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 $|0\rangle$.

$$\begin{aligned} \langle \Phi | a^\dagger_{\mathbf{p}} a_{\mathbf{p}} | \Phi \rangle &= \int \mathrm{d}^3\mathbf{p}_1 \ldots \mathrm{d}^3\mathbf{p}_A \langle \Phi | \mathbf{p}_1 \mathbf{p}_2 \ldots \mathbf{p}_A \rangle \langle \mathbf{p}_1 \mathbf{p}_2 \ldots \mathbf{p}_A | a^\dagger_{\mathbf{p}} a_{\mathbf{p}} | \Phi \rangle & (3) \\ &= \int \mathrm{d}^A\mathbf{p}_1 \ldots \mathrm{d}^3\mathbf{p}_A \langle \Phi | \mathbf{p}_1 \mathbf{p}_2 \ldots \mathbf{p}_A \rangle \langle 0 | a_{\mathbf{p}_1} a_{\mathbf{p}_2} \ldots a_{\mathbf{p}_A} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} | \Phi \rangle & (4) \end{aligned}$$

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

$$\begin{aligned} \langle 0 | a_{\mathbf{p}_1} a_{\mathbf{p}_2} \ldots a_{\mathbf{p}_A} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} | \Phi \rangle &= \langle 0 | a_{\mathbf{p}_1} a_{\mathbf{p}_2} \ldots \delta(\mathbf{p} - \mathbf{p}_A) a_{\mathbf{p}} | \Phi \rangle - \langle 0 | a_{\mathbf{p}_1} a_{\mathbf{p}_2} \ldots a_{\mathbf{p}_{A-1}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}_A} a_{\mathbf{p}} | \Phi \rangle & (5) \\ &= \delta(\mathbf{p} - \mathbf{p}_A) \langle \mathbf{p}_1 \mathbf{p}_2 \ldots \mathbf{p} | \Phi \rangle - \delta(\mathbf{p} - \mathbf{p}_{A-1}) \langle 0 | a_{\mathbf{p}_1} \ldots a_{\mathbf{p}_{A-2}} a_{\mathbf{p}_A} a_{\mathbf{p}} | \Phi \rangle & (6) \\ &+ \langle 0 | a_{\mathbf{p}_1} \ldots a_{\mathbf{p}_{A-2}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}_{A-1}} a_{\mathbf{p}_A} a_{\mathbf{p}} | \Phi \rangle & (7) \\ &= \delta(\mathbf{p} - \mathbf{p}_A) \langle \mathbf{p}_1 \mathbf{p}_2 \ldots \mathbf{p}_A | \Phi \rangle + \delta(\mathbf{p} - \mathbf{p}_{A-1}) \langle \mathbf{p}_1 \ldots \mathbf{p}_{A-2} \mathbf{p}_{A-1} \mathbf{p}_A | \Phi \rangle & (8) \\ &+ \langle 0 | a_{\mathbf{p}_1} \ldots a_{\mathbf{p}_{A-2}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}_{A-1}} a_{\mathbf{p}_A} a_{\mathbf{p}} | \Phi \rangle \qquad = \ldots & (9) \\ &= \sum_{i=1}^{A} \delta(\mathbf{p} - \mathbf{p}_i) \langle \mathbf{p}_1 \ldots \mathbf{p}_A | \Phi \rangle + (-1)^A \underbrace{\langle 0 | a^\dagger_{\mathbf{p}} a_{\mathbf{p}_1} \ldots a_{\mathbf{p}_A} a_{\mathbf{p}} | \Phi \rangle}_{=0} & (10) \end{aligned}$$

Hence,

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

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,

$$a^\dagger_{\mathbf{p}} a_{\mathbf{p}} |\Phi\rangle = a^\dagger_{\mathbf{p}} a_{\mathbf{p}} |\alpha_1 \alpha_2 \ldots \alpha_A\rangle = a^\dagger_{\mathbf{p}} a_{\mathbf{p}} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_A} |0\rangle \tag{13}$$

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,

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

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

The conjugate gives,

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

Hence,

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

$$= \sum_{i}\phi^{\dagger}_{\alpha_i}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p}) \tag{20}$$

Which is exactly the same result as before.

So the one body momentum distribution is given by,

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

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

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

The class calculates all the coefficients,

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

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,

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

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,

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

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,

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

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

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

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

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

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 $\hat{\delta}^{[1]}_{m_t} = (1 + (2m_t)\hat{t}_{i,0})/2$ we get,

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

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

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

We now investigate the effect of the insertion of the isospin-projection operator $\hat{\delta}^{[i]}_{m_t}$ 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 $\langle T M_T | \hat{\vec{\tau}}_1 \cdot \hat{\vec{\tau}}_2 \hat{\delta}^{[i]}_{m_t} | T' M'_T \rangle$ 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),

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

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

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

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,

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

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

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

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. 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. $\frac{2}{A}\sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A|B\rangle$ for a pp and/or nn pair(s) (isospin $M_T = \pm 1$)
  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 $R_{nl}(r) = N_{nl}\nu^{\frac{l+3/2}{2}} r^l e^{-\nu r^2/2} L^{l+1/2}_n(\nu r^2)$ and $\nu = M_N\omega/\hbar$,

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

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 $\hat{n}^{[1]}_{s,t}(\vec{p})$. s is the spin projection of the nucleon and t the isospin projection.

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

The one-body momentum operator is given by,

$$\begin{aligned}\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1) = |\vec{p}_1 s_1 t_1\rangle\langle\vec{p}_1 s_1 t_1| &= \sum_{s_2,t_2}\int \mathrm{d}^3\vec{p}_2\, n^{[2]}_{\substack{s_1,t_1\\s_2,t_2}}(\vec{p}_1,\vec{p}_2)\\ &= \sum_{s_2,t_2}\int \mathrm{d}^3\vec{p}_2\, |\vec{p}_1 s_1 t_1, \vec{p}_2 s_2 t_2\rangle\langle\vec{p}_1 s_1 t_1, \vec{p}_2 s_2 t_2|\end{aligned}$$

Hence,

Do spin projection before inserting coordinates

$$\begin{aligned}\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle &= \sum_{s_2,t_2}\int \mathrm{d}^3\vec{p}_2\,\langle A|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger|\vec{p}_1 s_1 t_1,\vec{p}_2 s_2 t_2\rangle\langle\vec{p}_1 s_1 t_1,\vec{p}_2 s_2 t_2|f_q\hat{\mathcal{O}}^q|A'\rangle\\ &= \sum_{s_2,t_2}\int \mathrm{d}^3\vec{p}_2 \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2\mathrm{d}^3\vec{r}_1{}'\mathrm{d}^3\vec{r}_2{}'\\ &\quad \langle A|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger|\vec{r}_1 s_1 t_1,\vec{r}_2 s_2 t_2\rangle\langle\vec{r}_1\vec{r}_2|\vec{p}_1\vec{p}_2\rangle\langle\vec{p}_1\vec{p}_2|\vec{r}_1{}'\vec{r}_2{}'\rangle\langle\vec{r}_1{}' s_1 t_1,\vec{r}_2{}' s_2 t_2|f_q\hat{\mathcal{O}}^q|A'\rangle\end{aligned}$$

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

$$\begin{aligned}\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \frac{1}{(2\pi)^6}\sum_{s_2,t_2}\int &\mathrm{d}^3\vec{p}_2\mathrm{d}^3\vec{R}_{12}\mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{R}_{12}'\mathrm{d}^3\vec{r}_{12}' e^{i\vec{p}_1\cdot(\vec{r}_1-\vec{r}_1{}')}e^{i\vec{p}_2\cdot(\vec{r}_2-\vec{r}_2{}')}\\ &\langle A|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger|\vec{R}_{12}s_1t_1,\vec{r}_{12}s_2t_2\rangle\langle\vec{R}_{12}'s_1t_1\vec{r}_{12}'s_2t_2|f_q\hat{\mathcal{O}}^q|A'\rangle\end{aligned}$$

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,

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

$$\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \frac{\sqrt{8}}{(2\pi)^3}\sum_{s_2,t_2}\int \mathrm{d}^3\vec{R}_{12}\mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}'_{12}e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}'_{12})}$$
$$\langle A|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger|\vec{R}_{12}s_1t_1,\vec{r}_{12}s_2t_2\rangle\,\langle\vec{R}'_{12}s_1t_1,\vec{r}'_{12}s_2t_2|f_q\hat{\mathcal{O}}^q|A'\rangle\Big|_{\vec{R}'_{12}=\vec{R}_{12}-\vec{r}_{12}+\vec{r}'_{12}}$$

Let us investigate the matrix element with the operators $\hat{\mathcal{O}}^{p,q}$ (central,tensor or spin-isospin) and the spin/isospin projections s_1,t_1,s_2,t_2 in detail:

$$\sum_{s_2,t_2}\langle A|\hat{\mathcal{O}}^{p\dagger}|s_1t_1,s_2t_2\rangle\,\langle s_1t_1,s_2t_2|\hat{\mathcal{O}}^q|A'\rangle$$

Using the expressions for $\hat{\mathcal{O}}^p\,|A'\rangle$ (??) this becomes,

$$\sum_{s_2,t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^q(S',T',j',l',l'_q)$$
$$\langle n(l_pS)jm_jNLM_LTM_T|s_1t_1,s_2t_2\rangle\,\langle s_1t_1,s_2t_2|n'(l'_qS')j'm'_jN'L'M'_LT'M'_T\rangle$$

with

$$\begin{aligned}\langle\frac{1}{2}s_1\frac{1}{2}s_2|(lS)jm_j\rangle &= \sum_{m_lm_s}\langle lm_lSm_S|jm_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|Sm_S\rangle\,|lm_l\rangle\\ &= \langle lm_lSm_S|jm_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|Sm_S\rangle\,|lm_l\rangle\Big|_{\substack{m_S=s_1+s_2\\ m_l=m_j-s_1-s_2}}\end{aligned}$$

We get,

$$\sum_{s_2,t_2}\langle A|\hat{\mathcal{O}}^{p\dagger}|s_1t_1,s_2t_2\rangle\,\langle s_1t_1,s_2t_2|\hat{\mathcal{O}}^q|A'\rangle =$$
$$\sum_{s_2,t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^q(S',T',j',l',l'_q)$$
$$\langle\frac{1}{2}t_1\frac{1}{2}t_2|TM_T\rangle\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|T'M'_T\rangle$$
$$\langle l_pm_{l_p}Sm_S|jm_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|Sm_S\rangle\,\langle l_pm_{l_p}|\,\langle l'_qm'_{l_q}S'm'_S|j'm'_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|S'm'_S\rangle\,|l'_qm'_{l_q}\rangle$$

$$\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \sum_{s_2,t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^q(S',T',j',l',l'_q)\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|TM_T\rangle\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|T'M'_T\rangle$$
$$\langle l_pm_{l_p}Sm_S|jm_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|Sm_S\rangle\,\langle l'_qm'_{l_q}S'm'_S|j'm'_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|S'm'_S\rangle$$
$$\frac{\sqrt{8}}{(2\pi)^3}\int\mathrm{d}^3\vec{R}_{12}\mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}'_{12}e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}'_{12})}f_p^\dagger(r_{12})f_q(r'_{12})$$
$$\psi^\dagger_{NLM_L}(\vec{R}_{12})\psi^\dagger_{nl_pm_{l_p}}(\vec{r}_{12})\psi_{N'L'M'_L}(\vec{R}'_{12})\psi_{n'l'_qm_{l'_q}}(\vec{r}'_{12})\Big|_{\substack{\vec{R}'_{12}=\vec{R}_{12}-\vec{r}_{12}+\vec{r}'_{12}\\ m_{l_p}=m_j-s_1-s_2\\ m_{l'_q}=m'_j-s_1-s_2}}$$

For the sake of brevity we define,

$$\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2) = \mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^{q}(S',T',j',l',l'_q)\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|TM_T\rangle\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|T'M'_T\rangle$$
$$\langle l_p m_{l_p} S m_S|j m_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|S m_S\rangle\,\langle l'_q m'_{l_q} S' m'_S|j' m'_j\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|S' m'_S\rangle$$

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

$$\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \sum_{s_2 t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$\frac{\sqrt{8}}{(2\pi)^3}\int \mathrm{d}^3\vec{R}_{12}\mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}\,'_{12}e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}\,'_{12})}f^\dagger_p(r_{12})f_q(r'_{12})\psi^\dagger_{nl_p m_{l_p}}(\vec{r}_{12})\psi_{n'l'_q m_{l'_q}}(\vec{r}\,'_{12})$$
$$\frac{1}{(2\pi)^3}\int \mathrm{d}^3\vec{P}_{12}\int \mathrm{d}^3\vec{P}\,'_{12}e^{-i\vec{P}_{12}\cdot\vec{R}_{12}}\phi^\dagger_{NLM_L}(\vec{P}_{12})e^{i\vec{P}\,'_{12}\cdot(\vec{R}_{12}-\vec{r}_{12}+\vec{r}\,'_{12})}\phi_{N'L'M'_L}(\vec{P}\,'_{12})$$
$$= \sum_{s_2 t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$\frac{\sqrt{8}}{(2\pi)^3}\int \mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}\,'_{12}e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}\,'_{12})}f^\dagger_p(r_{12})f_q(r'_{12})\psi^\dagger_{nl_p m_{l_p}}(\vec{r}_{12})\psi_{n'l'_q m'_{l_q}}(\vec{r}\,'_{12})$$
$$\int \mathrm{d}^3\vec{P}_{12}e^{-i\vec{P}_{12}\cdot(\vec{r}_{12}-\vec{r}\,'_{12})}\phi^\dagger_{NLM_L}(\vec{P}_{12})\phi_{N'L'M'_L}(\vec{P}_{12})$$

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 $\psi_{nlm_l}(\vec{r}) = R_{nl}(r)Y_{lm_l}(\Omega_r)$,

$\psi_{nlm_l}(\vec{p}) = \Pi_{nl}(p) Y_{lm_l}(\Omega_p)$.

$$\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$\frac{\sqrt{8}}{(2\pi)^3} \int \mathrm{d}^3\vec{R}_{12}\mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}'_{12} e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}'_{12})} f^\dagger_p(r_{12}) f_q(r'_{12}) \psi^\dagger_{nl_p m_{l_p}}(\vec{r}_{12}) \psi_{n'l'_q m_{l'_q}}(\vec{r}'_{12})$$
$$\frac{1}{(2\pi)^3} \int \mathrm{d}^3\vec{P}_{12} \int \mathrm{d}^3\vec{P}'_{12} e^{-i\vec{P}_{12}\cdot\vec{R}_{12}} \phi^\dagger_{NLM_L}(\vec{P}_{12}) e^{i\vec{P}'_{12}\cdot(\vec{R}_{12}-\vec{r}_{12}+\vec{r}'_{12})} \phi_{N'L'M'_L}(\vec{P}'_{12})$$
$$= \sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$\frac{\sqrt{8}(4\pi)^4}{(2\pi)^3} \int \mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}'_{12} f^\dagger_p(r_{12}) f_q(r'_{12}) R_{nl_p}(r_{12}) Y^*_{l_p m_{l_p}}(\Omega_{r_{12}}) R_{n'l'_q}(r'_{12}) Y_{l'_q m_{l'_q}}(\Omega_{r'_{12}})$$
$$\sum_{km_k} i^k j_k(\sqrt{2}p_1 r_{12}) Y^*_{km_k}(\Omega_{p_1}) Y_{km_k}(\Omega_{r_{12}})$$
$$\sum_{k'm'_k} i^{-k'} j_{k'}(\sqrt{2}p_1 r'_{12}) Y_{k'm'_k}(\Omega_{p_1}) Y^*_{k'm'_k}(\Omega_{r'_{12}})$$
$$\int \mathrm{d}^3\vec{P}_{12} \Pi_{NL}(P_{12}) Y^*_{LM_L}(\Omega_{P_{12}}) \Pi_{N'L'}(P_{12}) Y_{L'M'_L}(\Omega_{P_{12}})$$
$$\sum_{Km_K} i^{-K} j_K(P_{12}r_{12}) Y^*_{Km_K}(\Omega_{P_{12}}) Y_{Km_K}(\Omega_{r_{12}})$$
$$\sum_{K'm'_K} i^{K'} j_{K'}(P_{12}r'_{12}) Y_{K'm'_K}(\Omega_{P_{12}}) Y^*_{K'm'_K}(\Omega_{r'_{12}})$$

$$\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$64\sqrt{2}\pi \sum_{km_k} \sum_{k'm'_k} \sum_{Km_K} \sum_{K'm'_K} i^{k-k'-K+K'} Y^*_{km_k}(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1})$$
$$\int \mathrm{d}P_{12}\, P^2_{12} \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12})$$
$$\int \mathrm{d}r_{12}\, r^2_{12} f^\dagger_p(r_{12}) R_{nl_p}(r_{12}) j_k(\sqrt{2}p_1 r_{12}) j_K(P_{12}r_{12})$$
$$\int \mathrm{d}r'_{12}\, r'^2_{12} f_q(r'_{12}) R_{n'l'_q}(r'_{12}) j_{k'}(\sqrt{2}p_1 r'_{12}) j_{K'}(P_{12}r'_{12})$$
$$\int \mathrm{d}^2\Omega_{r_{12}} Y^*_{l_p m_{l_p}}(\Omega_{r_{12}}) Y_{km_k}(\Omega_{r_{12}}) Y_{Km_K}(\Omega_{r_{12}})$$
$$\int \mathrm{d}^2\Omega_{r'_{12}} Y_{l'_q m_{l'_q}}(\Omega_{r'_{12}}) Y^*_{k'm'_k}(\Omega_{r'_{12}}) Y^*_{K'm'_K}(\Omega_{r'_{12}})$$
$$\int \mathrm{d}^2\Omega_{P_{12}} Y^*_{LM_L}(\Omega_{P_{12}}) Y_{L'M'_L}(\Omega_{P_{12}}) Y^*_{Km_K}(\Omega_{P_{12}}) Y_{K'm'_K}(\Omega_{P_{12}})$$

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

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

and,

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

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

$$\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = &\sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2) \\
&64\sqrt{2}\pi \sum_{km_k} \sum_{k'm'_k} \sum_{KM_K} \sum_{K'M'_K} i^{k-k'-K+K'}\, Y^*_{km_k}(\Omega_{p_1}) Y_{k'm'_k}(\Omega_{p_1}) \\
&\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl_p}(p_1,P_{12}) \chi^{k'K'}_{q,n'l'_q}(p_1,P_{12}) \\
&\sqrt{\frac{(2k+1)(2K+1)}{4\pi(2l_p+1)}} \langle km_k KM_K|l_p m_{l_p}\rangle \langle k0K0|l_p0\rangle \\
&\sqrt{\frac{(2k'+1)(2K'+1)}{4\pi(2l'_q+1)}} \langle k'm'_k K'M'_K|l'_q m_{l'_q}\rangle \langle k'0K'0|l'_q0\rangle \\
&\sum_{JM_J} \sqrt{\frac{(2L+1)(2K+1)}{4\pi(2J+1)}} \langle LM_L KM_K|JM_J\rangle \langle L0K0|J0\rangle \\
&\sqrt{\frac{(2L'+1)(2K'+1)}{4\pi(2J+1)}} \langle L'M'_L K'M'_K|JM_J\rangle \langle L'0K'0|J0\rangle
\end{aligned}$$

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

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle = &\sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2) \\
&\frac{4\sqrt{2}}{\pi} \sum_{k m_k} \sum_{k' m'_k} \sum_{K M_K} \sum_{K' M'_K} i^{k-k'-K+K'} Y^*_{k m_k}(\Omega_{p_1}) Y_{k' m'_k}(\Omega_{p_1}) \\
&\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl_p}(p_1,P_{12}) \chi^{k'K'}_{q,n'l'_q}(p_1,P_{12}) \\
&\frac{\hat{k}\hat{k}'\hat{K}\hat{K}'}{\hat{l}_p \hat{l}'_q} \langle k m_k K M_K | l_p m_{l_p}\rangle \langle k0K0|l_p 0\rangle \langle k' m'_k K' M'_K | l'_q m_{l'_q}\rangle \langle k'0K'0|l'_q 0\rangle \\
&\sum_{J M_J} \frac{\hat{L}\hat{L}'\hat{K}\hat{K}'}{\hat{J}^2} \langle L M_L K M_K | J M_J\rangle \langle L0K0|J0\rangle \langle L' M'_L K' M'_K | J M_J\rangle \langle L'0K'0|J0\rangle
\end{aligned}
$$

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

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(p_1)|A'\rangle = &\sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2) \\
&\frac{4\sqrt{2}}{\pi} \sum_{k m_k} \sum_{K M_K} \sum_{K' M'_K} i^{-K+K'} \\
&\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl_p}(p_1,P_{12}) \chi^{kK'}_{q,n'l'_q}(p_1,P_{12}) \\
&\frac{\hat{k}^2\hat{K}\hat{K}'}{\hat{l}_p \hat{l}'_q} \langle k m_k K M_K | l_p m_{l_p}\rangle \langle k0K0|l_p 0\rangle \langle k m_k K' M'_K | l'_q m_{l'_q}\rangle \langle k0K'0|l'_q 0\rangle \\
&\sum_{J M_J} \frac{\hat{L}\hat{L}'\hat{K}\hat{K}'}{\hat{J}^2} \langle L M_L K M_K | J M_J\rangle \langle L0K0|J0\rangle \langle L' M'_L K' M'_K | J M_J\rangle \langle L'0K'0|J0\rangle
\end{aligned}
$$

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

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

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(p_1)|A'\rangle = &\sum_{s_2 t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2) \\
&\frac{4\sqrt{2}}{\pi} \sum_{k m_k} \sum_{K M_K} \sum_{K' M'_K} i^{-K+K'} (-1)^{m_{l_p}+m_{l'_q}} \\
&\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12}) \Pi_{N'L'}(P_{12}) \chi^{kK\dagger}_{p,nl_p}(p_1,P_{12}) \chi^{kK'}_{q,n'l'_q}(p_1,P_{12}) \\
&\hat{k}^2\hat{K}\hat{K}'\hat{l}_p\hat{l}'_q \begin{pmatrix} k & K & l_p \\ m_k & M_K & -m_{l_p} \end{pmatrix} \begin{pmatrix} k & K & l_p \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & K' & l'_q \\ m_k & M'_K & -m_{l'_q} \end{pmatrix} \begin{pmatrix} k & K' & l'_q \\ 0 & 0 & 0 \end{pmatrix} \\
&\sum_{J M_J} \hat{L}\hat{L}'\hat{K}\hat{K}'\hat{J}^2 \begin{pmatrix} L & K & J \\ M_L & M_K & M_J \end{pmatrix} \begin{pmatrix} L & K & J \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L' & K' & J \\ M'_L & M'_K & M_J \end{pmatrix} \begin{pmatrix} L' & K' & J \\ 0 & 0 & 0 \end{pmatrix}
\end{aligned}
$$

Where we flipped the sign of M_J as it as a summation index. Writing $\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$ explicitly gives,

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(p_1)|A'\rangle = &\sum_{s_2 t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1} \mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^{q}(S',T',j',l',l'_q) \\
&(-1)^{M_T+M'_T+M_S+M'_S}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T\\ t_1 & t_2 & -M_T\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T'\\ t_1 & t_2 & -M'_T\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & S\\ s_1 & s_2 & -M_S\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & S'\\ s_1 & s_2 & -M'_S\end{pmatrix} \\
&(-1)^{l_p+l'_q-S-S'+m_j+m'_j}\hat{j}\hat{j}'\begin{pmatrix}l_p & S & j\\ m_{l_p} & m_S & m_j\end{pmatrix}\begin{pmatrix}l'_q & S' & j'\\ m_{l'_q} & m'_S & m'_j\end{pmatrix} \\
&\frac{4\sqrt{2}}{\pi}\sum_{km_k}\sum_{KM_K}\sum_{K'M'_K} i^{-K+K'}(-1)^{m_{l_p}+m_{l'_q}} \\
&\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{kK\dagger}_{p,nl_p}(p_1,P_{12})\chi^{kK'}_{q,n'l'_q}(p_1,P_{12}) \\
&\hat{k}^2\hat{K}\hat{K}'\hat{l}_p\hat{l}'_q\begin{pmatrix}k & K & l_p\\ m_k & M_K & -m_{l_p}\end{pmatrix}\begin{pmatrix}k & K & l_p\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}k & K' & l'_q\\ m_k & M'_K & -m_{l'_q}\end{pmatrix}\begin{pmatrix}k & K' & l'_q\\ 0 & 0 & 0\end{pmatrix} \\
&\sum_{JM_J}\hat{L}\hat{L}'\hat{K}\hat{K}'\hat{J}^2\begin{pmatrix}L & K & J\\ M_L & M_K & M_J\end{pmatrix}\begin{pmatrix}L & K & J\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}L' & K' & J\\ M'_L & M'_K & M_J\end{pmatrix}\begin{pmatrix}L' & K' & J\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}
$$

If we are not interested in a specific spin contribution we get,

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle = \sum_{s_1}\langle A|\hat{n}^{[1]}_{s_1,t_1}(p_1)|A'\rangle = &\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1} \mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^{q}(S,T',j',l',l'_q) \\
&\sum_{t_2}(-1)^{M_T+M'_T}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T\\ t_1 & t_2 & -M_T\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T'\\ t_1 & t_2 & -M'_T\end{pmatrix} \\
&(-1)^{l_p+l'_q+m_j+m'_j}\hat{j}\hat{j}'\begin{pmatrix}l_p & S & j\\ m_{l_p} & m_S & m_j\end{pmatrix}\begin{pmatrix}l'_q & S & j'\\ m_{l'_q} & m_S & m'_j\end{pmatrix} \\
&\frac{4\sqrt{2}}{\pi}\sum_{km_k}\sum_{KM_K}\sum_{K'M'_K} i^{-K+K'}(-1)^{m_{l_p}+m_{l'_q}} \\
&\int \mathrm{d}P_{12}\, P_{12}^2 \Pi_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{kK\dagger}_{p,nl_p}(p_1,P_{12})\chi^{kK'}_{q,n'l'_q}(p_1,P_{12}) \\
&\hat{k}^2\hat{K}\hat{K}'\hat{l}_p\hat{l}'_q\begin{pmatrix}k & K & l_p\\ m_k & M_K & -m_{l_p}\end{pmatrix}\begin{pmatrix}k & K & l_p\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}k & K' & l'_q\\ m_k & M'_K & -m_{l'_q}\end{pmatrix}\begin{pmatrix}k & K' & l'_q\\ 0 & 0 & 0\end{pmatrix} \\
&\sum_{JM_J}\hat{L}\hat{L}'\hat{K}\hat{K}'\hat{J}^2\begin{pmatrix}L & K & J\\ M_L & M_K & M_J\end{pmatrix}\begin{pmatrix}L & K & J\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}L' & K' & J\\ M'_L & M'_K & M_J\end{pmatrix}\begin{pmatrix}L' & K' & J\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}
$$

To make the comparison with (D.37) easier we swap variables: $JM_J \to qm_q$, $KM_K \to km_k$, $K'M_K' \to k'm_k'$, $km_k \to l_1m_{l_1}$

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(p_1)|A'\rangle = &\sum_{l_p=|j-1|}^{j+1}\sum_{l_q'=|j'-1|}^{j'+1} \mathrm{O}^{p\dagger}(S,T,j,l,l_p)\mathrm{O}^{q}(S,T',j',l',l_q') \\
&\sum_{t_2}(-1)^{M_T+M_T'}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T\\ t_1 & t_2 & -M_T\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T'\\ t_1 & t_2 & -M_T'\end{pmatrix} \\
(-1)^{l_p+l_q'+m_j+m_j'}\hat{j}\hat{j}' &\begin{pmatrix}l_p & S & j\\ m_{l_p} & m_S & m_j\end{pmatrix}\begin{pmatrix}l_q' & S & j'\\ m_{l_q'} & m_S & m_j'\end{pmatrix}\frac{4\sqrt{2}}{\pi}\sum_{l_1m_{l_1}}\sum_{km_k}\sum_{k'm_k'} i^{-k+k'}(-1)^{m_{l_p}+m_{l_q'}} \\
&\int \mathrm{d}P_{12}\, P_{12}^2\Pi_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{l_1k\dagger}_{p,nl_p}(p_1,P_{12})\chi^{l_1k'}_{q,n'l_q'}(p_1,P_{12}) \\
\hat{l}_1^2\hat{k}^2\hat{k}'^2\hat{l}_p\hat{l}_q'\hat{L}\hat{L}' &\begin{pmatrix}l_p & l_1 & k\\ -m_{l_p} & m_{l_1} & m_k\end{pmatrix}\begin{pmatrix}l_p & l_1 & k\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_q' & l_1 & k'\\ -m_{l_q'} & m_{l_1} & m_k'\end{pmatrix}\begin{pmatrix}l_q' & l_1 & k'\\ 0 & 0 & 0\end{pmatrix} \\
&\sum_{qm_q}\hat{q}^2\begin{pmatrix}L & k & q\\ M_L & m_k & m_q\end{pmatrix}\begin{pmatrix}L & k & q\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}L' & k' & q\\ M_L' & m_k' & m_q\end{pmatrix}\begin{pmatrix}L' & k' & q\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}
$$

Finally we make use of the fact that m_{l_1} and m_k are sum indices to flip their sign and

$$
\begin{pmatrix}l_p & l_1 & k\\ -m_{l_p} & -m_{l_1} & -m_k\end{pmatrix} = \begin{pmatrix}l_p & l_1 & k\\ -m_{l_p} & -m_{l_1} & -m_k\end{pmatrix}
$$

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 (I think Maarten intended to write L, L' in stead of L_A, L_B).

$$
\begin{aligned}
\langle A|\hat{n}^{[1]}_{s_1,t_1}(p_1)|A'\rangle = &\mathcal{M}^{p,q}_{AA'}(s_1,t_1)\frac{4\sqrt{2}}{\pi}\sum_{l_1m_{l_1}}\sum_{km_k}\sum_{k'm_k'}(-1)^{l+l'-S-S'+m_j+m_j'} i^{L_A-L_B+k'-k}\hat{l}_1^2\hat{k}^2\hat{k}'^2\hat{l}\hat{l}'\hat{L}\hat{L}'\hat{j}\hat{j}' \\
&\int \mathrm{d}P_{12}\, P_{12}^2\Pi_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{l_1k\dagger}_{p,nl}(p_1,P_{12})\chi^{l_1k'}_{q,n'l'}(p_1,P_{12}) \\
&\sum_{m_lm_S}\begin{pmatrix}l & S & j\\ m_l & m_S & -m_j\end{pmatrix}\begin{pmatrix}l & l_1 & k\\ m_l & m_{l_1} & m_k\end{pmatrix}\begin{pmatrix}l & l_1 & k\\ 0 & 0 & 0\end{pmatrix} \\
&\sum_{m_l'm_S'}\begin{pmatrix}l' & S' & j'\\ m_l' & m_S' & -m_j'\end{pmatrix}\begin{pmatrix}l' & l_1 & k'\\ m_l' & m_{l_1} & m_k'\end{pmatrix}\begin{pmatrix}l' & l_1 & k'\\ 0 & 0 & 0\end{pmatrix} \\
&\sum_{qm_q}\begin{pmatrix}L' & k & q\\ M_L' & m_k & m_q\end{pmatrix}\begin{pmatrix}L' & k & q\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}L & k' & q\\ M_L & m_k' & m_q\end{pmatrix}\begin{pmatrix}L & k' & q\\ 0 & 0 & 0\end{pmatrix}
\end{aligned}
$$

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.

7.1 The matrix element $\mathcal{M}^{p,q}_{AA'}(s_1,t_1)$

Let us now look into the factorized matrix element $\mathcal{M}^{p,q}_{AA'}(s_1,t_1)$ in the one-body momentum distribution . Note that we implicitly assumed that the operators $\mathcal{O}^{p,q}$ do not change the quantum numbers of the orbital wave functions, $n(lS)jm_jNLM_L$ (the quantum numbers involved in the radial integrals). More explicitly,

$$
\hat{\mathcal{O}}^p\,|n(lS)jm_jNLM_L\rangle = \mathrm{O}^p(n,l,S,j,m_j,N,L,M_L)\,|n(lS)jm_jNLM_L\rangle
$$

If not it is impossible to factorize $\mathcal{M}^{p,q}_{AA'}(s_1,t_1)$ as is done in (above (??)). We now investigate this in detail to make sure this is the case. For the central and spin-isospin operators $\hat{\mathcal{O}} = \mathbb{1}, \vec{\sigma}_1\cdot\vec{\sigma_2}\vec{\tau}_1\cdot\vec{\tau}_2$ this is trivially valid,

$$\begin{aligned}\mathbb{1}\,|n(lS)jm_jNLM_L\rangle &= |n(lS)jm_jNLM_L\rangle\\ \vec{\sigma}_1\cdot\vec{\sigma_2}\vec{\tau}_1\cdot\vec{\tau}_2\,|n(lS)jm_jNLM_L\rangle &= [2S(S+1)-3]\,|n(lS)jm_jNLM_L\rangle\,\vec{\tau}_1\cdot\vec{\tau}_2\end{aligned}$$

The case for the tensor operator $\hat{S}_{12} = 2\left[3\frac{\vec{S}\cdot\vec{r}_{12}}{r_{12}^2} - \vec{S}^2\right]$ requires a bit more work. As it only operates on the total spin S and the (unit) relative coordinate r_{12} we only write out the ket $|(lS)jm_j\rangle$ and drop $|n\rangle\,|NLM_L\rangle$.

Maybe one can use something like a general thing that scalar operators cannot change quantum numbers but let us proof it explicitly for our case.

$$\begin{aligned}\hat{S}_{12}\,|(lS)jm_j\rangle &= \sum_{l'S'j'm_j'}|(l'S')j'm_j'\rangle\,\langle(l'S')j'm_j'|\,\hat{S}_{12}\,|(lS)jm_j\rangle\\ &= \sum_{l'S'j'm_j'}|(l'S')j'm_j'\rangle\,2\delta_{jj'}\delta_{m_jm_j'}(-1)^{S+j}\sqrt{120}\,\hat{l}\hat{l}'\begin{pmatrix} l & l' & 2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l & l' & 2\\ S' & S & j\end{Bmatrix}\delta_{jj'}\delta_{m_jm_j'}\delta_{SS'}\delta_{S1}\\ &= \sum_{l'=|j-1|}^{j+1}|(l'S)jm_j\rangle\,(-1)^{S+j}\sqrt{120}\,\hat{l}\hat{l}'\begin{pmatrix} l & l' & 2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l & l' & 2\\ S & S & j\end{Bmatrix}\delta_{S1}\\ &= \sum_{l'=|j-1|}^{j+1}\mathrm{S}_{12}(S,j,l,l')\,|(l'S)jm_j\rangle\end{aligned}$$

Where we have made use of the unity,

$$\begin{aligned}\sum_{lSjm_j}|(lS)jm_j\rangle\,\langle(lS)jmj| &= \sum_{lSjm_j}\sum_{m_lm_S}\sum_{m_l'm_S'}\langle lm_lSm_S|jm_j\rangle\,|lm_lSm_S\rangle\,\langle jm_j|lm_l'Sm_S'\rangle\,\langle lm_l'Sm_S'|\\ &= \sum_{lS}\sum_{m_lm_S}\sum_{m_l'm_S'}|lm_lSm_S\rangle\,\langle lm_l'Sm_S'|\sum_{jm_j}\langle lm_lSm_S|jm_j\rangle\,\langle jm_j|lm_l'Sm_S'\rangle\\ &= \sum_{lS}\sum_{m_lm_S}|lm_lSm_S\rangle\,\langle lm_lSm_S| = \mathbb{1}\end{aligned}$$

Summarizing we can write,

$$\hat{\mathcal{O}}^p\,|n(lS)jm_jNLM_LTM_T\rangle = \sum_{l'=|j-1|}^{j+1}\mathrm{O}^p(S,T,j,l,l')\,|n(l'S)jm_jNLM_LTM_T\rangle$$

With

$$\begin{aligned}\hat{\mathcal{O}}^p = \mathbb{1} &\Rightarrow \mathrm{O}^p(S,T,j,l,l') = \delta_{ll'}\\ \hat{\mathcal{O}}^p = \vec{\sigma}_1\cdot\vec{\sigma_2}\vec{\tau}_1\cdot\vec{\tau}_2 &\Rightarrow \mathrm{O}^p(S,T,j,l,l') = [2S(S+1)-3][2T(T+1)-3]\delta_{ll'}\\ \hat{\mathcal{O}}^p = \hat{S}_{12} &\Rightarrow \mathrm{O}^p(S,T,j,l,l') = \mathrm{S}_{12}(S,j,l,l')\end{aligned}$$

7.2 Isospin projection part

Let us investigate the expression,

$$\sum_{t_2}\langle\frac{1}{2}t_1\frac{1}{2}t_2|TM_T\rangle\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|T'M_T'\rangle = \sum_{t_2}(-1)^{M_T+M_T'}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T\\ t_1 & t_2 & -M_T\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & T'\\ t_1 & t_2 & -M_T'\end{pmatrix}$$

separately as in Maartens code the 3j symbols do not appear but some `if, else` magic is employed. We will cover the 3 cases for $|TM_T\rangle, |T'M'_T\rangle \in \{|11\rangle, |10\rangle, |1-1\rangle, |00\rangle\}$, leading to 10 ($\frac{4\cdot5}{2}$) possible combinations:

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\mp1\rangle = 0$$

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle = \delta_{t_1,\pm\frac{1}{2}}$$

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle = 0$$

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle = 0$$

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle = \frac{1}{2}$$

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle = \mathrm{sgn}(t_1)\frac{1}{2} = t_1$$

$$\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle = \frac{1}{2}$$

Yes, there are 10 terms here above if you take the $\pm$-signs into account. The first line only counts for 1, the second, third and fourth lines each represent 2 different combinations. Together with the last 3 single combinations that makes $1+6+3=10$. Note that all the non zero terms have $M_T = M'_T$, and we may effectively include a δ_{M_T,M'_T} (which is done in Maarten's Code):

```
if( t != 0 ) {
    if( t == -MT  )
        continue;
    if( MT == 0 ) {
        preifactor*= 0.5;
        if( TA != TB ) preifactor *= t;
    }
}
if( t == 0 && TA != TB ) {
    continue;
}
```

`t` is equal to $2t_1$. A value of `t=0` means summing over t_1 resulting in $\delta_{TT'}\delta_{M_TM'_T}$.

8 Fourier transform of HO wave functions

The HO Shrödinger equation is given by

$$\left(-\frac{\hbar^2}{2m_N}\nabla^2 + \frac{1}{2}m_N\omega^2r^2 - E\right)\psi(\vec{r}) = 0$$

With $\nu = \frac{m_N\omega}{\hbar}$ (units 1/fm^2) and writing E in units $\hbar\omega$ ($E \rightarrow \hbar\omega E$),

$$\left(-\frac{1}{2}\nabla^2 + \frac{1}{2}\nu^2r^2 - \nu E\right)\psi(\vec{r}) = 0$$

With solutions

$$\psi_{nlm}(r) = \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})}\nu^{l+\frac{3}{2}}\right]^{\frac{1}{2}} r^l e^{-\frac{\nu r^2}{2}} L_n^{l+\frac{1}{2}}(\nu r^2) Y_{lm}(\Omega_r)$$

The HO Shrödinger equation in momentum space is obtained by using $\hat{\vec{r}} = i\hbar\vec{\nabla}_{\vec{p}}$,

$$\left(\frac{p^2}{2m_N} - \frac{1}{2}m_N\hbar^2\omega^2\nabla^2 - E\right)\phi(\vec{p}) = 0$$

Defining $\nu' = 1/\nu = \frac{\hbar}{m_N\omega}$ and writing the energy E again in units of $\hbar\omega$ ($E \to \hbar\omega E$),

$$\left(-\frac{1}{2}\frac{\hbar^2}{\nu'}\nabla^2 + \frac{\nu'}{\hbar^2}p^2 - E\right)\phi(\vec{p}) = 0$$

If we define $\vec{p}$ in units $\hbar$ so that the dimension of $\vec{p}$ becomes 1/fm we get ($\vec{p} \to \hbar\vec{p}$),

$$\left(-\frac{1}{2}\nabla^2 + \nu'^2 p^2 - \nu' E\right)\phi(\vec{p}) = 0$$

This has exactly the same form as the Shrödinger equation in r-space. The solutions are,

$$\phi_{nlm}(p) = \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})}\nu'^{l+\frac{3}{2}}\right]^{\frac{1}{2}} p^l e^{-\frac{\nu' p^2}{2}} L_n^{l+\frac{1}{2}}(\nu' p^2) Y_{lm}(\Omega_p)$$

If you don't believe in the trick $\hat{\vec{r}} = i\hbar\vec{\nabla}_p$, we can also show this in a slightly more elaborate way, starting from the r-space Shrödinger equation and write (we will now explicitly put the $\hbar$'s in the exponents, this is generally omitted) $\psi_{nlm}(\vec{r})$ as $\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\phi_{nlm}(\vec{p})$,

$$\left(-\frac{1}{2}\nabla^2 + \frac{1}{2}\nu^2 r^2 - \nu E\right)\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\phi_{nlm}(\vec{p}) = 0$$

Noting that $\vec{r}\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\psi_{nlm}(\vec{p})$ can be written as,

$$\begin{aligned}
\vec{r}\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\psi_{nlm}(\vec{p}) &= \frac{\hbar}{i}\int \mathrm{d}^3\vec{p}\left(\vec{\nabla}_p e^{i\vec{p}\cdot\vec{r}/\hbar}\right)\phi_{nlm}(\vec{p}) \\
&= \frac{\hbar}{i}\left[e^{i\vec{p}\cdot\vec{r}/\hbar}\phi_{nlm}(\vec{p})\right]_{-\infty}^{+\infty} - \frac{\hbar}{i}\int \mathrm{d}^3\vec{p}\,e^{i\vec{p}\cdot\vec{r}/\hbar}\left(\vec{\nabla}_p\phi_{nlm}(\vec{p})\right) \\
&= i\hbar\int \mathrm{d}^3\vec{p}\,e^{i\vec{p}\cdot\vec{r}/\hbar}\left(\vec{\nabla}_p\phi_{nlm}(\vec{p})\right)
\end{aligned}$$

and $\vec{\nabla}\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\phi_{nlm}(\vec{p}) = \int \mathrm{d}^3\vec{p}\frac{i}{\hbar}\vec{p}e^{i\vec{p}\cdot\vec{r}}\phi_{nlm}(\vec{p})$, we get,

$$\begin{aligned}
&\left(-\frac{1}{2}\nabla^2 + \frac{1}{2}\nu^2 r^2 - \nu E\right)\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\phi_{nlm}(\vec{p}) = 0 \\
\Rightarrow &\int \mathrm{d}^3\vec{p}e^{i\vec{p}\cdot\vec{r}/\hbar}\left(\frac{1}{2}\frac{p^2}{\hbar^2} - \frac{1}{2}\nu^2\hbar^2\nabla_{\vec{p}}^2 - \nu E\right)\phi_{nlm}(\vec{p}) = 0
\end{aligned}$$

As this last line must be true for all $\vec{r}$ we must have that,

$$\left(\frac{1}{2}\frac{p^2}{\hbar^2} - \frac{1}{2}\nu^2\hbar^2\nabla_{\vec{p}}^2 - \nu E\right)\phi_{nlm}(\vec{p}) = 0$$

Again redefining $\vec{p}$ in units $\hbar$ so that its dimension becomes 1/fm instead of MeV/c. We get,

$$\begin{aligned}
&\left(-\frac{1}{2}\nabla_{\vec{p}}^2 + \frac{1}{2}\frac{1}{\nu^2}p^2 - \frac{1}{\nu}E\right)\phi_{nlm}(\vec{p}) = 0 \\
\Rightarrow &\left(-\frac{1}{2}\nabla_{\vec{p}}^2 + \frac{1}{2}\nu'^2 p^2 - \nu' E\right)\phi_{nlm}(\vec{p}) = 0
\end{aligned}$$

which is exactly what we set out to prove! But let us try a even more elaborate way by taking the Fourier transform of the wave function in r-space!

$$\begin{aligned}\phi_{nlm}(\vec{p}) &= \frac{1}{(2\pi)^{\frac{3}{2}}}\int \mathrm{d}^3\vec{r}\, e^{-i\vec{p}\cdot\vec{r}}\psi_{nlm}(\vec{r}) \\ &= \frac{1}{(2\pi)^{\frac{3}{2}}}\left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})}\nu^{l+\frac{3}{2}}\right]^{\frac{1}{2}}\int \mathrm{d}^3\vec{r}\, e^{-i\vec{p}\cdot\vec{r}} r^l e^{-\frac{\nu r^2}{2}} L_n^{l+\frac{1}{2}}(\nu r^2) Y_{lm}(\Omega_r)\end{aligned}$$

For the sake of conciseness We define $N_{nl} = \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})}\nu^{l+\frac{3}{2}}\right]^{\frac{1}{2}}$. We use the plane wave expansion $e^{-i\vec{p}\cdot\vec{r}} = (4\pi)\sum_{km_k}(-i)^k j_k(pr) Y^*_{km_k}(\Omega_r) Y_{km_k}(\Omega_p)$.

$$\begin{aligned}\phi_{nlm}(\vec{p}) &= \frac{1}{(2\pi)^{\frac{3}{2}}}\int \mathrm{d}^3\vec{r}\, e^{-i\vec{p}\cdot\vec{r}}\psi_{nlm}(\vec{r}) \\ &= N_{nl}\frac{4\pi}{(2\pi)^{\frac{3}{2}}}\sum_{km_k}(-i)^k Y_{km_k}(\Omega_p)\int \mathrm{d}r\, r^2 j_k(pr) r^l e^{-\frac{\nu r^2}{2}} L_n^{l+\frac{1}{2}}(\nu r^2)\int \mathrm{d}^2\Omega_r\, Y^*_{km_k}(\Omega_r) Y_{lm}(\Omega_r) \\ &= N_{nl}\sqrt{\frac{2}{\pi}}(-i)^l Y_{lm}(\Omega_p)\int \mathrm{d}r\, r^2 j_l(pr) r^l e^{-\frac{\nu r^2}{2}} L_n^{l+\frac{1}{2}}(\nu r^2)\end{aligned}$$

Using the expansion of the spherical bessel function $j_l(x)$ and the generalized Laguerre polynomials $L_n^{l+\frac{1}{2}}(x)$,

$$\begin{aligned}j_l(x) &= \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(x) = \sqrt{\frac{\pi}{2x}}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(k+l+3/2)}\left(\frac{x}{2}\right)^{2k+l+1/2} \\ &= \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(x) = \sqrt{\frac{\pi}{2x}}\left(\frac{x}{2}\right)^{l+\frac{1}{2}} e^{-t}\sum_{k=0}^{\infty}\frac{t^k}{\Gamma(k+l+3/2)} L_k^{l+\frac{1}{2}}\left(\frac{x^2}{4t}\right) \\ L_n^{l+\frac{1}{2}}(x) &= \sum_{j=0}^{n}(-1)^j\begin{pmatrix} n+l+1/2 \\ n-j\end{pmatrix}\frac{x^j}{j!} = \sum_{j=0}^{n}(-1)^j\frac{\Gamma(n+l+3/2)}{\Gamma(j+l+3/2)(n-j)!}\frac{x^j}{j!}\end{aligned}$$

Making the "inspired" choice $t = \frac{p^2}{2\nu}$ we get,

$$\phi_{nlm}(\vec{p}) = N_{nl}(-i)^l p^l Y_{lm}(\Omega_p) e^{-\frac{p^2}{2\nu}} 2^{-l-\frac{1}{2}}\sum_{k=0}^{\infty}\frac{\left(\frac{p^2}{2\nu}\right)^k}{\Gamma(k+l+3/2)}\int \mathrm{d}r\, r^{2+2l} L_k^{l+\frac{1}{2}}(\frac{\nu r^2}{2}) e^{-\frac{\nu r^2}{2}} L_n^{l+\frac{1}{2}}(\nu r^2)$$

Changing the integration variable r to $x = \nu r^2$ gives,

$$\begin{aligned}\phi_{nlm}(\vec{p}) = N_{nl}(-i)^l p^l Y_{lm}(\Omega_p) e^{-\frac{p^2}{2\nu}} 2^{-l-\frac{3}{2}}\nu^{-l-\frac{3}{2}} \\ \sum_{k=0}^{\infty}\frac{\left(\frac{p^2}{2\nu}\right)^k}{\Gamma(k+l+3/2)}\int \mathrm{d}x\, x^{l+\frac{1}{2}} e^{-\frac{x}{2}} L_k^{l+\frac{1}{2}}(x/2)\, L_n^{l+\frac{1}{2}}(x)\end{aligned}$$

Using the identity (`Applied Mathematics Letters 16 (2003) 1131-1136, equation (19)`) [1].

$$\int_0^{+\infty}\mathrm{d}x\, x^{\alpha} e^{-\sigma x} L_n^{\alpha}(\lambda x) L_k^{\alpha}(\sigma x) = \frac{\Gamma(\alpha+n+1)}{\sigma^{\alpha+n+1}}\frac{(\sigma-\lambda)^{n-k}}{(n-k)!}\frac{\lambda^k}{k!}$$

[1] Remarks on Some Associated Laguerre Integral Results.
http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.99.2040&rep=rep1&type=pdf

With $\alpha = l + 1/2, \sigma = 1/2, \lambda = 1$ we get,

$$\phi_{nlm}(\vec{p}) = N_{nl}(-i)^l p^l Y_{lm}(\Omega_p) e^{-\frac{p^2}{2\nu}} 2^{-l-\frac{3}{2}} \nu^{-l-\frac{3}{2}}$$
$$\sum_{k=0}^{\infty} \frac{\left(\frac{p^2}{2\nu}\right)^k}{\Gamma(k+l+3/2)} \frac{\Gamma(n+l+3/2)}{(1/2)^{n+l+3/2}} \frac{\left(-\frac{1}{2}\right)^{n-k}}{(n-k)!} \frac{1}{k!}$$
$$= N_{nl}(-i)^l p^l Y_{lm}(\Omega_p) e^{-\frac{p^2}{2\nu}} \nu^{-l-\frac{3}{2}}$$
$$(-1)^n \sum_{k=0}^{n} \frac{(-1)^k}{k!} \left(\frac{p^2}{\nu}\right)^k \frac{\Gamma(n+l+3/2)}{(n-k)!\Gamma(k+l+3/2)}$$
$$= \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})} \nu^{l+\frac{3}{2}}\right]^{\frac{1}{2}} (-i)^l p^l Y_{lm}(\Omega_p) e^{-\frac{p^2}{2\nu}} \nu^{-l-\frac{3}{2}} (-1)^n L_n^{l+\frac{1}{2}}(\frac{p^2}{\nu})$$

Note that we have applied a somewhat dirty trick we truncated the sum $\sum_{k=0}^{\infty} \ldots 1/(n-k)! \ldots$ to $\sum_{k=0}^{n} \ldots 1/(n-k)! \ldots$. The reasoning is that the factorial of a negative integer diverges to $\pm\infty$. Because the negative integer factorial appears in the denominator for $k > n$ we can truncate the sum to $k = n$. With $\nu' = 1/\nu$ the final solution becomes,

$$\phi_{nlm}(\vec{p}) = (-i)^l(-1)^n \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})} \nu'^{l+\frac{3}{2}}\right]^{\frac{1}{2}} p^l Y_{lm}(\Omega_p) e^{-\frac{\nu' p^2}{2}} L_n^{l+\frac{1}{2}}(\nu' p^2)$$

Which is the expected result except for the phase factor $(-i)^l(-1)^n = i^{2n+3l}$.