Note for the Breit Hamiltonian

I. INTRO

The goal here is to get the expression for

$$\langle ab : JM|H_{\mathrm{Breit}}|cd : JM\rangle. \tag{1}$$

Here, the single-particle basis a indicates the set of the quantum numbers; $\{n_a, l_a, j_a, m_a\}$ radial quantum number n_a, orbital angular momentum l_a, total angular momentum j_a and its z component m_a. The state $|ab : JM\rangle$ means the two angular momentum $|j_a m_a\rangle$ and $|j_b m_b\rangle$ couples to $|JM\rangle$:

$$|ab : J\rangle = \sum_{m_a m_b} \left(\begin{array}{cc|c} j_a & j_b & J \\ m_a & m_b & M \end{array} \right) |a\rangle \otimes |b\rangle. \tag{2}$$

Note that I omit the M dependence hereafter because the Hamiltonian has the rotational symmetry and does not depend on M.

II. MATHEMATICAL INGREDIENTS

In this section, I provide the definitions and formulas used in following derivations. For some of non-trivial formulas, the derivations will be given.

A. Basis function

The basis function we used in this note is

$$\phi_{n_a l_a j_a m_a}(\mathbf{r}) = \langle \mathbf{r}|a\rangle = R_{n_a l_a}(r) \sum_{m_{l_a} m_{s_a}} \left(\begin{array}{cc|c} l_a & 1/2 & j_a \\ m_{l_a} & m_{s_a} & m_a \end{array} \right) Y^{l_a}_{m_{l_a}}(\widehat{\mathbf{r}})\chi_{m_{s_a}}, \tag{3}$$

with the radial wave function $R_{nl}(r)$, spherical harmonics $Y_{lm}(\widehat{\mathbf{r}})$, and spinor χ_{m_s}. The radial wave function should be properly chosen.

B. Wigner-Eckart theorem

The matrix element of the spherical tensor operator T^{λ}_{μ} can be

$$\langle J'M'|T^{\lambda}_{\mu}|JM\rangle = (-1)^{J'-M'} \begin{pmatrix} J' & \lambda & J \\ -M' & \mu & M \end{pmatrix} \langle J'||T^{\lambda}||J\rangle. \tag{4}$$

This is quite useful because the M dependence can be factored out using the $3j$ symbol. The object $\langle J'||T^{\lambda}||J\rangle$ is known as the reduced matrix element. There are a lot of formula involving the reduced matrix elements.

C. Formulas involving the reduced matrix elements

$$\langle \alpha' J'||1||\alpha J\rangle = \sqrt{[J]}\delta_{\alpha'\alpha}\delta_{J'J} \tag{5}$$

$$\langle \alpha' J'||J||\alpha J\rangle = \sqrt{J(J+1)(2J+1)}\delta_{\alpha'\alpha}\delta_{J'J} \tag{6}$$

$$\langle \alpha' J' || [T^{k_1} T^{k_2}]^k || \alpha J \rangle = (-1)^{J'+k+J} \sqrt{[k]} \sum_{\alpha'' J''} \left\{ \begin{array}{ccc} k_1 & k_2 & k \\ J & J' & J'' \end{array} \right\} \langle \alpha' J' || T^{k_1} || \alpha'' J'' \rangle \langle \alpha'' J'' || T^{k_2} || \alpha J \rangle \tag{7}$$

$$\begin{aligned} &\langle \alpha_1' J_1' \alpha_2' J_2' J' || [T^{k_1}(1) T^{k_2}(2)]^k || \alpha_1 J_1 \alpha_2 J_2 J \rangle \\ &= \sqrt{[J'][k][J]} \left\{ \begin{array}{ccc} J_1' & J_2' & J' \\ J_1 & J_2 & J \\ k_1 & k_2 & k \end{array} \right\} \langle \alpha_1' J_1' || T^{k_1}(1) || \alpha_1 J_1 \rangle \langle \alpha_2' J_2' || T^{k_2}(2) || \alpha_2 J_2 \rangle \end{aligned} \tag{8}$$

$$\begin{aligned} &\langle \alpha_1' J_1' \alpha_2' J_2' J | T^k(1) \cdot T^k(2) | \alpha_1 J_1 \alpha_2 J_2 J \rangle \\ &= (-1)^{J_2'+J+J_1} \left\{ \begin{array}{ccc} J_1' & J_2' & J \\ J_2 & J_1 & k \end{array} \right\} \langle \alpha_1' J_1' || T^k(1) || \alpha_1 J_1 \rangle \langle \alpha_2' J_2' || T^k(2) || \alpha_2 J_2 \rangle \end{aligned} \tag{9}$$

$$\begin{aligned} &\langle \alpha_1' J_1' \alpha_2' J_2' J || [T^k(1) T^k(2)]^0 | \alpha_1 J_1 \alpha_2 J_2 J \rangle \\ &= \frac{(-1)^{J_2'+J+J_1+k}}{\sqrt{[k]}} \left\{ \begin{array}{ccc} J_1' & J_2' & J \\ J_2 & J_1 & k \end{array} \right\} \langle \alpha_1' J_1' || T^k(1) || \alpha_1 J_1 \rangle \langle \alpha_2' J_2' || T^k(2) || \alpha_2 J_2 \rangle \end{aligned} \tag{10}$$

$$\begin{aligned} &\langle \alpha_1' J_1' \alpha_2' J_2' J' || T^k(1) || \alpha_1 J_1 \alpha_2 J_2 J \rangle \\ &= (-1)^{J_1'+J_2'+J'+k} \sqrt{[J'][J]} \left\{ \begin{array}{ccc} J_1' & J' & J_2' \\ J & J_1 & k \end{array} \right\} \langle \alpha_1' J_1' || T^k(1) || \alpha_1 J_1 \rangle \delta_{\alpha_2' \alpha_2} \delta_{J_2' J_2} \end{aligned} \tag{11}$$

$$\begin{aligned} &\langle \alpha_1' J_1' \alpha_2' J_2' J' || T^k(2) || \alpha_1 J_1 \alpha_2 J_2 J \rangle \\ &= (-1)^{J_1'+J_2+J'+k} \sqrt{[J'][J]} \left\{ \begin{array}{ccc} J_2' & J' & J_1' \\ J & J_2 & k \end{array} \right\} \langle \alpha_2' J_2' || T^k(2) || \alpha_2 J_2 \rangle \delta_{\alpha_1' \alpha_1} \delta_{J_1' J_1} \end{aligned} \tag{12}$$

D. Formulas involving the spherical harmonics

$$Y_{m_1}^{l_1}(\theta,\phi) Y_{m_2}^{l_2}(\theta,\phi) = \sum_{l_3} \sqrt{\frac{[l_1][l_2]}{4\pi [l_3]}} Y_{m_3}^{l_3}(\theta,\phi) \left(\begin{array}{cc|c} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{array} \right) \left(\begin{array}{cc|c} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{array} \right) \tag{13}$$

$$\langle l' || Y^k || l \rangle = (-1)^{l'} \sqrt{\frac{[l'][k][l]}{4\pi}} \left(\begin{array}{ccc} l' & k & l \\ 0 & 0 & 0 \end{array} \right) \tag{14}$$

$$\langle l' \frac{1}{2} j' || Y^k || l \frac{1}{2} j \rangle = (-1)^{j-1/2+k} \sqrt{\frac{[j'][k][j]}{4\pi}} \left(\begin{array}{ccc} j' & k & j \\ -1/2 & 0 & 1/2 \end{array} \right) \frac{1}{2} [1 + (-1)^{l+l'+k}] \tag{15}$$

E. Vector of spherical tensor

Rearranging the unit vectors so the transformation law of the spherical tensor is satisfied, we have

$$\boldsymbol{\chi}_+ = -\sqrt{\frac{1}{2}} (\mathbf{e}_x + i \mathbf{e}_y), \tag{16}$$

$$\boldsymbol{\chi}_0 = \mathbf{e}_z, \tag{17}$$

$$\boldsymbol{\chi}_- = \sqrt{\frac{1}{2}}(\mathbf{e}_x - i\mathbf{e}_y). \tag{18}$$

Note that transformation from $\{\mathbf{e}_i\}$ to $\{\boldsymbol{\chi}_i\}$ is unitary but not orthogonal. So, we have to redefine the inner product so it does not change under the rotation:

$$\boldsymbol{\chi}_\mu \cdot \boldsymbol{\chi}_{\mu'} = (-1)^\mu \delta_{\mu',-\mu} \tag{19}$$

Using this new basis vector, an arbitrary vector can be

$$\mathbf{A} = \sum_\mu (-1)^\mu A_\mu \boldsymbol{\chi}_{-\mu} \tag{20}$$

Note that the ∇ can be defined in the same manner. Then, the gradient of the arbitrary function can be

$$\nabla\phi(\mathbf{r}) = \sum_{lm} \nabla f(r) Y^l_m(\widehat{\mathbf{r}}) \tag{21}$$

Now the problem is to get the expression of $\nabla f(r)Y^l_m(\widehat{\mathbf{r}})$. Recalling

$$\nabla = \widehat{\mathbf{r}}\frac{\partial}{\partial r} - \frac{i}{r}(\widehat{\mathbf{r}} \times \mathbf{L}), \tag{22}$$

we have to work with $\widehat{\mathbf{r}}Y^l_m$ and $\widehat{\mathbf{r}} \times \mathbf{L}Y^l_m$.

1. $\widehat{\mathbf{r}}Y^l_m$

Using the definition of the unit vector and Eq. (13), it is

$$\begin{aligned}
\widehat{\mathbf{r}}Y^l_m &= \sum_\mu (-1)^\mu \sqrt{\frac{4\pi}{3}} Y^1_\mu Y^l_m \boldsymbol{\chi}_{-\mu} \\
&= \sum_\mu (-1)^\mu \sum_\lambda \sqrt{\frac{[l]}{[\lambda]}} \left(\begin{array}{cc|c} 1 & l & \lambda \\ \mu & m & m+\mu \end{array}\right) \left(\begin{array}{cc|c} 1 & l & \lambda \\ 0 & 0 & 0 \end{array}\right) Y^\lambda_{m+\mu} \boldsymbol{\chi}_{-\mu} \\
&= -\sum_\mu \sum_\lambda \left(\begin{array}{cc|c} \lambda & 1 & l \\ m+\mu & -\mu & m \end{array}\right) \left(\begin{array}{cc|c} 1 & l & \lambda \\ 0 & 0 & 0 \end{array}\right) Y^\lambda_{m+\mu} \boldsymbol{\chi}_{-\mu} \\
&= -\sum_\mu \sum_\lambda \left(\begin{array}{cc|c} 1 & l & \lambda \\ 0 & 0 & 0 \end{array}\right) [Y^\lambda \boldsymbol{\chi}]^l_m.
\end{aligned} \tag{23}$$

Applying

$$\left(\begin{array}{cc|c} 1 & l & l-1 \\ 0 & 0 & 0 \end{array}\right) = -\sqrt{\frac{l}{[l]}},\ \left(\begin{array}{cc|c} 1 & l & l+1 \\ 0 & 0 & 0 \end{array}\right) = \sqrt{\frac{l+1}{[l]}}, \tag{24}$$

we have

$$\widehat{\mathbf{r}}Y^l_m = \sqrt{\frac{l}{[l]}}[Y^{l-1}\boldsymbol{\chi}]^l_m - \sqrt{\frac{l+1}{[l]}}[Y^{l+1}\boldsymbol{\chi}]^l_m. \tag{25}$$

2. $\widehat{\mathbf{r}} \times \mathbf{L}Y^l_m$

First, let us focusing on $\mathbf{L}Y^l_m$:

$$\mathbf{L}Y^l_m = \sum_\mu (-1)^\mu \boldsymbol{\chi}_{-\mu} L_\mu Y^l_m$$

$$= \sqrt{l(l+1)}\sum_{\mu}\left(\begin{array}{cc|c} l & 1 & l \\ m & \mu & m+\mu \end{array}\right)(-1)^{\mu}\boldsymbol{\chi}_{-\mu}Y^{l}_{m+\mu}$$
$$= \sqrt{l(l+1)}[Y^{l}\boldsymbol{\chi}]^{l}_{m} \tag{26}$$

Next, $\widehat{\mathbf{r}}\times[Y^{l}\boldsymbol{\chi}]^{l}_{m}$

$$\begin{aligned}
\widehat{\mathbf{r}}\times[Y^{l}\boldsymbol{\chi}]^{l}_{m} &= \sum_{\mu\nu}\sqrt{\frac{4\pi}{3}}(-1)^{\nu}Y^{1}_{-\nu}\left(\begin{array}{cc|c} l & 1 & l \\ m-\mu & \mu & m \end{array}\right)Y^{l}_{m-\mu}(\boldsymbol{\chi}_{\nu}\times\boldsymbol{\chi}_{\mu}) \\
&= \sum_{\mu\nu}\sqrt{\frac{4\pi}{3}}(-1)^{\nu}Y^{1}_{-\nu}\left(\begin{array}{cc|c} l & 1 & l \\ m-\mu & \mu & m \end{array}\right)Y^{l}_{m-\mu}i\sqrt{2}\left(\begin{array}{cc|c} 1 & 1 & 1 \\ \nu & \mu & \nu+\mu \end{array}\right)\boldsymbol{\chi}_{\nu+\mu} \\
&= i\sqrt{2}\sum_{\mu\nu}\sum_{\lambda}(-1)^{\nu}\sqrt{\frac{[l]}{[\lambda]}}\left(\begin{array}{cc|c} l & 1 & l \\ m-\mu & \mu & m \end{array}\right)\left(\begin{array}{cc|c} 1 & 1 & 1 \\ \nu & \mu & \nu+\mu \end{array}\right) \\
&\quad\times\left(\begin{array}{cc|c} 1 & l & \lambda \\ -\nu & m-\mu & m-\nu-\mu \end{array}\right)\left(\begin{array}{cc|c} 1 & l & \lambda \\ 0 & 0 & 0 \end{array}\right)Y^{\lambda}_{m-\nu-\mu}\boldsymbol{\chi}_{\nu+\mu} \\
&= i\sqrt{2}\sum_{\mu\nu}\sum_{\lambda\lambda'}(-1)^{\nu}\sqrt{\frac{[l]}{[\lambda]}}\left(\begin{array}{cc|c} 1 & l & \lambda \\ 0 & 0 & 0 \end{array}\right)\left(\begin{array}{cc|c} l & 1 & l \\ m-\mu & \mu & m \end{array}\right)\left(\begin{array}{cc|c} 1 & 1 & 1 \\ \nu & \mu & \nu+\mu \end{array}\right) \\
&\quad\times\left(\begin{array}{cc|c} 1 & l & \lambda \\ -\nu & m-\mu & m-\nu-\mu \end{array}\right)\left(\begin{array}{cc|c} \lambda & 1 & \lambda' \\ m-\nu-\mu & \nu+\mu & m \end{array}\right)[Y^{\lambda}\boldsymbol{\chi}]^{\lambda'}_{m} \\
&= i\left[\sqrt{\frac{l+1}{[l]}}[Y^{l-1}\boldsymbol{\chi}]^{l}_{m}+\sqrt{\frac{l}{[l]}}[Y^{l+1}\boldsymbol{\chi}]^{l}_{m}\right]
\end{aligned} \tag{27}$$

Then, we have

$$\widehat{\mathbf{r}}\times\mathbf{L}Y^{l}_{m} = i\left[(l+1)\sqrt{\frac{l}{[l]}}[Y^{l-1}\boldsymbol{\chi}]^{l}_{m}+l\sqrt{\frac{l+1}{[l]}}[Y^{l+1}\boldsymbol{\chi}]^{l}_{m}\right] \tag{28}$$

Using Eqs. (25) and (28), we have

$$\nabla f(r)Y^{l}_{m} = \sqrt{\frac{l}{[l]}}\left(\frac{\partial f}{\partial r}+\frac{(l+1)f}{r}\right)[Y^{l-1}\boldsymbol{\chi}]_{lm}-\sqrt{\frac{l+1}{[l]}}\left(\frac{\partial f}{\partial r}-\frac{lf}{r}\right)[Y^{l+1}\boldsymbol{\chi}]_{lm}, \tag{29}$$

or

$$\begin{aligned}
\nabla_{\mu}f(r)Y^{l}_{m} &= -\sqrt{\frac{l}{[l-1]}}\left(\frac{\partial f}{\partial r}+\frac{(l+1)f}{r}\right)\left(\begin{array}{cc|c} l & 1 & l-1 \\ m & \mu & m+\mu \end{array}\right)Y^{l-1}_{m+\mu} \\
&\quad+\sqrt{\frac{l+1}{[l+1]}}\left(\frac{\partial f}{\partial r}-\frac{lf}{r}\right)\left(\begin{array}{cc|c} l & 1 & l+1 \\ m & \mu & m+\mu \end{array}\right)Y^{l+1}_{m+\mu}.
\end{aligned} \tag{30}$$

The combination of Eq. (30) and the expansion formula of $1/r_{12}$,

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} = \sum_{lm}\frac{4\pi}{[l]}(-1)^{m}Y^{l}_{m}(1)Y^{l}_{-m}(2)\left(\frac{r_2^{l}}{r_1^{l+1}}\Theta(r_1-r_2)+\frac{r_1^{l}}{r_2^{l+1}}\Theta(r_2-r_1)\right) \tag{31}$$

is useful. Note that $\Theta(x)$ is the step function and is 1 (0) for $x>0$ ($x<0$), and the shorthand notation $Y^{l}_{m}(1)=Y^{l}_{m}(\widehat{\mathbf{r}}_1)$ is used. For example, we can calculate

$$\begin{aligned}
\frac{[\mathbf{r}_{12}]^{1}_{\mu}}{r_{12}^{3}} &= -\nabla_{\mu}(1)\frac{1}{r_{12}} \\
&= -\sum_{lm}(-1)^{m}\frac{4\pi}{[l]}\nabla_{\mu}(1)\left(\frac{r_2^{l}}{r_1^{l+1}}\Theta(r_1-r_2)+\frac{r_1^{l}}{r_2^{l+1}}\Theta(r_2-r_1)\right)Y^{l}_{m}(1)Y^{l}_{-m}(2)
\end{aligned}$$

$$= \sum_l 4\pi(-1)^l \sqrt{\frac{(l+1)}{3}} \frac{r_2^l}{r_1^{l+2}} \Theta(r_1 - r_2)[Y^{l+1}(1)Y^l(2)]^1_\mu$$

$$+ \sum_l 4\pi(-1)^l \sqrt{\frac{l}{3}} \frac{r_1^{l-1}}{r_2^{l+1}} \Theta(r_2 - r_1)[Y^{l-1}(1)Y^l(2)]^1_\mu. \quad (32)$$

Also, combining

$$\begin{aligned}
[(\mathbf{s}(1)\cdot\nabla(1))(\mathbf{s}(2)\cdot\nabla(2))]\frac{1}{r_{12}} &= \sum_{\mu_1\mu_2}(-1)^{\mu_1+\mu_2} s_{-\mu_1}(1)s_{-\mu_2}(2)\nabla_{\mu_1}(1)\nabla_{\mu_2}(2)\frac{1}{r_{12}} \\
&= \sum_{\mu_1\mu_2}(-1)^{\mu_1+\mu_2} s_{-\mu_1}(1)s_{-\mu_2}(2)\nabla_{\mu_1}(1)\frac{[\mathbf{r}_{12}]^1_{\mu_2}}{r_{12}^3} \\
&= \sum_{\mu_1\mu_2}(-1)^{\mu_1+\mu_2} s_{-\mu_1}(1)s_{-\mu_2}(2)\left[\frac{(-1)^{\mu_1}\delta_{\mu_1-\mu_2}}{r_{12}^3} - 3\frac{[\mathbf{r}_{12}]^1_{\mu_1}[\mathbf{r}_{12}]^1_{\mu_2}}{r_{12}^5}\right] \\
&= \frac{\mathbf{s}(1)\cdot\mathbf{s}(2)}{r_{12}^3} - 3\frac{(\mathbf{s}(1)\cdot\mathbf{r}_{12})(\mathbf{s}(2)\cdot\mathbf{r}_{12})}{r_{12}^5},
\end{aligned} \quad (33)$$

and Eq. (31), we have

$$\begin{aligned}
\frac{\mathbf{s}(1)\cdot\mathbf{s}(2)}{r_{12}^3} - 3\frac{(\mathbf{s}(1)\cdot\mathbf{r}_{12})(\mathbf{s}(2)\cdot\mathbf{r}_{12})}{r_{12}^5} &= \sum_{\mu_1\mu_2}(-1)^{\mu_1+\mu_2} s_{-\mu_1}(1)s_{-\mu_2}(2) \\
&\times \sum_{lm} 4\pi(-1)^m [l] \sqrt{\frac{l(l+1)}{[l-1][l+1]}} \\
&\times \left[\frac{r_2^{l-1}}{r_1^{l+2}}\Theta(r_1-r_2)\left(\begin{array}{cc|c} l & 1 & l+1 \\ m & \mu_1 & m+\mu_1 \end{array}\right)\left(\begin{array}{cc|c} l & 1 & l-1 \\ -m & \mu_2 & -m+\mu_2 \end{array}\right) Y^{l+1}_{m+\mu_1}(1)Y^{l-1}_{-m+\mu_2}(2) + (1\leftrightarrow 2)\right] \\
&= 4\pi\sum_l \left[(-1)^l\sqrt{l(l+1)[l]}[[Y^{l+1}(1)s(1)]^l[Y^{l-1}(2)s(2)]^l]^0 \frac{r_2^{l-1}}{r_1^{l+2}}\Theta(r_1-r_2) + (1\leftrightarrow 2)\right].
\end{aligned} \quad (34)$$

III. BREIT HAMILTONIAN

The derivation of the Breit Hamiltonian should be discussed somewhere else. The Hamiltonian is

$$\begin{aligned}
H_{\text{Breit}} &= H_{\text{Kinetic}} + H_{\text{Coul,1}} + H_{\text{Coul,2}} \\
&+ H_{p^4} + H_{\text{Darwin,1}} + H_{\text{LS,1}} + H_{\text{Darwin,2}} + H_{\text{Spin contact}} + H_{\text{Orbit orbit}} + H_{\text{LS,2}} + H_{\text{Spin dipole}}
\end{aligned} \quad (35)$$

Each term is given as

$$H_{\text{Kinetic}} = \sum_i \frac{\mathbf{p}_i^2}{2}, \quad (36)$$

$$H_{\text{Coul,1}} = -\sum_i \frac{Z}{r_i}, \quad (37)$$

$$H_{\text{Coul,2}} = \sum_{i<j} \frac{1}{r_{ij}}, \quad (38)$$

$$H_{p^4} = -\alpha^2 \sum_i \frac{\mathbf{p}_i^4}{8}, \quad (39)$$

$$H_{\text{Darwin,1}} = \alpha^2 \frac{\pi Z}{2} \sum_i \delta(\mathbf{r}_i), \quad (40)$$

$$H_{\text{LS,1}} = \alpha^2 \frac{Z}{2} \sum_i (L_i \cdot s_i)\frac{1}{r_i^3}, \quad (41)$$

$$H_{\text{Darwin},2} = -\alpha^2 \pi \sum_{i<j} \delta(\mathbf{r}_{ij}), \tag{42}$$

$$H_{\text{Spin contact}} = -\alpha^2 \frac{8\pi}{3} \sum_{i<j} (s_i \cdot s_j) \delta(\mathbf{r}_{ij}), \tag{43}$$

$$H_{\text{Orbit orbit}} = -\frac{\alpha^2}{2} \sum_{i<j} \left[(\mathbf{p}_i \cdot \mathbf{p}_j) \frac{1}{r_{ij}^3} + \frac{\mathbf{r}_{ij}}{r_{ij}^3} \cdot (\mathbf{r}_{ij} \cdot \mathbf{p}_i) \mathbf{p}_j \right], \tag{44}$$

$$H_{\text{LS},2} = \frac{\alpha^2}{2} \sum_{i<j} \frac{1}{r_{ij}^3} [\mathbf{s}_i \cdot (2\mathbf{r}_{ij} \times \mathbf{p}_j - \mathbf{r}_{ij} \times \mathbf{p}_i)], \tag{45}$$

$$H_{\text{Spin dipole}} = \alpha^2 \sum_{i<j} \left[\frac{\mathbf{s}_i \cdot \mathbf{s}_j}{r_{ij}^3} - 3 \frac{(\mathbf{s}_i \cdot \mathbf{r}_{ij})(\mathbf{s}_j \cdot \mathbf{r}_{ij})}{r_{ij}^5} \right]. \tag{46}$$

Here, the atomic unit is used, and α is the fine structure constant $\approx 1/137$.

IV. ONE-BODY TERMS

Here, the matrix elements of one-body terms are given. All the one-body terms are trivial.

A. Kinetic term

$$\boxed{\langle a | H_{\text{Kinetic}} | b \rangle = -\frac{1}{2} \int dr r^2 R^*_{n_a l_a}(r) \Delta R_{n_b l_b}(r) \delta_{l_a l_b} \delta_{j_a j_b}.} \tag{47}$$

B. Coolomb term

$$\boxed{\langle a | H_{\text{Coul},1} | b \rangle = -Z \int dr r R^*_{n_a l_a}(r) R_{n_b l_b}(r) \delta_{l_a l_b} \delta_{j_a j_b}.} \tag{48}$$

C. Relativistic correction for kinetic term

$$\boxed{\langle a | H_{p^4} | b \rangle = -\frac{\alpha^2}{8} \int dr r^2 R^*_{n_a l_a}(r) \Delta\Delta R_{n_b l_b}(r) \delta_{l_a l_b} \delta_{j_a j_b}.} \tag{49}$$

D. Darwin term

$$\boxed{\langle a | H_{\text{Darwin},1} | b \rangle = \alpha^2 \frac{Z}{8} R^*_{n_a l_a}(0) R_{n_b l_b}(0) \delta_{l_a 0} \delta_{l_b 0} \delta_{j_a j_b}.} \tag{50}$$

E. Spin-orbit term

$$\boxed{\langle a|H_{\mathrm{LS},1}|b\rangle = \alpha^2 \frac{Z}{4}\left[j_a(j_a+1) - l_a(l_a+1) - \frac{3}{4}\right]\int dr R^*_{n_a l_a}(r)\frac{1}{r}R_{n_b l_b}(r)\delta_{l_a l_b}\delta_{j_a j_b}.} \tag{51}$$

V. TWO-BODY TERMS

Here, the matrix elements of two-body terms are given.

A. Coulomb term

Using Eqs. (31), the matrix element is trivial:

$$\langle ab:J|H_{\mathrm{Coul}}|cd:J\rangle = (-1)^{j_b+J+j_c}\sum_L \frac{4\pi}{[L]}\left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} F_L(a,b,c,d)\langle j_a||Y^L||j_c\rangle\langle j_b||Y^L||j_d\rangle, \tag{52}$$

$$F_L(a,b,c,d) = \int dr_1 dr_2 r_1^2 r_2^2 R^*_{n_a l_a}(r_1)R^*_{n_b l_b}(r_2)\frac{r_<^L}{r_>^{L+1}}R_{n_c l_c}(r_1)R_{n_d l_d}(r_2). \tag{53}$$

Note that $\langle j_a||Y^L||j_c\rangle$ is given in Eq. (15).

B. Darwin term

Recalling

$$\delta(\mathbf{r}_{12}) = \frac{\delta(r_1-r_2)}{r_1^2}\sum_{lm}(-1)^m Y^l_m(1)Y^l_{-m}(2), \tag{54}$$

The matrix element is

$$\boxed{\langle ab:J|H_{\mathrm{Darwin},2}|cd:J\rangle = -\alpha^2\pi(-1)^{j_b+J+j_c}F(a,b,c,d)\sum_L [L]\left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\}\langle j_a||Y^L||j_c\rangle\langle j_b||Y^L||j_d\rangle,} \tag{55}$$

with

$$\boxed{F(a,b,c,d) = \int dr r^2 R^*_{n_a l_a}(r)R^*_{n_b l_b}(r)R_{n_c l_c}(r)R_{n_d l_d}(r).} \tag{56}$$

C. Spin-spin contact term

Similarly to the two-body Darwin term, we have

$$\begin{aligned}\langle ab:J|H_{\mathrm{Spin\ contact}}|cd:J\rangle = \alpha^2\frac{8\pi}{3}(-1)^{j_b+J+j_c}F(a,b,c,d)\sum_L(-1)^L \\ \times\sum_K\left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & K \end{array}\right\}\langle j_a||[Y^L s]^K||j_c\rangle\langle j_b||[Y^L s]^K||j_d\rangle,\end{aligned} \tag{57}$$

with

$$\boxed{\langle j_a||[Y^L s]^K||j_c\rangle = \sqrt{[j_a][K][j_c]}\left\{\begin{array}{ccc} l_a & 1/2 & j_a \\ l_b & 1/2 & j_b \\ L & 1 & K \end{array}\right\}\langle l_a||Y^L||l_c\rangle\sqrt{\frac{3}{2}}.} \tag{58}$$

Here, $\langle l_a||Y^L||l_c\rangle$ is already given in Eq. (14).

D. Spin-spin dipole term

Using Eq. (34), the matrix element is

$$\boxed{\begin{aligned}\langle ab:J|H_{\text{Spin dipole}}|cd:J\rangle = 4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{matrix} j_a & j_b & J \\ j_d & j_c & L\end{matrix}\right\}\sqrt{L(L+1)} \\ \times\left[G_L(a,b,c,d)\langle j_a||[Y^{L+1}s]^L||j_c\rangle\langle j_c||[Y^{L-1}s]^L||j_d\rangle + (a\leftrightarrow b,\ c\leftrightarrow d)\right],\end{aligned}} \tag{59}$$

with

$$\boxed{G_L = \int dr_1 dr_2 \Theta(r_1-r_2) R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2)\frac{r_2^{L+1}}{r_1^L} R_{n_c l_c}(r_1) R_{n_d l_d}(r_2)} \tag{60}$$

E. Spin-orbit term

The spin-orbit term is a bit tedious:

$$\begin{aligned}H_{\text{LS},2} &= \frac{\alpha^2}{2}\sum_{i<j}\frac{1}{r_{ij}^3}[\mathbf{s}_i\cdot(2\mathbf{r}_{ij}\times\mathbf{p}_j - \mathbf{r}_{ij}\times\mathbf{p}_i)] = \frac{\alpha^2}{2}\sum_{i<j}\left(\frac{\mathbf{r}_{ij}}{r_{ij}^3}\times\mathbf{p}_i\right)\cdot(2\mathbf{s}_i+\mathbf{s}_j) \\ &= -i\sqrt{6}\alpha^2\sum_{i<j}\left\{\left[\left[\left(-\nabla_i\frac{1}{r_{ij}}\right)p_i\right]^1 s_i\right]^0 - \frac{1}{2}(i\leftrightarrow j)\right\}\end{aligned} \tag{61}$$

Then, using Eq. (32), the term is

$$\begin{aligned}\left[\left[\left(-\nabla_i\frac{1}{r_{ij}}\right)p_i\right]^1 s_i\right]^0 &= 4\pi\sum_L(-1)^L\sqrt{\frac{L+1}{3}}\frac{r_j^L}{r_i^{L+2}}\Theta(r_i-r_j)[[[Y^{L+1}(i)Y^L(j)]^1 p(i)]^1 s(i)]^0 \\ &+ 4\pi\sum_L(-1)^L\sqrt{\frac{L}{3}}\frac{r_i^{L-1}}{r_j^{L+1}}\Theta(r_j-r_i)[[[Y^{L-1}(i)Y^L(j)]^1 p(i)]^1 s(i)]^0.\end{aligned} \tag{62}$$

Applying

$$\left\{\begin{matrix} l & 1 & l \\ 1 & l-1 & 1\end{matrix}\right\} = -\sqrt{\frac{1}{6}}\sqrt{\frac{l+1}{l[l]}},\ \left\{\begin{matrix} l & 1 & l-1 \\ 1 & l-1 & 1\end{matrix}\right\} = \sqrt{\frac{1}{6}}\sqrt{\frac{l-1}{l[l-1]}}, \tag{63}$$

the angular parts are

$$\begin{aligned}[[[Y^{L+1}(i)Y^L(j)]^1 p(i)]^1 s(i)]^0 &= -\sqrt{\frac{L}{2(L+1)}}[[[Y^{L+1}(i)p(i)]^L s(i)]^L Y^L(j)]^0 \\ &+ \sqrt{\frac{(L+2)}{2(L+1)}}[[[Y^{L+1}(i)p(i)]^{L+1} s(i)]^L Y^L(j)]^0\end{aligned} \tag{64}$$

$$\begin{aligned}[[[Y^{L-1}(i)Y^L(j)]^1 p(i)]^1 s(i)]^0 &= -\sqrt{\frac{L-1}{2L}}[[[Y^{L-1}(i)p(i)]^{L-1} s(i)]^L Y^L(j)]^0 \\ &+ \sqrt{\frac{(L+1)}{2L}}[[[Y^{L-1}(i)p(i)]^L s(i)]^L Y^L(j)]^0.\end{aligned} \tag{65}$$

Recalling

$$\mathbf{p}_\mu = -i\sqrt{\frac{4\pi}{3}}\left[Y^1_\mu\frac{\partial}{\partial r} - \frac{\sqrt{2}}{r}[Y^1 L]^1_\mu\right], \tag{66}$$

and

$$\begin{pmatrix} l+1 & 1 \\ 0 & 0 \end{pmatrix}\begin{vmatrix} l \\ 0 \end{pmatrix} = -\sqrt{\frac{l+1}{[l+1]}}, \quad \begin{pmatrix} l-1 & 1 \\ 0 & 0 \end{pmatrix}\begin{vmatrix} l \\ 0 \end{pmatrix} = \sqrt{\frac{l}{[l-1]}} \tag{67}$$

we have

$$[Y^{L+1}p]^L = i\sqrt{\frac{L+1}{[L]}}Y^L\partial + i\sqrt{\frac{L}{[L]}}[Y^L L]^L\frac{1}{r}, \tag{68}$$

$$[Y^{L+1}p]^{L+1} = i\sqrt{\frac{L+2}{[L+1]}}[Y^L L]^{L+1}\frac{1}{r} + i\sqrt{\frac{L+1}{[L+1]}}[Y^{L+2}L]^{L+1}\frac{1}{r}, \tag{69}$$

$$[Y^{L-1}p]^{L-1} = i\sqrt{\frac{L}{[L-1]}}[Y^{L-2}L]^{L-1}\frac{1}{r} + i\sqrt{\frac{L-1}{[L-1]}}[Y^L L]^{L-1}\frac{1}{r}, \tag{70}$$

$$[Y^{L-1}p]^L = -i\sqrt{\frac{L}{[L]}}Y^L\partial + i\sqrt{\frac{(L+1)}{[L]}}[Y^L L]^L\frac{1}{r} \tag{71}$$

Plug in Eqs. (64)–(71) for Eq.(62), we have

$$\begin{aligned}
\left[\left[\left(-\nabla_i\frac{1}{r_{ij}}\right)p_i\right]^1 s_i\right]^0 &= 4\pi\frac{i}{\sqrt{6}}\sum_L(-1)^L\frac{r_j^L}{r_i^{L+2}}\Theta(r_i-r_j) \\
&\times\Bigg[-\sqrt{\frac{L(L+1)}{[L]}}[[Y^L(i)s(i)]^L Y^L(j)]^0\partial(i) - \sqrt{\frac{L^2}{[L]}}[[R^{L,L}(i)s(i)]^L Y^L(j)]^0\frac{1}{r_i} \\
&+\sqrt{\frac{(L+2)^2}{[L+1]}}[[R^{L,L+1}(i)s(i)]^L Y^L(j)]^0\frac{1}{r_i} + \sqrt{\frac{(L+1)(L+2)}{[L+1]}}[[R^{L+2,L+1}(i)s(i)]^L Y^L(j)]^0\frac{1}{r_i}\Bigg] \\
&+4\pi\frac{i}{\sqrt{6}}\sum_L(-1)^L\frac{r_i^{L-1}}{r_j^{L+1}}\Theta(r_j-r_i) \\
&\times\Bigg[-\sqrt{\frac{L(L+1)}{[L]}}[[Y^L(i)s(i)]^L Y^L(j)]^0\partial(i) + \sqrt{\frac{(L+1)^2}{[L]}}[[R^{L,L}(i)s(i)]^L Y^L(j)]^0\frac{1}{r_i} \\
&-\sqrt{\frac{L(L-1)}{[L-1]}}[[R^{L-2,L-1}(i)s(i)]^L Y^L(j)]^0\frac{1}{r_i} + \sqrt{\frac{(L-1)^2}{[L-1]}}[[R^{L,L-1}(i)s(i)]^L Y^L(j)]^0\frac{1}{r_i}\Bigg]
\end{aligned} \tag{72}$$

Then, the Hamiltonian is

$$\begin{aligned}
H_{\mathrm{LS},2} &= 4\pi\alpha^2\sum_{i<j}\sum_L(-1)^L\left(-\sqrt{\frac{L(L+1)}{[L]}}\right)[[Y^L(i)s(i)]^L Y^L(j)]^0\left[\frac{r_j^L}{r_i^{L+2}}\Theta(r_i-r_j)+\frac{r_i^{L-1}}{r_j^{L+1}}\Theta(r_j-r_i)\right]\partial(i) \\
&+4\pi\alpha^2\sum_{i<j}\sum_L(-1)^L\frac{1}{[L]}[[R^{L,L}(i)s(i)]^L Y^L(j)]^0\left[-L\frac{r_j^L}{r_i^{L+3}}\Theta(r_i-r_j)+(L+1)\frac{r_i^{L-1}}{r_j^{L+2}}\Theta(r_j-r_i)\right] \\
&+4\pi\alpha^2\sum_{i<j}\sum_L(-1)^L(L+2)\sqrt{\frac{1}{[L+1]}}[[R^{L,L+1}(i)s(i)]^L Y^L]^0\frac{r_j^L}{r_i^{L+3}}\Theta(r_i-r_j) \\
&+4\pi\alpha^2\sum_{i<j}\sum_L(-1)^L\sqrt{\frac{(L+1)(L+2)}{[L+1]}}[[R^{L+2,L+1}(i)s(i)]^L Y^L]^0\frac{r_j^L}{r_i^{L+3}}\Theta(r_i-r_j) \\
&-4\pi\alpha^2\sum_{i<j}\sum_L(-1)^L\sqrt{\frac{L(L-1)}{[L-1]}}[[R^{L-2,L-1}(i)s(i)]^L Y^L]^0\frac{r_i^{L-2}}{r_j^{L+1}}\Theta(r_j-r_i) \\
&+4\pi\alpha^2\sum_{i<j}\sum_L(-1)^L(L-1)\sqrt{\frac{1}{[L-1]}}[[R^{L-1,L}(i)s(i)]^L Y^L]^0\frac{r_i^{L-2}}{r_j^{L+1}}\Theta(r_j-r_i)
\end{aligned}$$

$$-\frac{1}{2}(i \leftrightarrow j). \tag{73}$$

Finally, the matrix element is

$$\boxed{\begin{aligned}
&\langle ab:J|H_{\mathrm{LS},2}|cd:J\rangle = -4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} \frac{\sqrt{L(L+1)}}{[L]} A_L(a,b,c,d)\langle j_a||[Y^L s]^L||j_b\rangle\langle j_b||Y^L||j_d\rangle \\
&+ 4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} \frac{1}{[L]\sqrt{[L]}} B_L(a,b,c,d)\langle j_a||[R^{L,L} s]^L||j_b\rangle\langle j_b||Y^L||j_d\rangle \\
&+ 4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} \frac{L+2}{\sqrt{[L][L+1]}} C_L(a,b,c,d)\langle j_a||[R^{L,L+1} s]^L||j_b\rangle\langle j_b||Y^L||j_d\rangle \\
&+ 4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} \sqrt{\frac{(L+1)(L+2)}{[L][L+1]}} C_L(a,b,c,d)\langle j_a||[R^{L+2,L+1} s]^L||j_b\rangle\langle j_b||Y^L||j_d\rangle \\
&- 4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} \sqrt{\frac{L(L-1)}{[L][L-1]}} D_L(a,b,c,d)\langle j_a||[R^{L-2,L-1} s]^L||j_b\rangle\langle j_b||Y^L||j_d\rangle \\
&+ 4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L \left\{\begin{array}{ccc} j_a & j_b & J \\ j_d & j_c & L \end{array}\right\} \sqrt{\frac{(L-1)^2}{[L][L-1]}} D_L(a,b,c,d)\langle j_a||[R^{L-1,L} s]^L||j_b\rangle\langle j_b||Y^L||j_d\rangle \\
&- \frac{1}{2}(a \leftrightarrow b, c \leftrightarrow d),
\end{aligned}} \tag{74}$$

with $R^{M,N} = [Y^M L]^N$. Here, the radial integrals are introduced as

$$
\boxed{
\begin{aligned}
A_L(a,b,c,d) &= \int dr_1 dr_2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[\frac{r_2^{L+2}}{r_1^L}\Theta(r_1 - r_2) + \frac{r_1^{L+1}}{r_2^{L-1}}\Theta(r_2 - r_1) \right] \partial(1) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \\
B_L(a,b,c,d) &= \int dr_1 dr_2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[-L\frac{r_2^{L+2}}{r_1^{L+1}}\Theta(r_1 - r_2) + (L+1)\frac{r_1^{L+1}}{r_2^{L}}\Theta(r_2 - r_1) \right] R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \\
C_L(a,b,c,d) &= \int dr_1 dr_2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \frac{r_2^{L+2}}{r_1^{L+1}}\Theta(r_1 - r_2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \\
D_L(a,b,c,d) &= \int dr_1 dr_2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \frac{r_1^{L+1}}{r_2^{L}}\Theta(r_2 - r_1) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2).
\end{aligned}
}
$$

(75)

(76)

(77)

(78)

Also, the single-particle matrix elements are

(79)

F. Orbit-orbit term

This term is the most nasty part:

$$
H_{\text{Orbit orbit}} = -\frac{\alpha^2}{2} \sum_{i<j} \left[\frac{1}{r_{ij}} (\mathbf{p}_i \cdot \mathbf{p}_j) + \frac{\mathbf{r}_{ij}}{r_{ij}^3} \cdot (\mathbf{r}_{ij} \cdot \mathbf{p}_i) \mathbf{p}_j \right], \tag{80}
$$

$$
= -\frac{\alpha^2}{2} \sum_{i<j} \left[\frac{1}{r_{ij}} \frac{4}{3} (\mathbf{p}_i \cdot \mathbf{p}_j) + \sqrt{5} \left[\frac{[r_{ij} r_{ij}]^2}{r_{ij}^3} [p_i p_j]^2 \right]^0 \right]. \tag{81}
$$

The tensor part involving coordinates is

$$
\begin{aligned}
\frac{[r_{12} r_{12}]^2}{r_{12}^3} = {}& 4\pi \sum_l (-1)^l \sqrt{\frac{8l(l+1)}{15[l-1][l][l+1]}} \left[\frac{r_2^l}{r_1^{l+1}} \Theta(r_1 - r_2) + \frac{r_1^l}{r_2^{l+1}} \Theta(r_2 - r_1) \right] [Y^l(1) Y^l(2)]^2 \\
&+ 4\pi \sum_l (-1)^l \sqrt{\frac{(l+1)(l+2)}{5[l+1]}} \left[\frac{r_2^l}{r_1^{l+1}} \Theta(r_1 - r_2) [Y^{l+2}(1) Y^l(2)]^2 + \frac{r_1^l}{r_2^{l+1}} \Theta(r_2 - r_1) [Y^l(1) Y^{l+2}(2)]^2 \right] \\
&- 4\pi \sum_l (-1)^l \sqrt{\frac{(l-1)l}{5[l-1]}} \left[\frac{r_2^l}{r_1^{l+1}} \Theta(r_1 - r_2) [Y^l(1) Y^{l-2}(2)]^2 + \frac{r_1^l}{r_2^{l+1}} \Theta(r_2 - r_1) [Y^{l-2}(1) Y^l(2)]^2 \right].
\end{aligned} \tag{82}
$$

Note that

$$
\begin{Bmatrix} l & 1 & l-1 \\ 2 & l-1 & 1 \end{Bmatrix} = \sqrt{\frac{1}{30} \frac{(l-1)[l-2]}{l[l-1][l]}}, \quad \begin{Bmatrix} l & 1 & l+1 \\ 2 & l-1 & 1 \end{Bmatrix} = \sqrt{\frac{1}{5[l]}}, \tag{83}
$$

$$
\begin{Bmatrix} l & 2 & l \\ 1 & l-1 & 1 \end{Bmatrix} = \sqrt{\frac{1}{30} \frac{(l+1)[l+1]}{l[l-1][l]}}, \quad \begin{Bmatrix} l & 2 & l-2 \\ 1 & l-1 & 1 \end{Bmatrix} = \sqrt{\frac{1}{5[l-1]}}, \tag{84}
$$

are used in the derivation. The inner product term is

$$\frac{1}{r_{12}}(\mathbf{p}_1\cdot\mathbf{p}_2) = -4\pi\sqrt{3}\sum_L \frac{(-1)^L}{[L]}\left(\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right)[Y^L(1)Y^L(2)]^0[p(1)p(2)]^0$$
$$= -4\pi\sum_{LK}\frac{(-1)^L}{[L]}\sqrt{[K]}\left(\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right)[Y^L(1)p(1)]^K[Y^L(2)p(2)]^K. \quad (85)$$

The rank 2 tensor term is

$$\left[\frac{[r_{ij}r_{ij}]^2}{r_{ij}^3}[p_ip_j]^2\right]^0 = 4\pi\sum_L(-1)^L\frac{2}{3\sqrt{5}}\frac{L+1}{[L]}\sqrt{\frac{1}{[L-1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]$$
$$\times[[Y^L(1)p(1)]^{L-1}[Y^L(2)p(2)]^{L-1}]^0$$
$$-4\pi\sum_L(-1)^L\frac{2}{3\sqrt{5}}\sqrt{\frac{1}{[L]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]$$
$$\times[[Y^L(1)p(1)]^{L}[Y^L(2)p(2)]^{L}]^0$$
$$+4\pi\sum_L(-1)^L\frac{2}{3\sqrt{5}}\frac{L}{[L]}\sqrt{\frac{1}{[L+1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]$$
$$\times[[Y^L(1)p(1)]^{L+1}[Y^L(2)p(2)]^{L+1}]^0$$
$$+4\pi\sum_L(-1)^L\sqrt{\frac{(L+1)(L+2)}{5[L+1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)[[Y^{L+2}(1)p(1)]^{L+1}[Y^L(2)p(2)]^{L+1}]^0\right.$$
$$\left.+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)[[Y^L(1)p(1)]^{L+1}[Y^{L+2}(2)p]^{L+1}]^0\right]$$
$$-4\pi\sum_L(-1)^L\sqrt{\frac{(L-1)L}{5[L-1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)[[Y^{L}(1)p(1)]^{L-1}[Y^{L-2}(2)p(2)]^{L-1}]^0\right.$$
$$\left.+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)[[Y^{L-2}(1)p(1)]^{L-1}[Y^{L}(2)p]^{L-1}]^0\right]. \quad (86)$$

Then, the Hamiltonian is

$$\frac{1}{r_{12}}(\mathbf{p}_1\cdot\mathbf{p}_2)+\frac{\mathbf{r}_{12}}{r_{12}^3}\cdot(\mathbf{r}_{12}\cdot\mathbf{p}_1)\mathbf{p}_2 = -4\pi\sum_L(-1)^L\frac{2(L-1)}{[L]\sqrt{[L-1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]$$
$$\times[[Y^L(1)p(1)]^{L-1}[Y^L(2)p(2)]^{L-1}]^0$$
$$-4\pi\sum_L(-1)^L\frac{2}{\sqrt{[L]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]$$
$$\times[[Y^L(1)p(1)]^{L}[Y^L(2)p(2)]^{L}]^0$$
$$-4\pi\sum_L(-1)^L\frac{2(L+2)}{[L]\sqrt{[L+1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]$$
$$\times[[Y^L(1)p(1)]^{L+1}[Y^L(2)p(2)]^{L+1}]^0$$
$$+4\pi\sum_L(-1)^L\sqrt{\frac{(L+1)(L+2)}{[L+1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)[[Y^{L+2}(1)p(1)]^{L+1}[Y^L(2)p(2)]^{L+1}]^0\right.$$
$$\left.+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)[[Y^L(1)p(1)]^{L+1}[Y^{L+2}(2)p]^{L+1}]^0\right]$$
$$-4\pi\sum_L(-1)^L\sqrt{\frac{(L-1)L}{[L-1]}}\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)[[Y^{L}(1)p(1)]^{L-1}[Y^{L-2}(2)p(2)]^{L-1}]^0\right.$$

$$+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)[[Y^{L-2}(1)p(1)]^{L-1}[Y^L(2)p]^{L-1}]^0\Bigg]. \tag{87}$$

Plugging in the coupling of spherical harmonics and momentum operator,

$$[Y^Lp]^{L-1}=i\sqrt{\frac{L}{[L-1]}}Y^{L-1}\partial+i\sqrt{\frac{L-1}{[L-1]}}[Y^{L-1}L]^{L-1}\frac{1}{r}, \tag{88}$$

$$[Y^Lp]^{L}=i\sqrt{\frac{L+1}{[L]}}[Y^{L-1}L]^{L}\frac{1}{r}+i\sqrt{\frac{L}{[L]}}[Y^{L+1}L]^{L}\frac{1}{r}, \tag{89}$$

$$[Y^Lp]^{L+1}=-i\sqrt{\frac{L+1}{[L+1]}}Y^{L+1}\partial+i\sqrt{\frac{L+2}{[L+1]}}[Y^{L+1}L]^{L+1}\frac{1}{r}, \tag{90}$$

we have

$$\begin{aligned}
&\frac{1}{r_{12}}(\mathbf{p}_1\cdot\mathbf{p}_2)+\frac{\mathbf{r}_{12}}{r_{12}^3}\cdot(\mathbf{r}_{12}\cdot\mathbf{p}_1)\mathbf{p}_2\\
&=4\pi\sum_L(-1)^L\frac{(L+1)(L+2)}{[L]\sqrt{[L+1]}}[Y^{L+1}(1)Y^{L+1}(2)]^0\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]\partial(1)\partial(2)\\
&-4\pi\sum_L(-1)^L\frac{L(L-1)}{[L]\sqrt{[L-1]}}[Y^{L-1}(1)Y^{L-1}(2)]^0\left[\frac{r_2^L}{r_1^{L+1}}\Theta(r_1-r_2)+\frac{r_1^L}{r_2^{L+1}}\Theta(r_2-r_1)\right]\partial(1)\partial(2)\\
&+4\pi\sum_L(-1)^L\frac{(L+2)\sqrt{L(L-1)}}{[L]\sqrt{[L-1]}}[Y^{L-1}(1)R^{L-1,L-1}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+1}}\Theta(r_1-r_2)\right]\partial(1)+(1\leftrightarrow 2)\\
&-4\pi\sum_L(-1)^L\frac{(L-1)\sqrt{L(L-1)}}{[L]\sqrt{[L-1]}}[R^{L-1,L-1}(1)Y^{L-1}(2)]^0\left[\frac{r_2^{L}}{r_1^{L+2}}\Theta(r_1-r_2)\right]\partial(2)-(1\leftrightarrow 2)\\
&+4\pi\sum_L(-1)^L\frac{(L-1)(L+2)}{[L]\sqrt{[L-1]}}[R^{L-1,L-1}(1)R^{L-1,L-1}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&-4\pi\sum_L(-1)^L\frac{(L+2)\sqrt{(L+1)(L+2)}}{[L]\sqrt{[L+1]}}[Y^{L+1}(1)R^{L+1,L+1}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+1}}\Theta(r_1-r_2)\right]\partial(1)-(1\leftrightarrow 2)\\
&+4\pi\sum_L(-1)^L\frac{(L-1)\sqrt{(L+1)(L+2)}}{[L]\sqrt{[L+1]}}[R^{L+1,L+1}(1)Y^{L+1}(2)]^0\left[\frac{r_2^{L}}{r_1^{L+2}}\Theta(r_1-r_2)\right]\partial(2)+(1\leftrightarrow 2)\\
&-4\pi\sum_L(-1)^L\frac{(L-1)(L+2)}{[L]\sqrt{[L+1]}}[R^{L+1,L+1}(1)R^{L+1,L+1}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2(L+1)}{[L]\sqrt{[L]}}[R^{L-1,L}(1)R^{L-1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2\sqrt{L(L+1)}}{[L]\sqrt{[L]}}[R^{L+1,L}(1)R^{L-1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2\sqrt{L(L+1)}}{[L]\sqrt{[L]}}[R^{L-1,L}(1)R^{L+1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2L}{[L]\sqrt{[L]}}[R^{L+1,L}(1)R^{L+1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&=-4\pi\sum_L(-1)^L[Y^L(1)Y^L(2)]^0\frac{L(L+1)}{\sqrt{[L]}}\left[\left(\frac{1}{[L-1]}\frac{r_2^{L-1}}{r_1^L}-\frac{1}{[L+1]}\frac{r_2^{L+1}}{r_1^{L+2}}\right)\Theta(r_1-r_2)\right.\\
&\qquad\left.+\left(\frac{1}{[L-1]}\frac{r_1^{L-1}}{r_2^L}-\frac{1}{[L+1]}\frac{r_1^{L+1}}{r_2^{L+2}}\right)\Theta(r_2-r_1)\right]\partial(1)\partial(2)
\end{aligned}$$

$$
\begin{aligned}
&-4\pi\sum_L(-1)^L[Y^L(1)R^{L,L}(2)]^0\sqrt{\frac{L(L+1)}{[L]}}\left[\left(\frac{L+3}{[L+1]}\frac{r_2^L}{r_1^{L+2}}-\frac{L+1}{[L-1]}\frac{r_2^{L-2}}{r_1^L}\right)\Theta(r_1-r_2)\partial(1)\right]-(1\leftrightarrow 2)\\
&+4\pi\sum_L(-1)^L[R^{L,L}(1)Y^L(2)]^0\sqrt{\frac{L(L+1)}{[L]}}\left[\left(\frac{L}{[L+1]}\frac{r_2^{L+1}}{r_1^{L+3}}-\frac{(L-2)}{[L-1]}\frac{r_2^{L-1}}{r_1^{L+1}}\right)\Theta(r_1-r_2)\partial(2)\right]+(1\leftrightarrow 2)\\
&-4\pi\sum_L(-1)^L[R^{L,L}(1)R^{L,L}(2)]^0\sqrt{\frac{1}{[L]}}\left[\left(\frac{L(L+3)}{[L+1]}\frac{r_2^L}{r_1^{L+3}}-\frac{(L-2)(L+1)}{[L-1]}\frac{r_2^{L-2}}{r_1^{L+1}}\right)\Theta(r_1-r_2)\right.\\
&\qquad\left.+\left(\frac{L(L+3)}{[L+1]}\frac{r_1^L}{r_2^{L+3}}-\frac{(L-2)(L+1)}{[L-1]}\frac{r_1^{L-2}}{r_2^{L+1}}\right)\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2(L+1)}{[L]\sqrt{[L]}}[R^{L-1,L}(1)R^{L-1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2\sqrt{L(L+1)}}{[L]\sqrt{[L]}}[R^{L+1,L}(1)R^{L-1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2\sqrt{L(L+1)}}{[L]\sqrt{[L]}}[R^{L-1,L}(1)R^{L+1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]\\
&+4\pi\sum_L(-1)^L\frac{2L}{[L]\sqrt{[L]}}[R^{L+1,L}(1)R^{L+1,L}(2)]^0\left[\frac{r_2^{L-1}}{r_1^{L+2}}\Theta(r_1-r_2)+\frac{r_1^{L-1}}{r_2^{L+2}}\Theta(r_2-r_1)\right]
\end{aligned}
\tag{91}
$$

Finally, the matrix element is

$$
\boxed{
\begin{aligned}
&\langle ab:J|H_{\text{Orbit orbit}}|cd:J\rangle=4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{L(L+1)}{2[L]}H_L(a,b,c,d)\langle j_a||Y^L||j_c\rangle\langle j_b||Y^L||j_d\rangle\\
&+4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{\sqrt{L(L+1)}}{2[L]}I_L(a,b,c,d)\langle j_a||Y^L||j_c\rangle\langle j_b||R^{L,L}||j_d\rangle+(a\leftrightarrow b,c\leftrightarrow d)\\
&-4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{\sqrt{L(L+1)}}{2[L]}J_L(a,b,c,d)\langle j_a||R^{L,L}||j_c\rangle\langle j_b||Y^L||j_d\rangle-(a\leftrightarrow b,c\leftrightarrow d)\\
&+4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{1}{2[L]}K_L(a,b,c,d)\langle j_a||R^{L,L}||j_c\rangle\langle j_b||R^{L,L}||j_d\rangle\\
&-4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{(L+1)}{[L]^2}M_L(a,b,c,d)\langle j_a||R^{L-1,L}||j_c\rangle\langle j_b||R^{L-1,L}||j_d\rangle\\
&-4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{\sqrt{L(L+1)}}{[L]^2}M_L(a,b,c,d)\langle j_a||R^{L+1,L}||j_c\rangle\langle j_b||R^{L-1,L}||j_d\rangle\\
&-4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{\sqrt{L(L+1)}}{[L]^2}M_L(a,b,c,d)\langle j_a||R^{L-1,L}||j_c\rangle\langle j_b||R^{L+1,L}||j_d\rangle\\
&-4\pi\alpha^2(-1)^{j_b+J+j_c}\sum_L\left\{\begin{array}{ccc}j_a&j_b&J\\j_d&j_c&L\end{array}\right\}\frac{L}{[L]^2}M_L(a,b,c,d)\langle j_a||R^{L+1,L}||j_c\rangle\langle j_b||R^{L+1,L}||j_d\rangle,
\end{aligned}
}
\tag{92}
$$

with the following radial integrals:

$$H_L(a,b,c,d) = \int dr_1 dr_2 r_1^2 r_2^2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[\left(\frac{1}{[L-1]} \frac{r_2^{L-1}}{r_1^L} - \frac{1}{[L+1]} \frac{r_2^{L+1}}{r_1^{L+2}} \right) \Theta(r_1 - r_2) + \left(\frac{1}{[L-1]} \frac{r_1^{L-1}}{r_2^L} - \frac{1}{[L+1]} \frac{r_1^{L+1}}{r_2^{L+2}} \right) \Theta(r_2 - r_1) \right] \partial(1)\partial(2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \tag{93}$$

$$I_L(a,b,c,d) = \int dr_1 dr_2 r_1^2 r_2^2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[\left(\frac{L+3}{[L+1]} \frac{r_2^{L}}{r_1^{L+2}} - \frac{L+1}{[L-1]} \frac{r_2^{L-2}}{r_1^{L}} \right) \Theta(r_1 - r_2) \right] \times \partial(1) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \tag{94}$$

$$J_L(a,b,c,d) = \int dr_1 dr_2 r_1^2 r_2^2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[\left(\frac{L}{[L+1]} \frac{r_2^{L+1}}{r_1^{L+3}} - \frac{L-2}{[L-1]} \frac{r_2^{L-1}}{r_1^{L+1}} \right) \Theta(r_1 - r_2) \right] \times \partial(2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \tag{95}$$

$$K_L(a,b,c,d) = \int dr_1 dr_2 r_1^2 r_2^2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[\left(\frac{L(L+3)}{[L+1]} \frac{r_2^{L}}{r_1^{L+3}} - \frac{(L-2)(L+1)}{[L-1]} \frac{r_2^{L-2}}{r_1^{L+1}} \right) \Theta(r_1 - r_2) + \left(\frac{L(L+3)}{[L+1]} \frac{r_1^{L}}{r_2^{L+3}} - \frac{(L-2)(L+1)}{[L-1]} \frac{r_1^{L-2}}{r_2^{L+1}} \right) \Theta(r_2 - r_1) \right] R_{n_c l_c}(r_1) R_{n_d l_d}(r_2), \tag{96}$$

$$M_L(a,b,c,d) = \int dr_1 dr_2 r_1^2 r_2^2 R^*_{n_a l_a}(r_1) R^*_{n_b l_b}(r_2) \left[\frac{r_2^{L-1}}{r_1^{L+2}} \Theta(r_1 - r_2) + \frac{r_1^{L-1}}{r_2^{L+2}} \Theta(r_2 - r_1) \right] R_{n_c l_c}(r_1) R_{n_d l_d}(r_2). \tag{97}$$