Notes on orbital correlations

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Abstract

In these notes we work out the implementation of Joe's orbital correlations.

Using the notation from Kevin's notes we will denote the Slater matrix with

$$S_{ki} = \langle k|\vec{r}_i s_i\rangle = \sum_{s=1}^{4} \langle k|\vec{r}_i s\rangle\langle s|s_i\rangle \equiv \sum_{s=1}^{4} \Phi(k,s,i) sp(s,i) \tag{1}$$

where we introduced matrices Φ and sp that are used in the code. The first one is returned by *getphi* the second represents the spinor.

Joe's idea is to apply correlations (tensor in this case) to the orbitals such that $\forall k$ we have

$$\begin{aligned} S_{ki} \to S'_{ki}(x) &= \left[1 + x\sum_{j}^{A} f(r_{ji})\hat{r}_{ji}\cdot\vec{\sigma}_i\right] S_{ki} \\ &= \left[1 + x\vec{t}_i\cdot\vec{\sigma}_i\right] S_{ki} = \sum_{s=1}^{4} \Phi(k,s,i)\left[1 + x\vec{t}_i\cdot\vec{\sigma}_i\right] sp(s,i) \end{aligned} \tag{2}$$

The $x = \pm 1$ field is summed over after antisymmetrization. It's effect is to remove terms that are odd in the correlation operator. For two particles we have in fact

$$\begin{aligned} \sum_x det\,[S'] &= \sum_x \left[S'_{11}(x)S'_{22}(x) - S'_{12}(x)S'_{21}(x)\right] \\ &= \sum_x \left[1 + x\vec{t}_1\cdot\vec{\sigma}_1\right]\left[1 + x\vec{t}_2\cdot\vec{\sigma}_2\right]\left[S_{11}S_{22} - S_{12}S_{21}\right] \\ &= \sum_x \left[1 + x\left(\vec{t}_1\cdot\vec{\sigma}_1 + \vec{t}_2\cdot\vec{\sigma}_2\right) + \vec{t}_1\cdot\vec{\sigma}_1\vec{t}_2\cdot\vec{\sigma}_2\right]\left[S_{11}S_{22} - S_{12}S_{21}\right] \\ &= 2\left[1 + \vec{t}_1\cdot\vec{\sigma}_1\vec{t}_2\cdot\vec{\sigma}_2\right]\left[S_{11}S_{22} - S_{12}S_{21}\right] \\ &= 2\left[1 + f^2(r_{21})\hat{r}_{21}\cdot\vec{\sigma}_1\hat{r}_{12}\cdot\vec{\sigma}_2\right] det\,[S] \\ &= 2\left[1 - f^2(r_{21})\hat{r}_{12}\cdot\vec{\sigma}_1\hat{r}_{12}\cdot\vec{\sigma}_2\right] det\,[S] \end{aligned} \tag{3}$$

where the minus sign in the last line comes from the opposite sign of $\hat{r}_{12}$ and $\hat{r}_{21}$. We can use the same strategy to implement $\vec{\sigma}\cdot\vec{\sigma}$ correlations using 8 more auxiliary fields

$$S_{ki} \to S'_{ki}(x) = \left[1 + \sum_{d}^{3}\sum_{j}^{A} g(r_{ji}) y_d \sigma_i^d\right] S_{ki} \tag{4}$$

which for 2 particles results in

$$\sum_{y_d} det\,[S'] = 8\left[1 + g^2(r_{21})\vec{\sigma}_1\cdot\vec{\sigma}_2\right] det\,[S]\ . \tag{5}$$

In the same way we can implement the isospin dependent tensor correlation using

$$S_{ki} \to S'_{ki}(x) = \left[1 + \sum_{d}^{3}\sum_{j}^{A} f_t(r_{ji})\hat{r}_{ji}\cdot\vec{\sigma}_i y_d \tau_i^d\right] S_{ki}\ . \tag{6}$$

The current implementation increases the number of determinant so that we have one for every value of the auxiliary field:

- 2 determinants for tensor: $\hat{r}_{12}\cdot\vec{\sigma}_1\hat{r}_{12}\cdot\vec{\sigma}_2$
- 16 determinant for tensor plus sigma: $\hat{r}_{12}\cdot\vec{\sigma}_1\hat{r}_{12}\cdot\vec{\sigma}_2 + \vec{\sigma}_1\cdot\vec{\sigma}_2$
- 8 determinants for tensor tau: $\hat{r}_{12}\cdot\vec{\sigma}_1\hat{r}_{12}\cdot\vec{\sigma}_2\vec{\tau}_1\cdot\vec{\tau}_2$

0.1 Off diagonal correlations

This ansatz for the correlations has however the drawback of adding spurious correlations among all particles, for instance for the $\vec{\sigma}_1\cdot\vec{\sigma}_2$ term we get

$$\left[1+\vec{\sigma}_i\cdot\vec{\sigma}_j\sum_{k\neq i}g(r_{ik})\sum_{l\neq j}g(r_{jl})\right] = \left[1+\vec{\sigma}_i\cdot\vec{\sigma}_j g(r_{ij})^2+\vec{\sigma}_i\cdot\vec{\sigma}_j\sum_{l,k\neq j,i}g(r_{ik})g(r_{jl})\right] \tag{7}$$

In order to cancel the last terms we add additional phases to the single-particle correlators that then we sum over. We start by defining a unique pair index as

$$P(i,j)=\begin{cases}\frac{(i-1)(i-2)}{2}+j-1 & i>j\\ \frac{-(j-1)(j-2)}{2}-i+1 & i<j\end{cases} \tag{8}$$

which for A particle takes values in

$$P(i,j)\in\left[-\frac{A(A-1)}{2}+1,\frac{A(A-1)}{2}-1\right]. \tag{9}$$

Note that the shift by 1 is only used to remove redundancy but is not strictly needed. We now define a new single-particle correlator of the form (using the tensor interaction for instance)

$$S_{ki}\to S'_{ki}(x)=\left[1+x\sum_{j}^{A}e^{i\frac{2\pi}{A(A-1)}P(i,j)m}f(r_{ji})\hat{r}_{ji}\cdot\vec{\sigma}_i\right]S_{ki} \tag{10}$$

By summing now over m we effectively cancel all off-diagonal contributions in the pair correlators while leaving a few for higher order correlations. In fact from the completeness of plane waves on an interval we have

$$\begin{aligned}\sum_{m}^{A(A-1)}e^{i\frac{2\pi}{A(A-1)}(P(i,j)+P(k,l))m} &= P\sum_{n=-\infty}^{n=\infty}\delta\left(P(i,j)+P(k,l)+nA(A-1)\right)\\ &\equiv P\delta_{i,l}\delta_{j,k}\end{aligned} \tag{11}$$

where the last line follows from our definition of $P(i,j)=-P(j,i)$ and from the fact the for pairs only the terms with $n=0$ are contributing in the infinite series on the first line. For 4 particle correlations also the terms with $n=\pm1$ will contribute leaving some spurious off-diagonal correlations. These however can be removed by increasing the number of phases used $A(A-1)\to 2A(A-1)$ and eventually using $A^2(A-1)$ phases we effectively remove all off-diagonal correlations up to A-body. This is however probably to expensive to do and in general shouldn't be needed since the importance of higher-order correlations should become small.

An alternative is to cancel the off-diagonal terms only approximately by using a fixed number of phases using a Dirichlet kernel

$$D(x+y)=\sum_{k=-n}^{n}e^{ik(x+y)}=\frac{sin\left((n+1/2)(x+y)\right)}{sin\left((x+y)/2\right)}\xrightarrow{n\to\infty}\delta(x+y) \tag{12}$$

where the convergence with n is unfortunately rather slow and in any case n should scale as A^2 to maintain a given accuracy though the prefactor could be smaller than 1. Our previous strategy is essentially equivalent to using D but making sure that the possible values of $(x+y)$ are always on the nodes of $sin\left((n+1/2)(x+y)\right)$.

0.2 Issues

For the alpha particle all of the above correlations work fine while for O^{16}

- the tensor is fine
- $\vec{\tau}_1 \cdot \vec{\tau}_2$ breaks T^2 and T_z
- $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ breaks J^2 and J_z
- the tensor tau again breaks T^2 and T_z

The plot Fig.1 shows the magnitude of the breaking for $\vec{\tau}_1 \cdot \vec{\tau}_2$ correlation in O^{16} as a function of the magnitude of the correlation coupling. I tried to fit the initial rise and is approximately compatible with $< g(r) >^6$ suggesting issues in the 6-body correlations that clearly are missing in the alpha particle. It remains to understand why this is happening.

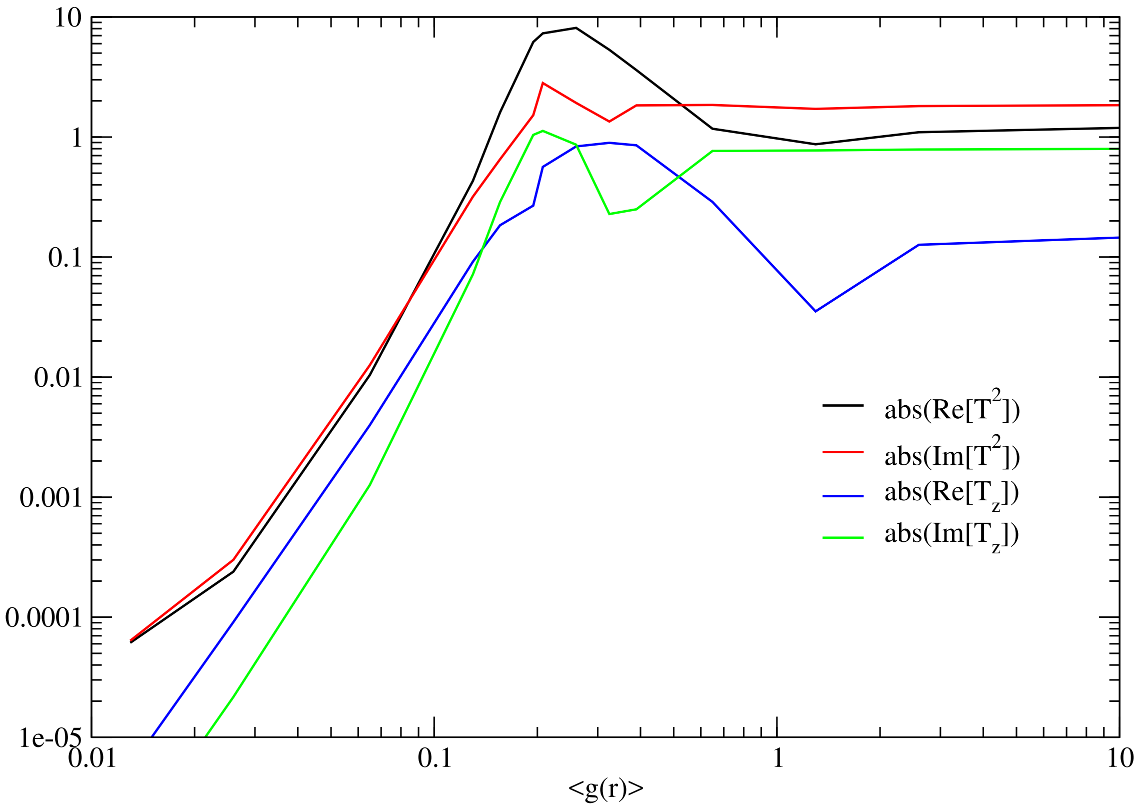

Figure 1: Absolute value of isospin breaking in O^{16}