AFDMC-TBF

Rong Chen
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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

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

for convenience just mark $\hat{r}_{ij}$ as $\hat{r}$.

the 4 and 6 operators can be combined as

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

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,

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

for the inner part, $(u^4_{ij}-u^6_{ij})\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + 3u^6_{ij}\boldsymbol{\sigma}_i\cdot\hat{r}_{ij}\boldsymbol{\sigma}_j\cdot\hat{r}_{ij}$, 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 $F_{ij} = \sum_p f^p_{ij} \hat{O}^p_{ij}$. For example, for v6' interaction we can write down

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

where

$$\begin{aligned} A^\tau_{ij} &= f^2_{ij} \\ A^\sigma_{ij} &= f^3_{ij}\delta_{\alpha\beta} + f^5_{ij}(3\hat{r}^\alpha_{ij}\hat{r}^\beta_{ij} - \delta_{\alpha\beta}) \\ A^{\sigma\tau}_{ij} &= f^4_{ij}\delta_{\alpha\beta} + f^6_{ij}(3\hat{r}^\alpha_{ij}\hat{r}^\beta_{ij} - \delta_{\alpha\beta}). \end{aligned} \tag{34}$$

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

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

And then F_{ij} can be written as

$$\begin{aligned} F_{ij} &= f^1_{ij} \\ &+ \sum_\alpha \sum_{k=1}^n (\tau_{i\alpha}\psi^\tau_{ik})\lambda^\tau_k(\tau_{j\alpha}\psi^\tau_{jk}) \\ &+ \sum_{\alpha\beta} \sum_{k=1}^n (\sigma_{i\alpha}\psi^\sigma_{ik})\lambda^\sigma_k(\sigma_{j\beta}\psi^\sigma_{jk}) \\ &+ \sum_{\alpha\beta\gamma} \sum_{k=1}^n (\sigma_{i\alpha}\tau_{i\gamma}\psi^{\sigma\tau}_{ik})\lambda^{\sigma\tau}_k(\sigma_{j\beta}\tau_{j\gamma}\psi^{\sigma\tau}_{jk}). \end{aligned} \tag{37}$$

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,

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

$$\hat{O}^{4} = \tau_x[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] \tag{38}$$

$$\hat{O}^{5} = \tau_y[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] \tag{39}$$

$$\hat{O}^{6} = \tau_z[\sigma_x vec(1,1) + \sigma_y vec(2,1) + \sigma_z vec(3,1)] \tag{40}$$

$$\hat{O}^{7} = \tau_x[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] \tag{41}$$

$$\hat{O}^{8} = \tau_y[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] \tag{42}$$

$$\hat{O}^{9} = \tau_z[\sigma_x vec(1,2) + \sigma_y vec(2,2) + \sigma_z vec(3,2)] \tag{43}$$

$$\hat{O}^{10} = \tau_x[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] \tag{44}$$

$$\hat{O}^{11} = \tau_y[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] \tag{45}$$

$$\hat{O}^{12} = \tau_z[\sigma_x vec(1,3) + \sigma_y vec(2,3) + \sigma_z vec(3,3)] \tag{46}$$

$$\hat{O}^{13} = \sigma_x vecs(1,1) + \sigma_y vecs(2,1) + \sigma_z vecs(3,1) \tag{47}$$

$$\hat{O}^{14} = \sigma_x vecs(1,2) + \sigma_y vecs(2,2) + \sigma_z vecs(3,2) \tag{48}$$

$$\hat{O}^{15} = \sigma_x vecs(1,3) + \sigma_y vecs(2,3) + \sigma_z vecs(3,3) \tag{49}$$

- 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.

$$d1b(s,i) = \sum_k S^{-1}_{ik} \langle k|\boldsymbol{r}_i s\rangle \tag{50}$$

$$d2b(s,js,ij) = f_{ij}\left[sxz(s,i,i)sxz(js,j,j) - sxz(js,j,i)sxz(s,i,j)\right] \tag{51}$$

$$\begin{aligned} d3b(s,js,ks,i,j,k) &= \frac{f_{ij}}{probijk(ijk)} \\ &\times \Big\{sxz(s,i,i)[sxz(js,j,j)sxz(ks,k,k) - sxz(ks,k,j)sxz(js,j,k)] \\ &+ sxz(s,i,j)sxz(js,j,k)sxz(ks,k,i) - sxz(js,j,i)sxz(ks,k,k) \\ &+ sxz(s,i,k)sxz(js,j,i)sxz(ks,k,j) - sxz(js,j,j)sxz(ks,k,i)\Big\} \end{aligned} \tag{52}$$

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

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

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

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

where

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

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).

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