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],

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

where the $\mathcal{O}_{ij}^p$'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 $t_{ij} = 3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij}\boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$. *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.

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

2 Evaluation the Trial Wave Function

To understand how to to this I'm going to just assume that $\mathcal{O}_{ij}^p$ 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.

$$\langle RS| \left[1 + f_1(r_{ij})\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right] |\Phi\rangle \tag{6}$$

$$= \det(S) + f_1(r_{ij}) \langle RS| \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j |\Phi\rangle \tag{7}$$

$$= \det(S) + f_1(r_{ij})\det(S') \tag{8}$$

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

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

Is this right?

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 Kevin Schmidt's writeup.

3.1 1-body spin-isospin operators

Here the idea is we want to calculate expectation values like

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

Now let's expand this the numerator term

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

where $\alpha_{is} = \langle s| \mathcal{O}_i |s_i\rangle$ and $\mathrm{d1b(s,i)} = \langle\Phi|R, s_1, \dots, s_{i-1}, s, s_{i+1}, \dots, s_A\rangle / \langle\Phi|R, s_1, \dots, s_A\rangle$. 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

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

I can't figure out why. Why is this? 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

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

Now let's expand this the numerator term

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

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

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

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

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

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

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

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

Rearranging this we can get the expectation value

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

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

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

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.

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].