AFDMC-TBF

Rong Chen
(Dated: June 10, 2015)

I. PROGRESS 2-26: SOME UNDERSTANDING ABOUT CORRELATOR.F90

A. the 15 operators in F_{ij}

The trial wave function can be written as

$$\langle \Psi_T | RS \rangle = \langle \Phi | \left[\prod_{i<j} f_c(r_{ij}) \right] \left[1 + \sum_{i<j} F_{ij} + \sum_{i<j<k} F_{ijk} \right] |RS\rangle. \tag{1}$$

For example, v6' interaction for the F_{ij}, we can write down

$$u_{ij}^1 + u_{ij}^2 \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + u_{ij}^3 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + u_{ij}^4 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + u_{ij}^5 (3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) + u_{ij}^6 (3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j, \tag{2}$$

for convenience just mark $\hat{r}_{ij}$ as $\hat{r}$.
the 4 and 6 operators can be combined as

$$\tau_{i\gamma}\tau_{j\gamma}\sigma_{i\alpha}\sigma_{j\beta} \underbrace{\left[(u_{ij}^4 - u_{ij}^6)\delta_{\alpha\beta} + 3u_{ij}^6 r_\alpha r_\beta \right]}_{\equiv A_{\alpha\beta}} = \lambda_\eta (\tau_{i\gamma}\sigma_{i\alpha}\phi_{\alpha\eta})(\tau_{j\gamma}\sigma_{j\beta}\phi_{\beta\eta}), \tag{3}$$

where the eigenvector matrix ϕ is orthogonal($\phi^T \phi = \mathbb{1}$) and eigenvalues are $\lambda_{1,2,3}$,

$$A\phi = \phi diag(\lambda_1, \lambda_2, \lambda_3). \tag{4}$$

The eigenvectors and eigenvalues can be calculated by using the matrixmod module.
In the code, the accordingly operators are

$$\begin{aligned}
\hat{O}^4 &= \tau_x[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] = \tau_x \sigma_\alpha \phi_{\alpha 1} && (5)\\
\hat{O}^5 &= \tau_y[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] = \tau_y \sigma_\alpha \phi_{\alpha 1} && (6)\\
\hat{O}^6 &= \tau_z[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] = \tau_z \sigma_\alpha \phi_{\alpha 1} && (7)\\
\hat{O}^7 &= \tau_x[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] = \tau_x \sigma_\alpha \phi_{\alpha 2} && (8)\\
\hat{O}^8 &= \tau_y[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] = \tau_y \sigma_\alpha \phi_{\alpha 2} && (9)\\
\hat{O}^9 &= \tau_z[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] = \tau_z \sigma_\alpha \phi_{\alpha 2} && (10)\\
\hat{O}^{10} &= \tau_x[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] = \tau_x \sigma_\alpha \phi_{\alpha 3} && (11)\\
\hat{O}^{11} &= \tau_y[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] = \tau_y \sigma_\alpha \phi_{\alpha 3} && (12)\\
\hat{O}^{12} &= \tau_z[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] = \tau_z \sigma_\alpha \phi_{\alpha 3}. && (13)
\end{aligned}$$

Obviously, $\phi_{\alpha\beta} = vec(\alpha, \beta)$.
On the other hand, the eigenvalues and eigenvector have their physical meaning and can be calculated directly. It is that,

$$\begin{aligned}
& u_{ij}^4 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + u_{ij}^6 (3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \\
= \; & \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \left[(u_{ij}^4 - u_{ij}^6) \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 3u_{ij}^6 \boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} \right],
\end{aligned} \tag{14}$$

for the inner part, $(u_{ij}^4 - u_{ij}^6)\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 3u_{ij}^6 \boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij}$, we can choose three basic directions (just like the x, y, z directions in the cartesian coordinates), $\hat{r}$, $\hat{r}_{\perp 1}$ and $\hat{r}_{\perp 2}$, and they are perpendicular with each other. For a given direction $\hat{r}$, the two perpendicular directions $\hat{r}_{\perp 1}$ and $\hat{r}_{\perp 2}$ can be easily chosen. Then for the inner part, we have

$$\begin{aligned}
\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j &= (\boldsymbol{\sigma}_i \cdot \hat{r})(\boldsymbol{\sigma}_j \cdot \hat{r}) + (\boldsymbol{\sigma}_i \cdot \hat{r}_{\perp 1})(\boldsymbol{\sigma}_j \cdot \hat{r}_{\perp 1}) + (\boldsymbol{\sigma}_i \cdot \hat{r}_{\perp 2})(\boldsymbol{\sigma}_j \cdot \hat{r}_{\perp 2}) \\
&= \sigma_{i\alpha} r_\alpha \sigma_{j\beta} r_\beta + \sigma_{i\alpha} r_{\perp 1\alpha} \sigma_{j\beta} r_{\perp 1\beta} + \sigma_{i\alpha} r_{\perp 2\alpha} \sigma_{j\beta} r_{\perp 2\beta}
\end{aligned} \tag{15}$$

and

$$\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} = \sigma_{i\alpha} r_\alpha \sigma_{j\beta} r_\beta, \tag{16}$$

where the α, β go through x, y, and z components. Combining those results, the inner part can be written as

$$\begin{aligned} & (u_{ij}^4 - u_{ij}^6)\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 3u_{ij}^6 \boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} \\ = \; & (u_{ij}^4 + 2u_{ij}^6)(\sigma_{i\alpha} r_\alpha)(\sigma_{j\beta} r_\beta) \\ + \; & (u_{ij}^4 - u_{ij}^6)(\sigma_{i\alpha} r_{\perp 1\alpha})(\sigma_{j\beta} r_{\perp 1\beta}) \\ + \; & (u_{ij}^4 - u_{ij}^6)(\sigma_{i\alpha} r_{\perp 2\alpha})(\sigma_{j\beta} r_{\perp 2\beta}). \end{aligned} \tag{17}$$

Then we have

$$\begin{aligned} & u_{ij}^4 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j + u_{ij}^6 (3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \\ = \; & \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \left[(u_{ij}^4 - u_{ij}^6)\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 3u_{ij}^6 \boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} \right] \\ = \; & (u_{ij}^4 + 2u_{ij}^6)[\tau_{i\gamma}(\sigma_{i\alpha} r_\alpha)][\tau_{j\gamma}(\sigma_{j\beta} r_\beta)] \\ + \; & (u_{ij}^4 - u_{ij}^6)[\tau_{i\gamma}(\sigma_{i\alpha} r_{\perp 1\alpha})][\tau_{j\gamma}(\sigma_{j\beta} r_{\perp 1\beta})] \\ + \; & (u_{ij}^4 - u_{ij}^6)[\tau_{i\gamma}(\sigma_{i\alpha} r_{\perp 2\alpha})][\tau_{j\gamma}(\sigma_{j\beta} r_{\perp 2\beta})], \end{aligned} \tag{18}$$

and compare with Eq.(3), we will know that

$$\begin{aligned} r_\alpha &= \phi_{\alpha 1} \\ \lambda_1 &= u_{ij}^4 + 2u_{ij}^6 \\ r_{\perp 1\alpha} &= \phi_{\alpha 2} \\ \lambda_2 &= u_{ij}^4 - u_{ij}^6 \\ r_{\perp 2\alpha} &= \phi_{\alpha 3} \\ \lambda_3 &= u_{ij}^4 - u_{ij}^6 = \lambda_2. \end{aligned} \tag{19}$$

Similarly, the 3 and 5 operators can be combined as

$$\begin{aligned} & u_{ij}^3 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + u_{ij}^5 (3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \\ = \; & (u_{ij}^3 - u_{ij}^5)\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 3u_{ij}^6 \boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} \\ = \; & 3u_{ij}^5 (\sigma_{i\alpha} r_\alpha)(\sigma_{j\beta} r_\beta) + (u_{ij}^3 - u_{ij}^5)\left[\sigma_{i\alpha} r_\alpha \sigma_{j\beta} r_\beta + \sigma_{i\alpha} r_{\perp 1\alpha} \sigma_{j\beta} r_{\perp 1\beta} + \sigma_{i\alpha} r_{\perp 2\alpha} \sigma_{j\beta} r_{\perp 2\beta} \right] \\ = \; & (u_{ij}^3 + 2u_{ij}^5)\sigma_{i\alpha} r_\alpha \sigma_{j\beta} r_\beta + (u_{ij}^3 - u_{ij}^5)\sigma_{i\alpha} r_{\perp 1\alpha} \sigma_{j\beta} r_{\perp 1\beta} + (u_{ij}^3 - u_{ij}^5)\sigma_{i\alpha} r_{\perp 2\alpha} \sigma_{j\beta} r_{\perp 2\beta}. \end{aligned} \tag{20}$$

And this gives the $\hat{O}^{13}$, $\hat{O}^{14}$ and $\hat{O}^{15}$. That is

$$\hat{O}^{13} = \sigma_x vecs(1,1) + \sigma_y vecs(2,1) + \sigma_z vecs(3,1) = \sigma_{i\alpha} r_\alpha \sigma_{j\beta} r_\beta \tag{21}$$

$$\hat{O}^{14} = \sigma_x vecs(1,2) + \sigma_y vecs(2,2) + \sigma_z vecs(3,2) = \sigma_{i\alpha} r_{\perp 1\alpha} \sigma_{j\beta} r_{\perp 1\beta} \tag{22}$$

$$\hat{O}^{15} = \sigma_x vecs(1,3) + \sigma_y vecs(2,3) + \sigma_z vecs(3,3) = \sigma_{i\alpha} r_{\perp 2\alpha} \sigma_{j\beta} r_{\perp 2\beta}. \tag{23}$$

On the other hand, still we can write down

$$\begin{aligned} & u_{ij}^3 \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + u_{ij}^5 (3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \\ = \; & \sigma_{i\alpha} \sigma_{j\beta} \underbrace{\left[3u_{ij}^5 r_\alpha r_\beta + (u_{ij}^3 - u_{ij}^5)\delta_{\alpha\beta} \right]}_{\equiv A_{\alpha\beta}} \\ = \; & \sigma_{i\alpha} A_{\alpha\beta} \sigma_{j\beta} \\ = \; & \sigma_{i\alpha} \psi_{\alpha\eta} \lambda_\eta \psi_{\beta\eta} \sigma_{j\beta} \\ = \; & \lambda_\eta (\sigma_{i\alpha} \psi_{\alpha\eta})(\sigma_{j\beta} \psi_{\beta\eta}). \end{aligned} \tag{24}$$

Again it gives $\hat{O}^{13}$, $\hat{O}^{14}$ and $\hat{O}^{15}$. Comparing with Eq.(20), we have

$$\begin{aligned}
r_\alpha &= \phi_{\alpha 1} \\
\lambda_1 &= u^3_{ij} + 2u^5_{ij} \\
r_{\perp 1\alpha} &= \phi_{\alpha 2} \\
\lambda_2 &= u^3_{ij} - u^5_{ij} \\
r_{\perp 2\alpha} &= \phi_{\alpha 3} \\
\lambda_3 &= u^3_{ij} - u^5_{ij} = \lambda_2 .
\end{aligned} \tag{25}$$

Finally,

$$\hat{O}^{1,2,3} = \tau_x, \tau_y, \tau_z \tag{26}$$

just taken from $u^2_{ij}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j = u^2_{ij}\tau_{i\alpha}\tau_{j\alpha}$.

So, until here, the meaning of the 15 operators in the code is clear. And the two-body correlation operator F_{ij} can be written as

$$F_{ij} = u^1_{ij} + u^2_{ij}\tau_{i\alpha}\tau_{j\alpha} + \lambda^{(\tau\sigma)}_\eta(\tau_{i\gamma}\sigma_{i\alpha}\phi_{\alpha\eta})(\tau_{j\gamma}\sigma_{j\beta}\phi_{\beta\eta}) + \lambda^{(\sigma)}_\eta(\sigma_{i\alpha}\psi_{\alpha\eta})(\sigma_{j\beta}\psi_{\beta\eta}) = u^1_{ij} + \sum_{p=1}^{15} f^p_{ij}\hat{O}^p_i\hat{O}^p_j \tag{27}$$

B. The cartesian 39 operators

On the other hand, a traditional way is to write this interaction as 39 operators. That is, we can write down

$$F_{ij} = u^1_{ij} + \sum_\alpha \tau_{i\alpha}A^\tau_{ij}\tau_{j\alpha} + \sum_{\alpha\beta}\sigma_{i\alpha}A^\sigma_{ij}\sigma_{j\beta} + \sum_{\alpha\beta\gamma}(\sigma_{i\alpha}\tau_{i\gamma})A^{\sigma\tau}_{ij}(\sigma_{j\beta}\tau_{j\gamma}), \tag{28}$$

where

$$A^\tau_{ij} = u^2_{ij} \tag{29}$$

$$A^\sigma_{ij} = u^3_{ij}\delta_{\alpha\beta} + u^5_{ij}(3\hat{r}^\alpha_{ij}\hat{r}^\beta_{ij} - \delta_{\alpha\beta}) \tag{30}$$

$$A^{\sigma\tau}_{ij} = u^4_{ij}\delta_{\alpha\beta} + u^6_{ij}(3\hat{r}^\alpha_{ij}\hat{r}^\beta_{ij} - \delta_{\alpha\beta}) \tag{31}$$

II. PROGRESS 2-18: SOME UNDERSTANDING ABOUT CORRELATOR.F90

A. two body correlation operator F_{ij}

The trial wave function can be written as

$$\langle \Psi_T | RS \rangle = \langle \Phi | \left[\prod_{i<j} f_c(r_{ij}) \right] \left[1 + \sum_{i<j} F_{ij} + \sum_{i<j<k} F_{ijk} \right] |RS\rangle, \tag{32}$$

Now, let us just look at $F_{ij} = \sum_p f_{ij}^p \hat{O}_{ij}^p$. For example, for v6' interaction we can write down

$$\begin{aligned} F_{ij} &= f_{ij}^1 \\ &+ \sum_{\alpha} \tau_{i\alpha} A_{ij}^{\tau} \tau_{j\alpha} \\ &+ \sum_{\alpha\beta} \sigma_{i\alpha} A_{ij}^{\sigma} \sigma_{j\beta} \\ &+ \sum_{\alpha\beta\gamma} (\sigma_{i\alpha}\tau_{i\gamma}) A_{ij}^{\sigma\tau} (\sigma_{i\beta}\tau_{i\gamma}), \end{aligned} \tag{33}$$

where

$$\begin{aligned} A_{ij}^{\tau} &= f_{ij}^2 \\ A_{ij}^{\sigma} &= f_{ij}^3 \delta_{\alpha\beta} + f_{ij}^5 (3\hat{r}_{ij}^{\alpha}\hat{r}_{ij}^{\beta} - \delta_{\alpha\beta}) \\ A_{ij}^{\sigma\tau} &= f_{ij}^4 \delta_{\alpha\beta} + f_{ij}^6 (3\hat{r}_{ij}^{\alpha}\hat{r}_{ij}^{\beta} - \delta_{\alpha\beta}). \end{aligned} \tag{34}$$

All the A matrices are real and symmetric and can be diagonalize by their real eigenvector matrices. For example,

$$A = \psi diag(\lambda_1, \lambda_2 ... \lambda_A) \psi^{\dagger} \tag{35}$$

where λ_i are the eigenvalues of A. ψ is $n \times n$ matrix where n is the particle number, and ψ is composed of the n $n \times 1$ column vectors of A. And therefore we can write down

$$A_{ij} = \sum_{k=1}^{n} \psi_{ik} \lambda_k \psi_{kj}^{\dagger} = \sum_{k=1}^{n} \psi_{ik} \lambda_k \psi_{jk}. \tag{36}$$

And then F_{ij} can be written as

$$\begin{aligned} F_{ij} &= f_{ij}^1 \\ &+ \sum_{\alpha} \sum_{k=1}^{n} (\tau_{i\alpha} \psi_{ik}^{\tau}) \lambda_k^{\tau} (\tau_{j\alpha} \psi_{jk}^{\tau}) \\ &+ \sum_{\alpha\beta} \sum_{k=1}^{n} (\sigma_{i\alpha} \psi_{ik}^{\sigma}) \lambda_k^{\sigma} (\sigma_{j\beta} \psi_{jk}^{\sigma}) \\ &+ \sum_{\alpha\beta\gamma} \sum_{k=1}^{n} (\sigma_{i\alpha}\tau_{i\gamma} \psi_{ik}^{\sigma\tau}) \lambda_k^{\sigma\tau} (\sigma_{j\beta}\tau_{j\gamma} \psi_{jk}^{\sigma\tau}). \end{aligned} \tag{37}$$

For a given i or j, there are 15 basic operators, which include $\tau_{\alpha}(3)$, $\sigma_{\alpha}(3)$ and $\sigma_{\alpha}\tau_{\beta}(9)$.

I have checked the code, and I found that in the correlator.f90, in subroutine v6tot, the 15 operators are,

$$
\begin{aligned}
\hat{O}^{1,2,3} &= \tau_x, \tau_y, \tau_z \\
\hat{O}^{4} &= \tau_x[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] && (38) \\
\hat{O}^{5} &= \tau_y[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] && (39) \\
\hat{O}^{6} &= \tau_z[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] && (40) \\
\hat{O}^{7} &= \tau_x[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] && (41) \\
\hat{O}^{8} &= \tau_y[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] && (42) \\
\hat{O}^{9} &= \tau_z[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] && (43) \\
\hat{O}^{10} &= \tau_x[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] && (44) \\
\hat{O}^{11} &= \tau_y[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] && (45) \\
\hat{O}^{12} &= \tau_z[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] && (46) \\
\hat{O}^{13} &= \sigma_x vecs(1,1) + \sigma_y vecs(2,1) + \sigma_z vecs(3,1) && (47) \\
\hat{O}^{14} &= \sigma_x vecs(1,2) + \sigma_y vecs(2,2) + \sigma_z vecs(3,2) && (48) \\
\hat{O}^{15} &= \sigma_x vecs(1,3) + \sigma_y vecs(2,3) + \sigma_z vecs(3,3) && (49)
\end{aligned}
$$

- But I would like to know what exactly are those vec=fstvec, vecs=fsvec, fij, ft, fstval, fsval.
- and what exactly does v6tot do?

B. g1bval, g2bval, g3bval

As to g1bval, g2bval, g3bval, they are updating d1b, d2b and d3b accordingly.

$$
\begin{aligned}
d1b(s,i) &= \sum_k S^{-1}_{ik} \langle k|\boldsymbol{r}_i s\rangle && (50) \\
d2b(s,js,ij) &= f_{ij}\,[sxz(s,i,i)sxz(js,j,j) - sxz(js,j,i)sxz(s,i,j)] && (51) \\
d3b(s,js,ks,i,j,k) &= \frac{f_{ij}}{probijk(ijk)} \\
&\times \Big\{ sxz(s,i,i)[sxz(js,j,j)sxz(ks,k,k) - sxz(ks,k,j)sxz(js,j,k)] \\
&+ sxz(s,i,j)sxz(js,j,k)sxz(ks,k,i) - sxz(js,j,i)sxz(ks,k,k) \\
&+ sxz(s,i,k)sxz(js,j,i)sxz(ks,k,j) - sxz(js,j,j)sxz(ks,k,i) \Big\} && (52)
\end{aligned}
$$

and $sp(s,i) = \langle s|s_i\rangle$.
d1b is defined in order to calculate $|S^{-1}S'|$ in $|S'|$. It is that

$$
\begin{aligned}
|S^{-1}S'| &= \sum_k S^{-1}_{ik} S'_{ki} \\
&= \sum_s \underbrace{\sum_k S^{-1}_{ik} \langle k|\boldsymbol{r}_i s\rangle}_{sxmallz(i,s,i)} \langle s|O|s_i\rangle && (53)
\end{aligned}
$$

d2b is defined in order to calculate $|S^{-1}S''|$ in $|S''|$. It is that

$$
\begin{aligned}
|S^{-1}S''| &= (\sum_k S^{-1}_{ik} S''_{ki})(\sum_k S^{-1}_{jk} S''_{kj}) - (\sum_k S^{-1}_{ik} S''_{kj})(\sum_k S^{-1}_{jk} S''_{ki}) \\
&= \sum_s \sum_{js} \langle s|O_i|s_i\rangle \langle js|O_j|s_j\rangle \big[sxz(s,i,i)sxz(js,j,j) - sxz(js,j,i)sxz(s,i,j)\big], && (54)
\end{aligned}
$$

where

$$
d2b(s,js,ij) \equiv f_{ij}\big[sxz(s,i,i)sxz(js,j,j) - sxz(js,j,i)sxz(s,i,j)\big] \quad (55)
$$

d3b is defined in order to calculate $|S^{-1}S'''|$ in $|S'''|$. Define $\boxed{\text{ij}} \equiv \sum_k S^{-1}_{ik} S'''_{kj}$. It is that

$$
\begin{aligned}
|S^{-1}S'''| &= \boxed{\text{ii}}\Big(\boxed{\text{jj}}\boxed{\text{kk}} - \boxed{\text{jk}}\boxed{\text{kj}}\Big) + \boxed{\text{ij}}\Big(\boxed{\text{ji}}\boxed{\text{kk}} - \boxed{\text{jk}}\boxed{\text{ki}}\Big) + \boxed{\text{ik}}\Big(\boxed{\text{jj}}\boxed{\text{kj}} - \boxed{\text{jj}}\boxed{\text{ki}}\Big) \\
&= \sum_{s,js,ks} spx(s,p,i)spx(js,p,j)spx(ks,p,k) \\
&\times \Big\{sxz(s,i,i)[sxz(js,j,j)sxz(ks,k,k) - sxz(ks,k,j)sxz(js,j,k)] \\
&+ sxz(s,i,j)sxz(js,j,k)sxz(ks,k,i) - sxz(js,j,i)sxz(ks,k,k) \\
&+ sxz(s,i,k)sxz(js,j,i)sxz(ks,k,j) - sxz(js,j,j)sxz(ks,k,i)\Big\}
\end{aligned}
\tag{56}
$$

The part in the { } is related with d3b.

- But why there is f_{ij} in d2b?
- And why there is $\frac{f_{ij}}{probijk(ijk)}$ in d3b?

C. sinvijz

in the note, sinvijz is defined as 4D sinvijz(s,n,m,p), but in the code it is 3D sinvijz(s,n,m).

[1] Stenven C. Pieper, V.R. Pandharipande, R.B. Wiringa, and J. Carlson, Phys. Rev. C**64** (2001).
[2] J. Carlson et al, RMP, arxiv:1412.3081v1.
[3] S. Gandolfi, A. Lovato, J. Carlson, and Kevin E. Schmidt, arxiv:1406.3388v1.
[4] Kevin E. Schmidt, Three-body potential notes.
[5] Kevin E. Schmidt, chiral.pdf