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,

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

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

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

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

$$\langle\Phi|a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}}|\Phi\rangle = \int \mathrm{d}^3\mathbf{p}_1 \dots \mathrm{d}^3\mathbf{p}_A \langle\Phi|\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A\rangle \langle\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A|a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}}|\Phi\rangle \tag{3}$$

$$= \int \mathrm{d}^A\mathbf{p}_1 \dots \mathrm{d}^3\mathbf{p}_A \langle\Phi|\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A\rangle \langle 0|a_{\mathbf{p}_1} a_{\mathbf{p}_2}\dots a_{\mathbf{p}_A} a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}}|\Phi\rangle \tag{4}$$

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

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

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

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

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

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

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

Hence,

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

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

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

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

$$a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}} |\Phi\rangle = a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}} |\alpha_1\alpha_2\dots\alpha_A\rangle = a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}} a^{\dagger}_{\alpha_1} a^{\dagger}_{\alpha_2}\dots a^{\dagger}_{\alpha_A} |0\rangle \tag{13}$$

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

$$a^\dagger_{\alpha_i} = \int \mathrm{d}^3\mathbf{k}\phi_{\alpha_i}(\mathbf{k})a^\dagger_k \tag{14}$$

$$\Rightarrow a_{\mathbf{p}}a^\dagger_{\alpha_i} = \int \mathrm{d}^3\mathbf{k}\phi_{\alpha_i}(\mathbf{k})a_{\mathbf{p}}a^\dagger_{\mathbf{k}} = \phi_{\alpha_i}(\mathbf{p}) - a^\dagger_{\alpha_i}a_{\mathbf{p}} \tag{15}$$

So,

$$\begin{aligned} a_{\mathbf{p}}\left|\Phi\right\rangle &= a_{\mathbf{p}}a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_A}\left|0\right\rangle = (\phi_{\alpha_1}(\mathbf{p}) - a^\dagger_{\alpha_1}a_{\mathbf{p}})a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_A}\left|0\right\rangle & (16)\\ &= \sum_{i=1}^{A}(-1)^{i-1}\phi_{\alpha_i}(\mathbf{p})\left|\alpha_1\dots\alpha_{i-1}\alpha_{i+1}\dots\alpha_A\right\rangle & (17)\end{aligned}$$

The conjugate gives,

$$\left\langle\Phi\right| a^\dagger_{\mathbf{p}} = \sum_{j=1}^{A}(-1)^{j-1}\left\langle\alpha_1\dots\alpha_{j-1}\alpha_{j+1}\dots\alpha_A\right|\phi^\dagger_{\alpha_j}(\mathbf{p}) \tag{18}$$

Hence,

$$\begin{aligned} \langle\Phi|a^\dagger_{\mathbf{p}}a_{\mathbf{p}}|\Phi\rangle &= \sum_{i,j=1}^{A}(-1)^{i+j}\phi^\dagger_{\alpha_j}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p})\underbrace{\langle\alpha_1\dots\alpha_{j-1}\alpha_{j+1}\dots\alpha_A|\alpha_1\dots\alpha_{i-1}\alpha_{i+1}\dots\alpha_A\rangle}_{=\delta_{ij}} & (19)\\ &= \sum_i \phi^\dagger_{\alpha_i}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p}) & (20)\end{aligned}$$

Which is exactly the same result as before.

So the one body momentum distribution is given by,

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

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,

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

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

$$|\alpha_1, \alpha_2\rangle_{\mathrm{nas}} \quad , |\alpha\rangle \equiv |nljm_j t m_t\rangle \tag{23}$$

The class calculates all the coefficients,

$$C^A_{\alpha_1\alpha_2} = \langle A \equiv \{nlSjm_j, NLM_L TM_T\} | \alpha_1 \alpha_2 \rangle \tag{24}$$

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 seperated. 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 brakets. The only function in this class is to calculate $C^A_{\alpha_1\alpha_2}$ using the formula,

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

It is easy to check that the result indeed depends on α_1, α_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,

$$\langle \alpha_1\alpha_2 | \hat{\mathcal{O}} | \alpha_1\alpha_2\rangle = \sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^B_{\alpha_1\alpha_2} \langle A | \hat{\mathcal{O}} | B\rangle \tag{26}$$

We want to calculate matrix elements as $\langle A|\hat{\mathcal{O}}|B\rangle$ only once. $|\alpha_1\alpha_2\rangle$ that map to the same A, B states should lookup the earlier calculated values for $\langle A|\hat{\mathcal{O}}|B\rangle$. In general the matrix element $\langle A|\hat{\mathcal{O}}|B\rangle$ 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 $\langle A|\hat{\mathcal{O}}|B\rangle$. The value for the transformation coefficients $C^{A,\dagger}_{\alpha_1,\alpha_2} C^{B}_{\alpha_1,\alpha_2}$ is stored in the second field of the map (`double`). So that the the summation over B (Eq. 26) is replaced by,

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

`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 $\hat{\wr}$ between the bras and kets.

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

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

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

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

$$\langle n(lS)jm_jNLM_LTM_T|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger f_q\hat{\mathcal{O}}^q|n'(l'S')j'm_j'N'L'M_L'T'M_T'\rangle$$

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

$$\delta_{NN'}\delta_{LL'}\delta_{M_LM_L'}\,\langle n(lS)jm_jTM_T|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger f_q\hat{\mathcal{O}}^q|n'(l'S')j'm_j'T'M_T'\rangle$$

Let us now take a look at the separate cases for $\delta_{NN'}\delta_{LL'}\delta_{M_LM_L'}\,\langle n(lS)jm_jTM_T|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger f_q\hat{\mathcal{O}}^q|n'(l'S')j'm_j'T'M_T'\rangle$,

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

$$\begin{aligned}&\delta_{NN'}\delta_{LL'}\delta_{M_LM_L'}\,\langle n(lS)jm_jTM_T|f_c(r_{12})|n'(l'S')j'm_j'T'M_T'\rangle\\ &\qquad\qquad = \delta_{NN'}\delta_{LL'}\delta_{M_LM_L'}\delta_{SS'}\delta_{jj'}\delta_{m_jm_j'}\delta_{TT'}\delta_{M_TM_T'}\delta_{ll'}\,\langle nl|f_c(r_{12})|n'l'\rangle\end{aligned}$$

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

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 $\nu = M_N\omega/\hbar$.

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

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, $L_n^l(r) = \sum_k a_{nl,k} r^k$,

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

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

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

$K = 2 + l + l' + \lambda + 2k + 2k'$. 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_λ is the λ'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 $b_\lambda = \delta_{\lambda,0}$, $b = 0$.

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

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

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

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

6 Matrix elements bis

Let us take a look at

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

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

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,

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

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

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

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

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

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

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

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,

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

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

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

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

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

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

$$\langle TM_T|\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2|T'M_T'\rangle$$

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\langle 1,\pm1|\hat{\delta}^{[1]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[1]}_{m_t}|1,\pm1\rangle = \langle 1,\pm1|\hat{\delta}^{[2]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[2]}_{m_t}|1,\pm1\rangle &= \delta_{\pm1,2m_t} \\
\langle 1,0|\hat{\delta}^{[1]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[1]}_{m_t}|1,0\rangle = \langle 0,0|\hat{\delta}^{[1]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[1]}_{m_t}|0,0\rangle &= -\frac{1}{2} \\
\langle 1,0|\hat{\delta}^{[1]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[1]}_{m_t}|0,0\rangle = \langle 0,0|\hat{\delta}^{[1]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[1]}_{m_t}|1,0\rangle &= -\frac{1}{2}2m_t \\
\langle 1,0|\hat{\delta}^{[2]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[2]}_{m_t}|1,0\rangle = \langle 0,0|\hat{\delta}^{[2]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[2]}_{m_t}|0,0\rangle &= -\frac{1}{2} \\
\langle 1,0|\hat{\delta}^{[2]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[2]}_{m_t}|0,0\rangle = \langle 0,0|\hat{\delta}^{[2]}_{m_t}\hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2\hat{\delta}^{[2]}_{m_t}|1,0\rangle &= \frac{1}{2}2m_t
\end{aligned}$$

These matrix element have been checked with a simple python program (`numpy.kron` ftw 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 $\langle 1, 0| \ldots |0, 0\rangle$ or $\langle 0, 0| \ldots |1, 0\rangle$ is involved.

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. $\frac{2}{A}\sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A|B\rangle$ for a pp and/or nn pair(s) (isospin $M_T = \pm1$)
  2. $\frac{1}{A}\sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A|B\rangle$ 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 $\sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A|B\rangle$ ...

  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` $\neq$ `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 $\sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A|B\rangle = \sum_A |C^{A}_{\alpha_1\alpha_2}|^2$ 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 $\sum_{\texttt{pair in pairs}}$ `norm::ob_get_me(pair,...)` 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}Al with 13 protons and 14 neutrons has an open $1d\frac{5}{2}$ 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

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

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

$$\chi^{kK}_{p,nl}(p_1, P) = \int \mathrm{d}r\, r^2 f_p(r) R_{nl}(r) j_k(\sqrt{2}p_1 r) j_K(Pr)$$

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 $\nu = M_N\omega/\hbar$,

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

Expanding the Generalized-Laguerre polynomials gives,

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

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

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

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 $\hat{n}^{[1]}(\vec{p})$.

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

The one-body momentum operator is given by,

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

Hence,

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

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

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

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,

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

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

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 $\mathcal{M}^{p,q}_{AA'}$.

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

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

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

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 $\psi_{nlm_l}(\vec{r}) = R_{nl}(r) Y_{lm_l}(\Omega_r)$, $\psi_{nlm_l}(\vec{p}) = \Pi_{NL}(p) Y_{lm_l}(\Omega_p)$, $\psi_{n(lS)jm_j}(\vec{r}) = R_{nl}(r) \mathcal{Y}_{(lS)jm_j}(\Omega_r)$.

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

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

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

$$
\chi^{kK}_{p,nl}(p_1, P) = \int \mathrm{d}r\, r^2 f_p(r) R_{nl}(r) j_k(\sqrt{2}p_1 r) j_K(Pr)
$$

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

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

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

and,

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

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

$$\begin{aligned}\langle A|\hat{n}^{[1]}(\vec{p}_1)|A'\rangle = \mathcal{M}^{p,q}_{AA'} 64\sqrt{2}\pi &\sum_{km_k}\sum_{k'm'_k}\sum_{KM_K}\sum_{K'M'_K} (-1)^{k'+K} i^{k+k'+K+K'}\, Y^*_{km_k}(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1}) \\ &\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl}(p_1, P_{12}) \chi^{k'K'}_{q,n'l'}(p_1, P_{12}) \\ &\sum_{m_l m_S} \langle lm_l Sm_S|jm_j\rangle \sqrt{\frac{(2l+1)(2K+1)}{4\pi(2k+1)}}\, \langle lm_l KM_K|km_k\rangle\, \langle l0K0|k0\rangle \\ &\sum_{m'_l m'_S} \langle l'm'_l S'm'_S|j'm'_j\rangle \sqrt{\frac{(2l'+1)(2K'+1)}{4\pi(2k'+1)}}\, \langle l'm'_l K'M'_K|k'm'_k\rangle\, \langle l'0K'0|k'0\rangle \\ &\sum_{JM_J} \sqrt{\frac{(2L'+1)(2K+1)}{4\pi(2J+1)}}\, \langle L'M'_L KM_K|JM_J\rangle\, \langle L'0K0|J0\rangle \\ &\sqrt{\frac{(2L+1)(2K'+1)}{4\pi(2J+1)}}\, \langle LM_L K'M'_K|JM\rangle\, \langle L0K'0|J0\rangle\end{aligned}$$

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

$$\langle A|\hat{n}^{[1]}(\vec{p}_1)|A'\rangle = \mathcal{M}^{p,q}_{AA'} \frac{4\sqrt{2}}{\pi} \sum_{km_k} \sum_{k'm'_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^{k'+K} i^{k+k'+K+K'} Y^*_{km_k}(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1})$$

$$\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl}(p_1, P_{12}) \chi^{k'K'}_{q,n'l'}(p_1, P_{12})$$

$$\sum_{m_l m_S} \langle l m_l S m_S | j m_j \rangle \frac{\hat{l}\hat{K}}{\hat{k}} \langle l m_l K M_K | k m_k \rangle \langle l 0 K 0 | k 0 \rangle$$

$$\sum_{m'_l m'_S} \langle l' m'_l S' m'_S | j' m'_j \rangle \frac{\hat{l}'\hat{K}'}{\hat{k}'} \langle l' m'_l K' M'_K | k' m'_k \rangle \langle l' 0 K' 0 | k' 0 \rangle$$

$$\sum_{JM_J} \frac{\hat{K}\hat{L}\hat{K}'\hat{L}'}{\hat{J}^2} \langle L' M'_L K M_K | J M_J \rangle \langle L' 0 K 0 | J 0 \rangle \langle L M_L K' M'_K | J M \rangle \langle L 0 K' 0 | J 0 \rangle$$

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

$$\langle A|\hat{n}^{[1]}(p_1)|A'\rangle = \mathcal{M}^{p,q}_{AA'} \frac{4\sqrt{2}}{\pi} \sum_{km_k} \sum_{KM_K} \sum_{K'M'_K} (-1)^{K} i^{K+K'}$$

$$\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl}(p_1, P_{12}) \chi^{kK'}_{q,n'l'}(p_1, P_{12})$$

$$\sum_{m_l m_S} \langle l m_l S m_S | j m_j \rangle \frac{\hat{l}\hat{K}}{\hat{k}} \langle l m_l K M_K | k m_k \rangle \langle l 0 K 0 | k 0 \rangle$$

$$\sum_{m'_l m'_S} \langle l' m'_l S' m'_S | j' m'_j \rangle \frac{\hat{l}'\hat{K}'}{\hat{k}} \langle l' m'_l K' M'_K | k m_k \rangle \langle l' 0 K' 0 | k 0 \rangle$$

$$\sum_{JM_J} \frac{\hat{K}\hat{L}\hat{K}'\hat{L}'}{\hat{J}^2} \langle L' M'_L K M_K | J M_J \rangle \langle L' 0 K 0 | J 0 \rangle \langle L M_L K' M'_K | J M_J \rangle \langle L 0 K' 0 | J 0 \rangle$$

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

$$\langle j_1 m_1 j_2 m_2 | J M \rangle = (-1)^{j_1 - j_2 + M} \hat{J} \begin{pmatrix} j1 & j2 & J \\ m_1 & m_2 & -M \end{pmatrix}$$

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

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

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

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

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

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.

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

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.