

Derivation of Trial Wave Function for Nuclear Monte Carlo

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1 Trial Wave Function

To obtain the trial wave function for nuclear Monte Carlo there are two parts, the antisymmetric long range part ($|\Phi\rangle$) and the symmetric short range correlation operator (\mathcal{F}). That is

$$|\psi_T\rangle = \mathcal{F} |\Phi\rangle. \quad (1)$$

The antisymmetric part is made up of single particle orbitals in the form of a slater determinant. It is the symmetric correlation operator that I am not sure about. By reading other papers this is what I have understood. If you ignore three-body correlations then

$$\mathcal{F} = \mathcal{S} \prod_{i < j} F_{ij}, \quad (2)$$

where

$$F_{ij} = \sum_p f^p(r_{ij}) \mathcal{O}_{ij}^p, \quad (3)$$

where \mathcal{S} is the symmetrization operator and $\mathcal{O}_{ij}^p = 1, \sigma_i \cdot \sigma_j, 3\sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j$ plus each of these terms times $\tau_i \cdot \tau_j$. To write this more like what other papers have written it I will pull the 1 term out of the sum and let $f^1(r_{ij}) = f^c(r_{ij})$ since that term is a central term and I will call $u_{ij}^p = f^p(r_{ij})/f^1(r_{ij})$. This gives us

$$F_{ij} = \sum_p f_c(r_{ij}) \left(1 + \sum_p u^p(r_{ij}) \right). \quad (4)$$

Putting all of these pieces together the trial wave function becomes

$$|\Phi_T\rangle = \left[\mathcal{S} \prod_{i < j} f_c(r_{ij}) \left(1 + \sum_p u^p(r_{ij}) \mathcal{O}_{ij}^p \right) \right] |\Phi\rangle. \quad (5)$$

When we spoke the trial general trial wave function was supposed to be

$$|\Phi_T\rangle = \left[\prod_{i < j} f_c(r_{ij}) \left(1 + \sum_{i < j} \sum_p u^p(r_{ij}) \mathcal{O}_{ij}^p \right) \right] |\Phi\rangle. \quad (6)$$

Where the only differences are \mathcal{S} in equation 5 and the double sum in equation 6. Does the double sum come from the symmetrization operator or am I just wrong with my derivation?