Three-body potential notes

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1 Notation

- Label the orbital states as $|k\rangle$ with a k index.
- The position and spin state of particle i is written $|\vec{r}_i\ s_i\rangle$.
- We store a particle spin state as the 4 numbers $\langle p\uparrow|s_i\rangle$, $\langle p\downarrow|s_i\rangle$, $\langle n\uparrow|s_i\rangle$, $\langle n\downarrow|s_i\rangle$, which is written as $\langle s|s_i\rangle$ with s running from 1 to 4 respectively.
- We use the matrix identity $\det S^{-1}S' = \frac{\det S'}{\det S}$ to calculate the determinant of the matrix S' when it has only a small number of columns diffrent from A. The unchanged columns give 1 on the diagonal and 0 on the off diagonals so that the determinant of C with $C = S^{-1}S'$ is given by the determinant of the determinant of the matrix C_{mn} where m and n only take values of the changed columns of S'.

2 Calculations

Here we deal with the case where the operators only change the spin state of the particles. The Slater matrix is

$$S_{ki} = \langle k|\vec{r}_i s_i\rangle = \sum_{s=1}^{4} \langle k|\vec{r}_i s\rangle\langle s|s_i\rangle \tag{1}$$

so a general matrix element of S' will be a linear combination of the orbital matrix elements $\langle k|\vec{r}_i s\rangle$. We therefore precompute

$$\mathrm{sxmallz(j,s,i)} \;=\; \sum_k S^{-1}_{jk}\langle k|\vec{r}_i, s\rangle \tag{2}$$

where s runs from 1 to 4. j and i run from 1 to the number of particles A. This quantity is then used for all subsequent determinant calculations. The original reason for having the spin as the middle index was to exploit the matrix multiply form. However, we can get a useful speed up by having the spin variable leftmost so that it has unit stride in inner loops, so we transpose this and write

$$\mathrm{sxz(s,i,j)} \;=\; \mathrm{sxmallz(j,s,i)} = \sum_k S^{-1}_{jk}\langle k|\vec{r}_i, s\rangle \tag{3}$$

The 2- and 3-body potentials are written in terms of products of linear combinations of the 15 operators for each particle, $\sigma_{\alpha i}$, $\tau_{\gamma i}$, $\sigma_{\alpha i}\tau_{\gamma i}$. We label these O_i^p, with p running from 1 to 15, and greek letters giving the cartesian components. Since these were the only operators in previous versions of the code, we calculated

$$\begin{aligned} \mathrm{sxmall(j,p,i)} &= \sum_k S^{-1}_{jk} \langle k|O_i^p|\vec{r}_i, s_i\rangle \\ &= \sum_{s=1}^{4}\sum_k S^{-1}_{jk}\langle k|\vec{r}_i s\rangle\langle s|O_i^p|s_i\rangle \,. \end{aligned} \tag{4}$$

In the code this is typically calculated as

$$\begin{aligned} \mathrm{spx(s,p,i)} &= \langle s|O_i^p|s_i\rangle \\ \mathrm{sxmall(j,p,i)} &= \sum_s \mathrm{sxmallz(j,s,i)\ spx(s,p,i)} \,. \end{aligned} \tag{5}$$

3 Correlated wave function

The correlated wave function has a sum of pair wise correlations. Each pairwise correlation is written as a sum of 12 (or 15, see below) products of two single particle operators. As in the code, these will be labeled i and j. In order to use the same single determinant code to calculate the energy, we need the equivalent of $\mathrm{sxmallz(m,s,n)}$ for the "Slater matrix"

$$S''_{km} = \left\{ \begin{array}{cc} S_{km} & m \neq i \text{ or } j \\ \langle k|\mathcal{O}_m^p|\vec{r}_m s_m\rangle & m = i \text{ or } m = j \end{array} \right. . \tag{6}$$

We require the inverse of this matrix S''^{-1} multiplied by the all possible "new orbitals" which will be

$$S''_{km}(s,p) = \left\{ \begin{array}{cc} \langle k|\vec{r}_m s\rangle & m \neq i \text{ or } j \\ \langle k|\mathcal{O}_m^p|\vec{r}_m s\rangle & \text{otherwise} \end{array} \right. . \tag{7}$$

In the code we have

$$\mathrm{sinvijz(s,n,m,p)} = \sum_k S''^{-1}_{mk} S''_{kn}(s,p) \tag{8}$$

which is the equivalent of $\mathrm{sxz(s,n,m)}$ for the p pair operator. $\mathrm{sinvijz(s,n,m,p)}$ is defined inside a pair loop and is recalculated for each ij pair. We calculate it and the ratio of determinants $\det S''/\det S$. Handing this array to the usual 2- or 3-body single determinant local energy routine, then hands back the correlated energy evaluated in the Slater determinant state S'', divided by the determinant of S''. Scaling this with the ratio of the determinants and the pair jastrow function gives the energy contribution for this part of the correlation operator.

To calculate $\sum_k S''^{-1}_{mk} S''_{kn}(s,p)$, we can write the usual expression for the updated inverse when two columns have been changed in terms of the old inverse. As shown below, multiplying this expression times $S''_{kn}(s,p)$ shows that all of the terms can be calculated from $\mathrm{sxmallz(m,s,n)}$ without using the old inverse matrix directly.

Looking at the case for a particular p, i, and j, along with column m changing. If m is not equal to i or j, i.e.

$$S'''_{kn} = \begin{cases} S_{kn} & n \neq i, j, \text{ or } m \\ \langle k|\mathcal{O}^p_m|\vec{r}_n s_n\rangle & n = i \text{ or } n = j \\ a_k & n = m \end{cases}, \tag{9}$$

where a_k is an arbitrary new column. We can calculate the updated inverse from

$$\begin{aligned} \frac{\det S''}{\det S} &= \det S^{-1} S'' \\ \frac{\det S'''}{\det S} &= \det S^{-1} S''' \\ \frac{\det S'''}{\det S''} &= \sum_k S''^{-1}_{mk} a_k \end{aligned} \tag{10}$$

In this case,

$$\frac{\det S'''}{\det S} = \det S^{-1} S''' = \det \begin{pmatrix} \sum_k S^{-1}_{ik}\langle k|\mathcal{O}^p_i|\vec{r}_i s_i\rangle & \sum_k S^{-1}_{ik}\langle k|\mathcal{O}^p_j|\vec{r}_j s_j\rangle & \sum_k S^{-1}_{ik} a_k \\ \sum_k S^{-1}_{jk}\langle k|\mathcal{O}^p_i|\vec{r}_i s_i\rangle & \sum_k S^{-1}_{jk}\langle k|\mathcal{O}^p_j|\vec{r}_j s_j\rangle & \sum_k S^{-1}_{jk} a_k \\ \sum_k S^{-1}_{mk}\langle k|\mathcal{O}^p_i|\vec{r}_i s_i\rangle & \sum_k S^{-1}_{mk}\langle k|\mathcal{O}^p_j|\vec{r}_j s_j\rangle & \sum_k S^{-1}_{mk} a_k \end{pmatrix} \tag{11}$$

For the case that $m = j$, we have

$$\frac{\det S'''}{\det S} = \det S^{-1} S''' = \det \begin{pmatrix} \sum_k S^{-1}_{ik}\langle k|\mathcal{O}^p_i|\vec{r}_i s_i\rangle & \sum_k S^{-1}_{ik} a_k \\ \sum_k S^{-1}_{jk}\langle k|\mathcal{O}^p_i|\vec{r}_i s_i\rangle & \sum_k S^{-1}_{jk} a_k \end{pmatrix}. \tag{12}$$

In the code once a particular pair i and j is chosen, we write

$$\begin{aligned} \mathrm{sxi(s,m,p)} &= \sum_k S^{-1}_{mk}\langle k|\mathcal{O}^p_i|\vec{r}_i s\rangle \\ \mathrm{di(m,p)} &= \sum_k S^{-1}_{mk}\langle k|\mathcal{O}^p_i|\vec{r}_i s_i\rangle \\ \mathrm{sxj(s,m,p)} &= \sum_k S^{-1}_{mk}\langle k|\mathcal{O}^p_j|\vec{r}_j s\rangle \\ \mathrm{dj(m,p)} &= \sum_k S^{-1}_{mk}\langle k|\mathcal{O}^p_j|\vec{r}_j s_j\rangle \end{aligned} \tag{13}$$

Eq. 11 can be written as

$$\frac{\det S'''}{\det S} = \det \begin{pmatrix} \mathrm{di(i,p)} & \mathrm{dj(i,p)} & \sum_k S^{-1}_{ik} a_k \\ \mathrm{di(j,p)} & \mathrm{dj(j,p)} & \sum_k S^{-1}_{jk} a_k \\ \mathrm{di(m,p)} & \mathrm{dj(m,p)} & \sum_k S^{-1}_{mk} a_k \end{pmatrix} \tag{14}$$

Combining these gives the updated inverse

$$S''^{-1}_{mk} = \frac{1}{\mathrm{di(i,p)dj(j,p) - di(j,p)dj(i,p)}} \begin{cases} \left[\mathrm{di(i,p)dj(j,p) - di(j,p)dj(i,p)}\right] S^{-1}_{mk} & \\ -\left[\mathrm{di(i,p)dj(m,p) - di(m,p)dj(i,p)}\right] S^{-1}_{jk} & m \neq i, m \neq j \\ +\left[\mathrm{di(j,p)dj(m,p) - di(m,p)dj(j,p)}\right] S^{-1}_{ik} & \\ \mathrm{dj(j,p)}S^{-1}_{ik} - \mathrm{dj(i,p)}S^{-1}_{jk} & m = i \\ \mathrm{di(i,p)}S^{-1}_{jk} - \mathrm{di(j,p)}S^{-1}_{ik} & m = j \end{cases} \tag{15}$$

As noted above, we want Eq. 8, so multiplying the inverse by $S''_{kn}(s,p)$ given in Eq. 7, and summing over k, the $\sum_k S^{-1}_{mk} S''_{kn}(s,p)$ become sxz terms if $n \neq i$ or $n \neq j$, and sxi or sxj terms if $n = i$ or $n = j$. At this point, the original inverse is no longer needed and the result can be built up from the original sxmallz or sxz array.

4 Operator breakup

We rewrite the v_6 2-body correlations and potentials as the sum of 15 (or 12 if there are no terms without $\vec{\tau}_i \cdot \vec{\tau}_j$ factors) operator products. That is we write these terms for pair ij as

$$\begin{aligned} &\sum_{\alpha\beta} \sigma_{i\alpha} V^{\sigma}_{\alpha\beta}(ij) \sigma_{j\beta} + \sum_{\alpha\beta\gamma} \sigma_{i\alpha} V^{\sigma\tau}(ij)_{\alpha\beta} \sigma_{j\beta} \tau_{i\gamma} \tau_{j\gamma} + \sum \gamma V^{\tau}(ij) \tau_{i\gamma} \tau_{j\gamma} \\ &= \sum_{p=1}^{3} V^{\sigma p}(ij) \mathcal{O}^{\sigma}_p(i) \mathcal{O}^{\sigma}_p(j) + \sum_{p=1}^{9} V^{\sigma\tau p}(ij) \mathcal{O}^{\sigma\tau}_p(i) \mathcal{O}^{\sigma\tau}_p(j) + \sum_{p=1}^{3} V^{\tau p}(ij) \mathcal{O}^{\tau}(i) \mathcal{O}^{\tau}(j) \end{aligned} \tag{16}$$

fix this. The notation is bad and wrong.

5 Application to the pairwise sum correlation