Calculating the Trial Wave Function for AFDMC

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1 Trial Wave Function

The trial wave function for AFDMC must be simple to evaluate. In the past the simple Slater determinant with pair-wise correlations has been used as shown in [1],

$$\langle RS|\Psi_T\rangle = \langle RS| \left[\prod_{i<j} f_c(r_{ij})\right] \left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij}\right] |\Phi\rangle\,, \tag{1}$$

where the $\mathcal{O}^p_{ij}$'s are $\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$, and $t_{ij}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, where $t_{ij} = 3\boldsymbol{\sigma}_i\cdot\hat{r}_{ij}\boldsymbol{\sigma}_j\cdot\hat{r}_{ij} - \boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$. *Question 1: Why weren't $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$ and t_{ij} used in this paper?*

My goal is to add the additional independent pair correlations.

$$\langle RS|\Psi_T\rangle = \langle RS| \left[\prod_{i<j} f_c(r_{ij})\right] \left[1 + \sum_{i<j}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij} + \sum_{i<j}\sum_{k<l}\sum_p f_p(r_{ij})\mathcal{O}^p_{ij}f_p(r_{kl})\mathcal{O}^p_{kl}\right] |\Phi\rangle\,, \tag{2}$$

2 Evaluation the Trial Wave Function

To understand how to to this I'm going to just assume that $\mathcal{O}^p_{ij}$ only contains the term $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$ and I'll start by looking at the trial wave function, equation 1, with only the linear term. So now

$$\langle RS|\Psi_T\rangle = \langle RS| \left[\prod_{i<j} f_c(r_{ij})\right] \left[1 + \sum_{i<j} f_1(r_{ij})\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\right] |\Phi\rangle\,. \tag{3}$$

Also since the central correlations don't change the states by any more than a multiplicative factor I am going to ignore that term as well. I will also just look at one term in the sum (a particular i and j value). So we are just looking at

$$\langle RS|\left[1 + f_1(r_{ij})\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\right]|\Phi\rangle\,. \tag{4}$$

Now we also know that the Slater determinant is defined as

$$\langle RS|\Phi\rangle = \det(S) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(R_1S_1) & \phi_2(R_1S_1) & \cdots & \psi_N(R_1S_1) \\ \phi_1(R_2S_2) & \phi_2(R_2S_2) & \cdots & \phi_N(R_2S_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(R_NS_N) & \phi_2(R_NS_N) & \cdots & \phi_N(R_NS_N) \end{vmatrix}, \tag{5}$$

where $\phi_i(R_jS_j) = \phi_i^r(R_j)\phi_i^s(S_j)$ and S is called the Slated Matrix.

Now lets look at equation 4 again for an example.

$$\begin{aligned}
&\langle RS| \left[1 + f_1(r_{ij})\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right] |\Phi\rangle && (6)\\
&= \det(S) + f_1(r_{ij}) \langle RS| \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j |\Phi\rangle && (7)\\
&= \det(S) + f_1(r_{ij})\det(S'') && (8)
\end{aligned}$$

Here S'' is the updated matrix. It only has two columns different than S and so we can get it's determinant of S'' easily once we have the determinant of S by using the fact that

$$\det(S_{ij}^{-1}S''_{jk}) = \frac{\det(S''_{jk})}{\det(S_{ij})}. \tag{9}$$

When we solve for $\det(S)$ we finish solving for the inverse, S^{-1} and the product $S_{ij}^{-1}S''_{jk}$ is 1 on the diagonal and 0 everywhere else except the two columns i and j. This makes the $\det(S_{ij}^{-1}S''_{jk})$ easy to solve for since it is simply the determinant of the submatrix. Thus once we have $\det(S)$ it is easier to solve for $\det(S'')$. All that is left is to do this over the pair loops and over each operator.

3 Implimentation in the code

Now how is this implimented into the code. The element of the Slater martix that corresponds to the k^{th} orbital and the i^{th} particle is given by

$$S_{ki} = \langle k|r_i, s_i\rangle = \sum_{s=1}^{4} \langle k|r_i, s\rangle \langle s|s_i\rangle . \tag{10}$$

From this you can see that a general Slater matrix can be written as a linear combination of matrix elements $\langle k|r_i, s\rangle$ and coefficients $\langle s|s_i\rangle$.

Therefore it's convenient to precompute

$$\mathrm{sxz(s,i,j)} = \mathrm{sxmallz(j,s,i)} = \sum_k S_{jk}^{-1} \langle k|r_i, s\rangle . \tag{11}$$

For example if we were computing the determinant of $S''_{ij} = \langle k|r_i, s'_i\rangle$ where the s'_i was changed is different from s_i on the changed columns, then the product matrix could be computed as

$$S_{jk}^{-1}S''_{ki} = \sum_{s=1}^{4}\left(\sum_k S_{jk}^{-1}\langle k|r_i, s\rangle\right)(\langle s|s_i\rangle) = \sum_{s=1}^{4}\mathrm{sxz(s,i,j)}\langle s|s_i\rangle . \tag{12}$$

Question 2: Is this how we use sxz?

I have looked at how to calculate the trial wave function with a correlation operator in the middle now lets look at how to do it with 1 and 2-body spin-isospin operators in the middle. Here I am mostly filling in gaps in my understanding of Kevin Schmidt's writeup.

3.1 1-body spin-isospin operators

Here the idea is we want to calculate expectation values like

$$\left\langle \sum_i \mathcal{O}_i \right\rangle = \frac{\langle\Phi| \sum_i \mathcal{O}_i |R,S\rangle}{\langle\Phi|R,S\rangle}. \tag{13}$$

Now let's expand this the numerator term

$$\begin{aligned}
\langle\Phi| \sum_i \mathcal{O}_i |R,S\rangle &= \langle\Phi| \sum_i \mathcal{O}_i |R, s_1, \ldots, s_A\rangle && (14)\\
&= \langle\Phi| \sum_i \sum_{s=1}^{4} |s\rangle \langle s| \mathcal{O}_i |R, s_1, \ldots, s_A\rangle && (15)\\
&= \langle\Phi| \sum_i \sum_{s=1}^{4} \langle s| \mathcal{O}_i |s_i\rangle |R, s_1, \ldots, s_{i-1}, s, s_{i+1}, \ldots, s_A\rangle && (16)\\
&= \langle\Phi| \sum_i \sum_{s=1}^{4} \alpha_{is} |R, s_1, \ldots, s_{i-1}, s, s_{i+1}, \ldots, s_A\rangle && (17)\\
&= \sum_i \sum_{s=1}^{4} \alpha_{is} \langle\Phi|R, s_1, \ldots, s_{i-1}, s, s_{i+1}, \ldots, s_A\rangle && (18)\\
&= \sum_i \sum_{s=1}^{4} \alpha_{is} \mathrm{d1b(s,i)} \langle\Phi|RS\rangle, && (19)
\end{aligned}$$

where $\alpha_{is} = \langle s| \mathcal{O}_i |s_i\rangle$ and $\mathrm{d1b(s,i)} = \langle\Phi|R, s_1, \ldots, s_{i-1}, s, s_{i+1}, \ldots, s_A\rangle / \langle\Phi|R, s_1, \ldots, s_A\rangle$. Rearranging this we can get the expectation value

$$\left\langle \sum_i \mathcal{O}_i \right\rangle = \sum_i \sum_{s=1}^{4} \alpha_{is} \mathrm{d1b(s,i)}. \tag{20}$$

Notice that we have

$$\mathrm{d1b(s,i)} = \mathrm{sxz(s,i,i)}. \tag{21}$$

Question 3: I can't figure out why. Why are these two equal? If it is easier to answer with regards to the d2b case then that works too.

3.2 2-body spin-isospin operators

Here the idea is we want to calculate expectation values like

$$\left\langle \sum_{i<j} \mathcal{O}_{ij} \right\rangle = \frac{\langle\Phi| \sum_{i<j} \mathcal{O}_{ij} |R,S\rangle}{\langle\Phi|R,S\rangle}. \tag{22}$$

Now let's expand this the numerator term

$$\langle\Phi|\sum_{i<j}\mathcal{O}_{ij}|R,S\rangle = \langle\Phi|\sum_{i<j}\mathcal{O}_{ij}|R,s_1,\ldots,s_A\rangle \tag{23}$$

$$= \langle\Phi|\sum_{i<j}\sum_{s=1}^{4}\sum_{s'=1}^{4}|s\rangle\langle s|s'\rangle\langle s'|\mathcal{O}_{ij}|R,s_1,\ldots,s_A\rangle \tag{24}$$

$$= \langle\Phi|\sum_{i<j}\sum_{s=1}^{4}\sum_{s'=1}^{4}\langle s,s'|\mathcal{O}_{ij}|s_i,s_j\rangle|R,s_1,\ldots,s_{i-1},s,s_{i+1},\ldots,s_{j-1},s',s_{j+1},\ldots,s_A\rangle \tag{25}$$

$$= \langle\Phi|\sum_{i<j}\sum_{s=1}^{4}\sum_{s'=1}^{4}\alpha_{ijs}|R,s_1,\ldots,s_{i-1},s,s_{i+1},\ldots,s_{j-1},s',s_{j+1},\ldots,s_A\rangle \tag{26}$$

$$= \sum_{i<j}\sum_{s=1}^{4}\sum_{s'=1}^{4}\alpha_{ijs}\langle\Phi|R,s_1,\ldots,s_{i-1},s,s_{i+1},\ldots,s_{j-1},s',s_{j+1},\ldots,s_A\rangle \tag{27}$$

$$= \sum_{i<j}\sum_{s=1}^{4}\sum_{s'=1}^{4}\alpha_{ijs}\mathrm{d2b}(\mathrm{s},\mathrm{s}',\mathrm{ij})\langle\Phi|RS\rangle\,, \tag{28}$$

where $\alpha_{ijs} = \langle s,s'|\mathcal{O}_{ij}|s_i,s_j\rangle$ and

$$\mathrm{d2b}(\mathrm{s},\mathrm{s}',\mathrm{ij}) = \langle\Phi|R,s_1,\ldots,s_{i-1},s,s_{i+1},\ldots,s_{j-1},s',s_{j+1},\ldots,s_A\rangle\,/\,\langle\Phi|R,s_1,\ldots,s_A\rangle\,. \tag{29}$$

Rearranging this we can get the expectation value

$$\left\langle\sum_{ij}\mathcal{O}_{ij}\right\rangle = \sum_{ij=1}^{((A-1)A)/2}\sum_{s=1}^{4}\sum_{s'=1}^{4}\alpha_{ijs}\mathrm{d2b}(\mathrm{s},\mathrm{s}',\mathrm{ij}), \tag{30}$$

and where the sum, $\sum_{ij}^{((A-1)A)/2}$ is essentially doing the same thing as $\sum_{i=1}^{A-1}\sum_{j=i+1}^{A}$ or $\sum_{i<j}$. Notice again that we have

$$\mathrm{d2b}(\mathrm{s},\mathrm{s}',\mathrm{ij}) = \det\begin{pmatrix}\mathrm{sxz}(\mathrm{s},\mathrm{i},\mathrm{i}) & \mathrm{sxz}(\mathrm{s},\mathrm{i},\mathrm{j})\\ \mathrm{sxz}(\mathrm{s}',\mathrm{j},\mathrm{i}) & \mathrm{sxz}(\mathrm{s}',\mathrm{j},\mathrm{j})\end{pmatrix} = \mathrm{sxz}(\mathrm{s},\mathrm{i},\mathrm{i})\mathrm{sxz}(\mathrm{s}',\mathrm{j},\mathrm{j}) - \mathrm{sxz}(\mathrm{s},\mathrm{i},\mathrm{j})\mathrm{sxz}(\mathrm{s}',\mathrm{j},\mathrm{i}). \tag{31}$$

Also Questions 3: I can't figure out why. Why is this? This doesn't need answered, I'll probably understand when I see the reason for the d1b case.

3.3 Inverse Update

Now in cases where we have two set's of operators like for example when we need to calculate the expectation value of the potential, there is the correlation operator and the potential operators. One of the operators is handled in the inner loop while the other is handeled in a more outer loop. We can include the second operator (set of operators) in the same way that the operators were included above except that we will now need to the inverse of the new Slater Matrix, S'^{-1}. To do this we need to update $\mathrm{sxz}(\mathrm{s},\mathrm{i},\mathrm{j})$.

References

[1] S. Gandolfi, A. Lovato, J. Carlson, and Kevin E. Schmidt. From the lightest nuclei to the equation of state of asymmetric nuclear matter with realistic nuclear interactions. 2014. arXiv:1406.3388v1 [nucl-th].