Notes on T^2 operator

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1 $\exp(-\alpha T^2)$ operator to decrease T^2 violating terms

The correlations violate T^2 and T_z. One solution to this is to multiply the correlations by a term $e^{-\alpha T^2}$ such that alpha is large enough to exponentially reduce the T^2 and T_z breaking. This added piece to the correlations would take the form

$$\exp\left(-\alpha T^2\right) = \exp\left(-\alpha \sum_\beta \sum_{i,j} \tau_{i\beta}\tau_{j\beta}\right). \tag{1}$$

The Hubbard-Stratanovich transformation can be used on these operators by writting them as an exponential of squared one-body operators.

$$\exp\left(-\alpha T^2\right) = \exp\left(-\alpha \sum_\beta \left(\sum_j \tau_{j\beta}\right)^2\right). \tag{2}$$

In a standard AFDMC calculation the sum over β would then be approximated by a product over β where the commutator terms are small as long as the factor α is small. However, α must be large in order to eliminate T^2 breaking terms from the wave function and thus this approximation can't be used. Instead we have used the identity

$$\exp\left(\sum_\beta A_\beta\right) = \mathcal{S}\prod_\beta \exp(A_\beta), \tag{3}$$

where the symmetrization operator $\mathcal{S} = \frac{1}{N!}\sum_\pi P_\pi$, permutes the cartesian coordinates $\beta = xyz$. With this identity and the Hubbard-Stratanovich transformation we can write the correlations as

$$\begin{aligned}
\exp\left(-\alpha \sum_\beta \left(\sum_j \tau_{j\beta}\right)^2\right) &= \mathcal{S}\prod_\beta \exp\left(-\alpha\left(\sum_j \tau_{j\beta}\right)^2\right) &(4)\\
&= \mathcal{S}\prod_\beta \int dx_\beta \exp\left(-x_\beta^2/2\right)\exp\left(i\sqrt{2\alpha}x_\beta \sum_j \tau_{j\beta}\right) &(5)\\
&\approx \mathcal{S}\prod_\beta \frac{1}{N}\sum_{n=1}^{N}\exp\left(i\sqrt{2\alpha}x_{n\beta}\sum_j \tau_{j\beta}\right), &(6)
\end{aligned}$$

where the sum over n is a sum over the N sampled configurations of the 3 auxiliary fields. The sum over i can be brought out of the exponential as a product because the operators on different particles all commute. Also the symmetrization operator can be written as a sum over the $3! = 6$ permutations of the β coordinates giving us

$$\frac{1}{6N}\prod_{j}\sum_{P(xyz)}\sum_{n=1}^{N}\exp\left(i\sqrt{2\alpha}x_{nx}\tau_{jx}\right)\exp\left(i\sqrt{2\alpha}x_{ny}\tau_{jy}\right)\exp\left(i\sqrt{2\alpha}x_{nz}\tau_{jz}\right) \tag{7}$$

The exponential operators on each particle look identical and can be written in a matrix representation as

$$\exp\left(i\sqrt{2\alpha}x_{nx}\tau_{jx}\right) = \begin{pmatrix} \cos(a_{xn}) & 0 & i\sin(a_{xn}) & 0 \\ 0 & \cos(a_{xn}) & 0 & i\sin(a_{xn}) \\ i\sin(a_{xn}) & 0 & \cos(a_{xn}) & 0 \\ 0 & i\sin(a_{xn}) & 0 & \cos(a_{xn}) \end{pmatrix} \tag{8}$$

$$\exp\left(i\sqrt{2\alpha}x_{ny}\tau_{jy}\right) = \begin{pmatrix} \cos(a_{yn}) & 0 & \sin(a_{yn}) & 0 \\ 0 & \cos(a_{y}) & 0 & \sin(a_{yn}) \\ -\sin(a_{yn}) & 0 & \cos(a_{yn}) & 0 \\ 0 & -\sin(a_{yn}) & 0 & \cos(a_{yn}) \end{pmatrix} \tag{9}$$

$$\exp\left(i\sqrt{2\alpha}x_{nz}\tau_{jz}\right) = \begin{pmatrix} e^{ia_{zn}} & 0 & 0 & 0 \\ 0 & e^{ia_{zn}} & 0 & 0 \\ 0 & 0 & e^{-ia_{zn}} & 0 \\ 0 & 0 & 0 & e^{-ia_{zn}} \end{pmatrix}, \tag{10}$$

where $a_{xn} = \sqrt{2\alpha}x_{xn}$, $a_{yn} = \sqrt{2\alpha}x_{yn}$, $a_{zn} = \sqrt{2\alpha}x_{zn}$ and in our basis the iso-spin matricies are

$$\tau_x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \qquad \tau_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \qquad \tau_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{11}$$

Owing to the clean matrix representation of these operators the symmetrized product of exponential operators can be written as one matrix,

$$\mathcal{M}_{jn} = \frac{1}{6}\sum_{P(xyz)} = \begin{pmatrix} A & 0 & B & 0 \\ 0 & A & 0 & B \\ C & 0 & D & 0 \\ 0 & C & 0 & D \end{pmatrix}, \tag{12}$$

where

$$A = e^{ia_{zn}}\cos(a_{xn})\sin(a_{yn}) \tag{13}$$
$$B = \cos(a_{zn})\left(i\cos(a_{yn})\sin(a_{xn}) + \cos(a_{xn})\sin(a_{yn})\right) \tag{14}$$
$$C = \cos(a_{zn})\left(i\cos(a_{yn})\sin(a_{xn}) - \cos(a_{xn})\sin(a_{yn})\right) \tag{15}$$
$$D = e^{-a_{zn}}\cos(a_{xn})\cos(a_{yn}). \tag{16}$$

This matrix can then be build and operated on each of the particles.

$$\exp\left(-\alpha T^2\right) \approx \frac{1}{N} \prod_{j=1}^{A} \sum_{n=1}^{N} \mathcal{M}_{jn} \tag{17}$$