

Here we elaborate the derivation of the Kohn-Sham ground energy (equation 7.91) with slightly more rigorous language of tensor product.

The totally symmetric or anti-symmetric multi-particle state  $|\Psi\rangle$  should be the totally symmetric or anti-symmetric combination of the tensor product states of each particle, i.e.,

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \eta_p |\phi_{p(1)}\rangle \otimes |\phi_{p(2)}\rangle \otimes \cdots \otimes |\phi_{p(N)}\rangle \quad (1)$$

where  $\eta_p = 1$  for symmetric states, and  $\eta_p = \epsilon_{p(1)p(2)\dots p(N)}$  for anti-symmetric states.

That  $|\Psi\rangle$  is normalized is guaranteed by requiring the set of  $\{|\phi_j\rangle\}$  to be orthonormal, in which case

$$\begin{aligned} \langle\Psi|\Psi\rangle &= \frac{1}{N!} \sum_{p,q \in S_N} (\eta_p \eta_q) \overbrace{(\langle\phi_{p(1)}|\phi_{q(1)}\rangle)}^{\delta_{p(1)q(1)}} \underbrace{(\langle\phi_{p(2)}|\phi_{q(2)}\rangle)}_{\delta_{p(2)q(2)}} \cdots \overbrace{(\langle\phi_{p(N)}|\phi_{q(N)}\rangle)}^{\delta_{p(N)q(N)}} \\ &= \frac{1}{N!} \sum_{p \in S_N} \eta_p^2 = 1 \end{aligned} \quad (2)$$

Thus, the wave function given by eq (7.88) should actually be written as

$$\begin{aligned} \langle\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N|\Psi\rangle &= \Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \\ &= \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \eta_p \phi_{p(1)}(\mathbf{x}_1) \phi_{p(2)}(\mathbf{x}_2) \cdots \phi_{p(N)}(\mathbf{x}_N) \end{aligned} \quad (3)$$

We also assume that each  $|\phi_j\rangle$  is an energy eigenstate satisfying eq (7.90), i.e.,

$$H_{KS}|\phi_j\rangle = \epsilon_j|\phi_j\rangle \quad (4)$$

Care must be taken to construct the multi-particle Hamiltonian  $H_{KS}^N$  from single particle Hamiltonian.  $H_{KS}^N$  should be written as

$$\begin{aligned} H_{KS}^N &= H_{KS} \otimes I \otimes \cdots \otimes I + \\ &\quad I \otimes H_{KS} \otimes I \otimes \cdots \otimes I + \\ &\quad \cdots + \\ &\quad I \otimes \cdots \otimes I \otimes H_{KS} \end{aligned} \quad (5)$$

In this spirit, we should have

$$\begin{aligned} \langle\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N|H_{KS}^N|\Psi\rangle &= (\langle\mathbf{x}_1| \otimes \langle\mathbf{x}_2| \otimes \cdots \otimes \langle\mathbf{x}_N|) H_{KS}^N \left( \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \eta_p |\phi_{p(1)}\rangle \otimes |\phi_{p(2)}\rangle \otimes \cdots \otimes |\phi_{p(N)}\rangle \right) \\ &= \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \eta_p \cdot \left[ \sum_{j=1}^N \phi_{p(1)}(\mathbf{x}_1) \cdots \epsilon_j \phi_{p(j)}(\mathbf{x}_j) \cdots \phi_{p(N)}(\mathbf{x}_N) \right] \\ &= \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \eta_p \left( \sum_j \epsilon_j \right) [\phi_{p(1)}(\mathbf{x}_1) \phi_{p(2)}(\mathbf{x}_2) \cdots \phi_{p(N)}(\mathbf{x}_N)] \\ &= \left( \sum_j \epsilon_j \right) \left[ \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \eta_p \phi_{p(1)}(\mathbf{x}_1) \phi_{p(2)}(\mathbf{x}_2) \cdots \phi_{p(N)}(\mathbf{x}_N) \right] \\ &= \left( \sum_j \epsilon_j \right) \langle\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N|\Psi\rangle \end{aligned} \quad (6)$$

which shows that  $|\Psi\rangle$  is an energy eigenstate of  $H_{KS}^N$  with eigenvalue  $\sum_j \epsilon_j$ , which gives eq (7.91).

Note that in this derivation, we assume all  $\phi_j$ s are distinct, but in fact they are allowed to be the same for  $i, j$  (even all  $N$  are allowed to be the same). When some of them are the same, the totally symmetric/anti-symmetric construction of  $|\Psi\rangle$  will be different than (1), see eq (7.63),(7.64) for example, but the remaining of the derivation still holds (with properly constructed  $|\Psi\rangle$ ).