Notes on the calculation of the correlated mixed expectation values

Kevin E. Schmidt
Department of Physics
Arizona State University
Tempe, AZ 85287 USA

June 1, 2015

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

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

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

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

3 Matrix elements of 1-, 2-, and 3-body spin-isospin operators

We need mixed expectations of various 1-, 2-, and 3-body spin-isospin operators to calculate the various terms in the local energy. Since the correlated trial wave function will be a linear combination of many terms, it is most efficient to organize the calculations so that the fewest operations are done in the inner loops.

3.1 1-body spin-isospin operators

We often would like to have the mixed expectation values of the 15 operators given by the components of $\sum_i \vec{\sigma}_i$, $\sum_i \vec{\tau}_i$, $\sum_i \vec{\sigma}_i\vec{\tau}_i$. Rather than calculate their matrix elements in the inner loops, it is more efficient to write a general 1-body spin/isospin operator operating on a walker $|s_1, s_2, ..., s_A\rangle$, as the linear combination of the $4A$ terms

$$\sum_i O_i|s_1, ..., s_A\rangle = \sum_{s=1}^{4} \alpha_{1s}|s, s_2, ..., s_A\rangle + \sum_{s=1}^{4} \alpha_{2s}|s_1, s, ..., s_A\rangle + ... \tag{4}$$

where $\alpha_{is} = \langle s|O_i|s_i\rangle$. The code then calculates the intermediate quantity given by the matrix elements

$$\mathrm{d1b(s,i)} = \frac{\langle\Phi|R, s_1, ..., s_{i-1}, s, s_{i+1}, ..., s_A\rangle}{\langle\Phi|R, s_1, ..., s_A\rangle}\,, \tag{5}$$

where d1b standards for "distribution 1-body" since this looks like a one-body spin projector distribution.

Given the sxz(s,i,j) corresponding to $|\Phi\rangle$, we have

$$\mathrm{d1b(s,i)} = \mathrm{sxz(s,i,i)}\,. \tag{6}$$

The full trial function will be expanded below in the equivalent of a linear combination of many different $\langle\Phi|$ pieces. These then give a full d1b(s,i) from the same linear combination of the separate ones.

Once the full d1b is calculated, the desired one-body operator mixed expectations are calculated from

$$\sum_{i=1}^{A}\sum_{s=1}^{4} \alpha_{is}\mathrm{d1b(s,i)}\,. \tag{7}$$

3.2 2-body spin-isospin operators

We now repeat the above analysis for 2-body operators. Since the pair 1-2 is equivalent to 2-1, we write the 2-body distributions we need given a particular $\langle\Phi|$ as

$$\mathrm{d2b(s,s',ij)} = \frac{\langle\Phi|R, s_1, ..., s_{i-1}, s, s_{i+1}, ..., s_{j-1}, s', s_{j+1}, ...s_A\rangle}{\langle\Phi|R, s_1, ..., s_A\rangle}\,, \tag{8}$$

where $i < j$, and ij runs from 1 to $A(A-1)/2$. The d2b contribution is calculated from the sxz as the corresponding 2×2 subdeterminant

$$\mathrm{d2b(s,s',ij)} = \det\begin{pmatrix} \mathrm{sxz(s,i,i)} & \mathrm{sxz(s,i,j)} \\ \mathrm{sxz(s',j,i)} & \mathrm{sxz(s',j,j)} \end{pmatrix}. \tag{9}$$

Just as for the 1-body case, there will a linear combination of such terms to give the full d2b result. Once this is calculated, the mixed expectation contribution of any two-body spin-isospin operator will be given by

$$\sum_{s=1}^{4}\sum_{s'=1}^{4}\sum_{ij=1}^{((A-1)A)/2} \mathrm{d2b(s,s',ij)}\langle ss'|O_{ij}|s_i s_j\rangle \tag{10}$$

3.3 3- or higher-body contributions

The generalization to higher-body operators should now be obvious. For example, for 3-body operators, we define a d3b(s,s',s",ijk) where s, s', and s'' are substitued for s_i, s_j, and s_k, $i < j < k$, and all 4^3 spin-isospin terms are calculated. The result will be the corresponding subdeterminants

$$\mathrm{d3b(s,s',s'',ijk)} = \det\begin{pmatrix} \mathrm{sxz(s,i,i)} & \mathrm{sxz(s,i,j)} & \mathrm{sxz(s,i,k)} \\ \mathrm{sxz(s',j,i)} & \mathrm{sxz(s',j,j)} & \mathrm{sxz(s',j,k)} \\ \mathrm{sxz(s'',k,i)} & \mathrm{sxz(s'',k,j)} & \mathrm{sxz(s'',k,k)} \end{pmatrix}, \tag{11}$$

and the contributions to the three-body mixed expectations are

$$\sum_{s=1}^{4}\sum_{s'=1}^{4}\sum_{s''=1}^{4}\sum_{ijk=1}^{((A-2)(A-1)A)/6} \mathrm{d3b(s,s',s'',ijk)}\langle ss's''|O_{ijk}|s_i s_j s_k\rangle\,. \tag{12}$$

I have seen some references to other calculations where physical quantities require the calculations of all the $m \times m$ subdeterminants of an $N \times N$ matrix. I have not found any mention of an optimal algorithm. Keep your eyes open for this since these are currently some of the most expensive parts of the code.

4 The correlated wave function

Initially a sum of pair operator correlations was used, and we used pair updates to the inverse matrix in sxz since we worried that using a sequence of single operator updates

might cause a division by zero or loss of precision from division by a small number, if the determinant of the matrix was zero for an unphysical intermediate state. This can easily happen if, for example, all the spinors have components of a single charge. An intermediate state with an s value having a flipped charge would be orthogonal to the model state and would give a zero determinant, even though flipping a second charge in the second operator of a pair would give a well defined result.

However, for realistic walkers, we have found that this division by zero does not occur. Therefore, we now use a sequence of single operator updates to obtain 1-, 2-, or more-particle additive correlations. This greatly simplifies the code, and makes it easy to add additional operators.

In order to use the same single determinant code described above to calculate the mixed expectations, we need the equivalent of sxz(s, m, n) for the "Slater matrix" (note this is no longer antisymmetric under interchange of particles since we only operate on particle i)

$$S'_{km} = \begin{cases} S_{km} & m \neq i \\ \langle k|O_i|\vec{r}_i s_i\rangle & m = i \end{cases} . \tag{13}$$

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

$$S'_{km}(s) = \begin{cases} \langle k|\vec{r}_m s\rangle & m \neq i \\ \langle k|O_i|\vec{r}_i s\rangle & m = i \end{cases} . \tag{14}$$

$$\mathrm{sxzi(s,n,m)} = \sum_k S'^{-1}_{mk} S'_{kn}(s) . \tag{15}$$

We can calculate the updated inverse in the usual way by calculating the ratio of determinants when two columns are changed to the original determinant in two ways where we first change column i to give S', and then column j to give S'',

$$\frac{\det S''}{\det S} = \frac{\det S'}{\det S} \sum_n S'^{-1}_{jn} S''_{nj} = \begin{cases} \sum_{nm} S^{-1}_{im} S''_{mi} S^{-1}_{jn} S''_{nj} - \sum_{nm} S^{-1}_{in} S''_{ni} S^{-1}_{jn} S''_{mi} & j \neq i \\ \sum_n S^{-1}_{in} S''_{nj} & j = i \end{cases} . \tag{16}$$

Realizing that $S''_{mi} = S'_{mi}$ when $j \neq i$, we equate the terms multiplying S''_{nj} to find usual result

$$S'^{-1}_{jn} = \begin{cases} S^{-1}_{jn} - \frac{\sum_m S^{-1}_{jm} S'_{mi}}{\sum_\ell S^{-1}_{i\ell} S'_{\ell i}} S^{-1}_{in} & j \neq i \\ \frac{S^{-1}_{in}}{\sum_m S^{-1}_{im} S'_{mi}} & j = i \end{cases} . \tag{17}$$

Multiplying we find

$$\mathrm{sxzi(s,n,m)} = \begin{cases} \mathrm{sxz(s,n,m)} - \frac{\sum_k S^{-1}_{mk} \langle k|O_i|\vec{r}_i s_i\rangle}{\sum_k S^{-1}_{ik} \langle k|O_i|\vec{r}_i s_i\rangle} \mathrm{sxz(s,n,i)} & n, m \neq i \\ \frac{\mathrm{sxz(s,n,i)}}{\sum_k S^{-1}_{ik} \langle k|O_i|\vec{r}_i s_i\rangle} & m = i; n \neq i \\ \sum_k S^{-1}_{mk} \langle k|O_i|\vec{r}_i s\rangle - \frac{\sum_k S^{-1}_{mk} \langle k|O_i|\vec{r}_i s_i\rangle}{\sum_k S^{-1}_{ik} \langle k|O_i|\vec{r}_i s_i\rangle} \sum_k S^{-1}_{ik} \langle k|O_i|\vec{r}_i s\rangle & n = i; m \neq i \\ \frac{\sum_k S^{-1}_{ik} \langle k|O_i|\vec{r}_i s\rangle}{\sum_k S^{-1}_{ik} \langle k|O_i|\vec{r}_i s_i\rangle} & n = m = i \end{cases} . \tag{18}$$

Writing the sums in terms of sxz(s,n,m), we define

$$\mathrm{opi(s,m)} = \sum_k S^{-1}_{mk} \langle k|O_i|\vec{r}_i s\rangle = \sum_{k,s'} S^{-1}_{mk} \langle k|\vec{r}_i s'\rangle \langle s'|O_i|s\rangle = \sum_{s'} \mathrm{sxz(s',i,m)} \langle s'|O_i|s\rangle \,. \quad (19)$$

The name opi is for "operator i." In the code, we have the function opmult that operates with the 15 possible cartesian 1-body spin-isospin operators (3 components of $\vec{\sigma}$, 3 components of $\vec{\tau}$, and 9 components fo $\vec{\sigma}\vec{\tau}$) to the right onto $|s\rangle$. We use this to operate to the left by taking the adjoint, operating and then taking the adjoint again. This amounts to taking the complex conjugate of sxz, applying the operator, and taking its complex conjugate again. Alternatively, the code could be changed to use the complex conjugate of the operator. Either one of these 15 operators if we are using cartesian components, or a linear combination of them defines opi(s,m). The other sum we need is where the right hand spinor is $|s_i\rangle$. We define

$$\mathrm{di(m)} = \sum_k S^{-1}_{mk} \langle k|O_i|\vec{r}_i s_i\rangle = \sum_s \mathrm{opi(s,m)} \langle s|s_i\rangle \quad (20)$$

where $\langle s|s_i\rangle$ are the walker spinor components sp(s,i). Since this is in some sense a ratio of determinants, the name di stands for "determinant i." Rewriting sxzi in terms of sxz, opi, and di, we have

$$\mathrm{sxzi(s,n,m)} = \begin{cases} \mathrm{sxz(s,n,m)} - \frac{\mathrm{di(m)}}{\mathrm{di(i)}} \mathrm{sxz(s,n,i)} & n, m \neq i \\ \frac{\mathrm{sxz(s,n,i)}}{\mathrm{di(i)}} & m = i; n \neq i \\ \mathrm{opi(s,m)} - \frac{\mathrm{di(m)}}{\mathrm{di(i)}} \mathrm{opi(s,i)} & n = i; m \neq i \\ \frac{\mathrm{opi(s,i)}}{\mathrm{di(i)}} & n = m = i \end{cases} . \quad (21)$$

Handing this new sxzi to the mixed expectation value routines will give the expectations with the modified $\langle\Phi|$ in the denominator. Therefore these results are multiplied by the ratio of the new to old determinants in order to be added to the d1b, d2b, and d3b sums.

At this point, 2-body, 3-body, etc. operators can be done by repeating the calculation above starting with sxzi and repeating the above update.

5 Calculation of just the wave function

If only the wave function for a new walker is needed, the code uses the machinery developed above to calculate d1b, d2b, d3b for just the single Slater determinant. The operator correlations are converted into the $p\uparrow$, $p\downarrow$, $n\uparrow$, $n\downarrow$ basis by operating on the walker spinors with the opmult(sp) routine, and then combining these with the operator correlations. For example a correlation containig $f_{\alpha\beta}(r_{ij})\sigma_{i\alpha}\sigma_{j\beta}$ is included by f2b(iz,jz,ij)=f2b(iz,jz,ij)+$f_{\alpha\beta}(r_{ij})$* spx(iz,α,i)*spx(jz,β,j). The determinant ratio is then given by sum(d2b*f2b) and similarly for 1- and 3-body correlations.

6 Breaking up the correlations

When operator mixed expectation values are needed, we will require the calculation of the d1b, d2b, d3b, etc. for every new sxz. Since these calculations will appear in the inner loop, we would like to break up the operator correlations in such a way to minimize their calls. On the other hand, updates of sxz require order A^2 operations. So we also want to minimize these updates.

The most straightforward break up of the v_6 correlations uses the cartesian components of the pauli spin-isospin operators. There are then 39 operator pairs for each particle, (3 from $\tau_\alpha \tau'_\alpha$, 9 from $\sigma_\alpha \sigma'_\beta$, and 27 from $\sigma_\alpha \sigma'_\beta \tau_\gamma \tau'_\gamma$). However, for any particle j, particle i can be operated on by just 15 operators $3\sigma_\alpha$, 3 τ_α, and 9 $\sigma_\alpha \tau_\beta$. Therefore, we can loop over the pair correlation with i the outer loop. For a given i value, we can calculate the 15 possible updates that give sxzi. In the inner j loop we then have 39 updates which each start from a precomputed sxzi. After the j updates, the d1b, d2b, d3b etc. can be calculated. The inner loop will therefore have roughly $39A^2/2$ updates, each costing A^2 operations itself, along with order A operations for d1b, A^2 operations for d2b, and A^3 operations for d3b.

An alternative method reduces the number of operator pairs by diagonalizing (or using singular value decomposition when the matrices are not symmetric) the coupling terms in the v_6 operators. For example the $\vec{\sigma}_i \cdot \vec{\sigma}_j$ and tensor components of the interaction can be written as

$$\sum_{\alpha\beta} \sigma_{i\alpha} A^{(ij)}_{\alpha\beta} \sigma_{j\beta} \,. \tag{22}$$

Finding the eigenvectors $\psi^{(n)}_\alpha$ and eigenvalues λ_n of the real symmetric matrix A, we can write this as

$$\sum_{\alpha\beta} \sigma_{i\alpha} A^{(ij)}_{\alpha\beta} \sigma_{j\beta} = \sum_n \left[\sum_\alpha \sigma_{i\alpha} \psi^{(n)}_\alpha \right] \left[\sum_\beta \sigma_{j\beta} \psi^{(n)}_\beta \right] \,. \tag{23}$$

and therefore define $O_i = \sum_\alpha \sigma_{i\alpha} \psi^{(n)}_\alpha$ $O_j = \sum_\beta \sigma_{j\beta} \psi^{(n)}_\beta$. In this way we can reduce the number of operator pairs from 39 to 15. There is a trade off however. Unlike the cartesian case, the O_i are different for each pair. Therefore both updates (unless someone can find a clever way to combine cartesian updates to get these updates) must be done in the j loop. We therefore reduce the number of updates from 39 to 30. We reduce the number of calls to d1b, d2b and d3b from 39 to 15.

For the case of 3-body anticommutator additive correlations, the A matrix above is no longer symmetric. However, this can be handled using singular value decomposition where we write

$$A_{\alpha\beta} = \sum_\gamma U_{\alpha\gamma} \Lambda_\gamma V_{\gamma\beta} \tag{24}$$

and everything above still goes through.