

$$V_{jk} = V_{kj}, \quad \sum_{j < k}^N V_{jk} = \frac{1}{2} \sum_j^N \sum_k^N V_{jk} \quad (j \neq k)$$

Applying the symmetric operator in both side of V expressed in first quantized form.

$$\begin{aligned} S^\pm \hat{V}_{tot} |\psi_{\nu_{\alpha_1}}(\mathbf{r}_1)\rangle |\psi_{\nu_{\alpha_2}}(\mathbf{r}_2)\rangle, \dots, |\psi_{\nu_{\alpha_N}}(\mathbf{r}_N)\rangle \\ = \hat{V}_{tot} a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger |0\rangle \\ = \frac{1}{2} \sum_{j \neq k}^N \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} \delta_{\nu_a, \nu_{\alpha_j}} \delta_{\nu_b, \nu_{\alpha_k}} |\psi_{\nu_{\alpha_1}}(\mathbf{r}_1)\rangle, \dots, |\psi_{\nu_c}(\mathbf{r}_j)\rangle, \dots, |\psi_{\nu_d}(\mathbf{r}_k)\rangle, \dots, |\psi_{\nu_{\alpha_N}}(\mathbf{r}_N)\rangle \\ = \frac{1}{2} \sum_{j \neq k}^N \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} \delta_{\nu_a, \nu_{\alpha_j}} \delta_{\nu_b, \nu_{\alpha_k}} (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots \underset{\substack{\uparrow \\ \text{jth}}}{a_{\nu_c}^\dagger} \dots \underset{\substack{\uparrow \\ \text{kth}}}{a_{\nu_d}^\dagger} \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \end{aligned}$$

To get the final result of summation, first, count each calculation process of equation term which stated as (a) for j and k indices,

$$= \frac{1}{2} \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} \underbrace{\left(\sum_j^N \sum_k^N \delta_{\nu_a, \nu_{\alpha_j}} \delta_{\nu_b, \nu_{\alpha_k}} (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots \underset{\substack{\uparrow \\ \text{jth}}}{a_{\nu_c}^\dagger} \dots \underset{\substack{\uparrow \\ \text{kth}}}{a_{\nu_d}^\dagger} \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \right)}_{\text{(a)}}$$

If the given operator represents a Coulomb interaction between two electrons, the difference compared to the case of single particle operator \hat{T} is a using fermionic creation operator c^\dagger and annihilation operator c instead of bosonic operators b^\dagger, b , due to the fermion property of electrons.

In the procedure below, all creation and annihilation operators a^\dagger and a are considered fermionic operators during the calculation, so it can be deduced that : $n_\alpha = 1$, and the range of a value of α is the same as the range of j, $1 \leq \alpha, j \leq N$.

The following 3 conditions are used to analyze the (a).

- (1) : $a^\dagger |0\rangle = a_j^\dagger a_i a_i^\dagger |0\rangle$
- (2) : $\{c_i, c_j^\dagger\} = \delta_{ij}, \quad [b_i, b_j^\dagger] = \delta_{ij}$
- (3) : if $\lambda = -\lambda, \quad \lambda = 0, \quad \text{if } \lambda \neq 0, \quad \lambda \neq -\lambda \quad (\lambda \text{ is a real number})$

First, counts each summation result for k indices, k=1,2,...,k'...,N.

$$\begin{aligned} \text{k=1} \quad & \delta_{\nu_b \nu_{\alpha_1}} (a_{\nu_d}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\ & = \delta_{\nu_b \nu_{\alpha_1}} \underbrace{(a_{\nu_d}^\dagger a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger)}_{\text{condition (1)}} |0\rangle \\ & = \delta_{\nu_b \nu_{\alpha_1}} a_{\nu_d}^\dagger a_{\nu_{\alpha_1}}^\dagger (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \rightarrow (1, \bigcirc) \end{aligned}$$

(1, \bigcirc) refers to the result of the calculation of the left side of the right-headed-arrow. A \bigcirc means that it is blank, the value will be given in the calculation process for j indices.

$$\begin{aligned} \text{k=2} \quad & \delta_{\nu_b \nu_{\alpha_2}} (a_{\nu_{\alpha_1}}^\dagger a_{\nu_d}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\ & = \delta_{\nu_b \nu_{\alpha_2}} \underset{\substack{\uparrow \\ \text{condition (2), by swapping the order}}}{(a_{\nu_{\alpha_1}}^\dagger a_{\nu_d}^\dagger)} a_{\nu_{\alpha_2}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger |0\rangle \end{aligned}$$

two operators are in ordered place, first one is in 1st place, and after 2nd place.

$$\begin{aligned} & = (-1) \delta_{\nu_b \nu_{\alpha_2}} a_{\nu_d}^\dagger (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\ & = (-1)^2 \delta_{\nu_b \nu_{\alpha_2}} a_{\nu_d}^\dagger a_{\nu_{\alpha_2}}^\dagger (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \dots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \rightarrow (2, \bigcirc) \end{aligned}$$

Notice that swapping the order of ν_d and ν_c is necessary because the overall summation process is equal to $\hat{V}_{tot} a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger |0\rangle > 0$, which requires the condition (3).

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$$\begin{aligned}
k=k' \quad & \delta_{\nu_b \nu_{\alpha_2}} (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \cdots a_{\nu_d}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = \delta_{\nu_b \nu_{\alpha_2}} \underbrace{(a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \cdots a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger)}_{k'-1 \text{ operators}} |0\rangle \\
& = (-1)^{k'-1} \delta_{\nu_b \nu_{\alpha_2}} a_{\nu_d}^\dagger (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{2(k'-1)} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_2}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \rightarrow (k', \bigcirc)
\end{aligned}$$

Successively, count the summation for the j index, where $k=k'$ and $j=1,2,\dots,j',\dots,N$

$$\begin{aligned}
k=k', j=1 \quad & (-1)^{2(k'-1)} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger (a_{\nu_c}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{2(k'-1)} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger (a_{\nu_c}^\dagger a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{2(k'-1)} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger a_{\nu_c}^\dagger a_{\nu_{\alpha_1}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{|2(k'-1)+1|} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} \underbrace{a_{\nu_d}^\dagger a_{\nu_c}^\dagger}_{\substack{\uparrow \quad \uparrow \\ \text{two operators are in ordered place}}} (a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_1}}^\dagger - \delta_{\nu_c \nu_{\alpha_1}}) a_{\nu_{\alpha_{k'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{|2(k'-1)+2|} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_c}^\dagger a_{\nu_d}^\dagger a_{\nu_{\alpha_1}}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& - \delta_{\nu_c \nu_{\alpha_1}} (\text{products of operators}) |0\rangle \rightarrow (k', 1)
\end{aligned}$$

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$$\begin{aligned}
k=k', j=j' \quad & (-1)^{2(k'-1)} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_c}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{2(k'-1)} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger \underbrace{(a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_c}^\dagger a_{\nu_{\alpha_{j'}}}^\dagger a_{\nu_{\alpha_{j'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger)}_{j'-1 \text{ operators}} |0\rangle \\
& = (-1)^{|2(k'-1)+2(j'-1)|} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger a_{\nu_c}^\dagger a_{\nu_{\alpha_{j'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_{j'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{|2(k'-1)+2(j'-1)+1|} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} \underbrace{a_{\nu_d}^\dagger a_{\nu_c}^\dagger}_{\substack{\uparrow \quad \uparrow \\ \text{two operators are in ordered place}}} (a_{\nu_{\alpha_{k'}}}^\dagger a_{\nu_{\alpha_{j'}}}^\dagger - \delta_{\nu_c \nu_{\alpha_{k'}}}) a_{\nu_{\alpha_{j'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_{j'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& = (-1)^{|2(k'-1)+2(j'-1)+2|} \delta_{\nu_a \nu_{\alpha_1}} \delta_{\nu_b \nu_{\alpha_{k'}}} a_{\nu_c}^\dagger a_{\nu_d}^\dagger a_{\nu_{\alpha_{k'}}}^\dagger a_{\nu_{\alpha_{j'}}}^\dagger (a_{\nu_{\alpha_1}}^\dagger \cdots a_{\nu_{\alpha_{k'}}}^\dagger \cdots a_{\nu_{\alpha_{j'}}}^\dagger \cdots a_{\nu_{\alpha_N}}^\dagger) |0\rangle \\
& - \delta_{\nu_c \nu_{\alpha_{k'}}} (\text{product of operators}) |0\rangle \rightarrow (k', j')
\end{aligned}$$

Now arrange each number set in a square formation, ordering (k,j) as k th row and j th column. The arranged form can be shown as a matrix, so let the corresponding matrix named A , then each number set (k,j) is an element of a matrix A_{kj} . The result of summation \textcircled{a} corresponds to the sum of all elements in matrix A .

$$A = \begin{pmatrix} 0 & (1,2) & (1,3) & \cdots & (1,N) \\ (2,1) & 0 & (2,3) & \cdots & (2,N) \\ \vdots & & & (k',j') & \\ (N,1) & (N,2) & (N,3) & \cdots & 0 \end{pmatrix}, \quad \textcircled{a} = \sum_j^N \sum_k^N A_{jk}$$

If $\nu_a = \nu'_j$ and $\nu_b = \nu_{k'}$, result of summation \textcircled{a} is the value of matrix element $A_{k'j'}$,

$$\begin{aligned}
& \frac{1}{2} \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} \left(\textcircled{a} \right) \\
&= \frac{1}{2} \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} \left(A_{k'j'} \right) \\
&= \frac{1}{2} \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} (-1)^{2(|k'-1|+|j'-1|+1)} c_{\nu_c}^\dagger c_{\nu_d}^\dagger c_{\nu_b} c_{\nu_a} (c_{\nu_1}^\dagger c_{\nu_2}^\dagger \cdots c_{\nu_N}^\dagger) |0\rangle \\
&\quad - \delta_{\nu_c \nu_{\alpha_{k'}}} (\text{product of operators}) |0\rangle
\end{aligned}$$

Since $\nu_c \neq \nu_b = \nu_{\alpha_{k'}}$, and $(-1)^{2(|k'-1|+|j'-1|+1)} = 1$,

$$= \frac{1}{2} \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} c_{\nu_c}^\dagger c_{\nu_d}^\dagger c_{\nu_b} c_{\nu_a} (c_{\nu_1}^\dagger c_{\nu_2}^\dagger \cdots c_{\nu_N}^\dagger) |0\rangle$$

Therefore,

$$V_{tot} = \frac{1}{2} \sum_{\nu_a \nu_b, \nu_c \nu_d} V_{\nu_c \nu_d, \nu_a \nu_b} c_{\nu_c}^\dagger c_{\nu_d}^\dagger c_{\nu_a} c_{\nu_b}$$