(\frac{K+1}{2}\right) (2B+1)^{-\frac{K+1}{2}} \end{aligned}$$

With  $K = 2 + l + l' + 2k + 2k' + \lambda + \lambda'$ .

## 6 Matrix elements bis

Let us take a look at

$$\langle S | \hat{\sigma}_1 \cdot \hat{\sigma}_2 | S' \rangle = 4 \langle S | \hat{s}_1 \cdot \hat{s}_2 | S' \rangle = 4 \langle S | \hat{S}^2 - \hat{s}_1^2 - \hat{s}_2^2 | S' \rangle = 2(S(S+1) - \frac{3}{4} - \frac{3}{4}) \delta_{SS'} = \delta_{SS'} (2S(S+1) - 3)$$

As we have 2 spin 1/2 particles  $S$  can be either 0, 1 resulting in  $\langle 1 | \hat{\sigma}_1 \cdot \hat{\sigma}_2 | 1 \rangle = 1$ ,  $\langle 0 | \hat{\sigma}_1 \cdot \hat{\sigma}_2 | 0 \rangle = -3$ .

Note that in the Maartens code the expression is modified to  $4S - 3$ , which is equivalent for  $S \in \{0, 1\}$ .

As this is independent of the spin projection  $M_S$  we have,

$$\langle SM_S | \hat{\sigma}_1 \cdot \hat{\sigma}_2 | S' M'_S \rangle = \delta_{SS'} \delta_{M_S M'_S} (2S(S+1) - 3)$$

Exactly the same derivation can be made for  $\hat{\tau}_1 \cdot \hat{\tau}_2$  leading to the same result.

$$\langle TM_T | \hat{\tau}_1 \cdot \hat{\tau}_2 | T' M'_T \rangle = \delta_{TT'} \delta_{M_T M'_T} (2T(T+1) - 3)$$

When selecting a specific isospin projection  $m_t = \pm 1/2$  (proton or neutron) of a nucleon this result changes however. The product  $\hat{\tau}_1 \cdot \hat{\tau}_2$  written in the spherical basis becomes,

$$\hat{\tau}_1 \cdot \hat{\tau}_2 = \hat{\tau}_{1,0} \hat{\tau}_{2,0} - \hat{\tau}_{1,+} \hat{\tau}_{2,-} - \hat{\tau}_{1,-} \hat{\tau}_{2,+} = \hat{\tau}_{1,0} \hat{\tau}_{2,0} + \frac{\hat{\tau}_1^+ \hat{\tau}_2^-}{2} + \frac{\hat{\tau}_1^- \hat{\tau}_2^+}{2}$$

Where  $\hat{\tau}^\pm$  are the raising/lowering operators. Transitioning to the operators  $\hat{t} = \hat{\tau}/2$  (analogues to the spin case  $\hat{S} = \hat{\sigma}/2$ ) with the properties,

$$\begin{aligned} \hat{t}_0 |t, m_t\rangle &= m_t |t, m_t\rangle \\ \hat{t}^\pm |t, m_t\rangle &= \sqrt{t(t+1) - m(m \pm 1)} |t, m_t \pm 1\rangle. \end{aligned}$$

we get

$$\hat{\tau}_1 \cdot \hat{\tau}_2 = 4\hat{t}_{1,0} \hat{t}_{2,0} + 2\hat{t}_1^+ \hat{t}_2^- + 2\hat{t}_1^- \hat{t}_2^+$$

Defining the isospin-projection operator acting on particle “ $i$ ” of the nucleon pair  $\hat{\delta}_{m_t}^{[1]} = (1 + (2m_t)\hat{t}_{i,0})/2$  we get,

$$\begin{aligned} \hat{\delta}_{m_t}^{[1]} |1, \pm 1\rangle &= \delta_{\pm 1, 2m_t} |1, \pm 1\rangle & \hat{\delta}_{m_t}^{[2]} |1, \pm 1\rangle &= \delta_{\pm 1, 2m_t} |1, \pm 1\rangle \\ \hat{\delta}_{m_t}^{[1]} |1, 0\rangle &= \frac{1}{\sqrt{2}} \left| \frac{1}{2}, m_t \right\rangle \otimes \left| \frac{1}{2}, -m_t \right\rangle & \hat{\delta}_{m_t}^{[2]} |1, 0\rangle &= \frac{1}{\sqrt{2}} \left| \frac{1}{2}, -m_t \right\rangle \otimes \left| \frac{1}{2}, m_t \right\rangle \\ \hat{\delta}_{m_t}^{[1]} |0, 0\rangle &= \frac{1}{\sqrt{2}} 2m_t \left| \frac{1}{2}, m_t \right\rangle \otimes \left| \frac{1}{2}, -m_t \right\rangle & \hat{\delta}_{m_t}^{[2]} |0, 0\rangle &= \frac{1}{\sqrt{2}} (-2m_t) \left| \frac{1}{2}, m_t \right\rangle \otimes \left| \frac{1}{2}, -m_t \right\rangle \end{aligned}$$

Note that  $\text{sgn}(m_t) \equiv 2m_t$  as  $m_t = \pm 1/2$ . It is straightforward to show that,

$$\begin{aligned} \langle 1, \pm 1 | \hat{\delta}_{m_t}^{[1]} | 1, \pm 1 \rangle &= \delta_{\pm 1, 2m_t} & \langle 1, \pm 1 | \hat{\delta}_{m_t}^{[2]} | 1, \pm 1 \rangle &= \delta_{\pm 1, 2m_t} \\ \langle 1, 0 | \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle = \frac{1}{2} & \langle 1, 0 | \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle = \frac{1}{2} \\ \langle 1, 0 | \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle = \frac{1}{2} 2m_t & \langle 1, 0 | \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle = \frac{1}{2} (-2m_t) \end{aligned}$$

We now investigate the effect of the insertion of the isospin-projection operator  $\hat{\delta}_{m_t}^{[i]}$  in

$$\langle TM_T | \hat{\tau}_1 \cdot \hat{\tau}_2 | T' M'_T \rangle$$

Note that  $\hat{\delta}_{m_t}^{[i]}$  and  $\hat{\tau}_1 \cdot \hat{\tau}_2$  are hermitian but do not commute. Hence the operator  $\hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[i]}$  is **not hermitian**.

$$\hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} |1, \pm 1\rangle = \delta_{\pm 1, 2m_t} |1, \pm 1\rangle$$

$$\begin{aligned} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} |1, 0\rangle &= \frac{1}{\sqrt{2}} \left( -|\frac{1}{2}, m_t\rangle \otimes |\frac{1}{2}, -m_t\rangle \right. \\ &\quad + (1 - 2m_t) |\frac{1}{2}, m_t + 1\rangle \otimes |\frac{1}{2}, -m_t - 1\rangle \\ &\quad \left. + (1 + 2m_t) |\frac{1}{2}, m_t - 1\rangle \otimes |\frac{1}{2}, -m_t + 1\rangle \right) \end{aligned}$$

$$\begin{aligned} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} |0, 0\rangle &= \frac{1}{\sqrt{2}} \left( -2m_t |\frac{1}{2}, m_t\rangle \otimes |\frac{1}{2}, -m_t\rangle \right. \\ &\quad + (2m_t - 1) |\frac{1}{2}, m_t + 1\rangle \otimes |\frac{1}{2}, -m_t - 1\rangle \\ &\quad \left. + (2m_t + 1) |\frac{1}{2}, m_t - 1\rangle \otimes |\frac{1}{2}, -m_t + 1\rangle \right) \end{aligned}$$

The non-zero matrix elements for  $\langle TM_T | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[i]} | T' M'_T \rangle$  are (one can make use of the fact that both  $\hat{\delta}_{m_t}^{[i]}$  and  $\hat{\tau}_1 \cdot \hat{\tau}_2$  are hermitian and let them act on the neighbouring bra or ket),

$$\begin{aligned} \langle 1, \pm 1 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, \pm 1 \rangle &= \delta_{\pm 1, 2m_t} & \langle 1, \pm 1 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, \pm 1 \rangle &= \delta_{\pm 1, 2m_t} \\ \langle 1, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle &= \frac{1}{2} & \langle 1, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle &= \frac{1}{2} \\ \langle 1, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle &= \frac{1}{2} 2m_t & \langle 1, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle &= -\frac{1}{2} 2m_t \\ \langle 0, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle &= -\frac{3}{2} 2m_t & \langle 0, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle &= \frac{3}{2} 2m_t \\ \langle 0, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle &= -\frac{3}{2} & \langle 0, 0 | \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle &= -\frac{3}{2} \end{aligned}$$

The non-zero matrix elements for  $\langle TM_T | \hat{\delta}_{m_t}^{[i]} \hat{\tau}_1 \cdot \hat{\tau}_2 | T' M'_T \rangle$  are,

$$\begin{aligned} \langle 1, \pm 1 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 1, \pm 1 \rangle &= \delta_{\pm 1, 2m_t} & \langle 1, \pm 1 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 1, \pm 1 \rangle &= \delta_{\pm 1, 2m_t} \\ \langle 1, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 1, 0 \rangle &= \frac{1}{2} & \langle 1, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 1, 0 \rangle &= \frac{1}{2} \\ \langle 1, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 0, 0 \rangle &= -\frac{3}{2} 2m_t & \langle 1, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 0, 0 \rangle &= \frac{3}{2} 2m_t \\ \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 1, 0 \rangle &= \frac{1}{2} 2m_t & \langle 0, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 1, 0 \rangle &= -\frac{1}{2} 2m_t \\ \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 0, 0 \rangle &= -\frac{3}{2} & \langle 0, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 | 0, 0 \rangle &= -\frac{3}{2} \end{aligned}$$

The non-zero matrix elements for  $\langle TM_T | \hat{\delta}_{m_t}^{[i]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[i]} | T' M'_T \rangle$  are,

$$\begin{aligned}
\langle 1, \pm 1 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, \pm 1 \rangle &= \langle 1, \pm 1 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, \pm 1 \rangle = \delta_{\pm 1, 2m_t} \\
\langle 1, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle = -\frac{1}{2} \\
\langle 1, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle = -\frac{1}{2} 2m_t \\
\langle 1, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle = -\frac{1}{2} \\
\langle 1, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle &= \langle 0, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle = \frac{1}{2} 2m_t
\end{aligned}$$

Note that the combinations of different isospin-projections are not necessarily zero when the operator  $\hat{\tau}_1 \cdot \hat{\tau}_2$  is involved,

$$\begin{aligned}
\langle 1, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle &= 1 & \langle 1, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle &= 1 \\
\langle 1, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle &= -2m_t & \langle 1, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle &= 2m_t \\
\langle 0, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 1, 0 \rangle &= 2m_t & \langle 0, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 1, 0 \rangle &= -2m_t \\
\langle 0, 0 | \hat{\delta}_{m_t}^{[1]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[1]} | 0, 0 \rangle &= -1 & \langle 0, 0 | \hat{\delta}_{m_t}^{[2]} \hat{\tau}_1 \cdot \hat{\tau}_2 \hat{\delta}_{m_t}^{[2]} | 0, 0 \rangle &= -1
\end{aligned}$$

These matrix element have been checked with a simple python program (`numpy.kron` for kronecker products). Note that all the matrix elements for  $i = 1, 2$  are the same expect for a minus sign whenever a combination like  $\langle 1, 0 | \dots | 0, 0 \rangle$  or  $\langle 0, 0 | \dots | 1, 0 \rangle$  is involved. Also note that all the matrix elements do not mix different  $M_T, M'_T$ , so we effectively have  $\delta_{M_T M'_T}$  everywhere.

## 6.1 norm\_ob : public operator\_virtual\_ob

Here we take a look at the calculation of the norm  $\mathcal{N}$  in `norm_ob.cpp`. Note that this class inherits from `operator_virtual_ob`, declaring general one body member functions.

- `norm_ob::get_me( Pair )`. This calculates the matrix element **meanfield** matrix element sum

1.  $\frac{2}{A} \sum_{AB} C_{\alpha_1 \alpha_2}^{A\dagger} C_{\alpha_1 \alpha_2}^B \langle A|B \rangle$  for a pp and/or nn pair(s) (isospin  $M_T = \pm 1$ )
2.  $\frac{1}{A} \sum_{AB} C_{\alpha_1 \alpha_2}^{A\dagger} C_{\alpha_1 \alpha_2}^B \langle A|B \rangle$  for a pn pair (isospin  $M_T = 0$ )

for a specific pair  $\alpha_1 \alpha_2$  passed trough `Pair`.

For now I have no clue why/how the factor  $\frac{2}{A}(\frac{1}{A})$  in front of  $\sum_{AB} C_{\alpha_1 \alpha_2}^{A\dagger} C_{\alpha_1 \alpha_2}^B \langle A|B \rangle \dots$

It is possible to filter on relative quantum numbers on  $n_A, l_A, n_B, l_B$ , selecting specific contributions `nAs, lAs, nBs, lBs` to the sum. A value of  $-1$  for these variables is interpreted as “all values allowed”. Trough the braket  $\langle A|B \rangle$  we already have  $n_A = n_B := n, l_A = l_B := l$ .

- if `(nAs > -1 && nBs > -1)` This forces `nAs = nBs = n`. So for `nAs ≠ nBs` we will get 0.
- if `(nAs == -1 && nBs > -1)` This forces `nBs = n`. Selecting a specific  $n = n_A = n_B$  contribution.
- if `(nAs > -1 && nBs == -1)` This forces `nAs = n`. Selecting a specific  $n = n_A = n_B$  contribution.
- if `(nAs == -1 && nBs == -1)` This makes no restrictions on  $n = n_A = n_B$ .

The exact same is valid for  $l = l_A = l_B$  and `lAs, lBs`. A few examples `(nAs, lAs, nBs, lBs)`:



- $(-1, 2, -1, -1)$  : allow all  $n = n_A = n_B$  values. Restriction on  $l = l_A = l_B = 2$ .
- $(-1, 2, -1, 2)$  : allow all  $n = n_A = n_B$  values. Restriction on  $l = l_A = l_B = 2$ .

As the unrestricted sum  $\sum_{AB} C_{\alpha_1\alpha_2}^{A\dagger} C_{\alpha_1\alpha_2}^B \langle A|B \rangle = \sum_A |C_{\alpha_1\alpha_2}^A|^2$  equals 1, the return value of `get_me` (for the unrestricted sum) is,

- $\frac{2}{A}$  with no restriction on the isospin (`norm_ob::norm_ob_params.t = 0`)
- $\frac{2}{A}$  for pp-pairs,  $\frac{1}{A}$  for pn-pairs and 0 for nn-pairs for a proton (`norm_ob::norm_ob_params.t = 1`)
- 0 for pp-pairs,  $\frac{1}{A}$  for pn-pairs and  $\frac{2}{A}$  for nn-pairs for a neutron (`norm_ob::norm_ob_params.t == -1`)

If we sum over all the pairs  $\sum_{\text{pair in pairs}} \text{norm::ob\_get\_me}(\text{pair}, \dots)$  we get,

- $\frac{A(A-1)}{2} \frac{2}{A} = A-1$  with no restriction on the isospin (`norm_ob::norm_ob_params.t = 0`)
- $\frac{Z(Z-1)}{2} \frac{2}{A} + NZ \frac{1}{A} + \frac{N(N-1)}{2} 0 = Z \frac{A-1}{A}$  for a proton (`norm_ob::norm_ob_params.t = 1`)
- $\frac{Z(Z-1)}{2} 0 + NZ \frac{1}{A} + \frac{N(N-1)}{2} \frac{2}{A} = N \frac{A-1}{A}$  for a neutron (`norm_ob::norm_ob_params.t == -1`)

**Open shellness not taken into account here. Must be done somewhere else (higher up)...**

For closed shell nuclei everything seems fine. For open shells however we get some strange results. For example  $^{27}\text{Al}$  with 13 protons and 14 neutrons has an open  $1d_{5/2}$  proton shell. Open-shell nuclei are treated as closed shell but the pairs in the open shells get a weight factor. This weight factor however is **not** present in the method `norm::ob_get_me(pair, ...)`. Hence as  $A = 27$  but the closed shell equivalent with  $A = 28$  causes the number of pairs to be  $28 \cdot 27/2$  instead of  $27 \cdot 26/2$ . We get

- $\frac{28 \cdot 27}{2} \frac{2}{27} = 28$  (`norm_ob::norm_ob_params.t = 0`)
- $\frac{14 \cdot 13}{2} \frac{2}{27} + \frac{14 \cdot 14}{27} = \frac{378}{27} = 14$  (`norm_ob::norm_ob_params.t = 1`)
- $\frac{14 \cdot 14}{27} + \frac{14 \cdot 13}{2} \frac{2}{27} = \frac{378}{27} = 14$  (`norm_ob::norm_ob_params.t == -1`)

- `norm_ob::get_me_corr_right( Pair )`.

## 6.2 density\_ob\_integrand3

Here we look at the file `density_ob_integrand3`.

## 6.3 density\_ob\_integrand\_cf

cf probably stands for correlation function. This class calculates integrals of the form

$$F_{p_1}(P) = \int dr r^{i+2} j_l\left(\frac{rP}{\sqrt{\nu}}\right) j_k\left(\frac{rp_1\sqrt{2}}{\sqrt{\nu}}\right) f\left(\frac{r}{\sqrt{\nu}}\right) e^{-\frac{r^2}{2}}$$

Where  $p$  is the one-body momentum and  $P$  is the c.m. momentum. This corresponds with the  $\chi$  symbols defined (??).

$$\chi_{p,nl}^{kK}(p_1, P) = \int dr r^2 f_p(r) R_{nl}(r) j_k(\sqrt{2}p_1 r) j_K(Pr)$$

With  $R_{nl}(r) = N_{nl} \nu^{\frac{l+3/2}{2}} r^l e^{-\nu r^2/2} L_n^{l+1/2}(\nu r^2)$  and  $\nu = M_N \omega / \hbar$ ,

$$\chi_{p,nl}^{kK}(p_1, P) = N_{nl} \nu^{\frac{l+3/2}{2}} \int dr r^{2+l} f_p(r) e^{-\nu r^2/2} L_n^{l+1/2}(\nu r^2) j_k(\sqrt{2}p_1 r) j_K(Pr)$$

Expanding the Generalized-Laguerre polynomials gives,

$$\chi_{p,nl}^{kK}(p_1, P) = N_{nl} \nu^{\frac{l+3/2}{2}} \sum_{i=0}^n a_{nl,i} \int dr r^{2+l} f_p(r) e^{-\nu r^2/2} (\nu r^2)^i j_k(\sqrt{2} p_1 r) j_K(Pr)$$

Changing variables  $r \rightarrow r/\sqrt{\nu}$  gives,

$$\chi_{p,nl}^{kK}(p_1, P) = N_{nl} \nu^{-\frac{3}{4}} \sum_{i=0}^n a_{nl,i} \int dr r^{2+l+2i} f_p(\nu^{-\frac{1}{2}} r) e^{-r^2/2} j_k(\nu^{-\frac{1}{2}} \sqrt{2} p_1 r) j_K(\nu^{-\frac{1}{2}} Pr)$$

This is exactly what is found in `density_ob_integrand_cf::integrand` and `density_ob_integrand_cf::get_value`. The integrals are stored in a map where the key field contains the order of the spherical Bessel functions  $k, K$  and is calculated as  $100k+K$ . It is necessary to assume that  $K < 100$ . The value field contains a two dimensional vector (`std::vector<std::vector<double>>`). The first dimension (index) corresponds with the power of  $r$  in the integrand and ranges from 0 to  $2n+l+2$ . The second dimension (index) corresponds with the different discretized values of  $P$ .

## 7 One body momentum distribution

We will look into one-body momentum distributions. A matrix element as calculated in the norm (??) is now extended by including the ony-body momentum operator  $\hat{n}^{[1]}(\vec{p})$ .

$$\hat{n}_{AA'}^{[1]}(p) = \langle A \equiv n(lS)j m_j N L M_L T M_T | \hat{\mathcal{O}}^{p\dagger} f_p^\dagger \hat{n}^{[1]}(\vec{p}) f_q \hat{\mathcal{O}}^q | A' \equiv n'(l'S')j' m'_j N' L' M'_L T' M'_T \rangle$$

The one-body momentum operator is given by,

$$\hat{n}^{[1]}(\vec{p}_1) = |\vec{p}_1\rangle \langle \vec{p}_1| = \int d^3 \vec{p}_2 n^{[2]}(\vec{p}_1, \vec{p}_2) = \int d^3 \vec{p}_2 |\vec{p}_1 \vec{p}_2\rangle \langle \vec{p}_1 \vec{p}_2|$$

Hence,

$$\begin{aligned} \langle A | \hat{n}^{[1]}(\vec{p}_1) | A' \rangle &= \int d^3 \vec{p}_2 \langle A | \hat{\mathcal{O}}^{p\dagger} f_p^\dagger | \vec{p}_1 \vec{p}_2 \rangle \langle \vec{p}_1 \vec{p}_2 | f_q \hat{\mathcal{O}}^q | A' \rangle \\ &= \int d^3 \vec{p}_2 d^3 \vec{r}_1 d^3 \vec{r}_2 d^3 \vec{r}'_1 d^3 \vec{r}'_2 \langle A | \hat{\mathcal{O}}^{p\dagger} f_p^\dagger | \vec{r}_1 \vec{r}_2 \rangle \langle \vec{r}_1 \vec{r}_2 | \vec{p}_1 \vec{p}_2 \rangle \langle \vec{p}_1 \vec{p}_2 | \vec{r}'_1 \vec{r}'_2 \rangle \langle \vec{r}'_1 \vec{r}'_2 | f_q \hat{\mathcal{O}}^q | A' \rangle \end{aligned}$$

With  $\langle \vec{r} | \vec{p} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{p} \cdot \vec{r}}$  and  $\vec{R}_{12} = \frac{\vec{r}_1 + \vec{r}_2}{\sqrt{2}}, \vec{r}_{12} = \frac{\vec{r}_1 - \vec{r}_2}{\sqrt{2}}$ .

$$\begin{aligned} \langle A | \hat{n}^{[1]}(\vec{p}_1) | A' \rangle &= \\ \frac{1}{(2\pi)^6} \int d^3 \vec{p}_2 d^3 \vec{R}_{12} d^3 \vec{r}_{12} d^3 \vec{R}'_{12} d^3 \vec{r}'_{12} e^{i\vec{p}_1 \cdot (\vec{r}_1 - \vec{r}'_1)} e^{i\vec{p}_2 \cdot (\vec{r}_2 - \vec{r}'_2)} \langle A | \hat{\mathcal{O}}^{p\dagger} f_p^\dagger | \vec{R}_{12} \vec{r}_{12} \rangle \langle \vec{R}'_{12} \vec{r}'_{12} | f_q \hat{\mathcal{O}}^q | A' \rangle \end{aligned}$$

With  $\vec{r}_1 - \vec{r}'_1 = \frac{\vec{R}_{12} + \vec{r}_{12} - \vec{R}'_{12} - \vec{r}'_{12}}{\sqrt{2}}, \vec{r}_2 - \vec{r}'_2 = \frac{\vec{R}_{12} - \vec{r}_{12} - \vec{R}'_{12} + \vec{r}'_{12}}{\sqrt{2}}$ , we have,

$$\int d^3 \vec{p}_2 e^{i\vec{p}_2 \cdot (\vec{r}_2 - \vec{r}'_2)} = (2\pi)^3 \sqrt{2}^3 \delta^{(3)}(\vec{R}_{12} - \vec{r}_{12} - \vec{R}'_{12} + \vec{r}'_{12})$$

$$\begin{aligned} \langle A | \hat{n}^{[1]}(\vec{p}_1) | A' \rangle &= \\ \frac{\sqrt{8}}{(2\pi)^3} \int d^3 \vec{R}_{12} d^3 \vec{r}_{12} d^3 \vec{r}'_{12} e^{i\sqrt{2}\vec{p}_1 \cdot (\vec{r}_{12} - \vec{r}'_{12})} \langle A | \hat{\mathcal{O}}^{p\dagger} f_p^\dagger | \vec{R}_{12} \vec{r}_{12} \rangle \langle \vec{R}'_{12} \vec{r}'_{12} | f_q \hat{\mathcal{O}}^q | A' \rangle \Big|_{\vec{R}'_{12} = \vec{R}_{12} - \vec{r}_{12} + \vec{r}'_{12}} \end{aligned}$$

We write out the explicit orbital wave functions. Let us denote the matrix element with the operators  $\hat{\mathcal{O}}^{p,q}$ ,  $\langle A|\hat{\mathcal{O}}^{p\dagger}\hat{\mathcal{O}}^q|A'\rangle$ , (central,tensor or spin-isospin) as  $\mathcal{M}_{AA'}^{p,q}$ .

$$\begin{aligned} \langle A|\hat{n}^{[1]}(\vec{p}_1)|A'\rangle = \\ \mathcal{M}_{AA'}^{p,q} \frac{\sqrt{8}}{(2\pi)^3} \int d^3\vec{R}_{12} d^3\vec{r}_{12} d^3\vec{r}'_{12} e^{i\sqrt{2}\vec{p}_1 \cdot (\vec{r}_{12} - \vec{r}'_{12})} f_p^\dagger(r_{12}) f_q(r'_{12}) \\ \psi_{NLM_L}^\dagger(\vec{R}_{12}) \psi_{n(lS)jm_j}^\dagger(\vec{r}_{12}) \psi_{N'L'M'_L}(\vec{R}'_{12}) \psi_{n'(l'S')j'm'_j}(\vec{r}'_{12}) \Big|_{\vec{R}'_{12} = \vec{R}_{12} - \vec{r}_{12} + \vec{r}'_{12}} \end{aligned}$$

Writing the wave functions as Fourier transformations  $\psi_{NLM_L}(\vec{R}_{12}) = 1/(2\pi)^{3/2} \int d^3\vec{P}_{12} e^{i\vec{P}_{12} \cdot \vec{R}_{12}} \phi_{NLM_L}(\vec{P}_{12})$ ,

$$\begin{aligned} \langle A|\hat{n}^{[1]}(\vec{p}_1)|A'\rangle = \\ \mathcal{M}_{AA'}^{p,q} \frac{\sqrt{8}}{(2\pi)^3} \int d^3\vec{R}_{12} d^3\vec{r}_{12} d^3\vec{r}'_{12} e^{i\sqrt{2}\vec{p}_1 \cdot (\vec{r}_{12} - \vec{r}'_{12})} f_p^\dagger(r_{12}) f_q(r'_{12}) \psi_{n(lS)jm_j}^\dagger(\vec{r}_{12}) \psi_{n'(l'S')j'm'_j}(\vec{r}'_{12}) \\ \frac{1}{(2\pi)^3} \int d^3\vec{P}_{12} \int d^3\vec{P}'_{12} e^{-i\vec{P}_{12} \cdot \vec{R}_{12}} \phi_{NLM_L}^\dagger(\vec{P}_{12}) e^{i\vec{P}'_{12} \cdot (\vec{R}_{12} - \vec{r}_{12} + \vec{r}'_{12})} \phi_{N'L'M'_L}(\vec{P}'_{12}) \\ = \mathcal{M}_{AA'}^{p,q} \frac{\sqrt{8}}{(2\pi)^3} \int d^3\vec{r}_{12} d^3\vec{r}'_{12} e^{i\sqrt{2}\vec{p}_1 \cdot (\vec{r}_{12} - \vec{r}'_{12})} f_p^\dagger(r_{12}) f_q(r'_{12}) \psi_{n(lS)jm_j}^\dagger(\vec{r}_{12}) \psi_{n'(l'S')j'm'_j}(\vec{r}'_{12}) \\ \int d^3\vec{P}_{12} e^{-i\vec{P}_{12} \cdot (\vec{r}_{12} - \vec{r}'_{12})} \phi_{NLM_L}^\dagger(\vec{P}_{12}) \phi_{N'L'M'_L}(\vec{P}_{12}) \end{aligned}$$

Using the plane wave expansion  $e^{i\vec{p} \cdot \vec{r}} = 4\pi \sum_{lm_l} i^l j_l(pr) Y_{lm_l}^*(\Omega_p) Y_{lm_l}(\Omega_r) = 4\pi \sum_{lm_l} i^l j_l(pr) Y_{lm_l}(\Omega_p) Y_{lm_l}^*(\Omega_r)$  and the fact that the isotropic harmonic oscillator wavefunctions factorize in  $\psi_{nlm_l}(\vec{r}) = R_{nl}(r) Y_{lm_l}(\Omega_r)$ ,  $\psi_{nlm_l}(\vec{p}) = \Pi_{NL}(p) Y_{lm_l}(\Omega_p)$ ,  $\psi_{n(lS)jm_j}(\vec{r}) = R_{nl}(r) \mathcal{Y}_{(lS)jm_j}(\Omega_r)$ .

$$\begin{aligned} \langle A|\hat{n}^{[1]}(\vec{p}_1)|A'\rangle = \\ \mathcal{M}_{AA'}^{p,q} \frac{\sqrt{8}}{(2\pi)^3} \int d^3\vec{R}_{12} d^3\vec{r}_{12} d^3\vec{r}'_{12} e^{i\sqrt{2}\vec{p}_1 \cdot (\vec{r}_{12} - \vec{r}'_{12})} f_p^\dagger(r_{12}) f_q(r'_{12}) \psi_{n(lS)jm_j}^\dagger(\vec{r}_{12}) \psi_{n'(l'S')j'm'_j}(\vec{r}'_{12}) \\ \frac{1}{(2\pi)^3} \int d^3\vec{P}_{12} \int d^3\vec{P}'_{12} e^{-i\vec{P}_{12} \cdot \vec{R}_{12}} \phi_{NLM_L}^\dagger(\vec{P}_{12}) e^{i\vec{P}'_{12} \cdot (\vec{R}_{12} - \vec{r}_{12} + \vec{r}'_{12})} \phi_{N'L'M'_L}(\vec{P}'_{12}) \\ = \mathcal{M}_{AA'}^{p,q} \frac{\sqrt{8}(4\pi)^4}{(2\pi)^3} \int d^3\vec{r}_{12} d^3\vec{r}'_{12} f_p^\dagger(r_{12}) f_q(r'_{12}) R_{nl}(r_{12}) \mathcal{Y}_{(lS)jm_j}^*(\Omega_{r_{12}}) R_{n'l'}(r'_{12}) \mathcal{Y}_{(l'S')j'm'_j}(\Omega_{r'_{12}}) \\ \sum_{km_k} i^k j_k(\sqrt{2}p_1 r_{12}) Y_{km_k}^*(\Omega_{p_1}) Y_{km_k}(\Omega_{r_{12}}) \\ \sum_{k'm'_k} (-i)^{k'} j_{k'}(\sqrt{2}p_1 r'_{12}) Y_{k'm'_k}(\Omega_{p_1}) Y_{k'm'_k}^*(\Omega_{r'_{12}}) \\ \int d^3\vec{P}_{12} \Pi_{NL}(P_{12}) Y_{LM_L}^*(\Omega_{P_{12}}) \Pi_{N'L'}(P_{12}) Y_{L'M'_L}(\Omega_{P_{12}}) \\ \sum_{K m_K} (-i)^K j_K(P_{12} r_{12}) Y_{K m_K}(\Omega_{P_{12}}) Y_{K m_K}^*(\Omega_{r_{12}}) \\ \sum_{K' m'_K} i^{K'} j_{K'}(P_{12} r'_{12}) Y_{K' m'_K}^*(\Omega_{P_{12}}) Y_{K' m'_K}(\Omega_{r'_{12}}) \end{aligned}$$

$$\begin{aligned}
\langle A | \hat{n}^{[1]}(\vec{p}_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} 64\sqrt{2}\pi \sum_{km_k} \sum_{k'm'_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^{k'+K} i^{k+k'+K+K'} Y_{km_k}^*(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1}) \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \\
&\int dr_{12} r_{12}^2 f_p^\dagger(r_{12}) R_{nl}(r_{12}) j_k(\sqrt{2}p_1 r_{12}) j_K(P_{12} r_{12}) \\
&\int dr'_{12} r_{12}'^2 f_q(r'_{12}) R_{n'l'}(r'_{12}) j_{k'}(\sqrt{2}p_1 r'_{12}) j_{K'}(P_{12} r'_{12}) \\
&\int d^2\Omega_{r_{12}} \mathcal{Y}_{(lS)jm_j}^*(\Omega_{r_{12}}) Y_{km_k}(\Omega_{r_{12}}) Y_{K m_K}^*(\Omega_{r_{12}}) \\
&\int d^2\Omega_{r'_{12}} \mathcal{Y}_{(l'S')j'm'_j}(\Omega_{r'_{12}}) Y_{k'm'_k}^*(\Omega_{r'_{12}}) Y_{K' m'_K}(\Omega_{r'_{12}}) \\
&\int d^2\Omega_{P_{12}} Y_{LM_L}^*(\Omega_{P_{12}}) Y_{L'M'_L}(\Omega_{P_{12}}) Y_{KM_K}(\Omega_{P_{12}}) Y_{K'M'_K}^*(\Omega_{P_{12}})
\end{aligned}$$

As in Eq. (D.38) we define,

$$\chi_{p,nl}^{kK}(p_1, P) = \int dr r^2 f_p(r) R_{nl}(r) j_k(\sqrt{2}p_1 r) j_K(P r)$$

Using the identity (see for example *Sakurai, modern quantum mechanics*)

$$Y_{lm}(\Omega) Y_{l'm'}(\Omega) = \sum_{LM} \sqrt{\frac{(2l+1)(2l'+1)}{4\pi(2L+1)}} \langle lml'm'|LM \rangle \langle l0l'0|L0 \rangle Y_{LM}(\Omega)$$

We can easily derive

$$\int d\Omega Y_{lm}(\Omega) Y_{l'm'}(\Omega) Y_{l''m''}^*(\Omega) = \sqrt{\frac{(2l+1)(2l'+1)}{4\pi(2l''+1)}} \langle lml'm'|l''m'' \rangle \langle l0l'0|l''0 \rangle ,$$

$$\begin{aligned}
\int d\Omega \mathcal{Y}_{(lS)jm_j}(\Omega) Y_{l'm'}(\Omega) Y_{l''m''}^*(\Omega) &= \\
&= \sum_{mm_S} \langle lmSm_S|jm_j \rangle \int d\Omega Y_{lm}(\Omega) Y_{l'm'}(\Omega) Y_{l''m''}^*(\Omega) \\
&= \sum_{mm_S} \langle lmSm_S|jm_j \rangle \sqrt{\frac{(2l+1)(2l'+1)}{4\pi(2l''+1)}} \langle lml'm'|l''m'' \rangle \langle l0l'0|l''0 \rangle
\end{aligned}$$

and,

$$\begin{aligned}
&\int d\Omega Y_{lm_l}(\Omega) Y_{l'm'_l}(\Omega) Y_{km_k}^*(\Omega) Y_{k'm'_k}^*(\Omega) \\
&= \int d\Omega \sum_{LM_L} \sqrt{\frac{(2l+1)(2l'+1)}{4\pi(2L+1)}} \langle lm_l l' m'_l | LM \rangle \langle l0l'0|L0 \rangle Y_{LM}(\Omega) \\
&\quad \sum_{KM_K} \sqrt{\frac{(2k+1)(2k'+1)}{4\pi(2K+1)}} \langle km_k k' m'_k | KM_K \rangle \langle k0k'0|K0 \rangle Y_{KM_K}^*(\Omega) \\
&= \sum_{LM_L} \sqrt{\frac{(2l+1)(2l'+1)}{4\pi(2L+1)}} \sqrt{\frac{(2k+1)(2k'+1)}{4\pi(2L+1)}} \langle lm_l l' m'_l | LM \rangle \langle l0l'0|L0 \rangle \langle km_k k' m'_k | LM_L \rangle \langle k0k'0|L0 \rangle
\end{aligned}$$

So we get for the one-body momentum matrix element,

$$\begin{aligned}
\langle A | \hat{n}^{[1]}(\vec{p}_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} 64\sqrt{2}\pi \sum_{km_k} \sum_{k'm'_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^{k'+K} i^{k+k'+K+K'} Y_{km_k}^*(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1}) \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{kK\dagger}(p_1, P_{12}) \chi_{q,n'l'}^{k'K'}(p_1, P_{12}) \\
&\sum_{m_l m_s} \langle l m_l S m_s | j m_j \rangle \sqrt{\frac{(2l+1)(2K+1)}{4\pi(2k+1)}} \langle l m_l K M_K | k m_k \rangle \langle l 0 K 0 | k 0 \rangle \\
&\sum_{m'_l m'_s} \langle l' m'_l S' m'_s | j' m'_j \rangle \sqrt{\frac{(2l'+1)(2K'+1)}{4\pi(2k'+1)}} \langle l' m'_l K' M'_K | k' m'_k \rangle \langle l' 0 K' 0 | k' 0 \rangle \\
&\sum_{JM_J} \sqrt{\frac{(2L'+1)(2K+1)}{4\pi(2J+1)}} \langle L' M'_L K M_K | J M_J \rangle \langle L' 0 K 0 | J 0 \rangle \\
&\sqrt{\frac{(2L+1)(2K'+1)}{4\pi(2J+1)}} \langle L M_L K' M'_K | J M \rangle \langle L 0 K' 0 | J 0 \rangle
\end{aligned}$$

Introducing the notation  $\hat{j} = \sqrt{2j+1}$  we get,

$$\begin{aligned}
\langle A | \hat{n}^{[1]}(\vec{p}_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} \frac{4\sqrt{2}}{\pi} \sum_{km_k} \sum_{k'm'_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^{k'+K} i^{k+k'+K+K'} Y_{km_k}^*(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1}) \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{kK\dagger}(p_1, P_{12}) \chi_{q,n'l'}^{k'K'}(p_1, P_{12}) \\
&\sum_{m_l m_s} \langle l m_l S m_s | j m_j \rangle \frac{\hat{l}\hat{K}}{\hat{k}} \langle l m_l K M_K | k m_k \rangle \langle l 0 K 0 | k 0 \rangle \\
&\sum_{m'_l m'_s} \langle l' m'_l S' m'_s | j' m'_j \rangle \frac{\hat{l}'\hat{K}'}{\hat{k}'} \langle l' m'_l K' M'_K | k' m'_k \rangle \langle l' 0 K' 0 | k' 0 \rangle \\
&\sum_{JM_J} \frac{\hat{K}\hat{L}\hat{K}'\hat{L}'}{\hat{j}^2} \langle L' M'_L K M_K | J M_J \rangle \langle L' 0 K 0 | J 0 \rangle \langle L M_L K' M'_K | J M \rangle \langle L 0 K' 0 | J 0 \rangle
\end{aligned}$$

Integration over the ob-momentum angle  $\Omega_{p_1}$  gives  $\delta_{kk'}\delta_{m_k m'_k}$ ,

$$\begin{aligned}
\langle A | \hat{n}^{[1]}(p_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} \frac{4\sqrt{2}}{\pi} \sum_{km_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^K i^{K+K'} \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{kK\dagger}(p_1, P_{12}) \chi_{q,n'l'}^{k'K'}(p_1, P_{12}) \\
&\sum_{m_l m_s} \langle l m_l S m_s | j m_j \rangle \frac{\hat{l}\hat{K}}{\hat{k}} \langle l m_l K M_K | k m_k \rangle \langle l 0 K 0 | k 0 \rangle \\
&\sum_{m'_l m'_s} \langle l' m'_l S' m'_s | j' m'_j \rangle \frac{\hat{l}'\hat{K}'}{\hat{k}'} \langle l' m'_l K' M'_K | k m_k \rangle \langle l' 0 K' 0 | k 0 \rangle \\
&\sum_{JM_J} \frac{\hat{K}\hat{L}\hat{K}'\hat{L}'}{\hat{j}^2} \langle L' M'_L K M_K | J M_J \rangle \langle L' 0 K 0 | J 0 \rangle \langle L M_L K' M'_K | J M_J \rangle \langle L 0 K' 0 | J 0 \rangle
\end{aligned}$$

To cross check this result with Maartens (D.37) we write the CGC coefficients as Wigner-3j symbols,

$$\begin{aligned}
\langle j_1 m_1 j_2 m_2 | JM \rangle &= (-1)^{j_1 - j_2 + M} \hat{J} \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix} \\
\langle A | \hat{n}^{[1]}(p_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} \frac{4\sqrt{2}}{\pi} \sum_{km_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^K i^{K+K'} \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{kK\uparrow}(p_1, P_{12}) \chi_{q,n'l'}^{kK'}(p_1, P_{12}) \\
&\sum_{m_l m_S} (-1)^{l-S+m_j} \hat{j} \begin{pmatrix} l & S & j \\ m_l & m_S & -m_j \end{pmatrix} \frac{\hat{l}\hat{K}}{\hat{k}} (-1)^{l-K+m_k} \hat{k} \begin{pmatrix} l & K & k \\ m_l & M_K & -m_k \end{pmatrix} (-1)^{l-K} \hat{k} \begin{pmatrix} l & K & k \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{m'_l m'_S} (-1)^{l'-S'+m'_j} \hat{j}' \begin{pmatrix} l' & S' & j' \\ m'_l & m'_S & -m'_j \end{pmatrix} \frac{\hat{l}'\hat{K}'}{\hat{k}'} (-1)^{l'-K'+m_k} \hat{k}' \begin{pmatrix} l' & K' & k \\ m'_l & M'_K & -m_k \end{pmatrix} (-1)^{l'-K'} \hat{k}' \begin{pmatrix} l' & K' & k \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{JM_J} \frac{\hat{K}\hat{L}\hat{K}'\hat{L}'}{\hat{J}^2} (-1)^{L'-K+M_J} \hat{J} \begin{pmatrix} L' & K & J \\ M'_L & M_K & -M_J \end{pmatrix} (-1)^{L'-K} \begin{pmatrix} L' & K & J \\ 0 & 0 & 0 \end{pmatrix} \\
&(-1)^{L-K'+M_J} \hat{J} \begin{pmatrix} L & K' & J \\ M_L & M'_K & -M_J \end{pmatrix} (-1)^{L-K'} \begin{pmatrix} L & K' & J \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

As  $m_k, M_J$  are sum indices we can safely flip the sign of these.

$$\begin{aligned}
\langle A | \hat{n}^{[1]}(p_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} \frac{4\sqrt{2}}{\pi} \sum_{km_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^{-K+l+l'-S-S'+m_j+m'_j} i^{K+K'} \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{kK\uparrow}(p_1, P_{12}) \chi_{q,n'l'}^{kK'}(p_1, P_{12}) \\
&\sum_{m_l m_S} \hat{j}\hat{l}\hat{K}\hat{k} \begin{pmatrix} l & S & j \\ m_l & m_S & -m_j \end{pmatrix} \begin{pmatrix} l & K & k \\ m_l & M_K & m_k \end{pmatrix} \begin{pmatrix} l & K & k \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{m'_l m'_S} \hat{j}'\hat{l}'\hat{K}'\hat{k}' \begin{pmatrix} l' & S' & j' \\ m'_l & m'_S & -m'_j \end{pmatrix} \begin{pmatrix} l' & K' & k \\ m'_l & M'_K & m_k \end{pmatrix} \begin{pmatrix} l' & K' & k \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{JM_J} \hat{K}\hat{L}\hat{K}'\hat{L}' \begin{pmatrix} L' & K & J \\ M'_L & M_K & M_J \end{pmatrix} \begin{pmatrix} L' & K & J \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & K' & J \\ M_L & M'_K & M_J \end{pmatrix} \begin{pmatrix} L & K' & J \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

To make the comparison with (D.37) easier we swap variables:  $JM_J \rightarrow qm_q$ ,  $KM_K \rightarrow km_k$ ,  $K'M'_K \rightarrow k'm'_k$ ,  $km_k \rightarrow l_1 m_{l_1}$

$$\begin{aligned}
\langle A | \hat{n}^{[1]}(p_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} \frac{4\sqrt{2}}{\pi} \sum_{l_1 m_{l_1}} \sum_{km_k} \sum_{k'm'_k} (-1)^{-k+l+l'-S-S'+m_j+m'_j} i^{k+k'} \\
&\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{l_1 k\uparrow}(p_1, P_{12}) \chi_{q,n'l'}^{l_1 k'}(p_1, P_{12}) \\
&\sum_{m_l m_S} \hat{j}\hat{l}\hat{k}\hat{l}_1 \begin{pmatrix} l & S & j \\ m_l & m_S & -m_j \end{pmatrix} \begin{pmatrix} l & k & l_1 \\ m_l & m_k & m_{l_1} \end{pmatrix} \begin{pmatrix} l & k & l_1 \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{m'_l m'_S} \hat{j}'\hat{l}'\hat{k}'\hat{l}_1 \begin{pmatrix} l' & S' & j' \\ m'_l & m'_S & -m'_j \end{pmatrix} \begin{pmatrix} l' & k' & l_1 \\ m'_l & m'_k & m_{l_1} \end{pmatrix} \begin{pmatrix} l' & k' & l_1 \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{qm_q} \hat{k}\hat{L}\hat{k}'\hat{L}' \begin{pmatrix} L' & k & q \\ M'_L & m_k & m_q \end{pmatrix} \begin{pmatrix} L' & k & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & k' & q \\ M_L & m'_k & m_q \end{pmatrix} \begin{pmatrix} L & k' & q \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

Finally we make use of

$$\begin{pmatrix} l & k & l_1 \\ m_l & m_k & m_{l_1} \end{pmatrix} \begin{pmatrix} l & k & l_1 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} l & l_1 & k \\ m_l & m_{l_1} & m_k \end{pmatrix} \begin{pmatrix} l & l_1 & k \\ 0 & 0 & 0 \end{pmatrix}$$

and compare our expression against (D.37) (using a final “trick”  $(-1)^{-k} = i^{-2k}$ ). Parts that are not found in (D.37) are colored **red**. Parts in (D.37) not appearing here are colored **blue**.

$$\begin{aligned} \langle A | \hat{n}^{[1]}(p_1) | A' \rangle &= \mathcal{M}_{AA'}^{p,q} \frac{4\sqrt{2}}{\pi} \sum_{l_1 m_{l_1}} \sum_{k m_k} \sum_{k' m'_k} (-1)^{l+l' - \textcolor{red}{S} - \textcolor{red}{S}' + m_j + m'_j} i^{\textcolor{blue}{L}_A + \textcolor{blue}{L}_B + k' - k} \hat{l}_1^2 \hat{k}^2 \hat{k}'^2 \hat{l} \hat{l}' \hat{L} \hat{L}' \hat{j} \hat{j}' \\ &\int dP_{12} P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi_{p,nl}^{l_1 k \dagger}(p_1, P_{12}) \chi_{q,n'l'}^{l_1 k'}(p_1, P_{12}) \\ &\sum_{m_l m_S} \begin{pmatrix} l & \textcolor{red}{S} & j \\ m_l & m_S & -m_j \end{pmatrix} \begin{pmatrix} l & l_1 & k \\ m_l & m_{l_1} & m_k \end{pmatrix} \begin{pmatrix} l & l_1 & k \\ 0 & 0 & 0 \end{pmatrix} \\ &\sum_{m'_l m'_S} \begin{pmatrix} l' & \textcolor{red}{S}' & j' \\ m'_l & m'_S & -m'_j \end{pmatrix} \begin{pmatrix} l' & l_1 & k' \\ m'_l & m_{l_1} & m'_k \end{pmatrix} \begin{pmatrix} l' & l_1 & k' \\ 0 & 0 & 0 \end{pmatrix} \\ &\sum_{q m_q} \begin{pmatrix} L' & k & q \\ M'_L & m_k & m_q \end{pmatrix} \begin{pmatrix} L' & k & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & k' & q \\ M_L & m'_k & m_q \end{pmatrix} \begin{pmatrix} L & k' & q \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

In the case that Maarten has simply omitted the LS coupling but than there should **not** be  $(-1)^{l+l'm_j+m'_j}$  as this stems from the 3j LS coupling symbol.