

# Hartree–Fock Wavefunction

$$\psi_{HF}(1,2,\dots,N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_i(1) & \varphi_i(2) & \varphi_i(N) \\ \varphi_j(1) & \varphi_j(2) & \varphi_j(N) \\ \vdots & \vdots & \vdots \\ \varphi_k(1) & \varphi_k(2) & \varphi_k(N) \end{vmatrix}$$

$$\psi_{HF} \equiv \hat{\mathcal{A}} \varphi_i(1) \varphi_j(2) \cdots \varphi_k(N)$$

where  $\hat{\mathcal{A}}$  is the antisymmetrizing operator

$$\varphi_i = \text{spin orbital} = \phi_i(\vec{r}) \begin{cases} \alpha \\ \beta \end{cases}$$

where  $\phi_i(\vec{r})$  is a spatial orbital  
and  $\alpha$  or  $\beta$  are the spin functions

$$\langle \varphi_i | \varphi_j \rangle = \delta_{ij} \text{ (orthonormal)}$$