Appendix A

An *aide-mémoire* on matrices

A.1 Definitions and notation

An $m \times n$ *matrix* $\mathbf{A} = (A_{ij})$; $i = 1, \ldots, m$; $j = 1, \ldots, n$; is an ordered array of mn numbers, which may be complex:

$$\mathbf{A} = \begin{pmatrix} A_{11} A_{12} \ldots A_{1n} \\ A_{21} A_{22} \ldots \\ \ldots\ldots\ldots\ldots\ldots \\ A_{m1} \ldots \quad A_{mn} \end{pmatrix}.$$

A_{ij} is the *element* of the ith row and jth column.

The *complex conjugate* of $\mathbf{A}$, written $\mathbf{A}^*$, is defined by

$$\mathbf{A}^* = (A^*_{ij}).$$

The *transpose* of $\mathbf{A}$, written $\mathbf{A}^{\mathrm{T}}$, is the $n \times m$ matrix defined by

$$A^{\mathrm{T}}_{ji} = A_{ij}.$$

The *Hermitian conjugate*, or *adjoint*, of $\mathbf{A}$, written $\mathbf{A}^\dagger$, is defined by

$$A^\dagger_{jt} = A^*_{ij} = A^{\mathrm{T}}_{ji}{}^*, \text{ or equivalently by} \mathbf{A}^\dagger = (\mathbf{A}^{\mathrm{T}})^*.$$

If λ, μ are complex numbers and $\mathbf{A}, \mathbf{B}$ are $m \times n$ matrices, $\mathrm{C} = \lambda\mathbf{A} + \mu\mathbf{B}$ is defined by

$$C_{ij} = \lambda A_{ij} + \mu B_{ij}.$$

Multiplication of the $m \times n$ matrix $\mathbf{A}$ by an $n \times l$ matrix $\mathbf{B}$ is defined by $\mathbf{AB} = \mathbf{C}$, where $\mathbf{C}$ is the $m \times l$ matrix given by

$$C_{ik} = A_{ij} B_{jk}.$$

We use the Einstein convention, that a repeated 'dummy' suffix is understood to be summed over, so that

$$A_{ij} B_{jk} \text{ means } \sum_{j=1}^{n} A_{ij} B_{jk}.$$

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Multiplication is associative: $(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$. If follows immediately from the definitions that

$$(\mathbf{AB})^* = \mathbf{A}^*\mathbf{B}^*, \ (\mathbf{AB})^{\mathrm{T}} = \mathbf{B}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}, \ (\mathbf{AB})^{\dagger} = \mathbf{B}^{\dagger}\mathbf{A}^{\dagger}.$$

Block multiplication: matrices may be subdivided into blocks and multiplied by a rule similar to that for multiplication of elements, provided that the blocks are compatible. For example,

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \mathbf{F} \end{pmatrix} = \begin{pmatrix} \mathbf{AE} + \mathbf{BF} \\ \mathbf{CE} + \mathbf{DF} \end{pmatrix}$$

provided that the l_1 columns of $\mathbf{A}$ and l_2 columns of $\mathbf{B}$ are matched by l_1 rows of $\mathbf{E}$ and l_2 rows of $\mathbf{F}$. The proof follows from writing out the appropriate sums.

A.2 Properties of $n \times n$ matrices

We now focus on 'square' $n \times n$ matrices. If $\mathbf{A}$ and $\mathbf{B}$ are $n \times n$ matrices, we can construct both $\mathbf{AB}$ and $\mathbf{BA}$. In general, matrix multiplication is non-commutative, i.e. in general, $\mathbf{AB} \neq \mathbf{BA}$.

The $n \times n$ *identity matrix* or *unit matrix* I is defined by $I_{ij} = \delta_{ij}$, where δ_{ij} is the Kronecker δ:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

From the rule for multiplication,

$$\mathbf{IA} = \mathbf{AI} = \mathbf{A}$$

for any $\mathbf{A}$. $\mathbf{A}$ is said to be *diagonal* if $A_{ij} = 0$ for $i \neq j$.

Determinants: with a square matrix $\mathbf{A}$ we can associate the *determinant* of $\mathbf{A}$, denoted by $\det \mathbf{A}$ or $|A_{ij}|$, and defined by

$$\det \mathbf{A} = \varepsilon_{ij\ldots t} A_{1i} A_{2j} \ldots A_{nt}$$

(remember the summation convention) where

$$\varepsilon_{ij\ldots t} = \begin{cases} 1 & \text{if } i, j, \ldots, t \text{ is an even permutation of } 1, 2, \ldots, n, \\ -1 & \text{if } i, j, \ldots, t \text{ is an odd permutation of } 1, 2, \ldots, n, \\ 0 & \text{otherwise.} \end{cases}$$

An important result is

$$\det(\mathbf{AB}) = \det \mathbf{A} \det \mathbf{B}.$$

Note also

$$\det \mathbf{A}^{\mathrm{T}} = \det \mathbf{A}, \quad \det \mathbf{I} = 1.$$

If $\det \mathbf{A} \neq 0$ the matrix $\mathbf{A}$ is said to be *non-singular*, and $\det \mathbf{A} \neq \mathbf{0}$ is a necessary and sufficient condition for a unique inverse $\mathbf{A}^{-1}$ to exist, such that

$$\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}.$$

Evidently,

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}.$$

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The trace of a matrix **A**, written Tr**A**, is the sum of its diagonal elements:

$$\mathrm{Tr}\mathbf{A} = A_{ii}.$$

It follows from the definition that

$$\mathrm{Tr}(\mathbf{AB}) = A_{ij}B_{ji} = B_{ji}A_{ij} = \mathrm{Tr}(\mathbf{BA}),$$

and hence

$$\mathrm{Tr}(\mathbf{ABC}) = \mathrm{Tr}(\mathbf{BCA}) = \mathrm{Tr}(\mathbf{CAB}).$$

A.3 Hermitian and unitary matrices

Hermitian and unitary matrices are square matrices of particular importance in quantum mechanics. In a matrix formulation of quantum mechanics, dynamical observables are represented by Hermitian matrices, while the time development of a system is determined by a unitary matrix.

A matrix **H** is *Hermitian* if it is equal to its Hermitian conjugate:

$$\mathbf{H} = \mathbf{H}^\dagger, \quad \text{or} \quad H_{ij} = H^*_{ji}.$$

The diagonal elements of a Hermitian matrix are therefore real, and an $n \times n$ Hermitian matrix is specified by $n + 2n(n-1)/2 = n^2$ real numbers.

A matrix **U** is *unitary* if

$$\mathbf{U}^{-1} = \mathbf{U}^\dagger, \quad \text{or} \quad \mathbf{UU}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbf{I}.$$

The product of two unitary matrices is also unitary.

A *unitary transformation* of a matrix **A** is a transformation of the form

$$\mathbf{A} \to \mathbf{A}' = \mathbf{UAU}^{-1} = \mathbf{UAU}^\dagger,$$

where **U** is a unitary matrix. The transformation preserves algebraic relationships:

$$(\mathbf{AB})' = \mathbf{A}'\mathbf{B}',$$

and Hermitian conjugation

$$(\mathbf{A}')^\dagger = \mathbf{UA}^\dagger\mathbf{U}^\dagger.$$

Also

$$\mathrm{Tr}\mathbf{A}' = \mathrm{Tr}\mathbf{A}, \quad \det\mathbf{A}' = \det\mathbf{A}.$$

An important theorem of matrix algebra is that, for each Hermitian matrix **H**, there exists a unitary matrix **U** such that

$$\mathbf{H}' = \mathbf{UHU}^{-1} = \mathbf{UHU}^\dagger = \mathbf{H}_D$$

is a real diagonal matrix.

A necessary and sufficient condition that Hermitian matrices $\mathbf{H}_1$ and $\mathbf{H}_2$ can be brought into the diagonal form by the same unitary transformation is

$$\mathbf{H}_1\mathbf{H}_2 - \mathbf{H}_2\mathbf{H}_1 = 0.$$

It follows from this (see Problem A.3) that a matrix **M** can be brought into diagonal form by a unitary transformation if and only if

$$\mathbf{MM}^\dagger - \mathbf{M}^\dagger\mathbf{M} = 0.$$

Note that unitary matrices satisfy this condition.

An arbitrary matrix **M** which does not satisfy this condition can be brought into real diagonal form by a generalised transformation involving two unitary matrices, $\mathbf{U}_1$ and $\mathbf{U}_2$ say, which may be chosen so that

$$\mathbf{U}_1\mathbf{M}\mathbf{U}_2^\dagger = \mathbf{M}_D$$

is diagonal (see Problem A.4).

If **H** is a Hermitian matrix, the matrix

$$\mathbf{U} = \exp(\mathrm{i}\mathbf{H})$$

is unitary. The right-hand side of this equation is to be understood as defined by the series expansion

$$\mathbf{U} = \mathbf{I} + (\mathrm{i}\mathbf{H}) + (\mathrm{i}\mathbf{H})^2/2! + \cdots$$

Then

$$\begin{aligned}\mathbf{U}^\dagger &= \mathbf{I} + (-\mathrm{i}\mathbf{H}^\dagger) + (-\mathrm{i}\mathbf{H}^\dagger)^2/2! + \cdots \\ &= \exp(-\mathrm{i}\mathbf{H}^\dagger) = \exp(-\mathrm{i}\mathbf{H}) = \mathbf{U}^{-1}\end{aligned}$$

(the operation of Hermitian conjugation being carried out term by term). Conversely, any unitary matrix **U** can be expressed in this form. Since an $n \times n$ Hermitian matrix is specified by n^2 real numbers, it follows that a unitary matrix is specified by n^2 real numbers.

A.4 A Fierz transformation

It is easy to show that any 2×2 matrix **M** with complex elements may be expressed as a linear combination of the matrices $\widetilde{\sigma}^\mu$.

$$\mathbf{M} = Z_\mu \widetilde{\sigma}^\mu,$$

and $\mathrm{Z}_\mu = \frac{1}{2}\mathrm{Tr}\,(\widetilde{\sigma}^\mu \mathbf{M})$, since $\mathrm{Tr}\,(\widetilde{\sigma}^\mu\widetilde{\sigma}^\nu) = 2\delta_{\mu\nu}$.

Consider the expression $g_{\mu\nu}\langle a^*|\widetilde{\sigma}^\mu|b\rangle\langle c^*|\widetilde{\sigma}^\nu|d\rangle$, where $|a\rangle$, $|b\rangle$, $|c\rangle$, $|d\rangle$ are two-component spinor fields. Using the result above, we can replace the matrix $|b\rangle\langle c^*|$ by

$$\begin{aligned}|b\rangle\langle c^*| &= \frac{1}{2}Tr(\widetilde{\sigma}^\lambda|b\rangle\langle c^*|)\widetilde{\sigma}^\lambda \\ &= -\frac{1}{2}\langle c^*|\widetilde{\sigma}^\lambda|b\rangle\widetilde{\sigma}^\lambda.\end{aligned}$$

The last step is evident on putting in the spinors indices, and the minus sign arises from the interchange of anticommuting spinor fields.

We now have

$$g_{\mu\nu}\langle a^*|\widetilde{\sigma}^\mu|b\rangle\langle c^*|\widetilde{\sigma}^\nu|d\rangle = -\frac{1}{2}g_{\mu\nu}\langle a^*|\widetilde{\sigma}^\mu\widetilde{\sigma}^\lambda\widetilde{\sigma}^\nu|d >< c^*|\widetilde{\sigma}^\lambda|b\rangle.$$

Using the algebraic identity

$$g_{\mu\nu}\widetilde{\sigma}^\mu\widetilde{\sigma}^\lambda\widetilde{\sigma}^\nu = -2g_{\rho\lambda}\widetilde{\sigma}^\rho,$$

gives $g_{\mu\nu}\langle a^*|\widetilde{\sigma}^\mu|b\rangle\langle c^*|\widetilde{\sigma}^\nu|d\rangle = g_{\rho\lambda}\langle a^*|\widetilde{\sigma}^\rho|d\rangle\langle c^*|\widetilde{\sigma}^\lambda|b\rangle$.

This is an example of a *Fierz transformation.*

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Problems

A.1 Show that

$$\varepsilon_{ij\ldots t} A_{\alpha i} A_{\beta j} \cdots A_{\nu t} = \varepsilon_{\alpha\beta\ldots\nu} \det \mathbf{A}.$$

A.2 Show that if $\mathbf{A}, \mathbf{B}$ are Hermitian, then $\mathrm{i}(\mathbf{AB} - \mathbf{BA})$ is Hermitian.

A.3 Show that an arbitrary square matrix $\mathbf{M}$ can be written in the form $\mathbf{M} = \mathbf{A} + \mathrm{i}\mathbf{B}$, where $\mathbf{A}$ and $\mathbf{B}$ are Hermitian matrices. Find $\mathbf{A}$ and $\mathbf{B}$ in terms of $\mathbf{M}$ and $\mathbf{M}^\dagger$. Hence show that $\mathbf{M}$ may be put into diagonal form by a unitary transformation if and only if $\mathbf{M}\mathbf{M}^\dagger - \mathbf{M}^\dagger\mathbf{M} = 0$.

A.4 If $\mathbf{M}$ is an arbitrary square matrix, show that $\mathbf{M}\mathbf{M}^\dagger$ is Hermitian and hence can be diagonalised by a unitary matrix $\mathbf{U}_1$, so that we can write

$$\mathbf{U}_1(\mathbf{M}\mathbf{M}^\dagger)\mathbf{U}_1{}^\dagger = \mathbf{M}_D{}^2$$

where $\mathbf{M}_D$ is diagonal with real diagonal elements ≥ 0. Suppose none are zero. Define the Hermitian matrix $\mathbf{H} = \mathbf{U}_1{}^\dagger \mathbf{M}_D \mathbf{U}_1$. Show that $\mathbf{V} = \mathbf{H}^{-1}\mathbf{M}$ is unitary. Hence show that

$$\mathbf{M} = \mathbf{U}_1{}^\dagger \mathbf{M}_D \mathbf{U}_2,$$

where $\mathbf{U}_2 = \mathbf{U}_1\mathbf{V}$ is a unitary matrix.