APPENDIX A

Reminding Matrices and Determinants

Matrices

Definition

A $n \times m$ matrix $\boldsymbol{A}$ represents a rectangular table of numbers[1] A_{ij} standing like soldiers in n perfect rows and m columns (index i tells us in which row, and index j tells us in which column the number A_{ij} is located):

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nm} \end{pmatrix}.$$

This notation allows us to operate the whole matrices (like troops), instead of specifying what happens to each number ("*soldier*") separately. If matrices were not invented, then the equations would be very long and clumsy, instead of short and clear.

Addition

Two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ may be *added*, if their dimensions n and m match. The result is matrix $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{B}$ (of the same dimensions as $\boldsymbol{A}$ and $\boldsymbol{B}$), where each element of $\boldsymbol{C}$ is a sum of the corresponding elements of $\boldsymbol{A}$ and $\boldsymbol{B}$:

$$C_{ij} = A_{ij} + B_{ij},$$

$$\text{e.g.,} \begin{pmatrix} 1 & -1 \\ -3 & 4 \end{pmatrix} + \begin{pmatrix} 2 & 1 \\ -2 & 3 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ -5 & 7 \end{pmatrix}.$$

Multiplying by a Number

A matrix may be multiplied by a number by multiplying every element of the matrix by this number: $c\boldsymbol{A} = \boldsymbol{B}$ with $B_{ij} = cA_{ij}$. E.g., $2\begin{pmatrix} 1 & -1 \\ 3 & -2 \end{pmatrix} = \begin{pmatrix} 2 & -2 \\ 6 & -4 \end{pmatrix}$.

[1] If instead of the numbers a matrix contained functions, then everything in this Appendix would remain valid (at particular values of the variables instead of the functions, we would have their values).

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Matrix Product

A product of two matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ is matrix $\boldsymbol{C}$, denoted by $\boldsymbol{C} = \boldsymbol{A}B$; its elements are calculated using elements of $\boldsymbol{A}$ and $\boldsymbol{B}$:

$$C_{ij} = \sum_{k=1}^{N} A_{ik} B_{kj},$$

where the number of the columns (N) of matrix $\boldsymbol{A}$ has to be equal to the number of rows in matrix $\boldsymbol{B}$. The resulting matrix $\boldsymbol{C}$ has the number of rows equal to the number of rows in $\boldsymbol{A}$ and the number of columns equal to the number of columns in $\boldsymbol{B}$. Let us see how it works in an example. The product $\boldsymbol{AB} = \boldsymbol{C}$:

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ \boldsymbol{A}_{21} & \boldsymbol{A}_{22} & \boldsymbol{A}_{23} & \boldsymbol{A}_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & \boldsymbol{B}_{13} & B_{14} & B_{15} & B_{16} & B_{17} \\ B_{21} & B_{22} & \boldsymbol{B}_{23} & B_{24} & B_{25} & B_{26} & B_{27} \\ B_{31} & B_{32} & \boldsymbol{B}_{33} & B_{34} & B_{35} & B_{36} & B_{37} \\ B_{41} & B_{42} & \boldsymbol{B}_{43} & B_{44} & B_{45} & B_{46} & B_{47} \end{pmatrix}$$
$$= \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} & C_{17} \\ C_{21} & C_{22} & \boldsymbol{C}_{23} & C_{24} & C_{25} & C_{26} & C_{27} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} & C_{37} \end{pmatrix};$$

e.g., C_{23} is the dot product of two vectors, or in matrix notation:

$$C_{23} = \begin{pmatrix} A_{21} & A_{22} & A_{23} & A_{24} \end{pmatrix} \cdot \begin{pmatrix} B_{13} \\ B_{23} \\ B_{33} \\ B_{43} \end{pmatrix}$$
$$= A_{21}B_{13} + A_{22}B_{23} + A_{23}B_{33} + A_{24}B_{43}.$$

At this point, note the following:

- The result of matrix multiplication depends in general on whether one has $\boldsymbol{AB}$ or $\boldsymbol{BA}$; i.e., in general,[2] $\boldsymbol{AB} \neq \boldsymbol{BA}$.
- Matrix multiplication satisfies the following relation (which is easy to check): $\boldsymbol{A}(\boldsymbol{BC}) = (\boldsymbol{AB})\boldsymbol{C}$; i.e., the parentheses do not count and we can write simply: $\boldsymbol{ABC}$.
- Often we will have multiplication of a square matrix $\boldsymbol{A}$ by a matrix $\boldsymbol{B}$ composed of one column. Then, using the rule of matrix multiplication, we obtain the matrix $\boldsymbol{C}$ in the form of a single column (with the number of elements identical to the dimension of $\boldsymbol{A}$):

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1m} \\ A_{21} & A_{22} & \dots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mm} \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_m \end{pmatrix} = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_m \end{pmatrix}.$$

[2] Note, however, that it may be that $\boldsymbol{AB} = \boldsymbol{BA}$.

Transposed Matrix

For a given matrix $\boldsymbol{A}$, we may define the transposed matrix $\boldsymbol{A}^T$ as $(\boldsymbol{A}^T)_{ij} = \boldsymbol{A}_{ji}$.

For example, if $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ -2 & 3 \end{pmatrix}$, then $\boldsymbol{A}^T = \begin{pmatrix} 1 & -2 \\ 2 & 3 \end{pmatrix}$.

If matrix $\boldsymbol{A} = \boldsymbol{BC}$, then $\boldsymbol{A}^T = \boldsymbol{C}^T\boldsymbol{B}^T$; i.e., the order of multiplication is reversed. Indeed, $(\boldsymbol{C}^T\boldsymbol{B}^T)_{ij} = \sum_k (\boldsymbol{C}^T)_{ik}(\boldsymbol{B}^T)_{kj} = \sum_k \boldsymbol{C}_{ki}\boldsymbol{B}_{jk} = \sum_k \boldsymbol{B}_{jk}\boldsymbol{C}_{ki} = (\boldsymbol{BC})_{ji} = (\boldsymbol{A}^T)_{ij}$.

Inverse Matrix

For some square matrices $\boldsymbol{A}$ (which will be called non-singular), we can define the so-called inverse matrix as $\boldsymbol{A}^{-1}$, which has the property $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \mathbf{1}$, where $\mathbf{1}$ stands for the unit matrix:

$\mathbf{1} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix}$. E.g., for the matrix $\boldsymbol{A} = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$ we can find $\boldsymbol{A}^{-1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}$.

For square matrices, $\boldsymbol{A}\mathbf{1} = \mathbf{1}\boldsymbol{A} = \boldsymbol{A}$.

If we cannot find $\boldsymbol{A}^{-1}$ (because it does not exist), then $\boldsymbol{A}$ is called a *singular matrix*. For example, the matrix $\boldsymbol{A} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ is singular. The inverse matrix for $\boldsymbol{A} = \boldsymbol{BC}$ is $\boldsymbol{A}^{-1} = \boldsymbol{C}^{-1}\boldsymbol{B}^{-1}$. Indeed, $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{BC}\boldsymbol{C}^{-1}\boldsymbol{B}^{-1} = \boldsymbol{B}\mathbf{1}\boldsymbol{B}^{-1} = \boldsymbol{B}\boldsymbol{B}^{-1} = \mathbf{1}$.

Adjoint, Hermitian, Symmetric Matrices

If the matrix $\boldsymbol{A}$ is transposed and all its elements are changed to their complex conjugates, then we obtain the *adjoint matrix* denoted as $\boldsymbol{A}^\dagger = (\boldsymbol{A}^T)^* = (\boldsymbol{A}^*)^T$. If for a square matrix we have $\boldsymbol{A}^\dagger = \boldsymbol{A}$, then $\boldsymbol{A}$ is called *Hermitian*. If $\boldsymbol{A}$ is real, then, of course, $\boldsymbol{A}^\dagger = \boldsymbol{A}^T$. In addition, if for a real square matrix $\boldsymbol{A}^T = \boldsymbol{A}$, then $\boldsymbol{A}$ is called *symmetric*. Examples: $\boldsymbol{A} = \begin{pmatrix} 1+i & 3-2i \\ 2+i & 3-i \end{pmatrix}$;
$\boldsymbol{A}^T = \begin{pmatrix} 1+i & 2+i \\ 3-2i & 3-i \end{pmatrix}$; $\boldsymbol{A}^\dagger = \begin{pmatrix} 1-i & 2-i \\ 3+2i & 3+i \end{pmatrix}$.

Matrix $\boldsymbol{A} = \begin{pmatrix} 1 & -i \\ i & -2 \end{pmatrix}$ represents an example of a Hermitian matrix because $\boldsymbol{A}^\dagger = \boldsymbol{A}$. Matrix $\boldsymbol{A} = \begin{pmatrix} 1 & -5 \\ -5 & -2 \end{pmatrix}$ is a symmetric matrix.

Unitary and Orthogonal Matrices

If for a square matrix $\boldsymbol{A}$ we have $\boldsymbol{A}^\dagger = \boldsymbol{A}^{-1}$, then $\boldsymbol{A}$ is called a *unitary* matrix. If $\boldsymbol{B}$ is Hermitian, then the matrix $\exp(i\boldsymbol{B})$ is unitary, where we define $\exp(i\boldsymbol{B})$ by using the Taylor expansion:

$\exp(i\boldsymbol{B}) = \mathbf{1} + i\boldsymbol{B} + \frac{1}{2!}(i\boldsymbol{B})^2 + \cdots$. Indeed, $[\exp(i\boldsymbol{B})]^\dagger = \mathbf{1} - i\boldsymbol{B}^T + \frac{1}{2!}(-i\boldsymbol{B}^T)^2 + \cdots = \mathbf{1} - i\boldsymbol{B} + \frac{1}{2!}(-i\boldsymbol{B})^2 + \cdots = \exp(-i\boldsymbol{B})$, while $\exp(i\boldsymbol{B})\exp(-i\boldsymbol{B}) = \mathbf{1}$.

If $\boldsymbol{A}$ is a real unitary matrix $\boldsymbol{A}^\dagger = \boldsymbol{A}^T$, then it is called *orthogonal* with the property $\boldsymbol{A}^T = \boldsymbol{A}^{-1}$. For example if $\boldsymbol{A} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$, then $\boldsymbol{A}^T = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \boldsymbol{A}^{-1}$. Indeed, $\boldsymbol{A}\boldsymbol{A}^T = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

Determinants

Definition

For any square matrix $\boldsymbol{A} = \{A_{ij}\}$, we may calculate a number called its *determinant* and denoted by $\det \boldsymbol{A}$ or $|\boldsymbol{A}|$. The determinant is computed by using the Laplace expansion

$$\det \boldsymbol{A} = \sum_i^N (-1)^{i+j} A_{ij}\bar{A}_{ij} = \sum_j^N (-1)^{i+j} A_{ij}\bar{A}_{ij},$$

where (N is the dimension of the matrix). Here, the result does not depend on which column j has been chosen in the first expression or which row i is the second expression. The symbol $\bar{A}_{ij}$ stands for the determinant of the matrix, which is obtained from $\boldsymbol{A}$ by removing the ith row and the jth column. Thus, we have defined a determinant (of dimension N) by saying that it is a certain linear combination of determinants (of dimension $N-1$). It is sufficient, then, to tell what we mean by the determinant that contains only one number c (i.e., having only one row and one column); this is simply $\det\, c \equiv c$.

For example, the matrix $\boldsymbol{A} = \begin{pmatrix} 1 & 0 & -1 \\ 2 & 2 & 4 \\ 3 & -2 & -3 \end{pmatrix}$;

and the determinant

$$\det \boldsymbol{A} = \begin{vmatrix} 1 & 0 & -1 \\ 2 & 2 & 4 \\ 3 & -2 & -3 \end{vmatrix} = (-1)^{1+1} \times 1 \times \begin{vmatrix} 2 & 4 \\ -2 & -3 \end{vmatrix} + (-1)^{1+2} \times 0 \times \begin{vmatrix} 2 & 4 \\ 3 & -3 \end{vmatrix}$$
$$+ (-1)^{1+3} \times (-1) \times \begin{vmatrix} 2 & 2 \\ 3 & -2 \end{vmatrix} = \begin{vmatrix} 2 & 4 \\ -2 & -3 \end{vmatrix} - \begin{vmatrix} 2 & 2 \\ 3 & -2 \end{vmatrix}$$
$$= (2 \times (-3) - 4 \times (-2)) - (2 \times (-2) - 2 \times 3) = 2 + 10 = 12.$$

In particular, $\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc.$

By repeating (i.e., expanding $\bar{A}_{ij}$, etc.) the Laplace expansion again and again, we arrive finally at a linear combination of products of the elements:

$$\det \boldsymbol{A} = \sum_P (-1)^p \hat{P}[A_{1\mathbf{1}} A_{2\mathbf{2}} \cdots A_{N\boldsymbol{N}}],$$

where the permutation operator $\hat{P}$ pertains to the second indices (shown in bold), and p is the parity of the permutation $\hat{P}$.

Slater Determinant

In this book, we will most often be dealing with determinants of the matrices, whose elements are functions, not numbers. In particular, the most important will be the so-called Slater determinants. A Slater determinant for the N electron system is built of the functions called *spinorbitals* $\phi_i(j),\ i = 1, 2, \ldots, N$, where the *symbol* j means the space and spin coordinates $(x_j, y_j, z_j, \sigma_j)$ of electron j:

$$\psi(1, 2, \ldots, N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1) & \phi_1(2) & \ldots & \phi_1(N) \\ \phi_2(1) & \phi_2(2) & \ldots & \phi_2(N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(1) & \phi_N(2) & \ldots & \phi_N(N) \end{vmatrix}.$$

After that, the Laplace expansion gives

$$\psi(1, 2, \ldots, N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^p \hat{P}[\phi_1(1)\phi_2(2) \cdots \phi_N(N)],$$

where the summation is over $N!$ permutations of the N electrons, $\hat{P}$ stands for the permutation operator that acts on the *arguments* of the product of the spinorbitals $[\phi_1(1)\phi_2(2) \cdots \phi_N(N)]$, and p is the parity of the permutation $\hat{P}$ (i.e., the number of the transpositions that change $[\phi_1(1)\phi_2(2) \cdots \phi_N(N)]$ into $\hat{P}[\phi_1(1)\phi_2(2) \cdots \phi_N(N)]$.

All the properties of determinants also pertain to the Slater determinants.

Some Useful Properties

- $\det \boldsymbol{A}^T = \det \boldsymbol{A}$.
- From the Laplace expansion, it follows that if one of the spinorbitals is composed of two functions $\phi_i = \xi + \zeta$, then the Slater determinant is a sum of the two Slater determinants, one with ξ instead of ϕ_i, and the second with ζ instead of ϕ_i.
- If we add to a row (column) any linear combination of other rows (columns), the value of the determinant does not change.

- If a row (column) is a linear combination of other rows (columns), then det $\boldsymbol{A} = 0$. In particular, if two rows (columns) are identical, then det $\boldsymbol{A} = 0$. Conclusion: in a Slater determinant, the spinorbitals have to be linearly independent; otherwise, the Slater determinant equals zero.
- If in a matrix $\boldsymbol{A}$ we exchange two rows (columns), then det $\boldsymbol{A}$ changes the sign. Conclusion: the exchange of the coordinates of any two electrons leads to the change of the sign of the Slater determinant (the Pauli exclusion principle).
- $\det(\boldsymbol{AB}) = \det \boldsymbol{A} \quad \det \boldsymbol{B}$.
- From the Laplace expansion, it follows that multiplying the determinant by a number is equivalent to multiplying an arbitrary row (column) by this number. Therefore, $\det(c\boldsymbol{A}) = c^N \det \boldsymbol{A}$, where N is the matrix dimension.[3]
- If matrix $\boldsymbol{U}$ is unitary then $\det \boldsymbol{U} = \exp(i\phi)$, where ϕ is a real number. This means that if $\boldsymbol{U}$ is an orthogonal matrix, then $\det \boldsymbol{U} = \pm 1$.

[3] Note that to multiply a matrix by a number, we have to multiply every element of the matrix by this number. However, to multiply a determinant by a number means to multiply by this number of one row (column).