LCA CODE MANUAL

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Contents

1 Definitions

A short (probably incomplete) overview of the quantities used in this manual, $\psi_{nlm_l}(\vec{r})$ are the $\vec{r}$-space solutions of the harmonic oscillator with parameter $\nu = m_N\omega/\hbar$,

$$\psi_{nlm_l}(\vec{r}) = R_{nl}(r) Y_{lm}(\Omega_r)\,, \tag{1}$$

$$R_{nl}(r) = \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})} \nu^{l+\frac{3}{2}} \right]^{\frac{1}{2}} r^l e^{-\frac{\nu r^2}{2}} L_n^{l+\frac{1}{2}}(\nu r^2)\,. \tag{2}$$

It is well known that the solutions $\phi_{nlm_l}(\vec{p})$ in $\vec{p}$-space are of the exact same form, where compared to the $\vec{r}$-space solution $\vec{r}$ is replaced by $\vec{p}$ and ν by $\nu' = 1/\nu$. However, when taking the explicit Fourier transformation, some (non-neglectable) phase factors appear (see Sec. 9),

$$\begin{aligned}
\phi_{nlm_l}(\vec{p}) &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int \mathrm{d}^3\vec{r} e^{-i\vec{p}\cdot\vec{r}} \psi_{nlm_l}(\vec{r}) && (3)\\
&= i^{-l}(-1)^n \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})} \nu'^{l+\frac{3}{2}} \right]^{\frac{1}{2}} p^l e^{-\frac{\nu' p^2}{2}} L_n^{l+\frac{1}{2}}(\nu' p^2) Y_{lm}(\Omega_p) && (4)\\
&= i^{-l}(-1)^n \Pi_{nl}(p) Y_{lm}(\Omega_p) \,, && (5)\\
\Pi_{nl}(p) &= \left[\frac{2n!}{\Gamma(n+l+\frac{3}{2})} \nu'^{l+\frac{3}{2}} \right]^{\frac{1}{2}} p^l e^{-\frac{\nu' p^2}{2}} L_n^{l+\frac{1}{2}}(\nu' p^2) && (6)
\end{aligned}$$

Here, the Laguerre polynomials are often expanded as follows,

$$\begin{aligned}
L_n^{l+\frac{1}{2}}(x) &= \sum_{i=0}^{n} a_{nl,i} x^i \,, \\
a_{nl,i} &= (-1)^i \frac{\Gamma(n+l+3/2)}{\Gamma(i+l+3/2)(n-i)!i!} && (7)
\end{aligned}$$

In the LCA a one-body operator $\widehat{\Omega}^{[1]} = \sum_i^A \widehat{\Omega}_i$ becomes,

$$\widehat{\Omega}^{[1],\,\mathrm{LCA}} = \widehat{\Omega}^{[1]} + \sum_{i,j \neq i}^{A} \left(\hat{l}_{ij}^\dagger \widehat{\Omega}_i + \widehat{\Omega}_i \hat{l}_{ij} + \hat{l}_{ij}^\dagger \widehat{\Omega}_i \hat{l}_{ij} \right) . \quad (8)$$

In similar vein, the LCA transforms a two-body operator $\widehat{\Omega}^{[2]} = \sum_{i<j} \widehat{\Omega}_{ij}$ to,

$$\begin{aligned}
&\widehat{\Omega}^{[2],\,\mathrm{LCA}} = \widehat{\Omega}^{[2]} \\
&\quad + \sum_{i<j}^{A} \left[\hat{l}_{ij}^\dagger \widehat{\Omega}_{ij} + \widehat{\Omega}_{ij} \hat{l}_{ij} + \hat{l}_{ij}^\dagger \widehat{\Omega}_{ij} \hat{l}_{ij} + \sum_{n \notin \{i,j\}}^{A} (\hat{l}_{in}^\dagger + \hat{l}_{jn}^\dagger) \widehat{\Omega}_{ij} + \widehat{\Omega}_{ij} (\hat{l}_{in} + \hat{l}_{jn}) + \hat{l}_{in}^\dagger \widehat{\Omega}_{ij} \hat{l}_{in} \right] . \quad (9)
\end{aligned}$$

To preserve normalization the normalisation denominator $\mathcal{N} = \langle \Phi | \widehat{\mathcal{G}}^\dagger \mathcal{G} | \Phi \rangle$, should be expanded to the same order in $\hat{l}$ as the numerator. The normalisation factor $\mathcal{N}$ can be calculated by replacing $\widehat{\Omega}_i$ with $\frac{1}{A}$ in Eq. (8) or $\widehat{\Omega}_{ij}$ with $\frac{2}{A(A-1)}$ in Eq. (9),

$$\begin{aligned}
\mathcal{N}^{[1]} &= 1 + \frac{2}{A} \sum_{i<j}^{A} \langle \alpha_i \alpha_j | \hat{l}_{ij}^\dagger + \hat{l}_{ij} + \hat{l}_{ij}^\dagger \hat{l}_{ij} | \alpha_i \alpha_j \rangle \,, && (10)\\
\mathcal{N}^{[2]} &= 1 + \frac{2(2A-3)}{A(A-1)} \sum_{i<j}^{A} \langle \alpha_i \alpha_j | \hat{l}_{ij}^\dagger + \hat{l}_{ij} + \hat{l}_{ij}^\dagger \hat{l}_{ij} | \alpha_i \alpha_j \rangle \,. && (11)
\end{aligned}$$

1.1 Rewriting Maartens summations, the simple way

The LCA summations derived in the previous section are at first glance not the same as found in Sec. 2.2 of [?]. Here it is shown that these are equivalent. In particular the equivalence of the Eqs. found in Camille's PHD thesis and (2.43),(2.45) of [?] is derived here. The derivation for the other summations is analogous. Starting from Eq. (2.43) of [?] with $\widehat{\Omega}_{ij} = \widehat{\Omega}_{ji}$ and $\hat{l}_{ij} = \hat{l}_{ji}$,

$$\widehat{\Omega}^{[2],1} = \sum_{i<j}^{A} \widehat{\Omega}_{ij} \hat{l}_{ij} + \sum_{i<j<k}^{A} \left(\widehat{\Omega}_{ij} \hat{l}_{ik} + \widehat{\Omega}_{ij} \hat{l}_{jk} + \widehat{\Omega}_{ik} \hat{l}_{ij} + \widehat{\Omega}_{ik} \hat{l}_{jk} + \widehat{\Omega}_{jk} \hat{l}_{ij} + \widehat{\Omega}_{jk} \hat{l}_{ik} \right) . \quad (12)$$

It is useful to note that there are $\frac{A(A-1)}{2} + A(A-1)(A-2) = A(A-1)(A-\frac{3}{2}) = A^3 - A^2 - 3\frac{A(A-1)}{2}$ individual terms in this summation. The sum indices i, j, k are reshuffled in such a way that each term contains $\widehat{\Omega}_{ij}$,

$$
\begin{aligned}
\widehat{\Omega}^{[2],1} = &\sum_{i<j}^{A} \widehat{\Omega}_{ij}\hat{l}_{ij} + \\
&\sum_{i<j<k}^{A} \widehat{\Omega}_{ij}\hat{l}_{ik} + \sum_{i<j<k}^{A} \widehat{\Omega}_{ij}\hat{l}_{jk} + \sum_{i<k<j}^{A} \widehat{\Omega}_{ij}\hat{l}_{ik} + \sum_{i<k<j}^{A} \widehat{\Omega}_{ij}\hat{l}_{jk} + \sum_{k<i<j}^{A} \widehat{\Omega}_{ij}\hat{l}_{ik} + \sum_{k<i<j}^{A} \widehat{\Omega}_{ij}\hat{l}_{jk} \\
&= \sum_{i<j}^{A} \widehat{\Omega}_{ij}\hat{l}_{ij} + \left(\sum_{i<j<k}^{A} + \sum_{i<k<j}^{A} + \sum_{k<i<j}^{A} \right) \widehat{\Omega}_{ij}\hat{l}_{ik} + \left(\sum_{i<j<k}^{A} + \sum_{i<k<j}^{A} + \sum_{k<i<j}^{A} \right) \widehat{\Omega}_{ij}\hat{l}_{jk} \\
&= \sum_{i<j}^{A} \widehat{\Omega}_{ij} \left(\hat{l}_{ij} + \sum_{k\notin\{i,j\}}^{A} \left[\hat{l}_{ik} + \hat{l}_{jk} \right] \right) . \qquad (13)
\end{aligned}
$$

It is easy to see that there are $\frac{A(A-1)}{2}(1 + 2(A-2)) = \frac{A(A-1)}{2} + A(A-1)(A-2)$ distinct terms, exactly the same as the original expression of Eq. (12). Eq. (13) appears in Eq. (9). The equivalence of the remaining contributions to Eq. (9) are derived in a completely similar fashion.

Remark, can be removed. As there are an equal number of distinct terms in the two equivalent summations: Eq. (13) and Eq. (12), I see no reason to use the arguably more obfuscated summation of Eq. (12).

At the cost of some readability Eq. (13) can be formulated shorter,

$$
\begin{aligned}
\widehat{\Omega}^{[2],1} &= \sum_{i<j}^{A} \widehat{\Omega}_{ij} \left(\hat{l}_{ij} + \sum_{k\notin\{i,j\}}^{A} \left[\hat{l}_{ik} + \hat{l}_{jk} \right] \right) = \frac{1}{2} \sum_{i\neq j}^{A} \widehat{\Omega}_{ij} \left(\hat{l}_{ij} + \sum_{k\notin\{i,j\}} \left[\hat{l}_{ik} + \hat{l}_{jk} \right] \right) \\
&= \sum_{i\neq j}^{A} \widehat{\Omega}_{ij} \left(\frac{\hat{l}_{ij}}{2} + \sum_{k\notin\{i,j\}}^{A} \hat{l}_{jk} \right) = \sum_{i\neq j}^{A} \widehat{\Omega}_{ij} \sum_{k\neq j}^{A} \hat{l}_{jk} (1 - \frac{\delta_{ik}}{2}) . \qquad (14)
\end{aligned}
$$

By going from $\sum_{i<j}^{A} = \sum_{i\neq j}^{A}$ introduced double counting of some terms was introduced, corrected by the factor $(1 - \frac{\delta_{ik}}{2})$. Eq. (14) has a total of $A(A-1)^2$ terms, an overhead $\frac{A(A-1)}{2}$ compared to Eq. (13). The relative increase is $\frac{A(A-1)^2}{A(A-1)(A-\frac{3}{2})} = 1 + \frac{1}{2A-3}$, about 1.048 for $A = 12$ and 1.003 for $A = 208$.

2 Momentum distributions

2.1 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,

$$
\hat{n}(p) = \frac{1}{(2\pi)^3} \int \mathrm{d}^2\Omega_{\mathbf{p}} a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}} \qquad (15)
$$

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

$$
\langle\Phi|\hat{n}(p)|\Phi\rangle = \frac{1}{(2\pi)^3} \int \mathrm{d}^2\Omega_{\mathbf{p}} \langle\Phi|a^{\dagger}_{\mathbf{p}} a_{\mathbf{p}}|\Phi\rangle \qquad (16)
$$

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

$$\langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \int \mathrm{d}^3\mathbf{p}_1 \dots \mathrm{d}^3\mathbf{p}_A \,\langle\Phi|\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A\rangle\,\langle\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle \tag{17}$$

$$= \int \mathrm{d}^A\mathbf{p}_1 \dots \mathrm{d}^3\mathbf{p}_A \,\langle\Phi|\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A\rangle\,\langle 0|a_{\mathbf{p}_1}a_{\mathbf{p}_2}\dots a_{\mathbf{p}_A}a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle \tag{18}$$

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

$$\langle 0|a_{\mathbf{p}_1}a_{\mathbf{p}_2}\dots a_{\mathbf{p}_A}a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \langle 0|a_{\mathbf{p}_1}a_{\mathbf{p}_2}\dots\delta(\mathbf{p}-\mathbf{p}_A)a_{\mathbf{p}}|\Phi\rangle - \langle 0|a_{\mathbf{p}_1}a_{\mathbf{p}_2}\dots a_{\mathbf{p}_{A-1}}a_{\mathbf{p}}^\dagger a_{\mathbf{p}_A}a_{\mathbf{p}}|\Phi\rangle \tag{19}$$

$$= \delta(\mathbf{p}-\mathbf{p}_A)\,\langle\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}|\Phi\rangle - \delta(\mathbf{p}-\mathbf{p}_{A-1})\,\langle 0|a_{\mathbf{p}_1}\dots a_{\mathbf{p}_{A-2}}a_{\mathbf{p}_A}a_{\mathbf{p}}|\Phi\rangle \tag{20}$$

$$+ \langle 0|a_{\mathbf{p}_1}\dots a_{\mathbf{p}_{A-2}}a_{\mathbf{p}}^\dagger a_{\mathbf{p}_{A-1}}a_{\mathbf{p}_A}a_{\mathbf{p}}|\Phi\rangle \tag{21}$$

$$= \delta(\mathbf{p}-\mathbf{p}_A)\,\langle\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A|\Phi\rangle + \delta(\mathbf{p}-\mathbf{p}_{A-1})\,\langle\mathbf{p}_1\dots\mathbf{p}_{A-2}\mathbf{p}_{A-1}\mathbf{p}_A|\Phi\rangle \tag{22}$$

$$+ \langle 0|a_{\mathbf{p}_1}\dots a_{\mathbf{p}_{A-2}}a_{\mathbf{p}}^\dagger a_{\mathbf{p}_{A-1}}a_{\mathbf{p}_A}a_{\mathbf{p}}|\Phi\rangle \qquad = \dots \tag{23}$$

$$= \sum_{i=1}^{A}\delta(\mathbf{p}-\mathbf{p}_i)\,\langle\mathbf{p}_1\dots\mathbf{p}_A|\Phi\rangle + (-1)^A \underbrace{\langle 0|a_{\mathbf{p}}^\dagger a_{\mathbf{p}_1}\dots a_{\mathbf{p}_A}a_{\mathbf{p}}|\Phi\rangle}_{=0} \tag{24}$$

Hence,

$$\langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \int \mathrm{d}^3\mathbf{p}_1 \dots \mathrm{d}^3\mathbf{p}_A \,\langle\Phi|\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A\rangle \sum_{i=1}^{A}\delta(\mathbf{p}-\mathbf{p}_i)\,\langle\mathbf{p}_1\mathbf{p}_2\dots\mathbf{p}_A|\Phi\rangle \tag{25}$$

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

$$\langle\Phi|a_{\mathbf{p}}^\dagger a_{\mathbf{p}}|\Phi\rangle = \sum_{i=1}^{A}|\,\langle\mathbf{p}|\phi_{\alpha_i}\rangle\,|^2 = \sum_{i=1}^{A}\phi_{\alpha_i}^\dagger(\mathbf{p})\phi_{\alpha_i}(\mathbf{p}) \tag{26}$$

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,

$$a_{\mathbf{p}}^\dagger a_{\mathbf{p}}\,|\Phi\rangle = a_{\mathbf{p}}^\dagger a_{\mathbf{p}}\,|\alpha_1\alpha_2\dots\alpha_A\rangle = a_{\mathbf{p}}^\dagger a_{\mathbf{p}}a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger\dots a_{\alpha_A}^\dagger\,|0\rangle \tag{27}$$

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

$$a_{\alpha_i}^\dagger = \int \mathrm{d}^3\mathbf{k}\phi_{\alpha_i}(\mathbf{k})a_k^\dagger \tag{28}$$

$$\Rightarrow a_{\mathbf{p}}a_{\alpha_i}^\dagger = \int \mathrm{d}^3\mathbf{k}\phi_{\alpha_i}(\mathbf{k})a_{\mathbf{p}}a_{\mathbf{k}}^\dagger = \phi_{\alpha_i}(\mathbf{p}) - a_{\alpha_i}^\dagger a_{\mathbf{p}} \tag{29}$$

So,

$$a_{\mathbf{p}}\,|\Phi\rangle = a_{\mathbf{p}}a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger\dots a_{\alpha_A}^\dagger\,|0\rangle = (\phi_{\alpha_1}(\mathbf{p}) - a_{\alpha_1}^\dagger a_{\mathbf{p}})a_{\alpha_2}^\dagger\dots a_{\alpha_A}^\dagger\,|0\rangle \tag{30}$$

$$= \sum_{i=1}^{A}(-1)^{i-1}\phi_{\alpha_i}(\mathbf{p})\,|\alpha_1\dots\alpha_{i-1}\alpha_{i+1}\dots\alpha_A\rangle \tag{31}$$

The conjugate gives,

$$\langle\Phi|\,a_{\mathbf{p}}^\dagger = \sum_{j=1}^{A}(-1)^{j-1}\,\langle\alpha_1\dots\alpha_{j-1}\alpha_{j+1}\dots\alpha_A|\,\phi_{\alpha_j}^\dagger(\mathbf{p}) \tag{32}$$

Hence,

$$\langle\Phi|a^\dagger_{\mathbf{p}}a_{\mathbf{p}}|\Phi\rangle = \sum_{i,j=1}^{A}(-1)^{i+j}\phi^\dagger_{\alpha_j}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p})\underbrace{\langle\alpha_1\ldots\alpha_{j-1}\alpha_{j+1}\ldots\alpha_A|\alpha_1\ldots\alpha_{i-1}\alpha_{i+1}\ldots\alpha_A\rangle}_{=\delta_{ij}} \tag{33}$$

$$= \sum_i \phi^\dagger_{\alpha_i}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p}) \tag{34}$$

Which is exactly the same result as before.
So the one body momentum distribution is given by,

$$\langle\Phi|\hat{n}(p)|\Phi\rangle = \sum_{i=1}^{A}\frac{1}{(2\pi)^3}\int \mathrm{d}^2\Omega_{\mathbf{p}}\phi^\dagger_{\alpha_i}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p}) \tag{35}$$

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,

$$\langle\Phi|\hat{n}(p)|\Phi\rangle = \frac{1}{A}\sum_{i=1}^{A}\frac{1}{(2\pi)^3}\int \mathrm{d}^2\Omega_{\mathbf{p}}\phi^\dagger_{\alpha_i}(\mathbf{p})\phi_{\alpha_i}(\mathbf{p}) \tag{36}$$

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, $n_1l_1j_1m_{j_1}, n_2l_2j_2m_{j_2}$ 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 $\langle n_1l_1n_2l_2;\Lambda|nlNL;\Lambda\rangle$ 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

$$|\alpha_1,\alpha_2\rangle_{\mathrm{nas}} \quad ,|\alpha\rangle \equiv |nljm_jtm_t\rangle \tag{37}$$

The class calculates all the coefficients,

$$C^{A}_{\alpha_1\alpha_2} = \langle A \equiv \{nlSjm_j, NLM_LTM_T\}|\alpha_1\alpha_2\rangle_{\mathrm{nas}} \tag{38}$$

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 $n_1 l_1 j_1 m_{j_1} m_{t_1} n_2 l_2 j_2 m_{j_2} m_{t_2} N L M_L n l S j m_j T M_T$, and calculates the coefficient given in Eq. (38). 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,

$$\sum_{JM_J} \sum_{\Lambda} \frac{1}{\sqrt{2}} [1 - (-1)^{l+S+T}] \langle t_1 m_{t_1} t_2 m_{t_2} | T M_T \rangle \langle j_1 m_{j_1} j_2 m_{j_2} | J M_J \rangle \langle j m_j L M_L | J M_J \rangle$$
$$\langle nlNL; \Lambda | n_1 l_1 n_2 l_2; \Lambda \rangle_{\mathrm{SMB}} \sqrt{2\Lambda + 1} \sqrt{2j+1} \left\{ \begin{array}{ccc} j & L & J \\ \Lambda & S & l \end{array} \right\}$$
$$\sqrt{2j_1 + 1} \sqrt{2j_2 + 1} \sqrt{2S + 1} \sqrt{2\Lambda + 1} \left\{ \begin{array}{ccc} l_1 & s_1 & j_1 \\ l_2 & s_2 & j_2 \\ \Lambda & S & J \end{array} \right\} \quad (39)$$

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,

$$\langle \alpha_1\alpha_2 | \hat{\mathcal{O}} | \alpha_1\alpha_2 \rangle = \sum_{AB} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A | \hat{\mathcal{O}} | B \rangle \quad (40)$$

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. 40) is replaced by,

$$\langle \alpha_1\alpha_2 | \hat{\mathcal{O}} | \alpha_1\alpha_2 \rangle = \sum_{A} \sum_{\texttt{Paircoef(A).links}} \texttt{link.strength} \langle A | \hat{\mathcal{O}} | B \rangle \quad (41)$$

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

Note that the "linked" rcm states $|A\rangle, |B\rangle$ both stem from the expansion of the same single particle state $|\alpha_1\alpha_2\rangle$. This means that the linked rcm states will have certain properties. For example, the parity of $|\alpha_1\alpha_2\rangle$ is given by $(-1)^{l_1+l_2}$, the parity of a rcm state is $(-1)^{l+L}$, with l the relative angular momentum and L the c.m. angular momentum. Conservation of parity means that $(-1)^{l_1+l_2} = (-1)^{l_A+L_A} = (-1)^{l_B+L_B}$. For example, for operators that do not change the total spin S (this is the case for the operators considered here), we have $S_A = S_B$, it then follows that

- if $T_A = T_B$ then l_A and l_B have the same even-odd parity because of $l+S+T=$ odd. From $l_A - l_B$ is even it then follows that $L_A - L_B$ is even, or L_A, L_B have the same even-odd parity.
- if $T_A \neq T_B$ then l_A and l_B have opposite even-odd parity. Resulting in the condition that L_A and L_B also must have different even-odd parity.

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,

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

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

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

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

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

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

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

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...)

$$\begin{aligned}
\langle nl|f_c(r_{12})|n'l'\rangle &= N_{nl}N_{n'l'}\nu^{\frac{l+l'+3}{2}} \sum_{kk'\lambda} a_{nl,k}a_{n'l',k'}b_\lambda \nu^{-\frac{3+l+l'+\lambda}{2}} \int \mathrm{d}r\, r^{2+l+l'} e^{-r^2} r^{2k} r^\lambda e^{-Br^2} r^{2k'} \\
&= N_{nl}N_{n'l'} \sum_{kk'\lambda} \nu^{-\frac{\lambda}{2}} a_{nl,k}a_{n'l',k'}b_\lambda \int \mathrm{d}r\, r^{2+l+l'+\lambda+2k+2k'} e^{-(B+1)r^2} \\
&= N_{nl}N_{n'l'} \sum_{kk'\lambda} \nu^{-\frac{\lambda}{2}} a_{nl,k}a_{n'l',k'}b_\lambda \frac{1}{2}\Gamma\left(\frac{K+1}{2}\right)(1+B)^{-\frac{K+1}{2}} \\
&= \frac{N_{nl}N_{n'l'}}{2} \sum_{kk'\lambda} \nu^{-\frac{\lambda}{2}} a_{nl,k}a_{n'l',k'}b_\lambda \Gamma\left(\frac{K+1}{2}\right)(1+B)^{-\frac{K+1}{2}} \qquad (42)
\end{aligned}$$

$K = 2 + l + l' + \lambda + 2k + 2k'$. 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. 42) can easily be checked, $\langle nl|1|n'l\rangle$ ($l = l'$ because of the orthonormality of the spherical harmonics), if we set $b_\lambda = \delta_{\lambda,0}$, $b = 0$.

$$\langle nl|1|n'l\rangle = \frac{N_{nl}N_{n'l}}{2} \sum_{kk'=0}^{nn'} a_{nl,k}a_{n'l,k'}\Gamma\left(\frac{3+2l+2k+2k'}{2}\right) \qquad (43)$$

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

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

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

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

6.1 norm_ob : public operator_virtual_ob

Here we take a look at the calculation of the norm $\mathcal{N}$ (see Eqs. (10,(11)) 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:

$$\frac{2}{A} \sum_{AB} \hat{\delta}_{t_1, n_A, l_A, n_B, l_B} C^{A\dagger}_{\alpha_1\alpha_2} C^{B}_{\alpha_1\alpha_2} \langle A|B\rangle = \frac{2}{A} \sum_{A} \hat{\delta}_{t_1, n_A, l_A} \left|C^{A}_{\alpha_1\alpha_2}\right|^2 \tag{44}$$

for a specific pair $|\alpha_1\alpha_2\rangle$ passed trough `Pair`. It is possible to filter on relative quantum numbers on n_A, l_A, n_B, l_B, represented by the operator $\hat{\delta}_{t_1,n_A,l_A,n_B,l_B}$. It selects 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`. See section 8.1 for more information. The following integral is calculated,

$$\int \mathrm{d}P_{12}\, P_{12}^2 \Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{l_1 k}_{p,nl_p}(p_1, P_{12})\chi^{l_1 k'}_{p,n'l'_q}(p_1, P_{12})$$

The symbols $\chi^{l_1 k}_{p,nl_p}(p_1, P_{12})$, $\chi^{l_1 k'}_{p,n'l'_q}(p_1, P_{12})$ are calculated in `density_ob_integrand_cf`. Hence this integrand takes two `density_ob_integrand_cf*` pointers. Additionally it takes the parameters, $n, l_p, k, m', l'_q, k', p_1, \nu,$ `index` (`nA,lA,la,nB,lB,l,k,nu,index` in the code). `index` corresponds to the power of P_{12} in the integrand. This is because the $\Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})$ are expanded in powers of P_{12}, again see 8.1 for more details.

6.3 density_ob_integrand_cf

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

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

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 operators acting on coupled states

For a one body operator sandwiched between antisymmetric A-particle states $|\alpha_1\alpha_2\ldots\alpha_A\rangle$ the following identity is valid,

$$\sum_{i=1}^{A} \langle\alpha_1\alpha_2\ldots\alpha_A|\hat{\mathcal{O}}_i|\alpha_1\alpha_2\ldots\alpha_A\rangle = A\,\langle\alpha_1\alpha_2\ldots\alpha_A|\hat{\mathcal{O}}_1|\alpha_1\alpha_2\ldots\alpha_A\rangle$$

In particle for two particles,

$$\sum_{i=1}^{2} \langle \alpha_1\alpha_2|\hat{\mathcal{O}}_i|\alpha_1\alpha_2\rangle = 2\,\langle \alpha_1\alpha_2|\hat{\mathcal{O}}_1|\alpha_1\alpha_2\rangle$$

We now investigate how this result changes if we let the one-body operator act on coupled states of two particles. More specifically we will look at the one-body momentum operator $\hat{n}^{[1],i}_{s_1,t_1}(\vec{p}_1)$. The square brackets [1] denote that this is a one-body operator. The number right next to that i symbolizes which particle it acts on. s,t denote the single-particle spin and isospin projections.

$$\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1) = \hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)\otimes \mathbb{1} = |\vec{p}_1 s_1 t_1\rangle\,\langle\vec{p}_1 s_1 t_1| \otimes \sum_{s_2,t_2}\int \mathrm{d}^3\,\vec{p}_2\,|\vec{p}_2 s_2 t_2\rangle\,\langle\vec{p}_2 s_2 t_2|$$

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

We will try to relate $\langle A|\hat{n}^{[1],2}_{s_1,t_1}(\vec{p}_1)|A'\rangle$ to $\langle A|\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)|A'\rangle$. We will see that the naive expectation that these are equal does not hold. This is caused by the fact that we are sandwiching the one-body operator between **coupled** states and not single-particle states.

$$\begin{aligned}
\langle A|\hat{n}^{[1],2}_{s_1,t_1}(\vec{p}_1)A'\rangle = \langle A|\mathbb{1}\otimes\hat{n}^{[1]}_{s_1,t_1}(\vec{p}_1)|A'\rangle &= \langle A|\left(\sum_{s_2,t_2}\int \mathrm{d}^3\,\vec{p}_2\,|\vec{p}_2 s_2 t_2\rangle\,\langle\vec{p}_2 s_2 t_2|\otimes|\vec{p}_1 s_1 t_1\rangle\,\langle\vec{p}_1 s_1 t_1|\right)|A'\rangle \\
&\propto \sum_{s_2,t_2}\int \mathrm{d}^3\,\vec{p}_2 \int \mathrm{d}^3\,\vec{r}_1 \mathrm{d}^3\,\vec{r}_1{}'\mathrm{d}^3\vec{r}_2\mathrm{d}^3\vec{r}_2{}' \\
&\quad \langle\widetilde{A}|\vec{r}_1\vec{r}_2\rangle\,\langle SM_S|\frac{1}{2}s_2\frac{1}{2}s_1\rangle\,\langle TM_T|\frac{1}{2}t_2\frac{1}{2}t_1\rangle\,\langle\vec{r}_1|\vec{p}_2\rangle\,\langle\vec{r}_2|\vec{p}_1\rangle \\
&\quad \langle\vec{r}_1{}'\vec{r}_2{}'|\widetilde{A}'\rangle\,\langle\frac{1}{2}s_2\frac{1}{2}s_1|S'M_S'\rangle\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|T'M_T'\rangle\,\langle\vec{p}_2|\vec{r}_1{}'\rangle\,\langle\vec{p}_1|\vec{r}_2{}'\rangle
\end{aligned}$$

Note that we used $\propto$ instead of the equality sign as we omit the LS-coupling for conciseness. This has no influence on the results. $\widetilde{A}$ symbolizes the coupled state without the spin and isospin part (with the LS-coupling omitted), $\widetilde{A} = |nlm_l NLM_L\rangle$. Using the identity,

$$\langle j_1 m_1, j_2 m_2|JM\rangle = (-1)^{j_1+j_2-J}\,\langle j_2 m_2, j_1 m_1|JM\rangle$$

we get

$$\begin{aligned}
\langle A|\hat{n}^{[1],2}_{s_1,t_1}(\vec{p}_1)A'\rangle \propto \sum_{s_2,t_2}\int \mathrm{d}^3\,\vec{p}_2 \int \mathrm{d}^3\,\vec{r}_1 \mathrm{d}^3\,\vec{r}_1{}'\mathrm{d}^3\vec{r}_2\mathrm{d}^3\vec{r}_2{}' \\
(-1)^{S+S'+T+T'} \\
\langle\widetilde{A}|\vec{r}_1\vec{r}_2\rangle\,\langle SM_S|\frac{1}{2}s_1\frac{1}{2}s_2\rangle\,\langle TM_T|\frac{1}{2}t_1\frac{1}{2}t_2\rangle\,\langle\vec{r}_1|\vec{p}_2\rangle\,\langle\vec{r}_2|\vec{p}_1\rangle \\
\langle\vec{r}_1{}'\vec{r}_2{}'|\widetilde{A}'\rangle\,\langle\frac{1}{2}s_1\frac{1}{2}s_2|S'M_S'\rangle\,\langle\frac{1}{2}t_1\frac{1}{2}t_2|T'M_T'\rangle\,\langle\vec{p}_2|\vec{r}_1{}'\rangle\,\langle\vec{p}_1|\vec{r}_2{}'\rangle
\end{aligned}$$

The part involving the spatial and momentum coordinates is not so straightforward,

$$\begin{aligned}
\int \mathrm{d}^3\,\vec{p}_2\,\langle\vec{r}_1|\vec{p}_2\rangle\,\langle\vec{r}_2|\vec{p}_1\rangle\,\langle\vec{p}_2|\vec{r}_1{}'\rangle\,\langle\vec{p}_1|\vec{r}_2{}'\rangle &= \delta(\vec{r}_1-\vec{r}_1{}')e^{i\vec{p}_1\cdot(\vec{r}_2-\vec{r}_2{}')} \\
&= \delta\left(\frac{\vec{R}_{12}-\vec{r}_{12}-\vec{R}_{12}'+\vec{r}_{12}'}{\sqrt{2}}\right)e^{-i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}_{12}')}
\end{aligned}$$

For $\langle A|\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)|A'\rangle$ we would get,

$$\int \mathrm{d}^3\,\vec{p}_2\,\langle\vec{r}_1|\vec{p}_1\rangle\,\langle\vec{r}_2|\vec{p}_2\rangle\,\langle\vec{p}_2|\vec{r}_2'\rangle\,\langle\vec{p}_1|\vec{r}_1'\rangle = \delta(\vec{r}_2-\vec{r}_2')e^{i\vec{p}_1\cdot(\vec{r}_1-\vec{r}_1')}$$
$$= \delta\left(\frac{\vec{R}_{12}+\vec{r}_{12}-\vec{R}_{12}'-\vec{r}_{12}'}{\sqrt{2}}\right)e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}_{12}')}$$

It is easy to see that the difference between $\langle A|\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)|A'\rangle$ and $\langle A|\hat{n}^{[1],2}_{s_1,t_1}(\vec{p}_1)|A'\rangle$ concerning the spatial coordinates is a sign flip of $\vec{r}_{12}$ and $\vec{r}_{12}'$, which can be intuitively understood. So to summarize,

$$\langle A|\hat{n}^{[1],2}_{s_1,t_1}(p_1)|A'\rangle = (-1)^{S+S'+T+T'}\,\langle A|\hat{n}^{[1],1}_{s_1,t_1}(p_1)\left[(\vec{r}_{12},\vec{r}_{12}')\to(-\vec{r}_{12},-\vec{r}_{12}')\right]|A'\rangle \tag{45}$$

Yes I agree that this is terrible notation but it should make the main message clear.

8 One body momentum distribution

We will look into one-body momentum distributions in more detail. A matrix element as calculated in the norm (??) is now extended by including the ony-body momentum operator $\hat{n}^{[1]}_{s,t}(\vec{p}) = \sum_i \hat{n}^{[1],i}_{s,t}(\vec{p})$. The square brackets [1] denote that this is a one-body operator. The number right next to that i symbolizes which particle it acts on. s is the spin projection of the nucleon and t the isospin projection. We will calculate the case where the momentum operator acts on "particle 1" first and then use the relation derived in Eq. (45) to get the expression for the case where the momentum operator acts on "particle 2".

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

The one-body momentum operator $\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)$ is given by,

$$\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1) = |\vec{p}_1s_1t_1\rangle\,\langle\vec{p}_1s_1t_1|\otimes\mathbb{1} = \sum_{s_2,t_2}\int\mathrm{d}^3\vec{p}_2\,n^{[2]}_{\substack{s_1,t_1\\s_2,t_2}}(\vec{p}_1,\vec{p}_2)$$
$$= \sum_{s_2,t_2}\int\mathrm{d}^3\vec{p}_2\,|\vec{p}_1s_1t_1,\vec{p}_2s_2t_2\rangle\,\langle\vec{p}_1s_1t_1,\vec{p}_2s_2t_2|$$

Hence,

$$\langle A|\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \sum_{s_2,t_2}\int\mathrm{d}^3\vec{p}_2\,\langle A|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger|\vec{p}_1s_1t_1,\vec{p}_2s_2t_2\rangle\,\langle\vec{p}_1s_1t_1,\vec{p}_2s_2t_2|f_q\hat{\mathcal{O}}^q|A'\rangle$$
$$= \sum_{s_2,t_2}\int\mathrm{d}^3\vec{p}_2\mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2\mathrm{d}^3\vec{r}_1'\mathrm{d}^3\vec{r}_2'$$
$$\langle A|\hat{\mathcal{O}}^{p\dagger}f_p^\dagger|\vec{r}_1s_1t_1,\vec{r}_2s_2t_2\rangle\,\langle\vec{r}_1\vec{r}_2|\vec{p}_1\vec{p}_2\rangle\,\langle\vec{p}_1\vec{p}_2|\vec{r}_1'\vec{r}_2'\rangle\,\langle\vec{r}_1's_1t_1,\vec{r}_2's_2t_2|f_q\hat{\mathcal{O}}^q|A'\rangle$$

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

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

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,

$$\int\mathrm{d}^3\vec{p}_2e^{i\vec{p}_2\cdot(\vec{r}_2-\vec{r}_2')} = (2\pi)^3\sqrt{2}^3\delta^{(3)}(\vec{R}_{12}-\vec{r}_{12}-\vec{R}_{12}'+\vec{r}_{12}')$$

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

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,

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

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

For the sake of brevity we define,

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

The c.m. wave functions $\psi_{NLM_L}(\vec{R}_{12})$, $\psi_{N'L'M'_L}(\vec{R}'_{12})$ are written as their inverse Fourier transformation (see Secs. 1,9),

$$\psi_{NLM_L}(\vec{R}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int \mathrm{d}^3\vec{P}e^{i\vec{P}\cdot\vec{R}}\phi_{NLM_L}(\vec{P}) \tag{46}$$
$$= i^{-L}(-1)^N(2\pi)^{-\frac{3}{2}}\int \mathrm{d}^3\vec{P}e^{i\vec{P}\cdot\vec{R}}\Pi_{NL}(P)Y_{LM_L}(\Omega_P)\,. \tag{47}$$

The one-body momentum distribution can then be written as,

$$\langle A|\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)|A'\rangle = \sum_{s_2t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$\frac{\sqrt{8}}{(2\pi)^3}\int \mathrm{d}^3\vec{R}_{12}\mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}'_{12}e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}'_{12})}f^{\dagger}_p(r_{12})f_q(r'_{12})\psi^{\dagger}_{nl_pm_{l_p}}(\vec{r}_{12})\psi_{n'l'_qm_{l'_q}}(\vec{r}'_{12})$$
$$\frac{1}{(2\pi)^3}\int \mathrm{d}^3\vec{P}_{12}\int \mathrm{d}^3\vec{P}'_{12}e^{-i\vec{P}_{12}\cdot\vec{R}_{12}}\phi^{\dagger}_{NLM_L}(\vec{P}_{12})e^{i\vec{P}'_{12}\cdot(\vec{R}_{12}-\vec{r}_{12}+\vec{r}'_{12})}\phi_{N'L'M'_L}(\vec{P}'_{12})$$
$$= \sum_{s_2t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1}\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$$
$$\frac{\sqrt{8}}{(2\pi)^3}\int \mathrm{d}^3\vec{r}_{12}\mathrm{d}^3\vec{r}'_{12}e^{i\sqrt{2}\vec{p}_1\cdot(\vec{r}_{12}-\vec{r}'_{12})}f^{\dagger}_p(r_{12})f_q(r'_{12})\psi^{\dagger}_{nl_pm_{l_p}}(\vec{r}_{12})\psi_{n'l'_qm'_{l_q}}(\vec{r}'_{12})$$
$$\int \mathrm{d}^3\vec{P}_{12}e^{-i\vec{P}_{12}\cdot(\vec{r}_{12}-\vec{r}'_{12})}\phi^{\dagger}_{NLM_L}(\vec{P}_{12})\phi_{N'L'M'_L}(\vec{P}_{12})$$

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

$\phi_{nlm_l}(\vec{p}) = i^{-l}(-1)^n \Pi_{nl}(p) Y_{lm_l}(\Omega_p)$ (see Secs. 1,9).

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

Rearranging the integrals results in

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

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

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

and,

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

The one-body momentum matrix element can then be written as,

$$\begin{aligned}
\langle A|\hat{n}^{[1],1}_{s_1,t_1}(\vec{p}_1)|A'\rangle = &\sum_{s_2t_2} \sum_{l_p=|j-1|}^{j+1} \sum_{l'_q=|j'-1|}^{j'+1} \mathcal{M}^{pq,l_pl'_q}_{AA'}(s_1,t_1,s_2,t_2) \\
&64\sqrt{2}\pi \sum_{km_k} \sum_{k'm'_k} \sum_{KM_K} \sum_{K'M'_K} i^{L-L'+k-k'-K+K'} Y^*_{km_k}(\Omega_{p_1})Y_{k'm'_k}(\Omega_{p_1}) \\
&(-1)^{N+N'} \int \mathrm{d}P_{12}\, P_{12}^2 \Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{kK\dagger}_{p,nl_p}(p_1,P_{12})\chi^{k'K'}_{q,n'l'_q}(p_1,P_{12}) \\
&\sqrt{\frac{(2k+1)(2K+1)}{4\pi(2l_p+1)}} \langle km_k KM_K|l_p m_{l_p}\rangle \langle k0K0|l_p0\rangle \\
&\sqrt{\frac{(2k'+1)(2K'+1)}{4\pi(2l'_q+1)}} \langle k'm'_k K'M'_K|l'_q m_{l'_q}\rangle \langle k'0K'0|l'_q0\rangle \\
&\sum_{JM_J} \sqrt{\frac{(2L+1)(2K+1)}{4\pi(2J+1)}} \langle LM_L KM_K|JM_J\rangle \langle L0K0|J0\rangle \\
&\sqrt{\frac{(2L'+1)(2K'+1)}{4\pi(2J+1)}} \langle L'M'_L K'M'_K|JM_J\rangle \langle L'0K'0|J0\rangle
\end{aligned}$$

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

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

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

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

To cross check this result with Maartens (D.37) we must go back a step and make another (debatably less logical) choice for contracting the spherical harmonics (note the subtle difference the complex conjugation choice of the spherical harmonics arising from the plane wave expansion).

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

$$
\begin{aligned}
\langle A|\hat{n}^{[1],1}_{s_1,t_1}(p_1)|A'\rangle = \sum_{s_2t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1} &\mathcal{M}^{pq,l_pl'_q}_{AA'}(s_1,t_1,s_2,t_2)\\
&64\sqrt{2}\pi\sum_{km_k}\sum_{Km_K}\sum_{K'm'_K} i^{L-L'-K+K'}\\
(-1)^{N+N'}\int &\mathrm{d}P_{12}\,P_{12}^2\Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{kK}_{p,nl_p}(p_1,P_{12})\chi^{kK'}_{p,n'l'_q}(p_1,P_{12})\\
&\int \mathrm{d}^2\Omega_{r_{12}}Y^*_{l_pm_{l_p}}(\Omega_{r_{12}})Y_{km_k}(\Omega_{r_{12}})Y^*_{Km_K}(\Omega_{r_{12}})\\
&\int \mathrm{d}^2\Omega_{r'_{12}}Y_{l'_qm_{l'_q}}(\Omega_{r'_{12}})Y^*_{km_k}(\Omega_{r'_{12}})Y_{K'm'_K}(\Omega_{r'_{12}})\\
&\int \mathrm{d}^2\Omega_{P_{12}}Y^*_{LM_L}(\Omega_{P_{12}})Y_{L'M'_L}(\Omega_{P_{12}})Y_{Km_K}(\Omega_{P_{12}})Y^*_{K'm'_K}(\Omega_{P_{12}})
\end{aligned}
$$

$$
\begin{aligned}
\langle A|\hat{n}^{[1],1}_{s_1,t_1}(p_1)|A'\rangle = \sum_{s_2t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1} &\mathcal{M}^{pq,l_pl'_q}_{AA'}(s_1,t_1,s_2,t_2)\\
&\frac{4\sqrt{2}}{\pi}\sum_{km_k}\sum_{Km_K}\sum_{K'm'_K} i^{L-L'-K+K'}\\
(-1)^{N+N'}\int &\mathrm{d}P_{12}\,P_{12}^2\Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{kK}_{p,nl_p}(p_1,P_{12})\chi^{kK'}_{p,n'l'_q}(p_1,P_{12})\\
&\frac{\hat{l}_p\hat{K}}{\hat{k}}\,\langle l_pm_{l_p}Km_K|km_k\rangle\,\langle l_p0K0|k0\rangle\\
&\frac{\hat{l}'_q\hat{K}'}{\hat{k}}\,\langle l'_qm_{l'_q}K'm'_K|km_k\rangle\,\langle l'_q0K'0|k0\rangle\\
\sum_{JM_J}\frac{\hat{L}\hat{K}'}{\hat{J}}\frac{\hat{L}'\hat{K}}{\hat{J}}\,&\langle LM_LK'm'_K|JM_J\rangle\,\langle L0K'0|JM_J\rangle\,\langle L'M'_LKm_K|J0\rangle\,\langle L'0K0|J0\rangle
\end{aligned}
$$

The CGC coefficients are written as Wigner-3j symbols,

$$
\langle j_1m_1j_2m_2|JM\rangle = (-1)^{j_1-j_2+M}\,\hat{J}\begin{pmatrix} j1 & j2 & J\\ m_1 & m_2 & -M\end{pmatrix},
$$

resulting in,

$$
\begin{aligned}
\langle A|\hat{n}^{[1],1}_{s_1,t_1}(p_1)|A'\rangle = \sum_{s_2t_2}\sum_{l_p=|j-1|}^{j+1}\sum_{l'_q=|j'-1|}^{j'+1} &\mathcal{M}^{pq,l_pl'_q}_{AA'}(s_1,t_1,s_2,t_2)\\
&\frac{4\sqrt{2}}{\pi}\sum_{km_k}\sum_{Km_K}\sum_{K'm'_K} i^{L-L'-K+K'}\\
(-1)^{N+N'}\int &\mathrm{d}P_{12}\,P_{12}^2\Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{kK}_{p,nl_p}(p_1,P_{12})\chi^{kK'}_{p,n'l'_q}(p_1,P_{12})\\
\hat{l}_p\hat{l}'_q\hat{K}\hat{K}'\hat{k}^2&\begin{pmatrix} l_p & K & k\\ m_{l_p} & m_K & m_k\end{pmatrix}\begin{pmatrix} l_p & K & k\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l'_q & K' & k\\ m_{l'_q} & m'_K & m_k\end{pmatrix}\begin{pmatrix} l'_q & K' & k\\ 0 & 0 & 0\end{pmatrix}\\
\sum_{JM_J}\hat{K}\hat{L}\hat{K}'\hat{L}'\hat{J}^2&\begin{pmatrix} L & K' & J\\ M_L & m'_K & M_J\end{pmatrix}\begin{pmatrix} L & K' & J\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} L' & K & J\\ M'_L & m_K & M_J\end{pmatrix}\begin{pmatrix} L' & K & J\\ 0 & 0 & 0\end{pmatrix}.
\end{aligned}
$$

The sign of the summation indices M_J and m_k have been flipped here, this is equivalent with simply rearranging the terms in the sums over M_J and m_k. Writing $\mathcal{M}^{pq,l_p l'_q}_{AA'}(s_1,t_1,s_2,t_2)$ explicitly gives,

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

If we are not interested in the spin decomposition of the one-body momentum matrix element, the spin s_1 can be summed over,

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

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

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

Finally we make use of

$$\begin{pmatrix} a & b & c \\ m_a & m_b & m_c \end{pmatrix} \begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} a & c & b \\ m_a & m_c & m_b \end{pmatrix} \begin{pmatrix} a & c & b \\ 0 & 0 & 0 \end{pmatrix}$$

and compare our expression against (D.37). Parts that are not found in (D.37) are colored red. Maarten uses the definition,

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

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. Maarten also omitted the sums over l_p and l'_q and picked a specific contribution l, l' which do not necessarily correspond with l, l' of the coupled states $|A\rangle, |A'\rangle$. The factor $(-1)^{N+N'}$ is absorbed in the way Maarten calculated the

$\Pi_{NL}(P_{12})$. Maartens definition of $\Pi_{NL}(P_{12})$ deviates slightly from our definition. This is detailed in Sec. 8.1.
If we now go back to the sum,

$$\begin{aligned}\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle &= \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle + \langle A|\hat{n}^{[1],2}_{t_1}(p_1)|A'\rangle \\ &= \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle + (-1)^{S+S'+T+T'}\,\langle A|\hat{n}^{[1],1}_{s_1,t_1}(p_1)\left[(\vec{r}_{12},\vec{r}^{\,\prime}_{12}) \to (-\vec{r}_{12},-\vec{r}^{\,\prime}_{12})\right]|A'\rangle\end{aligned}$$

A closer look at the above derivation shows that the effect of $(\vec{r}_{12},\vec{r}^{\,\prime}_{12}) \to (-\vec{r}_{12},-\vec{r}^{\,\prime}_{12})]$ translates into a sign switch in $i^{k-k'} \to i^{k'-k}, i^{K'-K} \to i^{K-K'}$. The phase factor $i^{L-L'}$ is connected to the c.m. coordinate R_{12} and is not affected. Suppose we are looking at a specific term in the summation over K,K'. (The dependence on $i^{k-k'}$ has vanished by integration over the solid angle of the one body momentum). The factors containing the imaginary unit i is explicitly written here.

$$\begin{aligned}\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} &= \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'}\left[i^{L-L'+K'-K} + (-1)^{S+S'+T+T'} i^{L-L'+K-K'}\right] \\ &= \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'}\, i^{L-L'+K'-K}\left[1 + (-1)^{S+S'+T+T'+K-K'}\right]\end{aligned}$$

The imaginary unit i is pulled out of the matrix element $\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'}$, and written explicitly. It can easily be checked that this means that $\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'}$ is real (that is, if the CondonShortley convention for the Clebsch-Gordan coefficients (CGC) is adopted, ensuring that the CGC are real).
As outlined in Sec. 4.3, A and A' have the same parity,

$$(-1)^{l+L} = (-1)^{l'+L'} \Leftrightarrow (-1)^{l+l'+L+L'} = 1 \Leftrightarrow (-1)^{l\pm l'} = (-1)^{L\pm L'}\,. \tag{48}$$

From the antisymmetry requirement of a fermion wave function it follows that $(-1)^{l+S+T} = -1$, hence,

$$(-1)^{S+S'+T+T'} = (-1)^2(-1)^{l+l'} = (-1)^{L+L'}\,. \tag{49}$$

This allows us to rewrite $\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'}$ as,

$$\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} = \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'}\, i^{L-L'+K'-K}\left[1 + (-1)^{L+L'+K-K'}\right]$$

An alternative expression can be derived using the fact that the correlation operators do not change the total spin S ($S = S'$),

$$\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} = \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'}\, i^{L-L'+K'-K}\left[1 + (-1)^{T+T'+K-K'}\right]$$

Let us take a look how this is, **IN A VERY OBFUSCATED WAY**, dealt with in Maarten's code. The powers of i, namely $i^{L-L'+K'-K}$ and $i^{L-L'+K-K'}$, are denoted `ipower1` and `ipower2` in Maarten's code.

```
int ipower1= (LA-LB+l-la)%4;
int ipower2= (LA-LB+la-l)%4;
double ifactor= preifactor;
if( TA == TB ) {
    if( GSL_IS_ODD( ipower1 ) ) {
        if( (ipower1+ipower2)%4 == 0 ) continue;
        else
            cerr << __FILE__ << __LINE__ << "IMAG" << endl;
    }
    if( fabs( ipower1) != fabs(ipower2) ) continue;
```

```
        if( ipower1 == 0 )
            ifactor *= 2;
        else
            ifactor*= -2;
    }
    if( TA != TB ) {
        if( GSL_IS_ODD( ipower1 ) ) {
            if( fabs((ipower1+ipower2)%4) == 2 ) continue;
            else
                cerr << __FILE__ << __LINE__ << "IMAG" << endl;

        }
        if( fabs( ipower1) == fabs(ipower2) ) continue;
        if( ipower1 == 0 )
            ifactor *= 2;
        else
            ifactor*= -2;
    }
```

First of all the modulo 4's you see appearing is because n in i^n can be changed by multiples of four for free. The variables `LA,LB,l,la` correspond to our L, L', K', K. Secondly note that as `ipower1` and `ipower2` are of the form $a+b$,$a-b$ with $a, b \in \mathbb{Z}$ we have that they both have the same parity (even or odd) (The modulo 4 does not change this fact).

- $T = T'$ (`TA==TB`)
  As we already have $S = S'$ and $l + S + T =$ odd, we have that $l \pm l'$ or equivalently $L \pm L'$ (`LA,LB`) is even,

$$\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} = \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'} i^{L-L'+K'-K}\left[1 + (-1)^{K-K'}\right] \tag{50}$$

  - `ipower1` is odd
    As $L \pm L'$ is even, this implies $K - K'$ is odd, from Eq. (50) it follows that the matrix element is zero. The check `(ipower1+ipower2) % 4 == 0` is automatically valid and not necessary,

$$\texttt{ipower1 + ipower2} = 2(L - L') \tag{51}$$

    As $L - L'$ is even, this is always a multiple of 4.
  - `ipower1` is even
    As $L \pm L'$ is even, this implies $K - K'$ is even as well. Eq. (50) then becomes,

$$\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} = \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'} 2i^{L-L'+K'-K}, \tag{52}$$

    where it ensured that $L-L'+K'-K$ is even, leading to a real result. If $L-L'+K'-K$ is a multiple of 4 a positive sign appears, otherwise a negative sign will survive. Additionally both `ipower1` and `ipower2` are even. Through the modulo 4 they can only equal -2,0, or 2. Next we have the check

```
if( fabs( ipower1) != fabs(ipower2) ) continue;
```

    We will show that this is unnecessary as well. Without loss of generality we can assume

$$\texttt{ipower1} = (2n + 2m)\%4$$
$$\texttt{ipower2} = (2n - 2m)\%4$$

With $n, m \in [-1, 0, 1]$. Larger ranges will be mapped back to $[-1, 0, 1]$ by the modulo %4 operator. $|\texttt{ipower1}| \neq |\texttt{ipower2}|$ implies that $\texttt{ipower1} = 0, \texttt{ipower2} = \pm 2$, or $\texttt{ipower1} = \pm 2, \texttt{ipower2} = 0$. It is straightforward to see that $\texttt{ipower1} = 0 \Leftrightarrow \texttt{ipower2} = 0$.

  * `ipower1 == 0`
    As we have just argued, this implies `ipower2 == 0` as well. $i^{\texttt{ipower1}} + i^{\texttt{ipower2}} = 1 + 1 = 2$, justifying the `ifactor *= 2;`
  * `ipower1 != 0` (corresponding to the `else` statement)
    We now have $\texttt{ipower1} = \pm 2$, $\texttt{ipower2} = \pm 2$, where the signs of `ipower1` and `ipower2` do not have to be the same. $i^{\texttt{ipower1}} + i^{\texttt{ipower2}} = (-1)^{\pm 1} + (-1)^{\pm 1} = -1 - 1 = -2$, hence the `ifactor *=-2;`

- $T \neq T'$, (`TA != TB`)
  Again using the argument that $l + S + T = \text{odd}$, $S = S'$ and the fact that $T, T' \in [0, 1]$ it is easy to see that this time $l \pm l'$ or $L \pm L'$ are odd.

$$\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} = \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'}\, i^{L-L'+K'-K}\left[1 - (-1)^{K-K'}\right] . \quad (53)$$

  - `ipower1` is odd
    As $L \pm L'$ is odd, this implies that $K' - K$ and $K - K'$ (`l-la` and `la-l`) are even. Eq. (53) is zero in this case. As we have that $\texttt{ipower1},\texttt{ipower2} \in [-3, -1, 1, 3]$, we can, without loss of generality, assume that $L - L'(\texttt{LA-LB}) = m$, $m \in [-1, 1]$, $K' - K(\texttt{l-la}) = 2n$, $n \in [-1, 0, 1]$. Hence $\texttt{ipower1 + ipower2} = 2m$, $m \in [-1, 1]$. Hence,

    ```
    if ( fabs((ipower1+ipower2)%4) == 2 )
    ```

    is always true here. $i^{\texttt{ipower1}} - i^{\texttt{ipower2}} = i^{\texttt{ipower1}} - i^{2m-\texttt{ipower1}} = i^{\texttt{ipower1}} - i^{\texttt{ipower1}} = 0$. Again the iteration is skipped in this case through the `continue` statement.
  - `ipower1` is even
    In this case $K - K'$ is odd and Eq. (53) becomes

$$\langle A|\hat{n}^{[1]}_{t_1}(p_1)|A'\rangle_{K,K'} = \langle A|\hat{n}^{[1],1}_{t_1}(p_1)|A'\rangle_{K,K'}\, 2i^{L-L'+K'-K} , \quad (54)$$

    here it ensured that $L - L' + K' - K$ is even, leading to a real result. If $L - L' + K' - K$ is a multiple of 4 a positive sign appears, otherwise a negative sign will survive. Here we have $\texttt{power1}, \texttt{power2} \in [-2, 0, 2]$. Next we have the check

    ```
    if( fabs( ipower1) == fabs(ipower2) ) continue;
    ```

    Without loss of generality we can write

$$\texttt{ipower1} = (2n + 1 + 2m + 1)\%4$$
$$\texttt{ipower2} = (2n + 1 - 2m - 1)\%4$$

    With $n, m \in [-1, 0, 1]$. It is an easy exercise to show that $\texttt{ipower1} = \pm\texttt{ipower2}$ implies that either n or m is equal to $-1/2$ which contradicts our starting point. This proves that $|\texttt{ipower1}| = |\texttt{ipower2}|$ is never true in this case.

    * `ipower1 == 0`
      As we have just argued, this implies $\texttt{ipower2} == \pm 2$. $i^{\texttt{ipower1}} - i^{\texttt{ipower2}} = 1 + 1 = 2$, justifying the `ifactor *= 2;`
    * `ipower1 != 0` (corresponding to the `else` statement)
      We now have $\texttt{ipower1} = \pm 2$, $\texttt{ipower2} = 0$. $i^{\texttt{ipower1}} - i^{\texttt{ipower2}} = (-1)^{\pm 1} - 1 = -2$, hence the `ifactor *=-2;`

THE MAIN MESSAGE
All this spaghetti code above of Maarten is equivalent with the simple one-liner:
`ifactor*` $= i^{L-L'+K'-K}\left[1+(-1)^{T+T'+K-K'}\right]$
or
`ifactor*` $= i^{L-L'+K'-K}\left[1+(-1)^{L+L'+K-K'}\right]$
ALL of the if-statements can be replaced by checking the antisymmetry $(-1)^{l+S+T} = (-1)^{l'+S'+T'} = -1$, the total spin-conservation $S = S'$ and the parity conservation $(-1)^{l+L} = (-1)^{l'+L'}$ as those are the only things used to make the above derivation.
WHY MAARTEN, WHHYYYYYYYYY??????????
TODO: Replace this in the code and test if I get the same results...

8.1 C.M. momentum integral

Let us take a closer a look at how the integral

$$\begin{aligned}(-1)^{N+N'} &\int \mathrm{d}P_{12}\, P_{12}^2 \Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{l_1 k}_{p,nl_p}(p_1,P_{12})\chi^{l_1 k'}_{p,n'l'_q}(p_1,P_{12}) \\ &= N_{NL}N_{N'L'}(-1)^{N+N'}\nu^{-\frac{L+L'+3}{2}} \int \mathrm{d}P_{12}\, P_{12}^2 P_{12}^L e^{-\frac{P_{12}^2}{2\nu}} L_N^{L+\frac{1}{2}}(P_{12}^2/\nu) P_{12}^{L'} e^{-\frac{P_{12}^2}{2\nu}} L_{N'}^{L'+\frac{1}{2}}(P_{12}^2/\nu) \\ &\qquad \chi^{l_1 k}_{p,nl_p}(p_1,P_{12})\chi^{l_1 k'}_{p,n'l'_q}(p_1,P_{12}) \end{aligned} \tag{55}$$

with $N_{NL} = [2n!/\Gamma(N+L+3/2)]^{1/2}$, is calculated. Note in particular the phase factor $(-1)^{N+N'}$, critical to the derivation. For the calculation of the above integral Maarten used a "somewhat more complicated approach", whereby the symmetry between the coordinate and momentum space of the HO is not exploited. The phase factor is hidden in Maarten's more complicated formulation. Expanding the generalized Laguerre polynomials in momentum space gives,

$$\begin{aligned}(-1)^{N+N'} &\int \mathrm{d}P_{12}\, P_{12}^2 \Pi^*_{NL}(P_{12})\Pi_{N'L'}(P_{12})\chi^{l_1 k}_{p,nl_p}(p_1,P_{12})\chi^{l_1 k'}_{p,n'l'_q}(p_1,P_{12}) \\ &= N_{NL}N_{N'L'}\nu^{-\frac{L+L'+3}{2}}(-1)^{N+N'}\sum_{i=0}^{N}\sum_{j=0}^{N'} a_{NL,i}a_{NL,j}\nu^{-i-j} \\ &\qquad \int \mathrm{d}P_{12}\, P_{12}^{2+L+L'+2i+2j} e^{-\frac{P_{12}^2}{\nu}} \chi^{l_1 k}_{p,nl_p}(p_1,P_{12})\chi^{l_1 k'}_{p,n'l'_q}(p_1,P_{12}) \end{aligned} \tag{56}$$

is calculated in the code. As discussed in (?????) the symbols $\chi^{l_1 k}_{p,nl_p}(p_1,P_{12})$ are calculated in `density_ob_integrand_cf`. The calculation of the c.m. momentum integral (Eq. (56)) is done in `density_ob_integrand3`. The integrand of (56) can be found in `density_ob_integrand3::integrand`.

$$P_{12}^2 P_{12}^{\mathrm{index}} e^{-\frac{P_{12}^2}{\nu}} \chi^{l_1 k}_{p,nl_p}(p_1,P_{12})\chi^{l_1 k'}_{p,n'l'_q}(p_1,P_{12})$$

Where the "index" (see code) is the power of the c.m. momentum (not including the P_{12}^2 of the Jacobian) $L + L' + 2i + 2j$.

ERROR: Maarten has extra summations, binomial coefficients, pochhammer symbols etc, of which I have no clue where they are coming from (see `density_ob_integrand3::add` @ line 34). If I read the code correctly it calculates the equation below, but I have no idea where it comes from... I was NOT able to derive this formula from the expression in appendix C.2 of Maartens thesis

`Maarten's expression in the c++ code:`

$$
\begin{aligned}
& N_{NL} N_{N'L'} \nu^{-\frac{L+L'+3}{2}} \sum_{i=0}^{N} \sum_{j=0}^{N} a_{NL,i} a_{N'L',j} 2^{i+j} \\
& \qquad \sum_{i'=0}^{i} \sum_{j'=0}^{j} (-2\nu)^{-i'-j'} \begin{pmatrix} i \\ i' \end{pmatrix} \begin{pmatrix} j \\ j' \end{pmatrix} (L+i'+\frac{3}{2})^{(i-i')} (L'+j'+\frac{3}{2})^{(j-j')} \\
& \qquad\qquad \int \mathrm{d}P_{12}\, P_{12}^{2+L+L'+2i'+2j'} e^{-\frac{P_{12}^2}{\nu}} \chi^{l_1 k}_{p,nl_p}(p_1, P_{12}) \chi^{l_1 k'}_{p,n'l'_q}(p_1, P_{12}) \qquad (57)
\end{aligned}
$$

We introduced the notation $a^{(n)} = \Gamma(a+n)/\Gamma(a)$ for the rising factorial or Pochhammer function. It is easy to see that eqs. (56) and (57) are equivalent if we can show that,

$$
(-1)^N \Pi_{NL}(P_{12}) = (-1)^N \sum_{i=0}^{N} a_{NL,i} \nu^{-i} P_{12}^{2i} = \sum_{i=0}^{N} a_{NL,i} 2^i \sum_{i'=0}^{i} (-2\nu)^{-i'} \begin{pmatrix} i \\ i' \end{pmatrix} (L+i'+\frac{3}{2})^{(i-i')} P_{12}^{2i'}
$$

The proof goes as follows:

$$
\begin{aligned}
& \sum_{i=0}^{N} a_{NL,i} 2^i \sum_{i'=0}^{i} (-2\nu)^{-i'} \begin{pmatrix} i \\ i' \end{pmatrix} (L+i'+\frac{3}{2})^{(i-i')} P_{12}^{2i'} \\
& \quad = \sum_{i=0}^{N} \frac{(-1)^i}{i!(N-i)!} \frac{\Gamma(N+L+3/2)}{\Gamma(i+L+3/2)} 2^i \sum_{i'=0}^{i} (-2\nu)^{-i'} \frac{i!}{i'!(i-i')!} \frac{\Gamma(L+i+3/2)}{\Gamma(L+i'+3/2)} P_{12}^{2i'} \\
& \qquad = \sum_{i=0}^{N} \sum_{i'=0}^{i} \frac{(-1)^i}{(N-i)! i'! (i-i')!} \frac{\Gamma(N+L+3/2)}{\Gamma(L+i'+3/2)} 2^i (-2\nu)^{-i'} P_{12}^{2i'}
\end{aligned}
$$

Changing the summation order to $i' \in [0, N], i \in [i', N]$ gives,

$$
\begin{aligned}
& \sum_{i'=0}^{N} \frac{(-1)^{i'}}{i'!(N-i')!} \frac{\Gamma(N+L+3/2)}{\Gamma(L+i'+3/2)} \nu^{-i'} P_{12}^{2i'} \sum_{i=i'}^{N} (-1)^i \frac{(N-i')!}{(N-i)!(i-i')!} 2^{i-i'} \\
& \qquad = (-1)^N \sum_{i'=0}^{N} a_{NL,i'} \nu^{-i'} P_{12}^{2i'} \sum_{i=i'}^{N} (-1)^{N-i} \frac{(N-i')!}{(N-i)!(i-i')!} 2^{i-i'}
\end{aligned}
$$

All we have to do now is to prove that

$$
\sum_{i=i'}^{N} (-1)^{N-i} \frac{(N-i')!}{(N-i)!(i-i')!} 2^{i-i'} = 1
$$

to get the equivalence of Eqs. (56) and (57). Defining $j = N-i$, $j' = N-i'$ gives,

$$
\sum_{j=j'}^{0} \frac{j'!}{j!(j'-j)!} (-1)^j 2^{j'-j} = \sum_{j=0}^{j'} \begin{pmatrix} j' \\ j \end{pmatrix} (-1)^j 2^{j'-j} = (-1+2)^{j'} = 1^{N-i} = 1
$$

This equivalence was checked in the code and found to be correct.

8.2 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,

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

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

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

8.3 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:

$$\begin{aligned}
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\mp1\rangle &= 0 \\
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle &= \delta_{t_1,\pm\frac{1}{2}} \\
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle &= 0 \\
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|1\pm1\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle &= 0 \\
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle &= \frac{1}{2} \\
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|10\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle &= \mathrm{sgn}(t_1)\frac{1}{2} = t_1 \\
\sum_{t_2} \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle \langle \frac{1}{2}t_1 \frac{1}{2}t_2|00\rangle &= \frac{1}{2}
\end{aligned}$$

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 $\delta_{M_T,M_T'}$ (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 $\delta_{TT'}\delta_{M_TM_T'}$.

9 Fourier transform of HO wave functions

The HO Shrödinger equation is given by

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

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

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

With solutions

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

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,

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

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,

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

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

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

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,

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

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].

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

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

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

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 $\nu' = 1/\nu$ and $(-i)^l = i^{-l}$ 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 $(-i)^l(-1)^n = i^{2n+3l}$.

[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