Notes on the Exponential Correlations

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1 Derive Exponential Wave Function

The most general form of the fully correlated wave function is the exponentially correlated wave function given by

$$|\Psi_T\rangle = \left[\prod_{i<j} f_c(r_{ij})\right] e^{\sum\limits_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p} |\Phi\rangle \tag{1}$$

The exponential is to maintain cluster decomposition of the wave function. The Jastrow spin-isospin independent correlations are handeled independent of my piece of the code and so I will ignore them here which effectively leaves me with

$$|\Psi_T\rangle = e^{\sum\limits_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p} |\Phi\rangle, \tag{2}$$

where the operators in the sum are the standard $v6'$ operators, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$, $\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, S_{ij} and $S_{ij}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, where $S_{ij}=3\boldsymbol{\sigma}_i\cdot\hat{r}_{ij}\boldsymbol{\sigma}_j\cdot\hat{r}_{ij}-\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$. In an effort to write this an a sum of squared single particle operators (to be used with the Hubbard Stratanovich transformation) these operators can be written in the form

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}_{ij}^p\right) = \exp\left(\frac{1}{2}\sum_{i\alpha,j\beta}\sigma_{i\alpha}A^{\sigma}_{i\alpha,j\beta}\sigma_{j\beta} + \frac{1}{2}\sum_{i\alpha,j\beta}\sigma_{i\alpha}A^{\sigma\tau}_{i\alpha,j\beta}\sigma_{j\beta}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j + \frac{1}{2}\sum_{i,j}A^{\tau}_{i,j}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\right). \tag{3}$$

These matricies are simply another way to write the $f^p(r_{ij})$ function. Writting the operators in this form is discussed in more detail in appendix A. In the code (in psicalc.f90) these matricies are actually called "ftau(npart,npart)", "fsig(3,npart,3,npart)" and "fsigtau(3,npart,3,npart)". These matricies are zero when $i=j$, symmetric and can be written in terms of their eigenvalues and vectors.

$$\sum_{j\beta} A^{\sigma}_{i\alpha,j\beta}\psi^{\sigma}_{n,j\beta} = \lambda^{\sigma}_n\psi^{\sigma}_{n,i\alpha} \tag{4}$$

$$\sum_{j\beta} A^{\sigma\tau}_{i\alpha,j\beta}\psi^{\sigma\tau}_{n,j\beta} = \lambda^{\sigma\tau}_n\psi^{\sigma\tau}_{n,i\alpha} \tag{5}$$

$$\sum_{j} A^{\tau}_{i,j}\psi^{\tau}_{n,j} = \lambda^{\tau}_n\psi^{\tau}_{n,i} \tag{6}$$

The operators can then be written as

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}^p_{ij}\right) = \exp\left(\frac{1}{2}\sum_{n=1}^{3A}\left(O^\sigma_n\right)^2\lambda^\sigma_n + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3A}\left(O^{\sigma\tau}_{n\alpha}\right)^2\lambda^{\sigma\tau}_n + \frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{A}\left(O^\tau_{n\alpha}\right)^2\lambda^\tau_n\right), \tag{7}$$

where the operators are given by

$$\begin{aligned} O^\sigma_n &= \sum_{j,\beta}\sigma_{j,\beta}\psi^\sigma_{n,j,\beta} \\ O^{\sigma\tau}_{n\alpha} &= \sum_{j,\beta}\tau_{j,\alpha}\sigma_{j,\beta}\psi^{\sigma\tau}_{n,j,\beta} \\ O^\tau_{n\alpha} &= \sum_{j}\tau_{j,\alpha}\psi^\tau_{n,j}. \end{aligned} \tag{8}$$

Now this is ready to use with the Hubbard Stratanovich transformation

$$e^{-\frac{1}{2}\lambda O^2} = \frac{1}{\sqrt{2\pi}}\int dx e^{-\frac{x^2}{2}+\sqrt{-\lambda}xO}. \tag{9}$$

Writting this set of correlation operators in a more compact way,

$$\exp\left(\sum_{i<j,p} f_p(r_{ij})\mathcal{O}^p_{ij}\right) = \exp\left(\frac{1}{2}\sum_{n=1}^{15A}\left(O_n\right)^2\lambda^\sigma_n\right) \tag{10}$$

allows for the application of the HS transformation, after breaking it into $15A$ exponentials and ignoring the commutation terms.

$$\exp\left(\frac{1}{2}\sum_{n=1}^{15A}\left(O_n\right)^2\lambda^\sigma_n\right) = \prod_{n=1}^{15A}\frac{1}{\sqrt{2\pi}}\int dx_n e^{-x_n^2/2}e^{\sqrt{\lambda_n}x_n O_n}. \tag{11}$$

The auxiliary fields can then be drawn from the gaussian distribution, $\exp\left(-x_n^2/2\right)$ and the correlations can be written as follows.

$$\Psi_T(R,S) = \langle RS|\prod_{n=1}^{15A}\frac{1}{N}\sum_{\{x_n\}}^{N}\frac{1}{\sqrt{2\pi}}e^{\sqrt{\lambda_n}x_n O_n}\left|\Phi\right\rangle. \tag{12}$$

2 Exponential of an Operator

To start I'll write down the exponential correlations in their full form. They look something like this

$$\prod_{n=1}^{15A}\frac{1}{\sqrt{2\pi}}\int dx_n e^{-x_n^2/2}e^{\sqrt{-\lambda_n}x_n O_n}. \tag{13}$$

This is after the Hubbard-Staratanovich transformation has been applied to the correlations so that the correlations can be sampled from single-particle operators. If they are sampled they take a form something like

$$\prod_{n=1}^{15A} \frac{1}{\sqrt{2\pi}} \sum_{x_n}^{N} \frac{1}{N} e^{\sqrt{-\lambda_n} x_n O_n}. \tag{14}$$

It might also be important to note that we have added plus-minus sampling to this. . . but I'll add that and the square root of the matrix stuff in later.

Now I will talk about each individual operator that we have in the correlations. The 15A operators are $\tau_{\alpha i}$ (3A), $\sigma_{\alpha i}$ (3A), and $\sigma_{\alpha i}\tau_{\beta j}$ (9A). Assuming the basis is $|p\uparrow, p\downarrow, n\uparrow, n\downarrow\rangle$ and stored as a column vector we can write the operators in matrix form as follows.

$$\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \tau_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \qquad \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\sigma_x\tau_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_x\tau_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_x\tau_z = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

$$\sigma_y\tau_x = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_y\tau_y = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \qquad \sigma_y\tau_z = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix}$$

$$\sigma_z\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \qquad \sigma_z\tau_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \qquad \sigma_z\tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Now those are easy enough to figure out if you just look at the pauli matricies on a simple spin-1/2 system. But what we really want is the exponential of these matricies with an extra factor up top that looks something like

$$e^{\sqrt{-\lambda_n} x_n O_n}. \tag{15}$$

I'm going to rewrite this with an i in it as

$$e^{i\gamma O_n}, \tag{16}$$

where the $\gamma = \sqrt{\lambda_n} x_n$, for each particular operator. In this way the exponentiated matricies can be written in terms of regular matricies. Plugging this into Mathematica I get the following.

$$e^{i\gamma\tau_x} = \begin{pmatrix} \cos\gamma & 0 & i\sin\gamma & 0 \\ 0 & \cos\gamma & 0 & i\sin\gamma \\ i\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & i\sin\gamma & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\tau_y} = \begin{pmatrix} \cos\gamma & 0 & \sin\gamma & 0 \\ 0 & \cos\gamma & 0 & \sin\gamma \\ -\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & -\sin\gamma & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\tau_z} = \begin{pmatrix} e^{i\gamma} & 0 & 0 & 0 \\ 0 & e^{i\gamma} & 0 & 0 \\ 0 & 0 & e^{-i\gamma} & 0 \\ 0 & 0 & 0 & e^{-i\gamma} \end{pmatrix}$$

$$e^{i\gamma\sigma_x} = \begin{pmatrix} \cos\gamma & i\sin\gamma & 0 & 0 \\ i\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & i\sin\gamma \\ 0 & 0 & i\sin\gamma & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_y} = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 & 0 \\ -\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & \sin\gamma \\ 0 & 0 & -\sin\gamma & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_z} = \begin{pmatrix} e^{i\gamma} & 0 & 0 & 0 \\ 0 & e^{-i\gamma} & 0 & 0 \\ 0 & 0 & e^{i\gamma} & 0 \\ 0 & 0 & 0 & e^{-i\gamma} \end{pmatrix}$$

$$e^{i\gamma\sigma_x\tau_x} = \begin{pmatrix} \cos\gamma & 0 & 0 & i\sin\gamma \\ 0 & \cos\gamma & i\sin\gamma & 0 \\ 0 & i\sin\gamma & \cos\gamma & 0 \\ i\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_x\tau_y} = \begin{pmatrix} \cos\gamma & 0 & 0 & \sin\gamma \\ 0 & \cos\gamma & \sin\gamma & 0 \\ 0 & -\sin\gamma & \cos\gamma & 0 \\ -\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_x\tau_z} = \begin{pmatrix} \cos\gamma & i\sin\gamma & 0 & 0 \\ i\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & -i\sin\gamma \\ 0 & 0 & -i\sin\gamma & \cos\gamma \end{pmatrix}$$

$$e^{i\gamma\sigma_y\tau_x} = \begin{pmatrix} \cos\gamma & 0 & 0 & \sin\gamma \\ 0 & \cos\gamma & -\sin\gamma & 0 \\ 0 & \sin\gamma & \cos\gamma & 0 \\ -\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_y\tau_y} = \begin{pmatrix} \cos\gamma & 0 & 0 & -i\sin\gamma \\ 0 & \cos\gamma & i\sin\gamma & 0 \\ 0 & i\sin\gamma & \cos\gamma & 0 \\ -i\sin\gamma & 0 & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_y\tau_z} = \begin{pmatrix} \cos\gamma & \sin\gamma & 0 & 0 \\ -\sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & \cos\gamma & -\sin\gamma \\ 0 & 0 & \sin\gamma & \cos\gamma \end{pmatrix}$$

$$e^{i\gamma\sigma_z\tau_x} = \begin{pmatrix} \cos\gamma & 0 & i\sin\gamma & 0 \\ 0 & \cos\gamma & 0 & -i\sin\gamma \\ i\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & -i\sin\gamma & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_z\tau_y} = \begin{pmatrix} \cos\gamma & 0 & \sin\gamma & 0 \\ 0 & \cos\gamma & 0 & -\sin\gamma \\ -\sin\gamma & 0 & \cos\gamma & 0 \\ 0 & \sin\gamma & 0 & \cos\gamma \end{pmatrix} e^{i\gamma\sigma_z\tau_z} = \begin{pmatrix} e^{i\gamma} & 0 & 0 & 0 \\ 0 & e^{-i\gamma} & 0 & 0 \\ 0 & 0 & e^{-i\gamma} & 0 \\ 0 & 0 & 0 & e^{i\gamma} \end{pmatrix}$$

A Write potential as squared ops for AFDMC

The spin-isospin dependent potential can be written in the form

$$V = \sum_p \sum_{i<j} u^p(\hat{r}_{ij}) \mathcal{O}^p_{ij}. \tag{17}$$

I'm going to just write this out in terms of the simplest set of terms, the $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$ terms.

$$\begin{aligned} V &= \sum_{i<j} u^\tau(\hat{r}_{ij}) \mathcal{O}^p_{ij} && (18) \\ &= \sum_{i<j} u^\tau(\hat{r}_{ij}) \left(\tau_{ix}\tau_{jx} + \tau_{iy}\tau_{jy} + \tau_{iz}\tau_{jz} \right) && (19) \\ &= \sum_{i<j} u^\tau(\hat{r}_{ij}) \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j && (20) \\ &= \sum_\alpha \sum_{i<j} u^\tau(\hat{r}_{ij}) \tau_{i\alpha}\tau_{j\alpha}. && (21) \end{aligned}$$

These can be rewritten in terms in a martix made of of the u values. In the case of the τ operators this is simple because $A^\tau_{i,j} = u^\tau(\hat{r}_{ij})$. If I rewrite the potential using this, and doing a full sum over all i and j and then dividing by 2 I get

$$V = \frac{1}{2} \sum_{\alpha,i,j} A^\tau_{i,j} \tau_{i\alpha}\tau_{j\alpha} \tag{22}$$

Now I want to write this matrix in terms of it's eigenvalues and eigenvectors, which are defined as

$$A^\tau \psi_n^\tau = \lambda_n^\tau \psi_n^\tau, \tag{23}$$

or if you want to write them in the matrix multiplication form

$$\sum_j A_{i,j}^\tau \psi_{n,j}^\tau = \lambda_n^\tau \psi_{n,i}^\tau. \tag{24}$$

Now I want to write out the A matrix in terms of it's eigenvalues and eigenvectors. I do this using eigenvector decompositon. This is defined as

$$A = Q\Lambda Q^{-1}, \tag{25}$$

where Q is the matrix of eigenvectors (so $Q_{ab} = \psi_{ab}$, the a^{th} eigenvector for the b^{th} particle, for example), and Λ is the diagonal matrix of eigenvalues (so $\Lambda_{ab} = \delta_{ab}\lambda_a$). I didn't prove this, but it's roughly believable when you consider the eigenvalue equation, and doing it for each component. Also, if Q is a symmetric square matrix, which it is for us, then you can write $Q^{-1} = Q^T$i. What we have in the potential is $A_{i,j}^\tau$, so we need to write the eigenvector decomposition in terms of the ij^{th} entry. This can be done by using the definitions of matrix multiplication.

$$(A\psi)_i = \sum_j A_{ij}\psi_j \tag{26}$$

$$(AB)_{ij} = \sum_\alpha A_{i\alpha}B_{\alpha j} \tag{27}$$

I'll now use these two equations to get A_{ij} from the definition of eigenvalue decomposition.

$$\begin{aligned}
A_{ij} &= \left(Q\Lambda Q^T\right)_{ij} && (28)\\
&= \sum_\alpha \sum_\beta Q_{i\beta}\Lambda_{\beta\alpha}Q_{\alpha j}^T && (29)\\
&= \sum_\alpha \sum_\beta Q_{i\beta}\delta_{\beta\alpha}\lambda_\alpha Q_{\alpha j}^T && (30)\\
&= \sum_\alpha \lambda_\alpha Q_{i\alpha}Q_{\alpha j}^T && (31)\\
&= \sum_\alpha \lambda_\alpha \psi_{i\alpha}\psi_{j\alpha} && (32)
\end{aligned}$$

Now plug this into the equation that we had earlier for the potential to get

$$\begin{aligned}
V &= \frac{1}{2}\sum_{\alpha,i,j} A_{i,j}^\tau \tau_{i\alpha}\tau_{j\alpha} && (33)\\
&= \frac{1}{2}\sum_{\alpha,i,j}\sum_n \lambda_n^\tau \psi_{i,n}\psi_{j,n}\tau_{i\alpha}\tau_{j\alpha} && (34)\\
&= \frac{1}{2}\sum_\alpha \sum_n \left(\mathcal{O}_{n\alpha}^\tau\right)^2 \lambda_n^\tau, && (35)
\end{aligned}$$

where

$$\mathcal{O}^{\tau}_{n\alpha} = \sum_i \tau_{i\alpha} \psi^{\tau}_n. \tag{36}$$

A similar analysis can be done for the $\mathcal{O}^{\sigma}_n$ and $\mathcal{O}^{\sigma\tau}_{n\alpha}$ operators.