EVALUATION OF EXPECTATION VALUES USING exp(S) METHOD. WITH APPLICATION TO ONE-BODY AND TWO-BODY DENSITY

by
J.H. Heisenberg
Dept. of Physics, University of New Hampshire, Durham, N.H. 03824
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In this document we work out the equations needed to evaluate any operator in the ground state described by the $exp(\mathbf{S})$ method. We assume the ground state is written as

$$|\tilde{0}\rangle = exp(\mathbf{S}^\dagger)|0\rangle \tag{1}$$

We define $\{\mathbf{C}_n^\dagger\}$ the complete set of *1p1h*, *2p2h*, ...,$ApAh$ excitations. Thus we can write the identity as

$$\mathbf{1} = |0><0| + \sum_n \mathbf{C}_n^\dagger |0><0|\mathbf{C}_n \tag{2}$$

The normalized expectation value $\bar{a}$ of any operator $\mathbf{A}$ can be worked out as

$$\bar{a} = \frac{\langle 0|exp(\mathbf{S})\mathbf{A}exp(\mathbf{S}^\dagger)|0\rangle}{\langle\tilde{0}|\tilde{0}\rangle} = \frac{\langle 0|exp(\mathbf{S})\mathbf{A}exp(-\mathbf{S})exp(\mathbf{S})exp(\mathbf{S}^\dagger)|0\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \tag{3}$$

Inserting a complete basis we obtain

$$\bar{a} = \langle 0|exp(\mathbf{S})\mathbf{A}exp(-\mathbf{S})|0\rangle + \sum_n \langle 0|exp(\mathbf{S})\mathbf{A}exp(-\mathbf{S})\mathbf{C}_n^\dagger|0\rangle \frac{\langle 0|exp(\mathbf{S})\mathbf{C}_n exp(\mathbf{S}^\dagger)|0\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \tag{4}$$

The expectation value on the right is by definition $\bar{c}_n$. Thus we can define the operator

$$\tilde{\mathbf{S}}^\dagger = \sum_n \bar{c}_n \mathbf{C}_n^\dagger \tag{5}$$

With this, the expectation value for any operator can be expressed as

$$\bar{a} = \langle 0|exp(\mathbf{S})\mathbf{A}exp(-\mathbf{S})(1+\tilde{\mathbf{S}}^\dagger)|0\rangle \tag{6}$$

An alternate way is obtained by inserting the complete set at a different point. We write

$$\begin{aligned}\bar{a} =& \frac{\langle 0|exp(\mathbf{S})exp(\mathbf{S}^\dagger)exp(-\mathbf{S}^\dagger)\mathbf{A}exp(\mathbf{S}^\dagger)|0\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \\ =& \langle 0|exp(-\mathbf{S}^\dagger)\mathbf{A}exp(\mathbf{S}^\dagger)|0\rangle + \sum_n \langle 0|\mathbf{C}_n exp(\mathbf{S}^\dagger)\mathbf{A}exp(-\mathbf{S}^\dagger)|0\rangle \frac{\langle 0|exp(\mathbf{S})\mathbf{C}_n^\dagger exp(\mathbf{S}^\dagger)|0\rangle}{\langle\tilde{0}|\tilde{0}\rangle} \\ =& \langle 0|(1+\tilde{\mathbf{S}})exp(-\mathbf{S}^\dagger)\mathbf{A}exp(\mathbf{S}^\dagger)|0\rangle\end{aligned} \tag{7}$$

It is obvious that this is just the adjoint expression of equation *5.* in particular we get

$$\bar{c}_n^* = \langle 0|exp(\mathbf{S})\mathbf{C}_n^\dagger exp(-\mathbf{S})(1+\tilde{\mathbf{S}}^\dagger)|0\rangle \tag{8}$$

The operators $\tilde{\mathbf{S}}^\dagger$ can be obtained by solving equation (5) and (8) in an iterative fashion.

Forms (6) or (7) are equivalent and it depends on the operator as to which form is simpler. If the operator can be expressed in terms of the operators $\mathbf{C}_n^\dagger$ the form (7) is preferable, whereas if the operator is given in terms of $\mathbf{C}_n$ the form (6) is preferable.

In lowest order one obtains:

$$\tilde{\mathbf{S}}_n^\dagger = \mathbf{S}_n^\dagger$$

Higher order corrections will be worked out below.

Equations determining the S-amplitudes:

The operator $\mathbf{S}_1$ is given in m-representation independent of m in terms of the spectroscopic amplitudes $\tilde{S}_{ph}$. We calculate the spectroscopic amplitudes as

$$\begin{aligned}
\tilde{S}_{ph} &= <0|\big[\mathbf{Z}_2, \mathbf{C}_{ph}^\dagger\big]\tilde{\mathbf{S}}_1^\dagger|0> \\
&- \frac{1}{\epsilon_{3p3h}} <0|\Big[\mathbf{V}^{tni}, \mathbf{C}_{ph}^\dagger\Big]\tilde{\mathbf{S}}_2^\dagger|0> \\
&- \frac{1}{\epsilon_{3p3h}} <0|\Big[\big[\mathbf{Z}_2, \mathbf{H}_{01}\big], \mathbf{C}_{ph}^\dagger\Big]\tilde{\mathbf{S}}_2^\dagger|0> \\
&- \frac{1}{2}\frac{1}{\epsilon_{3p3h}} <0|\Big[\mathbf{Z}_2, \big[\mathbf{Z}_2, \mathbf{C}_{ph}^\dagger\big]\Big]\ \big[\mathbf{H}_{10}, \mathbf{Z}_2^\dagger\big]|0> \\
&- \frac{1}{2}\frac{1}{\epsilon_{3p3h}} <0|\Big[\mathbf{Z}_2, \big[\mathbf{Z}_2, \mathbf{C}_{ph}^\dagger\big]\Big]\ \mathbf{V}^{tni\ \dagger}|0>
\end{aligned}$$

We use the expansion for the evaluation of $\tilde{\mathbf{S}}_2^\dagger$:

$$\begin{aligned}
\tilde{S}_{p_1h_1,p_2h_2} &= <0|\big[\mathbf{Z}_2, \mathbf{C}_{p_1h_1,p_2h_2}^\dagger\big]|0> \\
&- <0|\Big[\big[\mathbf{Z}_2, \mathbf{H}_{01}\big], \mathbf{C}_{p_1h_1,p_2h_2}^\dagger\Big]\tilde{\mathbf{S}}_1^\dagger|0> /(\epsilon_{3p3h}) \\
&- <0|\big[\mathbf{V}^{tni}, \mathbf{C}_{p_1h_1,p_2h_2}^\dagger\big]\tilde{\mathbf{S}}_1^\dagger|0> /(\epsilon_{3p3h}) \\
&+ \frac{1}{2} <0|\Big[\mathbf{Z}_2, \big[\mathbf{Z}_2, \mathbf{C}_{p_1h_1,p_2h_2}^\dagger\big]\Big]\tilde{\mathbf{S}}_2^\dagger|0> \\
&+ ....
\end{aligned}$$

We approximate $\tilde{\mathbf{S}}_3^\dagger$ by:

$$\begin{aligned}
\tilde{S}_{3p3h} &= <0|\big[\mathbf{Z}_3, \mathbf{C}_{3p3h}^\dagger\big]|0> \\
&+ \frac{1}{2} <0|\Big[\mathbf{Z}_2, \big[\mathbf{Z}_2, \mathbf{C}_{3p3h}^\dagger\big]\Big]\tilde{\mathbf{S}}_1^\dagger|0> \\
&+ ....
\end{aligned}$$

and $\tilde{\mathbf{S}}_4^\dagger$ by:

$$\begin{aligned}
S_{4p4h} &= <0|\big[\mathbf{Z}_4, \mathbf{C}_{4p4h}^\dagger\big]|0> \\
&+ \frac{1}{2} <0|\Big[\mathbf{Z}_2, \big[\mathbf{Z}_2, \mathbf{C}_{4p4h}^\dagger\big]\Big]\tilde{\mathbf{S}}_2^\dagger|0> \\
&+ ....
\end{aligned}$$

These expectation values need be evaluated and are subject to possibly further truncations. Explicitly we use:

Terms contributing to $\mathbf{S}_2$

Further, we define the density matrix here as:

$$d(h_n, h_m) = +\frac{1}{2}\frac{2\ell+1}{2j_{h_n}+1}\sum_{p_2h_2,p_1} Z^{\ell}_{p_1h_n,p_2h_2} S^{\ell}_{p_1h_m,p_2h_2}$$

and

$$d(p_n,p_m) = +\frac{1}{2}\frac{2\ell+1}{2j_{p_n}+1}\sum_{p_2h_2,h_1} Z^{\ell}_{p_nh_1,p_2h_2}S^{\ell}_{p_mh_1,p_2h_2}$$

<u>*Term C*</u>: $\frac{1}{2} < 0|\Big[\mathbf{Z}_2, \big[\mathbf{Z}_2, \mathbf{C}^{\dagger}_{p_1h_1,p_2h_2}\big]\Big]\tilde{\mathbf{S}}^{\dagger}_2|0>$:

<u>*Term C,1*</u>

$$\Delta S_{p_ih_i,p_jh_j} = -\frac{1}{2}Z_{p_1h_1,p_jh_2}Z_{p_ih_i,p_4h_j}S_{p_1h_1,p_4h_2}$$

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = -d(p_j,p_4)Z^{\lambda}_{p_ih_i,p_4h_j}$$

<u>*Term C,2*</u>

$$\Delta S_{p_ih_i,p_jh_j} = -\frac{1}{2}Z_{p_1h_i,p_2h_2}Z_{p_ih_3,p_jh_j}S_{p_1h_3,p_2h_2}$$

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = -d(h_i,h_3)Z^{\lambda}_{p_ih_3,p_jh_j}$$

<u>*Term C,3*</u>

$$\Delta S_{p_ih_i,p_jh_j} = -\frac{1}{2}Z_{p_1h_j,p_2h_2}Z_{p_ih_i,p_jh_3}S_{p_1h_3,p_2h_2}$$

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = -d(h_j,h_3)Z^{\lambda}_{p_ih_i,p_jh_3}$$

<u>*Term C,4*</u>

$$\Delta S_{p_ih_i,p_jh_j} = -\frac{1}{2}Z_{p_1h_1,p_ih_2}Z_{p_4h_i,p_jh_j}S_{p_1h_1,p_4h_2}$$

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = -d(p_i,p_4)Z^{\lambda}_{p_4h_i,p_jh_j}$$

<u>*Term C,5*</u>

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = Z^{\lambda}_{p_1h_1,p_jh_j}Z^{\lambda}_{p_ih_i,p_2h_2}S^{\lambda}_{p_1h_1,p_2h_2}$$

<u>*Term C,6*</u>

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = \sum_{\ell}(-)^{(\ell+\lambda)}(2\ell+1)\begin{Bmatrix} p_j & h_j & \lambda \\ p_i & h_i & \ell \end{Bmatrix} Z^{\ell}_{p_jh_i,p_1h_2}Z^{\ell}_{p_ih_j,p_2h_1}S^{\ell}_{p_1h_2,p_2h_1}$$

<u>*Term C,7*</u>

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = \frac{1}{4}\sum_{K}(-)^{(K+1)}(2K+1)\begin{Bmatrix} p_j & h_j & \lambda \\ h_i & p_i & K \end{Bmatrix} Z^{K}_{p_1h_1,h_ih_j}Z^{K}_{p_ip_j,h_1h_2}S^{K}_{p_1p_2,h_1h_2}$$

<u>*Term B*</u>: $- < 0|\big[\mathbf{V}^{tni}, \mathbf{C}^{\dagger}_{p_1h_1,p_2h_2}\big]\tilde{\mathbf{S}}^{\dagger}_1|0 > /(\epsilon_{3p3h})$:

<u>*Term B,1*</u>

$$\Delta S^{\lambda}_{p_ih_i,p_jh_j} = -\tilde{\mathbf{S}}_{ph}\big(V^{tni,\lambda}_{h,h_1,h_2;p,p_1,p_2} - V^{tni,\lambda}_{h,h_1,h_2;p,p_2,p_1}\big)/(\epsilon_{ph}+\epsilon_{p_1h_1}+\epsilon_{p_2h_2})$$

Contributions to $\mathbf{S}_1$

Term 3.a

$$\Delta S_{ph} = \{ \sum_\ell (-\frac{1}{2})(2\ell+1) Z^\ell_{p_1h_1,p_2h_2} \frac{S^\ell_{p_3h_1,p_2h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} \} \langle ph|V^{\lambda=0}|p_3p_1\rangle \frac{(-)^{k_p}}{\sqrt{2k_p}} \frac{(-)^{k_{p_2}}}{\sqrt{2k_{p_2}}}$$

Term 3.e

$$\Delta S_{ph} = \{ \sum_\ell (+\frac{1}{2})(2\ell+1) Z^\ell_{p_1h_1,p_2h_2} \frac{S^\ell_{p_1h_3,p_2h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} \} \langle ph|V^{\lambda=0}|h_3h_1\rangle \frac{(-)^{k_p}}{\sqrt{2k_p}} \frac{(-)^{k_{h_1}}}{\sqrt{2k_{h_1}}}$$

Term 3.b

$$\Delta S_{ph} = \{ \sum_\ell (-\frac{1}{2})(2\ell+1) \langle p_1h_1|V^\ell|p_3p_2\rangle \frac{S^\ell_{p_1h_1,p_2h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} \} Z^{\lambda=0}_{p_3h_2,ph} \frac{(-)^{k_p}}{\sqrt{2k_p}} \frac{(-)^{k_{p_3}}}{\sqrt{2k_{p_3}}}$$

Term 3.f

$$\Delta S_{ph} = \{ \sum_\ell (+\frac{1}{2})(2\ell+1) \langle p_1h_1|V^\ell|h_2h_3\rangle \frac{S^\ell_{p_1h_1,p_2h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} \} Z^{\lambda=0}_{p_2h_3,ph} \frac{(-)^{k_p}}{\sqrt{2k_p}} \frac{(-)^{k_{p_2}}}{\sqrt{2k_{p_2}}}$$

Term 3.c

$$\Delta S_{ph} = \{ \sum_\ell (-)(2\ell+1) \frac{S^\ell_{p_1h_1,p_2h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} Z^\ell_{p_2h_2,p_3h} \langle p_1h_1|V^\ell|p_3p\rangle \}$$

Term 3.g

$$\Delta S_{ph} = \{ \sum_\ell (+)(2\ell+1) \frac{S^\ell_{p_1h_1,p_2h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} Z^\ell_{p_2h_2,ph_3} \langle p_1h_1|V^\ell|hh_3\rangle \}$$

Term 3.d

$$\Delta S_{ph} = \{ \sum_K (+\frac{1}{4})(2K+1) \frac{S^K_{p_1p_2,h_1h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} Z^K_{p_3p,h_1h_2} \langle p_1p_2|V^K|p_3h\rangle \}$$

Term 3.h

$$\Delta S_{ph} = \{ \sum_K (-\frac{1}{4})(2K+1) \frac{S^K_{p_1p_2,h_1h_2}}{\epsilon_{p_1h_1}+\epsilon_{p_2h_2}+\epsilon_{ph}} Z^K_{p_1p_2,h_3h} \langle h_1h_2|V^K|h_3p\rangle \}$$

Term 1.a

$$\Delta S_{ph} = Z^0_{ph,p'h'} S_{p'h'} \sqrt{\frac{2j_{p'}+1}{2j_p+1}} (-)^{(k_p+k_{p'})}$$

Evaluation of one-body density

Any one-body operator $\mathbf{A}$ can be written in the form

$$\mathbf{A} = \sum_{ab} A_{ab} \mathbf{a}_a^\dagger \mathbf{a}_b$$

We can break this up into four cases:

$$\mathbf{A} = \sum_{ph} A_{ph} \mathbf{a}_p^\dagger \mathbf{a}_h + \sum_{ph} A_{hp} \mathbf{a}_h^\dagger \mathbf{a}_p + \sum_{h_1 h_2} A_{h_1 h_2} \mathbf{a}_{h_1}^\dagger \mathbf{a}_{h_2} + \sum_{p_1 p_2} A_{p_1 p_2} \mathbf{a}_{p_1}^\dagger \mathbf{a}_{p_2}$$

Thus the expectation $\langle A \rangle$ value of $\mathbf{A}$ can be written as

$$\langle A \rangle = \sum_{ab} A_{ab} S_{ab}$$

where

$$S_{ab} = \langle \mathbf{a}_a^\dagger \mathbf{a}_b \rangle = \langle \mathbf{a}_b^\dagger \mathbf{a}_a \rangle^*$$

Thus we need to compute the three expectation values: S_{h_1,h_2}, S_{p_1,p_2}, and $S_{p,h}$, which we compute according to

$$\begin{aligned} S_{p_1,p_2} &= + < \left[\mathbf{S}_2, \mathbf{a}_{p_1}^\dagger \mathbf{a}_{p_2}\right] \tilde{\mathbf{S}}_2^\dagger > + < \left[\mathbf{S}_3, \mathbf{a}_{p_1}^\dagger \mathbf{a}_{p_2}\right] \tilde{\mathbf{S}}_3^\dagger > \\ S_{h_1,h_2} &= + < \mathbf{a}_{h_1}^\dagger \mathbf{a}_{h_2} > + < \left[\mathbf{S}_2, \mathbf{a}_{h_1}^\dagger \mathbf{a}_{h_2}\right] \tilde{\mathbf{S}}_2^\dagger > + < \left[\mathbf{S}_3, \mathbf{a}_{h_1}^\dagger \mathbf{a}_{h_2}\right] \tilde{\mathbf{S}}_3^\dagger > \\ S_{p,h}^* &= + < \tilde{\mathbf{a}}_h^\dagger \mathbf{a}_p \tilde{\mathbf{S}}_1^\dagger > \end{aligned}$$

Here we have made use of the fact that any double commutator with this one-body operator vanishes.

Term: $\langle \rho S_1^\dagger \rangle$

$$\Delta\rho(r) = \sum (2\ell + 1) 2 \tilde{S}_{ph}^{(1)} R_p(r) R_h(r)$$

We now discuss the angular momentum coupling for the density operator. Consistent with the definition of matrix elements we introduce the 'Ring'-phase in the density. Following Heisenberg and Blok we find including this phase

$$\rho_{a,b}^\lambda(r) = (-)^{(\lambda+1)} \sqrt{\frac{(2j_a+1)(2j_b+1)}{4\pi}} \langle j_a \ 1/2 \ j_b \ -1/2 | \lambda 0 \rangle R_a(r) R_b(r)$$

In particular for $\lambda = 0$ we find

$$\rho_{a,b}^0(r) = (-)^{(j_a+1/2)} \sqrt{\frac{2j_a+1}{4\pi}} R_a(r) R_b(r) = (-)^{(j_a+1/2)} \sqrt{\frac{2j_a+1}{4\pi}} \rho_{a,b}(r)$$

where $\rho_{a,b}(r) = R_a(r) R_b(r)$ is the radial density. To simplify the expressions we leave out the factor $\sqrt{1/4\pi}$ in all the terms.

Term 1: $\langle \rho \rangle$

$$\rho(r) = \sum_h \rho_{h,h}(r) = \sum_h \ (2j_h + 1) \ R_h^2(r) \tag{1.a}$$

$$\rho(r) = \sum_h (-)^{j_h+1/2} \sqrt{2j_h+1} \rho_{h,h}^0(r)$$

Term 2: $\langle [Z_2, \rho] S_2^\dagger \rangle$

$$\Delta\rho(r) = +\rho_{p_1,p_2}(r)\frac{1}{2}\sum_\ell(2\ell+1)Z^\ell_{p_1h_1,p_3h_3}S^\ell_{p_2h_1,p_3h_3} = \rho_{p_1,p_2}(r)\ (2j_{p_1}+1)\ d(p_1,p_2) \tag{2.a}$$

$$\Delta\rho(r) = -\rho_{h_2,h_1}(r)\frac{1}{2}\sum_\ell(2\ell+1)Z^\ell_{p_1h_1,p_3h_3}S^\ell_{p_1h_2,p_3h_3} = -\rho_{h_2,h_1}(r)\ (2j_{h_1}+1)\ d(h_1,h_2) \tag{2.b}$$

Note: density matrix is not necessarily symmetric. However, since the trace of this density matrix vanishes, the normalization of ρ is not changed.

Evaluation of two-body density

In this part we evaluate the contributions to the two-body density in the nuclear ground state. We assume that in m-representation the operator can be written as

$$\rho^{op}(\vec{r}_1,\vec{r}_2) = \sum_{ab,cd}\rho_{abcd}\ \mathbf{abd^{-1}c^{-1}} = \sum_{ab,cd}\langle ac^{-1}|\rho|db^{-1}\rangle\ \mathbf{abd^{-1}c^{-1}} = \sum_{ab,cd}\rho_{ac}(\vec{r}_1)\ \rho_{db}(\vec{r}_2)\ \mathbf{abd^{-1}c^{-1}}$$

All angular momentum coupled quantities are expected to contain the "Ring"-phase. We couple these matrix elements identically to the ph-ph matrix element without the exchange term in order to be consistent with the phase convention. For the angular momentum coupled density we get

$$\langle(a\bar{b})_\lambda|\rho^{\lambda\mu}|(c\bar{d})_\lambda\rangle = \sum_{m_am_bm_cm_d}(-)^{k_b+m_b+k_d-m_d}(-)^{k_a+k_c}\langle j_am_aj_b-m_b|\lambda\mu\rangle\langle j_cm_cj_d-m_d|\lambda\mu\rangle\langle a\bar{b}|\rho|c\bar{d}\rangle$$

We can factorize the matrix element as

$$\langle a\bar{b}|\rho|c\bar{d}\rangle = \big(R_a(r_1)R_b(r_1)Y^*_{l,m}(\hat{r}_1)\langle j_a,m_a|Y_{l,m}|j_bm_b\rangle\big)\big(R_c(r_2)R_d(r_2)Y_{l,m}(\hat{r}_2)\langle j_d,m_d|Y^*_{l,m}|j_cm_c\rangle\big)$$

Writing the matrix elements as reduced matrix elements

$$\begin{aligned}\langle(a\bar{b})_\lambda|\rho^{\lambda\mu}|(c\bar{d})_\lambda\rangle =& \Big((-)^{k_a}R_a(r_1)R_b(r_1)\frac{1}{\sqrt{2\lambda+1}}\langle j_a\|Y_{\lambda\mu}\|j_b\rangle Y^*_{\lambda\mu}(\hat{r}_1)\Big)\\ &\times\Big((-)^{k_c}R_c(r_2)R_d(r_2)\frac{1}{\sqrt{2\lambda+1}}\langle j_c\|Y_{\lambda\mu}\|j_d\rangle Y_{\lambda\mu}(\hat{r}_2)\Big)\end{aligned}$$

For convenience we define the one-body multipole density as

$$\begin{aligned}\frac{1}{\hat{\lambda}}\rho^\lambda_{ab}(r) &= (-)^{k_a}R_a(r)R_b(r)\frac{1}{\hat{\lambda}}\langle j_a\|Y_{\lambda\mu}\|j_b\rangle\\ &= (-)^{\lambda+1}\frac{\hat{j}_a\hat{j}_b}{\hat{\lambda}}\langle j_a1/2j_b-1/2|\lambda 0\rangle R_a(r)R_b(r)\end{aligned}$$

if $\ell_a+\ell_b+\lambda$ is even. This density is zero otherwise.

For a spherically symmetric (spin=0) nucleus it is more relevant to calculate $\rho(r_1,r_2,\theta_{12})$ which we will express in angular momentum coupling. In spherical nuclei this matrix element will always occur as a sum over μ so that we can write

$$\rho^\lambda_{ab,cd}(r_1,r_2,\theta_{12}) = \sum_\mu\rho^{\lambda;\mu}_{ab,cd}(\vec{r}_1,\vec{r}_2) = \rho^\lambda_{ab}(r_1)\rho^\lambda_{cd}(r_2)\ \frac{1}{2\lambda+1}\sum_\mu Y^*_{\lambda\mu}(\hat{r}_1)Y_{\lambda\mu}(\hat{r}_2)$$

with

$$\rho^{\lambda}_{ab,cd}(r_1,r_2,\theta_{12}) = \rho^{\lambda}_{ab}(r_1)\rho^{\lambda}_{cd}(r_2)P_\lambda(cos\theta_{12})$$

Expectation values:

The expectation value of this operator can be written in the following series of expectation values in the bare ground state in which we number the terms consecutively:

$$\begin{aligned}
&+ < \rho > + < \rho\tilde{\mathbf{S}}_1^\dagger > + < \rho\tilde{\mathbf{S}}_2^\dagger > \\
&+ < \left[\mathbf{S}_2, \rho\right] > \\
&+ < \left[\mathbf{S}_2, \rho\right] \tilde{\mathbf{S}}_1^\dagger > + < \left[\mathbf{S}_2, \rho\right] \tilde{\mathbf{S}}_2^\dagger > + < \left[\mathbf{S}_2, \rho\right] \tilde{\mathbf{S}}_3^\dagger > + < \left[\mathbf{S}_2, \rho\right] \tilde{\mathbf{S}}_4^\dagger > \\
&+ < \left[\mathbf{S}_3, \rho\right] \tilde{\mathbf{S}}_1^\dagger > + < \left[\mathbf{S}_3, \rho\right] \tilde{\mathbf{S}}_2^\dagger > + < \left[\mathbf{S}_3, \rho\right] \tilde{\mathbf{S}}_3^\dagger > + < \left[\mathbf{S}_3, \rho\right] \tilde{\mathbf{S}}_4^\dagger > \\
&+ \frac{1}{2} < \left[\mathbf{S}_2, \left[\mathbf{S}_2, \rho\right]\right] \tilde{\mathbf{S}}_2^\dagger > + \frac{1}{2} < \left[\mathbf{S}_2, \left[\mathbf{S}_2, \rho\right]\right] \tilde{\mathbf{S}}_3^\dagger > + \frac{1}{2} < \left[\mathbf{S}_2, \left[\mathbf{S}_2, \rho\right]\right] \tilde{\mathbf{S}}_4^\dagger >
\end{aligned}$$

We can simplify these terms using the symmetries for adjoint operators as stated in the write-up. Thus we can restrict the density operator as

$$\begin{aligned}
\rho = \rho_{ac}(1)\rho_{db}(2)\Big[&\mathbf{a}^\dagger_{a=h}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=h}\mathbf{a}_{c=h} + \mathbf{a}^\dagger_{a=p}\mathbf{a}^\dagger_{b=p}\mathbf{a}_{d=p}\mathbf{a}_{c=p} \\
&+\mathbf{a}^\dagger_{a=h}\mathbf{a}^\dagger_{b=p}\mathbf{a}_{d=p}\mathbf{a}_{c=h} + \mathbf{a}^\dagger_{a=p}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=h}\mathbf{a}_{c=p} \\
&+2\mathbf{a}^\dagger_{a=h}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=p}\mathbf{a}_{c=h} + 2\mathbf{a}^\dagger_{a=p}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=p}\mathbf{a}_{c=h} \\
&+2\mathbf{a}^\dagger_{a=h}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=h}\mathbf{a}_{c=p} + 2\mathbf{a}^\dagger_{a=h}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=p}\mathbf{a}_{c=p} \\
&+2\mathbf{a}^\dagger_{a=h}\mathbf{a}^\dagger_{b=p}\mathbf{a}_{d=p}\mathbf{a}_{c=p} + 2\mathbf{a}^\dagger_{a=p}\mathbf{a}^\dagger_{b=h}\mathbf{a}_{d=p}\mathbf{a}_{c=p}\Big]
\end{aligned}$$

Using these symmetries we find that we can write the same series as

$$\begin{aligned}
&+ < \rho > + < \left[\mathbf{S}_2, \rho\right] \tilde{\mathbf{S}}_2^\dagger > + < \left[\mathbf{S}_3, \rho\right] \tilde{\mathbf{S}}_3^\dagger > + \frac{1}{2} < \left[\mathbf{S}_2, \left[\mathbf{S}_2, \rho\right]\right] \tilde{\mathbf{S}}_4^\dagger > \\
&+ < \tilde{\rho}\tilde{\mathbf{S}}_1^\dagger > + < \left[\mathbf{S}_2, \tilde{\rho}\right] \tilde{\mathbf{S}}_3^\dagger > + < \left[\mathbf{S}_3, \tilde{\rho}\right] \tilde{\mathbf{S}}_4^\dagger > \\
&+ < \tilde{\rho}\tilde{\mathbf{S}}_2^\dagger >
\end{aligned}$$

where $\tilde{\rho}$ is the symmetrized density:

$$\tilde{\rho} = \sum\big(\rho_{ac}(1)\rho_{db}(2) + \rho_{ac}(2)\rho_{db}(1)\big)\mathbf{a}^\dagger_a\mathbf{a}^\dagger_b\mathbf{a}_d\mathbf{a}_c$$

Contributions from bare hf-ground state:

<u>*Term 1a*</u>

$$\rho_{h_1h_1,h_2h_2}$$

In angular momentum coupling, sum over m's:

$$\begin{aligned}
\rho(r_1,r_2,\theta_{12}) &= \sum_{h_1,h_2}(-)^{(k_{h_1}+k_{h_2})}\hat{j}_{h_1}\rho^0_{h_1h_1}(r_1)\hat{j}_{h_2}\rho^0_{h_2h_2}(r_2)P_0(cos\theta_{12}) \\
&= \sum_{h_1h_2}\ (2j_{h_1}+1)R^2_{h_1}(r_1)\ (2j_{h_2}+1)R^2_{h_2}(r_2)
\end{aligned}$$

This term has the structure $\rho_{hf}(1) * \rho_{hf}(2)$. Here ρ_{hf} is the bare hartree-fock one-body density. We can include all higher order one-body density terms by adding

$$\Delta\rho(r_1,r_2,\theta_{12}) = \Delta\rho(r_1)\rho_{hf}(r_2) + \rho_{hf}(r_1)\Delta\rho(r_2)$$

where $\Delta\rho$ is the difference between the full one-body density minus the bare hartree-fock one-body density. In turn, in higher order terms we have to exclude those terms where in the operator ρ_{abcd} a connects with c or b connects with d. However, we still have to consider the exchange terms where a connects with d and b connects with c (see e.g. terms 8g-8j).

Term 1b

$$-\rho_{h_1h_2,h_1h_2}$$

In angular momentum coupling, sum over m's:

$$\Delta\rho(r_1, r_2, \theta_{12}) = -\sum_{h_1,h_2}\sum_{\ell}\rho^{\ell}_{h_1h_2}(r_1)\rho^{\ell}_{h_1h_2}(r_2)P_{\ell}(cos\theta_{12})$$

(No contribution in pn or np densities)

Contributions linear in Z or S:

For all following terms we imply a summation over all orbits appearing twice in any expression.

Term 2

In angular momentum coupling, sum over m's (factor 2 is due to symmetry , see above):

$$\Delta\rho(r_1, r_2, \theta_{12}) = \sum_{\lambda} S^{\lambda}_{p_1h_1,p_2h_2}\left[\rho^{\lambda}_{h_1p_1}(r_1)\rho^{\lambda}_{p_2h_2}(r_2) + \rho^{\lambda}_{p_1h_1}(r_1)\rho^{\lambda}_{h_2p_2}(r_2)\right]P_{\lambda}(cos\theta_{12})$$

Contributions quadratic in Z or S:

Term 8a

$$\frac{1}{2}Z_{p_1p_2h_1h_2}S_{p_3p_4h_1h_2}\rho_{p_1p_3}(r_1)\rho_{p_4p_2}(r_2)$$

In angular momentum coupling, sum over m's and all exchanges:

$$\Delta\rho(r_1, r_2, \theta_{12}) = \frac{1}{8}\sum_{K,\ell}(-)^{K+1}(2K+1)\begin{Bmatrix} p_1 & p_3 & \ell \\ p_4 & p_2 & K \end{Bmatrix} S^K_{p_3p_4,h_1h_2}Z^K_{p_1p_2,h_1h_2}$$
$$\left[\rho^{\ell}_{p_2p_4}(r_1)\rho^{\ell}_{p_3p_1}(r_2) + \rho^{\ell}_{p_1p_3}(r_1)\rho^{\ell}_{p_4p_2}(r_2)\right]P_{\ell}(cos\theta_{12})$$
$$+\frac{1}{8}\sum_{K,\ell}(-)^{1}(2K+1)\begin{Bmatrix} p_1 & p_4 & \ell \\ p_3 & p_2 & K \end{Bmatrix} S^K_{p_3p_4,h_1h_2}Z^K_{p_1p_2,h_1h_2}$$
$$\left[\rho^{\ell}_{p_2p_3}(r_1)\rho^{\ell}_{p_4p_1}(r_2) + \rho^{\ell}_{p_1p_4}(r_1)\rho^{\ell}_{p_3p_2}(r_2)\right]P_{\ell}(cos\theta_{12})$$

Term 8b

$$\frac{1}{2}Z_{p_1p_2h_1h_2}S_{p_1p_2h_3h_4}\rho_{h_3h_1}(r_1)\rho_{h_2h_4}(r_2)$$

In angular momentum coupling, sum over m's:

$$\Delta\rho(r_1, r_2, \theta_{12}) = \frac{1}{8}\sum_{K,\ell}(-)^{K+1}(2K+1)\begin{Bmatrix} h_1 & h_3 & \ell \\ h_4 & h_2 & K \end{Bmatrix} S^K_{p_1p_2,h_3h_4}Z^K_{p_1p_2,h_1h_2}$$
$$\left[\rho^{\ell}_{h_2h_4}(r_1)\rho^{\ell}_{h_3h_1}(r_2) + \rho^{\ell}_{h_1h_3}(r_1)\rho^{\ell}_{h_4h_2}(r_2)\right]P_{\ell}(cos\theta_{12})$$
$$+\frac{1}{8}\sum_{K,\ell}(-)^{1}(2K+1)\begin{Bmatrix} h_1 & h_4 & \ell \\ h_3 & h_2 & K \end{Bmatrix} S^K_{p_1p_2,h_3h_4}Z^K_{p_1p_2,h_1h_2}$$
$$\left[\rho^{\ell}_{h_2h_3}(r_1)\rho^{\ell}_{h_4h_1}(r_2) + \rho^{\ell}_{h_1h_4}(r_1)\rho^{\ell}_{h_3h_2}(r_2)\right]P_{\ell}(cos\theta_{12})$$

Term 8d

$$Z_{p_1p_2h_1h_2}S_{p_3p_2h_3h_2}\rho_{p_1h_1}(r_1)\rho_{p_3h_3}(r_2)$$

In angular momentum coupling, sum over m's:

$$\Delta\rho(r_1,r_2,\theta_{12}) = Z^{\ell}_{p_1h_1,p_2h_2} S^{\ell}_{p_3h_3,p_2h_2} \rho^{\ell}_{p_1h_1}(r_1)\rho^{\ell}_{p_3h_3}(r_2) P_\ell(cos\theta_{12})$$

<u>*Term 8e*</u>

$$Z_{p_1p_2h_1h_2} S_{p_3p_2h_3h_2} \rho_{h_3p_3}(r_1)\rho_{h_1p_1}(r_2)$$

In angular momentum coupling, sum over m's:

$$\Delta\rho(r_1,r_2,\theta_{12}) = Z^{\ell}_{p_1h_1,p_2h_2} S^{\ell}_{p_3h_3,p_2h_2} \rho^{\ell}_{h_3p_3}(r_1)\rho^{\ell}_{h_1p_1}(r_2) P_\ell(cos\theta_{12})$$

<u>*Term 8c*</u>

$$-Z_{p_1p_2h_1h_2} S_{p_3p_2h_3h_2} \rho_{p_1p_3}(r_1)\rho_{h_1h_3}(r_2)$$

In angular momentum coupling, sum over m's:

$$\Delta\rho(r_1,r_2,\theta_{12}) = Z^{k}_{p_1h_1,p_2h_2} S^{k}_{p_3h_3,p_2h_2} (-)^{\ell+k}(2k+1) \begin{Bmatrix} p_1 & p_3 & \ell \\ h_3 & h_1 & k \end{Bmatrix} \rho^{\ell}_{p_1p_3}(r_1)\rho^{\ell}_{h_1h_3}(r_2) P_\ell(cos\theta_{12})$$

<u>*Term 8f*</u>

$$-Z_{p_1p_2h_1h_2} S_{p_3p_2h_3h_2} \rho_{h_3h_1}(r_1)\rho_{p_3p_1}(r_2)$$

In angular momentum coupling, sum over m's:

$$\Delta\rho(r_1,r_2,\theta_{12}) = Z^{k}_{p_1h_1,p_2h_2} S^{k}_{p_3h_3,p_2h_2} (-)^{\ell+k}(2k+1) \begin{Bmatrix} p_1 & p_3 & \ell \\ h_3 & h_1 & k \end{Bmatrix} \rho^{\ell}_{h_3h_1}(r_1)\rho^{\ell}_{p_3p_1}(r_2) P_\ell(cos\theta_{12})$$

<u>*Terms 8g-8j*</u>

$$\begin{aligned}\Delta\rho(r_1,r_2,\theta_{12}) = &- d(p_1,p_3)\sum_\ell \rho^{\ell}_{p_1h_1}(r_1)\rho^{\ell}_{p_3h_1}(r_2) P_\ell(cos\theta_{12}) \\ &- d(p_1,p_3)\sum_\ell \rho^{\ell}_{p_3h_1}(r_1)\rho^{\ell}_{p_1h_1}(r_2) P_\ell(cos\theta_{12}) \\ &+ d(h_1,h_3)\sum_\ell \rho^{\ell}_{h_1h_2}(r_1)\rho^{\ell}_{h_3h_2}(r_2) P_\ell(cos\theta_{12}) \\ &+ d(h_1,h_3)\sum_\ell \rho^{\ell}_{h_3h_2}(r_1)\rho^{\ell}_{h_1h_2}(r_2) P_\ell(cos\theta_{12})\end{aligned}$$

Here we left out terms implicitly included by the corrections in term (1)
Contributions from third order terms:
<u>*Term 6a*</u>

$$\Delta\rho(r_1,r_2,\theta_{12}) = 2\ S_{ph}[\rho_{hp}(r_1)\rho_{h_sh_s}(r_2) + \rho_{ph}(r_2)\rho_{h_sh_s}(r_1)]$$

This term is included through *term 1*, see note.
<u>*Term 6b*</u>

$$\begin{aligned}\Delta\rho(r_1,r_2,\theta_{12}) = -S_{ph}\Big[&\rho^{\ell}_{h_sp}(r_1)\rho^{\ell}_{h_sh}(r_2) + \rho^{\ell}_{hh_s}(r_1)\rho^{\ell}_{ph_s}(r_2) + \\ &+\rho^{\ell}_{ph_s}(r_1)\rho^{\ell}_{hh_s}(r_2) + \rho^{\ell}_{h_sh}(r_1)\rho^{\ell}_{h_sp}(r_2)\Big] P_\ell(cos\theta_{12})\end{aligned}$$

<u>*Term 9:*</u> Contributions from $< [\mathbf{S}_2,\tilde\rho]\ \tilde{\mathbf{S}}_3^\dagger >$
<u>*Term 9a*</u>

$$\begin{aligned}\Delta\rho(r_1,r_2,\theta_{12}) = -\langle p_d\bar h_b|V^\ell|p_5\bar p_c\rangle einv(p_a,p_5,\omega=\epsilon_{p_ch_b}+\epsilon_{p_d}) \\ \big(\rho^{\ell}_{p_ap_c}(r_1)\rho^{\ell}_{p_dh_b}(r_2) + \rho_{h_bp_d}(r_1)\rho_{p_cp_a}(r_2)\big) P_\ell(cos\theta_{12})\end{aligned}$$

<u>*Term 9b*</u>

$$\begin{aligned}\Delta\rho(r_1,r_2,\theta_{12}) = -\langle p_d\bar h_b|V^\ell|h_a\bar h_3\rangle einv(h_c,h_3,\omega=\epsilon_{p_ch_b}+\epsilon_{p_d}) \\ \big(\rho^{\ell}_{h_ah_c}(r_1)\rho^{\ell}_{p_dh_b}(r_2) + \rho_{h_bp_d}(r_1)\rho_{h_ch_a}(r_2)\big) P_\ell(cos\theta_{12})\end{aligned}$$

Term 9c

$$\Delta\rho(r_1,r_2,\theta_{12}) = d(h_c,p_5,\omega=\epsilon_{p_dh_b}+\epsilon_{h_a})\tilde{S}_{p_5h_a,p_dh_b}\big(\rho_{h_ah_c}(r_1)\rho_{p_dh_b}(r_2)+\rho_{h_bp_d}(r_1)\rho_{h_ch_a}(r_2)\big)P_\ell(cos\theta_{12})$$

Term 9d

$$\Delta\rho(r_1,r_2,\theta_{12}) = d(p_a,h_3,\omega=\epsilon_{p_dh_b}+\epsilon_{p_c})\tilde{S}_{p_ch_3,p_dh_b}\big(\rho_{p_ap_c}(r_1)\rho_{p_dh_b}(r_2)+\rho_{h_bp_d}(r_1)\rho_{p_cp_a}(r_2)\big)P_\ell(cos\theta_{12})$$

where we used the definitions

$$einv(p_a,p_5,\omega) = \frac{2\ell+1}{2j_{p_a}+1}\frac{Z^\ell_{p_ah_1,p_2h_2}\tilde{S}^\ell_{p_5h_1,p_2h_2}}{\epsilon_{p_2h_2}+\epsilon_{h_1}+\omega}$$

$$einv(h_c,h_3,\omega) = \frac{2\ell+1}{2j_{h_c}+1}\frac{Z^\ell_{p_1h_c,p_2h_2}\tilde{S}^\ell_{p_1h_3,p_2h_2}}{\epsilon_{p_2h_2}+\epsilon_{p_1}+\omega}$$

$$d(h_c,p_5,\omega) = -\frac{2\ell+1}{2j_{h_c}+1}\frac{Z^\ell_{p_1h_c,p_2h_2}\langle p_2\bar{h}_2|V^\ell|p_5\bar{p}_1\rangle}{\epsilon_{p_2h_2}+\epsilon_{p_1}+\omega}$$

$$d(p_a,h_3,\omega) = -\frac{2\ell+1}{2j_{p_a}+1}\frac{Z^\ell_{p_ah_1,p_2h_2}\langle p_2\bar{h}_2|V^\ell|h_1\bar{h}_3\rangle}{\epsilon_{p_2h_2}+\epsilon_{h_1}+\omega}$$

The dominant contribution from $\tilde{S}_4$ is $\langle\Big[Z_2,\big[Z_2,\rho\big]\Big]Z_2^\dagger Z_2^\dagger\rangle$ giving rise to
Term 10
which is obtained making the replacements in *term 8a* and *term 8b*

$$\begin{aligned}
Z^K_{p_1p_2,h_1h_2} &\to Z^K_{p_1p_2,h_1h_2} - \frac{1}{2}d^{ZZ}(p_1,p_5)Z^K_{p_5p_2,h_1h_2} - \frac{1}{2}d^{ZZ}(p_2,p_5)Z^K_{p_1p_5,h_1h_2}\\
S^K_{p_3p_4,h_1h_2} &\to S^K_{p_3p_4,h_1h_2} - \frac{1}{2}d^{ZZ}(p_3,p_5)S^K_{p_5p_4,h_1h_2} - \frac{1}{2}d^{ZZ}(p_4,p_5)S^K_{p_3p_5,h_1h_2}\\
Z^K_{p_1p_2,h_1h_2} &\to Z^K_{p_1p_2,h_1h_2} - \frac{1}{2}d^{ZZ}(h_1,h_5)Z^K_{p_1p_2,h_5h_2} - \frac{1}{2}d^{ZZ}(h_2,h_5)Z^K_{p_1p_2,h_1h_5}\\
S^K_{p_1p_2,h_3h_4} &\to S^K_{p_1p_2,h_3h_4} - \frac{1}{2}d^{ZZ}(h_3,h_5)S^K_{p_1p_2,h_5h_4} - \frac{1}{2}d^{ZZ}(h_4,h_5)S^K_{p_1p_2,h_3h_5}
\end{aligned}$$