Permutation group and determinants
(Dated: September 19, 2018)
I. SYMMETRIES OF MANY-PARTICLE FUNCTIONS

Since electrons are fermions, the electronic wave functions have to be antisymmetric. This chapter will show how to achieve this goal. The notion of antisymmetry is related to permutations of electrons’ coordinates. Therefore we will start with the discussion of the permutation group and then introduce the permutation-group-based definition of determinant, the zeroth-order approximation to the wave function in theory of many fermions. This definition, in contrast to that based on the Laplace expansion, relates clearly to properties of fermionic wave functions. The determinant gives an \(N\)-particle wave function built from a set of \(N\) one-particle waves functions and is called Slater’s determinant.

II. PERMUTATION (SYMMETRIC) GROUP

*Definition of permutation group:* The permutation group, known also under the name of symmetric group, is the group of all operations on a set of \(N\) distinct objects that order the objects in all possible ways. The group is denoted as \(S_N\) (we will show that this is a group below). We will call these operations permutations and denote them by symbols \(\sigma_i\). For a set consisting of numbers 1, 2, \ldots, \(N\), the permutation \(\sigma_i\) orders these numbers in such a way that \(k\) is at \(j\)th position. Often a better way of looking at permutations is to say that permutations are all mappings of the set 1, 2, \ldots, \(N\) onto itself: \(\sigma_i(k) = j\), where \(j\) has to go over all elements.

*Number of permutations:* The number of permutations is \(N!\). Indeed, we can first place each object at positions 1, so there are \(N\) possible placements. For each case, we can place one of the remaining \(N-1\) objects at the second positions, so that the number of possible arrangements is now \(N(N-1)\). Continuing in this way, we prove the theorem.

*Example:* For three numbers: 1, 2, 3, there are the following 3! = 6 arrangements: 123, 132, 213, 231, 312, 321.

*Notation:* One can use the following “matrix” to denote permutations:

\[
\sigma = \begin{pmatrix}
1 & 2 & \ldots & k & \ldots & N \\
\sigma(1) & \sigma(2) & \ldots & \sigma(k) & \ldots & \sigma(N)
\end{pmatrix}
\]

The order of columns in the matrix above is convenient, but note that if the columns were ordered differently, this would still be the same permutation. Another way if writing a permutation is to include only the second row. An example of a permutation in this notation is

\[
\sigma = \begin{pmatrix}
1 & 2 & 3 & 4 \\
3 & 4 & 1 & 2
\end{pmatrix}
\]
**Multiplication:** We define the operation of multiplication within the set of permutations as \((\sigma \circ \sigma')(k) = \sigma(\sigma'(k))\). For example, if

\[
\sigma_1 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 1 & 2 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 3 & 1 \end{pmatrix}
\]

then

\[
\sigma_2 \circ \sigma_1 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 1 & 2 & 4 \end{pmatrix}.
\]

**Symmetric group:** We can now check if these operations satisfy the group postulates

- **Closure:** \(\sigma \circ \sigma' \in S_N\). The proof is obvious since the product of permutations gives a number from the set, therefore is a permutation.

- **Existence of unity** \(I\): this is the permutation \(\sigma_I(k) = k\).

- **Existence of inverse**, i.e., for each \(\sigma\) there exists \(\sigma^{-1}\) such that \(\sigma \circ \sigma^{-1} = I\). Clearly, the inverse can be defined such that if \(\sigma(k) = j\), then \(\sigma^{-1}(j) = k\).

- **Multiplications are associative:**

\[
\sigma_3 \circ (\sigma_2 \circ \sigma_1) = (\sigma_3 \circ \sigma_2) \circ \sigma_1.
\]

Proof is in a homework problem.

**\(\sigma \circ S_N = S_N\):** One important theorem resulting from these definitions is that the set of products of a single permutation with all elements of \(S_N\) is equal to \(S_N\)

\[
\sigma \circ S_N = S_N.
\]

Proof: Due to closure, the only possibility of not reproducing the whole group is that two different elements of \(S_N\) are mapped by \(\sigma\) onto the same element:

\[
\sigma \circ \sigma' = \sigma'' = \sigma \circ \sigma''.
\]

Multiplying this equation by \(\sigma^{-1}\), we get \(\sigma' = \sigma''\) which contradicts our assumption.

**\(\{\sigma^{-1}\} = S_N\):** Another theorem states that \(\{\sigma^{-1}\} = S_N\). This is equivalent to saying that \(\sigma\) and \(\sigma^{-1}\) are in one-to-one correspondence. Indeed, assume that there are two permutations that are inverse to \(\sigma\): \(\sigma_1 \circ \sigma = I = \sigma_2 \circ \sigma\). Multiplying this by \(\sigma^{-1}\) from the right, we get that \(\sigma_1 = \sigma_2\).

**Transpositions:** A transposition is the simplest possible permutation other than \(\sigma_I\), i.e., a permutation involving only two elements:

\[
\tau = \tau_{ij} = (ij) = \begin{cases} \sigma(i) = j \\ \sigma(j) = i \\ \sigma(k) = k \quad \text{for} \quad k \neq i, j \end{cases} = \begin{pmatrix} 1 & 2 & \ldots & i & \ldots & j & \ldots & N \\ 1 & 2 & \ldots & j & \ldots & i & \ldots & N \end{pmatrix}.
\]
**Permutation as product of transpositions:** One important property of permutations is that each permutation can be written as a product of transpositions. To prove that any permutation can be written as a product of transpositions, we just construct such a product. For a permutation $\sigma$ written as

$$\sigma = \begin{pmatrix} 1 & 2 & \ldots & k & \ldots & N \\ i_1 & i_2 & \ldots & i_k & \ldots & i_N \end{pmatrix}$$

(1)

first find $i_1$ in the set $\{1, 2, \ldots, N\}$ and then transpose it with 1 (unless $i_1 = 1$, in which case do nothing). This maps $i_1 \leftrightarrow 1$. Then consider the set with $i_1$ removed, find $i_2$, and transpose it with the number in the second position (it will be 2 if the first transposition did not affect this place). Continuing in this way, we get the mapping of expression (1) which proves the theorem. The decomposition of a permutation into transposition is not unique as we can always add $\tau_{ij} \tau_{ij} = 1$. As an example, consider

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 3 & 2 \end{pmatrix}.$$

We first look for $i_1 = 2$ and then transpose it with 1:

$$1234 \tau_{12} \rightarrow 2134 \tau_{14} \rightarrow 2431$$

where in the second step we looked for $i_2 = 4$ and transposed it with the element in the second positions, i.e., with 1. Then we looked for $i_3 = 3$ and did nothing. Therefore, $\sigma$ can be written as

$$\sigma = \tau_{14} \circ \tau_{12}.$$

Let us check explicitly that the right-hand side indeed gives $\sigma$

$$\sigma(1) = \tau_{14}(\tau_{12}(1)) = \tau_{14}(2) = 2; \quad \sigma(2) = \tau_{14}(\tau_{12}(2)) = \tau_{14}(1) = 4;$$

$$\sigma(3) = \tau_{14}(\tau_{12}(3)) = \tau_{14}(3) = 3; \quad \sigma(4) = \tau_{14}(\tau_{12}(4)) = \tau_{14}(4) = 1.$$

**Parity of permutation:** Although the number of transpositions in a decomposition is not unique, this number is always either odd or even for a given permutation. The proof of this important theorem is given as a homework. Thus, $(-1)^{\pi_\sigma}$, where $\pi_\sigma$ is the number of permutations in an arbitrary decomposition, is always 1 or $-1$ for a given permutation and we can classify each permutation as either odd or even. We say that each permutation has a definitive parity.

**Parity of inverse permutation:** One theorem concerning the parity of permutations is that that $(-1)^{\pi_\sigma} = (-1)^{\pi_{\sigma^{-1}}}$, i.e., that a permutation and its inverse have the same parity. To prove it, first note that

$$(\sigma_1 \circ \sigma_2)^{-1} = \sigma_2^{-1} \sigma_1^{-1}$$
which is obvious if we multiply on the left with $\sigma_1 \circ \sigma_2$. We can write $\sigma$ as

$$\sigma = \tau_1 \circ \tau_2 \circ \cdots \circ \tau_r.$$ 

Then

$$\sigma^{-1} = \tau_r^{-1} \circ \tau_{r-1}^{-1} \circ \cdots \circ \tau_1^{-1}.$$ 

Thus, $\pi_\sigma = \pi_{\sigma^{-1}}$. Note that $\tau_{ij}^{-1} = \tau_{ji}$, but this is not needed for the proof.

III. DETERMINANT

**Definition of determinant:** For a general $N \times N$ matrix $A$ with elements $a_{ij}$, the determinant is defined as

$$|A| \equiv \det A = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{vmatrix} = \sum_\sigma (-1)^{\pi_\sigma} a_{\sigma(1)1} a_{\sigma(2)2} \cdots a_{\sigma(N)N} \quad (2)$$

where the sum is over all permutations of numbers 1 to $N$ and $\pi_\sigma$ is the parity of the permutation. There are several important theorems involving determinants that we will now prove.

**Determinant is invariant to matrix transposition:** Show that that

$$|A| = |A^T|,$$

which also means that the definition (2) can be written as

$$|A| = \sum_\sigma (-1)^{\pi_\sigma} a_{1\sigma(1)} a_{2\sigma(2)} \cdots a_{N\sigma(N)}. \quad (3)$$

**Proof.** Using notation $A^T = A' = \{a'_{ij}\}$, we can write the definition (2) as

$$|A^T| = \sum_\sigma (-1)^{\pi_\sigma} a'_{\sigma(1)1} a'_{\sigma(2)2} \cdots a'_{\sigma(N)N} = \sum_\sigma (-1)^{\pi_\sigma} a_{1\sigma(1)} a_{2\sigma(2)} \cdots a_{N\sigma(N)}$$

(since $a'_{ij} = a_{ji}$). Note that term with a given $\sigma$ in the equation written above is not the same as the term with the same $\sigma$ in Eq. (2) since $a_{ij} \neq a_{ji}$. Let us reshuffle the terms in the last equations in such a way that the factor with $\sigma(i) = 1$ is in the first position (we can do it since product does not depend on the order of factors). There must be one such a factor $a_{i\sigma(i)}$ since $\sigma(i)$ runs over the numbers 1, 2, ..., $N$. Denote this value of $i$ in a given term by $i_1$ so that $a_{i\sigma(i)} = a_{i_11}$ and move this factor to the first position in the product to get

$$a_{1\sigma(1)} a_{2\sigma(2)} \cdots a_{i_11} \cdots a_{N\sigma(N)} = a_{i_11} a_{2\sigma(2)} \cdots a_{i_1-1\sigma(i_1-1)} a_{i_1+1\sigma(i_1+1)} a_{N\sigma(N)}$$
Next, look for $\sigma(i) = 2 = \sigma(i_2)$ and move $a_{i_2}$ to the second position in the product. Continuing, one eventually gets
\[ a_{1\sigma(1)}a_{2\sigma(2)} \cdots a_{\sigma(N)N} = a_{i_1}a_{i_2}a_{i_3} \cdots a_{i_k} \cdots a_{i_N}. \] (4)

The set $i_1, i_2, \ldots, i_N$ is a permutation $\tilde{\sigma}$: $\tilde{\sigma}(k) = i_k$. Note that $\tilde{\sigma} \neq \sigma$ in general. Thus, we have
\[ \sigma(i_k) = k \text{ and } i_k = \tilde{\sigma}(k) \Rightarrow (\sigma \circ \tilde{\sigma})(k) = \sigma(\tilde{\sigma}(k)) = k. \]

Thus, $\tilde{\sigma} = \sigma^{-1}$. Therefore, if we sum all possible terms on the right-hand side of Eq. (4), we sum over all permutations of $S_N$ (as shown earlier, $\{\sigma^{-1}\} = S_N$). The only remaining issue is the sign. The sign is right since we have proved that the parity of $\sigma$ and $\sigma^{-1}$ is the same. This completes the proof. \[\square\]

Interchange of columns: The next important theorem says that if one interchanges two columns (or rows) in a determinant, the value of the determinant changes sign
\[ |A_{i \leftrightarrow j}| = -|A| \]
where $A_{i \leftrightarrow j}$ denotes a matrix with such interchange.

Proof. We can assume without loss of generality that $i < j$. Denote:
\[ A = \{a_{kl}\} \quad A_{i \leftrightarrow j} = \{a'_{kl}\} \]
\[ a'_{kl} = a_{kl} \text{ if } l \neq i, j, \quad k = 1, \ldots, N \] (5)
\[ a'_{ki} = a_{kj}, \quad a'_{kj} = a_{ki}, \quad k = 1, \ldots, N \] (6)

We will expand $|A|$ and $|A_{i \leftrightarrow j}|$ and try to identify identical terms in both expansions, ignoring the sign for now. The expansion of $|A|$ is
\[ |A| = \sum_{\sigma} (-1)^{\pi_\sigma} a_{\sigma(1)1}a_{\sigma(2)2} \cdots a_{\sigma(N)N} \]
where $\sigma$ is here some fixed permutation of $1, 2, \cdots N$. The expansion of $|A_{i \leftrightarrow j}|$ is
\[ |A_{i \leftrightarrow j}| = \sum_{\tilde{\sigma}} (-1)^{\pi_{\tilde{\sigma}}} a'_{\tilde{\sigma}(1)1}a'_{\tilde{\sigma}(2)2} \cdots a'_{\tilde{\sigma}(i)i} \cdots a'_{\tilde{\sigma}(j)j} \cdots a'_{\tilde{\sigma}(N)N} \]
where we use tilde to distinguish the two summations, but both $\sigma$ and $\tilde{\sigma}$ run over the same $S_N$. Now pick one term from the expansion of $|A|$ and find an identical term (containing the same product of matrix elements) in the expansion of $|A_{i \leftrightarrow j}|$. First we see that we should choose $\tilde{\sigma}$ that is the same as $\sigma$ on $k$ other than $i$ or $j$:
\[ \tilde{\sigma}(k) = \sigma(k) \text{ for } k \neq i, j. \]
Check: due to Eq. (5), \( a'_{\sigma(k)k} = a_{\sigma(k)k} \) if \( k \neq i, j \). For the two remaining factors, we choose
\[
\tilde{\sigma}(i) = \sigma(j) \quad \text{and} \quad \tilde{\sigma}(j) = \sigma(i)
\]
Check: due to Eq. (6),
\[
a'_{\tilde{\sigma}(i)i} = a_{\tilde{\sigma}(i)i} = a_{\sigma(j)i},
\]
\[
a'_{\tilde{\sigma}(j)j} = a_{\tilde{\sigma}(j)j} = a_{\sigma(i)j}.
\]
This can be done for all \( N! \) terms in both expansions, so that there is one to one correspondence between the terms, modulo sign.

To find the sign, realize that \( \tilde{\sigma}(k) = (\sigma \circ \tau_{ij})(k) = \begin{cases} \sigma(k) & k \neq i, j \\ (\sigma \circ \tau_{ij})(k) & k = i \text{ or } j \end{cases} \)

The upper line says that if \( k \neq i, j \), \( \tau_{ij} \) has no effect. The lower one is equivalent to the choice of \( \tilde{\sigma} \) that we made earlier since \( \tilde{\sigma}(i) = (\sigma \circ \tau_{ij})(i) = \sigma(\tau_{ij}(i)) = \sigma(j) \) and similarly for \( j \). Thus, the permutations \( \tilde{\sigma} \) and \( \sigma \) differ by one transposition and therefore \( (-1)^{\pi_{\tilde{\sigma}}} = -(-1)^{\pi_{\sigma}} \), which proves the theorem.

**Linear combination of column vectors:** Another theorem states that if a column of a matrix is a linear combination of two (or more) column matrices (vectors), the determinant of this matrix is equal to the linear combination of determinants, each containing one of these column matrices:
\[
|A(a_j = \beta b + \gamma c)| = \beta |A(a_j = b)| + \gamma |A(a_j = c)|. \tag{7}
\]
The proof follows from the fact that the definition of determinant implies that each term in the expansion (2) contains exactly one element from each column and each row. Thus, each term contains the factor \( \beta b_i + \gamma c_i \) and can be written as a sum of two terms. Pulling the coefficients in front of determinants proves the theorem.

**Determinant of a product of matrices:** One more theorem which is the subject of a homework is that the determinant of a product of two matrices is the product of determinants:
\[
|AB| = |A||B|.
\]

**Determinant of unitary matrix:** This theorem formulated above can be used to prove that the determinant of a unitary matrix, i.e., a matrix with the property \( UU^\dagger = I \), where the dagger denotes a matrix which is transformed and complex conjugated, is a complex number of modulus 1. Indeed
\[
1 = |UU^\dagger| = |U||U^\dagger| = |U||U^T|^* = |U||U^*| = |z|^2
\]
where we used the theorem about the determinant of a transformed matrix.

Laplace expansion of determinant: Finally, a homework problem shows that the determinant of $A$ can be computed using the so-called Laplace’s expansion

$$|A| = \sum_i (-1)^{i+j} a_{ij} |M_{ij}| = \sum_j (-1)^{i+j} a_{ij} |M_{ij}|,$$

where the matrix $M_{ij}$ is obtained from matrix $A$ by removing the $i$th row and $j$th column.