

#### 0.17.4 Coupling of SF diagrams

The coupling to spherical CC of the SF diagrams are simplified by the fact that we are reallyt just interested in reduced matrix elements. Sticking with the notation of article 1, we have that  $J_A$ ,  $M_A$ ,  $J_{A-1}$ ,  $M_{A-1}$ ,  $j$  and  $m$  have a fixed, predetermined value. This information will be used to simplify the coupled diagrams

##### Left A-1, right A

The first diagram is very simple

$$\begin{aligned} l^i r_0 &= \langle i | l^{J_{A-1}} | \rangle r_0 = (00 J_{A-1} M_{A-1} | j m) \langle i | l^{J_{A-1}} | \rangle r_0 \\ &= \delta_{j J_{A-1}} \delta_{m M_{A-1}} \langle i | l^{J_{A-1}} | \rangle r_0 \end{aligned} \quad (405)$$

In general, all diagrams that contain either  $r_0$  or  $l_0$  are expected to be particularly simple, since the  $A$ -body solution is represented by the reference determinant in those cases. Note that  $i$  is here the unsummed index, corresponding to the externally imposed orbit, so that  $j_i = j$  and  $m_i = m$ . In the following we will always substitute the angular momentum quantum labels of the unsummed index with  $j$  and  $m$  without commenting it.

To couple the next diagram we use the trick of rewriting s.p. orbits in a ket as s.p. holes in the bra side of the matrix elements. This operation can be related to cross coupling of the matrix element as in reference [?]:

$$\begin{aligned} l_a^{ij} r_j^a &= \langle i j | l^{A-1} | a \rangle \langle a | r^A | j \rangle = \langle i | l^{A-1} | a j^{-1} \rangle \langle a j^{-1} | r^A | \rangle \\ &= \sum_{J_{aj} M_{aj}} \sum_{J'_{aj} M'_{aj}} (j_a m_a j_j - m_j | J_{aj} M_{aj}) (j_a m_a j_j - m_j | J'_{aj} M'_{aj}) \\ &\quad \times (-1)^{j_j - m_j} (-1)^{j_j - m_j} \langle i | l^{A-1} | a j^{-1}; J_{aj} M_{aj} \rangle \langle a j^{-1}; J'_{aj} M'_{aj} | r^A | \rangle \\ &= \sum_{J_{aj} M_{aj}} \sum_{J'_{aj} M'_{aj}} \delta_{J_{aj} J'_{aj}} \delta_{M_{aj} M'_{aj}} \\ &\quad \times \langle i | l^{A-1} | a j^{-1}; J_{aj} M_{aj} \rangle \langle a j^{-1}; J'_{aj} M'_{aj} | r^A | \rangle \\ &= \sum_{J_{aj} M_{aj}} \langle i | l^{A-1} | (a j^{-1}) \rangle \langle (a j^{-1}) | r^A | \rangle \end{aligned} \quad (406)$$

Notice that the implicit sum over the m-scheme orbitals  $j$  and  $a$  implies an implicit sum over the projections  $m_j$  and  $m_a$ . Since there is no dependency on those projections in the above expression except in the Clebsch-Gordan coefficient, we can employ the orthogonality relation of C-Gs and obtain the final equation above. For each C-G that couples a hole and a particle, we get a phase  $(-1)^{j_j - m_j}$ . Here we got this phase twice, so we could have ignored it. We also introduced a shorter notation for the coupled state,

$$|(ab)\rangle \equiv |ab; J_{ab} M_{ab}\rangle. \quad (407)$$

But we can go further, the coupling of the  $a$  and  $j$  orbits allows us to introduce reduced matrix elements via the Wigner-Eckardt theorem.

$$\begin{aligned}
l_a^{ij} r_j^a &= \sum_{J_{aj} M_{aj}} \langle i | l^{A-1} | (aj^{-1}) \rangle \langle (aj^{-1}) | r^A | \rangle \\
&= \sum_{J_{aj} M_{aj}} (J_{aj} M_{aj} J_{A-1} M_{A-1} | jm) (00 J_A M_A | J_{aj} M_{aj}) \\
&\quad \times \langle i | l^{A-1} | (aj^{-1}) \rangle \langle (aj^{-1}) | r^A | \rangle \\
&= (J_A M_A J_{A-1} M_{A-1} | jm) \\
&\quad \times \sum_{(aj)} \delta_{J_{aj} J_A} \delta_{M_{aj} M_A} \langle i | l^{A-1} | (aj^{-1}) \rangle \langle (aj^{-1}) | r^A | \rangle \quad (408)
\end{aligned}$$

The implicit sum over m-scheme orbits  $a$  and  $j$  carries through to the final expression where we choose to state it explicitly as the sum over J-scheme configurations  $(aj^{-1})$ .

In the diagrams corresponding to the removal of a particle above fermi, the removed orbit is denoted by  $a$ , so that we have  $j = j_a$  and  $m = m_a$ . The equations are:

$$\begin{aligned}
l_i^a t_i^a r_0 &= \langle a | t^0 | i \rangle \langle i | l^{J_{A-1}} | \rangle r_0 \\
&= (j_i m_i 00 | jm) (00 J_{A-1} M_{A-1} | j_i m_i) \langle a | t^0 | i \rangle \langle i | l^{J_{A-1}} | \rangle r_0 \\
&= (00 J_{A-1} M_{A-1} | jm) \sum_i \delta_{j j_i} \delta_{m m_i} \langle a | t^0 | i \rangle \langle i | l^{J_{A-1}} | \rangle r_0 \quad (409)
\end{aligned}$$

The sum over  $i$  collapses to a sum over nodes due to the delta functions.

$$\begin{aligned}
l_i^a r_i^a &= \langle a | r^{J_A} | i \rangle \langle i | l^{J_{A-1}} | \rangle \\
&= (j_i m_i J_A M_A | jm) (00 J_{A-1} M_{A-1} | j_i m_i) \langle a | r^{J_A} | i \rangle \langle i | l^{J_{A-1}} | \rangle \\
&= (J_{A-1} M_{A-1} J_A M_A | jm) \\
&\quad \times \sum_i \delta_{J_{A-1} j_i} \delta_{M_{A-1} m_i} \langle a | r^{J_A} | i \rangle \langle i | l^{J_{A-1}} | \rangle \quad (410)
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2} l_b^{ij} t_{ij}^{ab} r_0 &= \frac{1}{2} \langle ab|t^0|ij\rangle \langle ij|l^{J_{A-1}}|b\rangle r_0 \\
&= \frac{1}{2} \langle a|t^0|ijb^{-1}\rangle \langle ijb^{-1}|l^{J_{A-1}}|\rangle r_0 \\
&= \frac{1}{2} \sum_{J_{ij} M_{ij}} \sum_{J_{ijb} M_{ijb}} \sum_{J'_{ij} M'_{ij}} \sum_{J'_{ijb} M'_{ijb}} \\
&\quad \times (j_i m_i j_j m_j | J_{ij} M_{ij}) (J_{ij} M_{ij} j_b - m_b | J_{ijb} M_{ijb}) (-1)^{j_b - m_b} \\
&\quad \times (j_i m_i j_j m_j | J'_{ij} M'_{ij}) (J'_{ij} M'_{ij} j_b - m_b | J'_{ijb} M'_{ijb}) (-1)^{j_b - m_b} \\
&\quad \times \langle a|t^0|((ij)b^{-1})\rangle \langle ((ij)b^{-1})|l^{J_{A-1}}|\rangle r_0 \tag{411}
\end{aligned}$$

$$= \frac{1}{2} \sum_{J_{ij} J_{ijb} M_{ijb}} \langle a|t^0|((ij)b^{-1})\rangle \langle ((ij)b^{-1})|l^{J_{A-1}}|\rangle r_0 \tag{412}$$

$$\begin{aligned}
&= \frac{1}{2} \sum_{J_{ij} J_{ijb} M_{ijb}} (J_{ijb} M_{ijb} 00 | jm) (00 J_{A-1} M_{A-1} | J_{ijb} M_{ijb}) \\
&\quad \times \langle a||t^0||((ij)b^{-1})\rangle \langle ((ij)b^{-1})||l^{J_{A-1}}||\rangle r_0 \\
&= (00 J_{A-1} M_{A-1} | jm) \frac{1}{2} \sum_{J_{ij}} \sum_{((ij)b)} \delta_{j J_{ijb}} \delta_{m M_{ijb}} \\
&\quad \times \langle a||t^0||((ij)b^{-1})\rangle \langle ((ij)b^{-1})||l^{J_{A-1}}||\rangle r_0 \tag{413}
\end{aligned}$$

Again we have chosen to explicitly state the sum over single particle orbitals in the form of J-scheme configurations. It is to be interpreted as the sum over J-scheme  $(ij)$  configurations and for each  $(ij)$  we perform a sum over three-body J-scheme configurations  $((ij)b)$ .

$$\begin{aligned}
l_b^{ij} t_i^a r_j^b &= \langle a|t^0|i\rangle \langle ij|l^{J_{A-1}}|b\rangle \langle b|r^{J_A}|j\rangle \\
&= \langle a|t^0|i\rangle \langle i|l^{J_{A-1}}|bj^{-1}\rangle \langle bj^{-1}|r^{J_A}|\rangle \\
&= \sum_{J_{bj} M_{bj}} \sum_{J'_{bj} M'_{bj}} (-1)^{j_j - m_j} (-1)^{j_j - m_j} \\
&\quad \times (j_b m_b j_j - m_j | J_{bj} M_{bj}) (j_b m_b j_j - m_j | J'_{bj} M'_{bj}) \\
&\quad \times (j_i m_i 00 | jm) \langle a||t^0||i\rangle \\
&\quad \times (00 J_A M_A | J_{bj} M_{bj}) \langle (bj^{-1})||r^{J_A}||\rangle \\
&\quad \times (J_{bj} M_{bj} J_{A-1} M_{A-1} | j_i m_i) \langle i|l^{J_{A-1}}|(bj^{-1})\rangle \\
&= (J_A M_A J_{A-1} M_{A-1} | jm) \\
&\quad \times \sum_{(bj^{-1})} \sum_i \delta_{j j_i} \delta_{m m_i} \delta_{J_A J_{bj}} \delta_{M_A M_{bj}} \\
&\quad \times \langle a||t^0||i\rangle \langle i|l^{J_{A-1}}|(bj^{-1})\rangle \langle (bj^{-1})||r^{J_A}||\rangle \tag{414}
\end{aligned}$$

$$\begin{aligned}
\frac{1}{2}l_b^{ij}r_{ij}^{ab} &= \langle ab|r^A|ij\rangle \langle ij|l^{A-1}|b\rangle \\
&= \langle a|r^A|ijb^{-1}\rangle \langle ijb^{-1}|l^{A-1}|\rangle \\
&= \sum_{J_{ij}M_{ij}} \sum_{J'_{ij}M'_{ij}} \sum_{J_{ijb}M_{ijb}} \sum_{J'_{ijb}M'_{ijb}} (-1)^{(j_b-m_b)} (-1)^{(j_b-m_b)} \\
&\quad \times (j_im_ij_jm_j|J_{ij}M_{ij}) (j_im_ij_jm_j|J'_{ij}M'_{ij}) \\
&\quad \times (J_{ij}M_{ij}j_b-m_b|J_{ijb}M_{ijb}) (J'_{ij}M'_{ij}j_b-m_b|J'_{ijb}M'_{ijb}) \\
&\quad \times \langle a|r^A|((ij)'b^{-1})'\rangle \langle ((ij)b^{-1})|l^{A-1}|\rangle \\
&= \sum_{J_{ij}} \sum_{J_{ijb}M_{ijb}} \delta_{J_{ij}J'_{ij}} \delta_{M_{ij}M'_{ij}} \delta_{J_{ijb}J'_{ijb}} \delta_{M_{ijb}M'_{ijb}} \\
&\quad \times (J_{ijb}M_{ijb}J_A M_A|jm) \langle a||r^A|((ij)b^{-1})\rangle \\
&\quad \times (00J_{A-1}M_{A-1}|J_{ijb}M_{ijb}) \langle ((ij)b^{-1})||l^{A-1}||\rangle \\
&= (J_{A-1}M_{A-1}J_A M_A|jm) \sum_{J_{ij}} \sum_{((ij)b)} \delta_{J_{A-1}J_{ijb}} \delta_{M_{A-1}M_{ijb}} \\
&\quad \times \langle a||r^A|((ij)b^{-1})\rangle \langle ((ij)b^{-1})||l^{A-1}||\rangle \tag{415}
\end{aligned}$$

Left **A**, right **A-1**

$$\begin{aligned}
l_a^i r_i &= \langle |r^{J_{A-1}}|i\rangle \langle i|l^{J_A}|a\rangle \\
&= (j_im_iJ_{A-1}M_{A-1}|00) (jmJ_A M_A|j_im_i) \langle ||r^{J_{A-1}}||i\rangle \langle i||l^{J_A}||a\rangle \\
&= (jmJ_A M_A|J_{A-1}-M_{A-1}) (-1)^{J_{A-1}+M_{A-1}} \hat{J}_{A-1}^{-1} \\
&\quad \times \sum_i \delta_{j_iJ_{A-1}} \delta_{-m_iM_{A-1}} \langle ||r^{J_{A-1}}||i\rangle \langle i||l^{J_A}||a\rangle \tag{416}
\end{aligned}$$

Again we see that the sum over orbitals  $i$  is reduced to a sum over nodes  $n_i$ .

$$\begin{aligned}
\frac{1}{2} l_{ab}^{ij} r_{ij}^b &= \frac{1}{2} \langle b | r^{J_{A-1}} | ij \rangle \langle ij | l^{J_A} | ab \rangle \\
&= \frac{1}{2} \langle | r^{J_{A-1}} | ijb^{-1} \rangle \langle ijb^{-1} | l^{J_A} | a \rangle \\
&= \frac{1}{2} \sum_{J_{ij}} \sum_{J_{ijb} M_{ijb}} (-1)^{(j_b - m_b)} (-1)^{(j_b - m_b)} \delta_{J_{ij} J'_{ij}} \delta_{M_{ij} M'_{ij}} \delta_{J_{ijb} J'_{ijb}} \delta_{M_{ijb} M'_{ijb}} \\
&\quad \times \langle | r^{J_{A-1}} | ((ij)b^{-1}) \rangle \langle ((ij)b^{-1}) | l^{J_A} | a \rangle \\
&= \frac{1}{2} \sum_{J_{ij}} \sum_{J_{ijb} M_{ijb}} (J_{ijb} M_{ijb} J_{A-1} M_{A-1} | 00) (jm J_A M_A | J_{ijb} M_{ijb}) \\
&\quad \times \langle | r^{J_{A-1}} | ((ij)b^{-1}) \rangle \langle ((ij)b^{-1}) | l^{J_A} | a \rangle \\
&= \frac{1}{2} (jm J_A M_A | J_{A-1} - M_{A-1}) (-1)^{J_{A-1} + M_{A-1}} \hat{J}_{A-1}^{-1} \\
&\quad \times \sum_{J_{ij}} \sum_{((ij)b)} \delta_{J_{ijb} J_{A-1}} \delta_{-M_{ijb} M_{A-1}} \\
&\quad \times \langle | r^{J_{A-1}} | ((ij)b^{-1}) \rangle \langle ((ij)b^{-1}) | l^{J_A} | a \rangle
\end{aligned} \tag{417}$$

The diagrams for a creation operator below fermi are

$$\begin{aligned}
l^0 r_i &= l^0 \langle | r^{J_{A-1}} | i \rangle \\
&= (jm J_{A-1} M_{A-1} | 00) l^0 \langle | r^{J_{A-1}} | i \rangle \\
&= (-1)^{j-m} \hat{j}^{-1} \delta_{j J_{A-1}} \delta_{-m M_{A-1}} l^0 \langle | r^{J_{A-1}} | i \rangle
\end{aligned} \tag{418}$$

$$\begin{aligned}
l_a^j r_{ij}^a &= \langle j | l^{J_A} | a \rangle \langle a | r^{J_{A-1}} | ij \rangle \\
&= \langle | l^{J_A} | aj^{-1} \rangle \langle aj^{-1} | r^{J_{A-1}} | i \rangle \\
&= \sum_{J_{aj} M_{aj}} \sum_{J'_{aj} M'_{aj}} \delta_{J_{aj} J'_{aj}} \delta_{M_{aj} M'_{aj}} \langle | l^{J_A} | (aj^{-1}) \rangle \langle (aj^{-1}) | r^{J_{A-1}} | i \rangle \\
&= \sum_{J_{aj} M_{aj}} (J_{aj} M_{aj} J_A M_A | 00) (jm J_{A-1} M_{A-1} | J_{aj} M_{aj}) \\
&\quad \times \langle | l^{J_A} | (aj^{-1}) \rangle \langle (aj^{-1}) | r^{J_{A-1}} | i \rangle \\
&= (-1)^{J_A + M_A} \hat{J}_A^{-1} (jm J_{A-1} M_{A-1} | J_A - M_A) \\
&\quad \times \sum_{(aj)} \delta_{J_{aj} J_A} \delta_{-M_{aj} M_A} \langle | l^{J_A} | (aj^{-1}) \rangle \langle (aj^{-1}) | r^{J_{A-1}} | i \rangle
\end{aligned} \tag{419}$$

$$\begin{aligned}
-l_a^j t_i^a r_j &= -\langle |r^{J_{A-1}}|j\rangle \langle j|l^{J_A}|a\rangle \langle a|t^0|i\rangle \\
&= -(j_j m_j J_{A-1} M_{A-1} |00\rangle (j_a m_a J_A M_A |j_j m_j\rangle (j m 00 |j_a m_a\rangle) \\
&\quad \times \langle ||r^{J_{A-1}}||j\rangle \langle j||l^{J_A}||a\rangle \langle a||t^0||i\rangle \\
&= -(-1)^{J_{A-1} M_{A-1}} \hat{J}_{A-1}^{-1} (j m J_A M_A |j_j m_j\rangle \sum_{aj} \delta_{j_j J_{A-1}} \delta_{-m_j M_{A-1}} \delta_{j j_a} \delta_{m m_a} \\
&\quad \times \langle ||r^{J_{A-1}}||j\rangle \langle j||l^{J_A}||a\rangle \langle a||t^0||i\rangle \tag{420}
\end{aligned}$$

$$\begin{aligned}
-\frac{1}{2} l_{ab}^{jk} t_i^a r_{jk}^b &= -\frac{1}{2} \langle b|r^{J_{A-1}}|jk\rangle \langle jk|l^{J_A}|ab\rangle \langle a|t^0|i\rangle \\
&= -\frac{1}{2} \langle |r^{J_{A-1}}|jkb^{-1}\rangle \langle jkb^{-1}|l^{J_A}|a\rangle \langle a|t^0|i\rangle \\
&= -\frac{1}{2} \sum_{J_{jk} M_{jk}} \sum_{J'_{jk} M'_{jk}} \sum_{J_{jkb} M_{jkb}} \sum_{J'_{jkb} M'_{jkb}} \\
&\quad \times (j_j m_j j_k m_k |J_{jk} M_{jk}\rangle (J_{jk} M_{jk} j_b - m_b |J_{jkb} M_{jkb}\rangle (-1)^{j_b - m_b} \\
&\quad \times (j_j m_j j_k m_k |J'_{jk} M'_{jk}\rangle (J'_{jk} M'_{jk} j_b - m_b |J'_{jkb} M'_{jkb}\rangle (-1)^{j_b - m_b} \\
&\quad \times \langle |r^{J_{A-1}}|((jk)b^{-1})\rangle \langle ((jk)'b^{-1})'|l^{J_A}|a\rangle \langle a|t^0|i\rangle \\
&= -\frac{1}{2} \sum_{J_{jk}} \sum_{J_{jkb} M_{jkb}} \delta_{J_{jk} J'_{jk}} \delta_{M_{jk} M'_{jk}} \delta_{J_{jkb} J'_{jkb}} \delta_{M_{jkb} M'_{jkb}} \\
&\quad \times \langle |r^{J_{A-1}}|((jk)b^{-1})\rangle \langle ((jk)b^{-1})'|l^{J_A}|a\rangle \langle a|t^0|i\rangle \\
&= -\frac{1}{2} \sum_{J_{jk}} \sum_{J_{jkb} M_{jkb}} \\
&\quad \times (J_{jkb} M_{jkb} J_{A-1} M_{A-1} |00\rangle (j_a m_a J_A M_A |J_{jkb} M_{jkb}\rangle (j m 00 |j_a m_a\rangle) \\
&\quad \times \langle ||r^{J_{A-1}}||((jk)b^{-1})\rangle \langle ((jk)b^{-1})||l^{J_A}||a\rangle \langle a||t^0||i\rangle \\
&= -\frac{1}{2} (-1)^{J_{A-1} + M_{A-1}} \hat{J}_{A-1}^{-1} (j m J_A M_A |J_{A-1} - M_{A-1}\rangle) \\
&\quad \times \sum_{J_{jk}} \sum_{((jk)b)} \delta_{J_{A-1} J_{jkb}} \delta_{-M_{A-1} M_{jkb}} \delta_{j j_a} \delta_{m m_a} \\
&\quad \times \langle ||r^{J_{A-1}}||((jk)b^{-1})\rangle \langle ((jk)b^{-1})||l^{J_A}||a\rangle \langle a||t^0||i\rangle \tag{421}
\end{aligned}$$

$$\begin{aligned}
-\frac{1}{2}l_{ab}^{jk}t_{ik}^{ab}r_j &= -\frac{1}{2}\langle|r^{JA-1}|j\rangle\langle jk|l^{JA}|ab\rangle\langle ab|t^0|ik\rangle \\
&= -\frac{1}{2}\langle|r^{JA-1}|j\rangle\langle j|l^{JA}|abk^{-1}\rangle\langle abk^{-1}|t^0|i\rangle \\
&= -\frac{1}{2}\sum_{J_{ab}M_{ab}}\sum_{J'_{ab}M'_{ab}}\sum_{J_{abk}M_{abk}}\sum_{J'_{abk}M'_{abk}} \\
&\quad \times (j_a m_a j_b m_b|J_{ab}M_{ab})(J_{ab}M_{ab}j_k - m_k|J_{abk}M_{abk})(-1)^{j_k - m_k} \\
&\quad \times (j_a m_a j_b m_b|J'_{ab}M'_{ab})(J'_{ab}M'_{ab}j_k - m_k|J'_{abk}M'_{abk})(-1)^{j_k - m_k} \\
&\quad \times \langle|r^{JA-1}|j\rangle\langle j|l^{JA}|((ab)k^{-1})\rangle\langle((ab)'k^{-1})'|t^0|i\rangle \\
&= -\frac{1}{2}\sum_{J_{ab}}\sum_{J_{abk}M_{abk}}\delta_{J_{ab}J'_{ab}}\delta_{M_{ab}M'_{ab}}\delta_{J_{abk}J'_{abk}}\delta_{M_{abk}M'_{abk}} \\
&\quad \times \langle|r^{JA-1}|j\rangle\langle j|l^{JA}|((ab)k^{-1})\rangle\langle((ab)k^{-1})|t^0|i\rangle \\
&= -\frac{1}{2}\sum_{J_{ab}}\sum_{J_{abk}M_{abk}} \\
&\quad \times (j_j m_j J_{A-1} M_{A-1}|00)(J_{abk}M_{abk}J_A M_A|j_j m_j)(j m 00|J_{abk}M_{abk}) \\
&\quad \times \langle||r^{JA-1}||j\rangle\langle j||l^{JA}||((ab)k^{-1})\rangle\langle((ab)k^{-1})||t^0||i\rangle \\
&= -\frac{1}{2}(-1)^{J_{A-1}+M_{A-1}}\hat{J}_{A-1}^{-1}(j m J_A M_A|J_{A-1}M_{A-1}) \\
&\quad \times \sum_{J_{ab}}\sum_{((ab)k)}\delta_{j_j J_{A-1}}\delta_{-m_j M_{A-1}}\delta_{j J_{abk}}\delta_{m M_{abk}} \\
&\quad \times \langle||r^{JA-1}||j\rangle\langle j||l^{JA}||((ab)k^{-1})\rangle\langle((ab)k^{-1})||t^0||i\rangle
\end{aligned} \tag{422}$$