Appendix A
Linear algebra basics

A.1 Linear spaces

Linear spaces consist of elements called *vectors*. Vectors are abstract mathematical objects, but, as the name suggests, they can be visualized as geometric vectors. Like regular numbers, vectors can be added together and subtracted from each other to form new vectors; they can also be multiplied by numbers. However, vectors cannot be multiplied or divided by one another as numbers can.

One important peculiarity of the linear algebra used in quantum mechanics is the so-called *Dirac notation* for vectors. To denote vectors, instead of writing, for example, $\vec{a}$, we write $|a\rangle$. We shall see later how convenient this notation turns out to be.

Definition A.1. A *linear (vector) space* $\mathbb{V}$ over a field[1] $\mathbb{F}$ is a set in which the following operations are defined:

1. Addition: for any two vectors $|a\rangle, |b\rangle \in \mathbb{V}$, there exists a unique vector in $\mathbb{V}$ called their sum, denoted by $|a\rangle + |b\rangle$.
2. Multiplication by a number ("scalar"): For any vector $|a\rangle \in \mathbb{V}$ and any number $\lambda \in \mathbb{F}$, there exists a unique vector in $\mathbb{V}$ called their product, denoted by $\lambda |a\rangle \equiv |a\rangle \lambda$.

These operations obey the following *axioms*.

1. Commutativity of addition: $|a\rangle + |b\rangle = |b\rangle + |a\rangle$.
2. Associativity of addition: $(|a\rangle + |b\rangle) + |c\rangle = |a\rangle + (|b\rangle + |c\rangle)$.
3. Existence of zero: there exists an element of $\mathbb{V}$ called $|\text{zero}\rangle$ such that, for any vector $|a\rangle$, $|a\rangle + |\text{zero}\rangle = |a\rangle$.[2]

A solutions manual for this appendix is available for download at
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[1] *Field* is a term from algebra which means a complete set of numbers. The sets of rational numbers $\mathbb{Q}$, real numbers $\mathbb{R}$, and complex numbers $\mathbb{C}$ are examples of fields. Quantum mechanics usually deals with vector spaces over the field of complex numbers.

[2] As an alternative notation for $|\text{zero}\rangle$, we some times use "0" but *not* "$|0\rangle$".

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4. Existence of the opposite element: For any vector $|a\rangle$ there exists another vector, denoted by $-|a\rangle$, such that $|a\rangle + (-|a\rangle) = |\text{zero}\rangle$.
5. Distributivity of vector sums: $\lambda(|a\rangle + |b\rangle) = \lambda|a\rangle + \lambda|b\rangle$.
6. Distributivity of scalar sums: $(\lambda + \mu)|a\rangle = \lambda|a\rangle + \mu|a\rangle$.
7. Associativity of scalar multiplication: $\lambda(\mu|a\rangle) = (\lambda\mu)|a\rangle$.
8. Scalar multiplication identity: For any vector $|a\rangle$ and number $1 \in \mathbb{F}$, $1 \cdot |a\rangle = |a\rangle$.

Definition A.2. *Subtraction* of vectors in a linear space is defined as follows:

$$|a\rangle - |b\rangle \equiv |a\rangle + (-|b\rangle).$$

Exercise A.1. Which of the following are linear spaces (over the field of complex numbers, unless otherwise indicated)?

a) $\mathbb{R}$ over $\mathbb{R}$? $\mathbb{R}$ over $\mathbb{C}$? $\mathbb{C}$ over $\mathbb{R}$? $\mathbb{C}$ over $\mathbb{C}$?
b) Polynomial functions? Polynomial functions of degree $\leq n$? $> n$?
c) All functions such that $f(1) = 0$? $f(1) = 1$?
d) All periodic functions of period T?
e) N-dimensional geometric vectors over $\mathbb{R}$?

Exercise A.2. Prove the following:

a) there is only one zero in a linear space;
b) if $|a\rangle + |x\rangle = |a\rangle$ for some $|a\rangle \in \mathbb{V}$, then $|x\rangle = |\text{zero}\rangle$;
c) for any vector $|a\rangle$ and for number $0 \in \mathbb{F}$, $0|a\rangle = |\text{zero}\rangle$;
d) $-|a\rangle = (-1)|a\rangle$;
e) $-|\text{zero}\rangle = |\text{zero}\rangle$;
f) for any $|a\rangle$, $-|a\rangle$ is unique;
g) $-(-|a\rangle) = |a\rangle$;
h) $|a\rangle = |b\rangle$ if and only if $|a\rangle - |b\rangle = 0$.

Hint: Most of these propositions can be proved by adding the same number to the two sides of an equality.

A.2 Basis and dimension

Definition A.3. A set of vectors $|v_i\rangle$ is said to be *linearly independent* if no nontrivial[2] *linear combination* $\lambda_1|v_1\rangle + \ldots + \lambda_N|v_N\rangle$ equals $|\text{zero}\rangle$.

Exercise A.3. Show that a set of vectors $\{|v_i\rangle\}$ is *not* linearly independent if and only if one of the $|v_i\rangle$ can be represented as a linear combination of others.

Exercise A.4. For linear spaces of geometric vectors, show the following:

a) For the space of vectors in a plane (denoted $\mathbb{R}^3$), any two vectors are linearly independent if and only if they are not parallel. Any set of three vectors is linearly dependent.

[3] That is, in which at least one of the coefficients is nonzero.

b) For the space of vectors in a three-dimensional space (denoted $\mathbb{R}^4$), any three non-coplanar vectors form a linearly independent set.

Hint: Recall that a geometric vector can be defined by its x, y and z components.

Definition A.4. A subset $\{|v_i\rangle\}$ of a vector space $\mathbb{V}$ is said to *span* $\mathbb{V}$ (or to be a *spanning set* for $\mathbb{V}$) if any vector in $\mathbb{V}$ can be expressed as a linear combination of the $|v_i\rangle$.

Exercise A.5. For the linear space of geometric vectors in a plane, show that any set of at least two vectors, of which at least two are non-parallel, forms a spanning set.

Definition A.5. A *basis* of $\mathbb{V}$ is any linearly independent spanning set. A *decomposition* of a vector relative to a basis is its expression as a linear combination of the basis elements.

The basis is a smallest subset of a linear space such that all other vectors can be expressed as a linear combination of the basis elements. The term "basis" may suggest that each linear space has only one basis — just as a building can have only one foundation. Actually, as we shall see, in any nontrivial linear space, there are infinitely many bases.

Definition A.6. The number of elements in a basis is called the *dimension* of $\mathbb{V}$. Notation: $\dim\mathbb{V}$.

Exercise A.6.* Prove that in a finite-dimensional space, all bases have the same number of elements.

Exercise A.7. Using the result of Ex. A.6, show that, in a finite-dimensional space,

a) any linearly independent set of $N = \dim\mathbb{V}$ vectors forms a basis;
b) any spanning set of $N = \dim\mathbb{V}$ vectors forms a basis.

Exercise A.8. Show that, for any element of $\mathbb{V}$, there exists only one decomposition into basis vectors.

Definition A.7. For a decomposition of the vector $|a\rangle$ into basis $\{|v_i\rangle\}$, viz.,

$$|a\rangle = \sum_i a_i |v_i\rangle\,, \tag{A.1}$$

we may use the notation

$$|a\rangle \simeq \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}. \tag{A.2}$$

This is called the *matrix form* of a vector, in contrast to the Dirac form (A.1). The scalars a_i are called the *coefficients* or *amplitudes* of the decomposition[3].

[4] We use the symbol $\simeq$ instead of $=$ when expressing vectors and operators in matrix form, e.g., in Eq. (A.2). This is to emphasize the difference: the left-hand side, a vector, is an abstract object

Exercise A.9. Let $|a\rangle$ be one of the elements, $|v_k\rangle$, of the basis $\{|v_i\rangle\}$. Find the matrix form of the decomposition of $|a\rangle$ into this basis.

Exercise A.10. Consider the linear space of two-dimensional geometric vectors. Such vectors are usually defined by two numbers (x,y), which correspond to their x and y components, respectively. Does this notation correspond to a decomposition into any basis? If so, which one?

Exercise A.11. Show the following:

a) For the linear space of geometric vectors in a plane, any two non-parallel vectors form a basis.
b) For the linear space of geometric vectors in a three-dimensional space, any three non-coplanar vectors form a basis.

Exercise A.12. Consider the linear space of two-dimensional geometric vectors. The vectors $\vec{a},\vec{b},\vec{c},\vec{d}$ are oriented with respect to the x axis at angles $0, 45^\circ, 90^\circ, 180^\circ$ and have lengths $2,1,3,1$, respectively. Do the pairs $\{\vec{a},\vec{c}\}$, $\{\vec{b},\vec{d}\}$, $\{\vec{a},\vec{d}\}$ form bases? Find the decompositions of the vector $\vec{b}$ in each of these bases. Express them in the matrix form.

Definition A.8. A subset of a linear space $\mathbb{V}$ that is a linear space on its own is called a *subspace* of $\mathbb{V}$.

Exercise A.13. In an arbitrary basis $\{|v_i\rangle\}$ in the linear space $\mathbb{V}$, a subset of elements is taken. Show that a set of vectors that are spanned by this subset is a subspace of $\mathbb{V}$.

For example, in the space of three-dimensional geometric vectors, any set of vectors within a particular plane or any set of vectors collinear to a given straight line form a subspace.

A.3 Inner Product

Although vectors cannot be multiplied together in the same way that numbers can, one can define a multiplication operation that maps any pair of vectors onto a number. This operation generalizes the scalar product that is familiar from geometry.

Definition A.9. For any two vectors $|a\rangle$, $|b\rangle \in \mathbb{V}$ we define an *inner (scalar) product*[5] — a number $\langle a|\, b\rangle \in \mathbb{C}$ such that:

1. For any three vectors $|a\rangle, |b\rangle, |c\rangle$, $\langle a|\,(|b\rangle + |c\rangle) = \langle a|\, b\rangle + \langle a|\, c\rangle$.
2. For any two vectors $|a\rangle, |b\rangle$ and number λ, $\langle a|\,(\lambda\,|b\rangle) = \lambda\,\langle a|\, b\rangle$.

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and is basis-independent, while the right-hand side is a set of numbers and depends on the choice of basis $\{|v_i\rangle\}$. However, in the literature, the equality sign is generally used for simplicity.

[5] The inner product of two vectors is sometimes called the *overlap* in the context of quantum physics.

3. For any two vectors $|a\rangle, |b\rangle$, $\langle a|\, b\rangle = \langle b|\, a\rangle^*$.
4. For any $|a\rangle$, $\langle a|\, a\rangle$ is a nonnegative real number, and $\langle a|\, a\rangle = 0$ if and only if $|a\rangle = 0$.

Exercise A.14. In geometry, the scalar product of two vectors $\vec{a} = (x_a, y_a)$ and $\vec{b} = (x_b, y_b)$ (where all components are real) is defined as $\vec{a} \cdot \vec{b} = x_a x_b + y_a y_b$. Show that this definition has all the properties listed above.

Exercise A.15. Suppose a vector $|x\rangle$ is written as a linear combination of some vectors $|a_i\rangle$: $|x\rangle = \sum_i \lambda_i |a_i\rangle$. For any other vector $|b\rangle$, show that $\langle b|\, x\rangle = \sum_i \lambda_i \langle b|\, a_i\rangle$ and $\langle x|\, b\rangle = \sum_i \lambda_i^* \langle a_i|\, b\rangle$.

Exercise A.16. For any vector $|a\rangle$, show that $\langle \text{zero}|\, a\rangle = \langle a|\, \text{zero}\rangle = 0$.

Definition A.10. $|a\rangle$ and $|b\rangle$ are said to be *orthogonal* if $\langle a|\, b\rangle = 0$.

Exercise A.17. Prove that a set of nonzero mutually orthogonal vectors is linearly independent.

Definition A.11. $\|\, |a\rangle \,\| = \sqrt{\langle a|\, a\rangle}$ is called the *norm (length)* of a vector. Vectors of norm 1 are said to be *normalized*. For a given vector $|a\rangle$, the quantity $\mathcal{N} = 1/\|\, |a\rangle \,\|$ (such that the vector $\mathcal{N}\, |a\rangle$ is normalized) is called the *normalization factor*.

Exercise A.18. Show that multiplying a vector by a *phase factor* $e^{i\phi}$, where ϕ is a real number, does not change its norm.

Definition A.12. A linear space in which an inner product is defined is called a *Hilbert space*.

A.4 Orthonormal Basis

Definition A.13. An *orthonormal basis* $\{|v_i\rangle\}$ is a basis whose elements are mutually orthogonal and have norm 1, i.e.,

$$\langle v_i|\, v_j\rangle = \delta_{ij}, \tag{A.3}$$

where δ_{ij} is the Kronecker symbol.

Exercise A.19. Show that any orthonormal set of N (where $N = \dim \mathbb{V}$) vectors forms a basis.

Exercise A.20. Show that, if $\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$ and $\begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix}$ are the decompositions of vectors $|a\rangle$ and $|b\rangle$ in an orthonormal basis, their inner product can be written in the form

$$\langle a|\, b\rangle = a_1^* b_1 + \ldots + a_N^* b_N. \tag{A.4}$$

Equation (A.4) can be expressed in matrix form using the "row-times-column" rule:

$$\langle a|\, b\rangle = \begin{pmatrix} a_1^* & \dots & a_N^* \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix}. \tag{A.5}$$

One context where we can use the above equations for calculating the inner product is ordinary spatial geometry. As we found in Ex. A.10, the coordinates of geometric vectors correspond to their decomposition into orthogonal basis $\{\hat{i}, \hat{j}\}$, so not surprisingly, their scalar products are given by Eq. (A.4).

Suppose we calculate the inner product of the same pair of vectors using Eq. (A.5) in two different bases. Then the right-hand side of that equation will contain different numbers, so it may seem that the inner product will also depend on the basis chosen. This is not the case, however: according to Defn. A.9, the inner product is defined for a pair of vectors, and is basis-independent.

Exercise A.21. Show that the amplitudes of the decomposition $\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$ of a vector $|a\rangle$ into an orthonormal basis can be found as follows:

$$a_i = \langle v_i|\, a\rangle\,. \tag{A.6}$$

In other words [see Eq. (A.1)],

$$|a\rangle = \sum_i \langle v_i|\, a\rangle\, |v_i\rangle\,. \tag{A.7}$$

Exercise A.22. Consider two vectors in a two-dimensional Hilbert space, $|\psi\rangle = 4\,|v_1\rangle + 5\,|v_2\rangle$ and $|\phi\rangle = -2\,|v_1\rangle + 3\mathrm{i}\,|v_2\rangle$, where $\{|v_1\rangle\,, |v_2\rangle\}$ is an orthonormal basis.

a) Show that the set $\{|w_1\rangle = (|v_1\rangle + \mathrm{i}\,|v_2\rangle)/\sqrt{2}, |w_2\rangle = (|v_1\rangle - \mathrm{i}\,|v_2\rangle)/\sqrt{2}\}$ is also an orthonormal basis.
b) Find the matrices of vectors $|\psi\rangle$ and $|\phi\rangle$ in both bases.
c) Calculate the inner product of these vectors in both bases using Eq. (A.5). Show that they are the same.

Exercise A.23. Show that, if $|a\rangle$ is a normalized vector and $\{a_i = \langle v_i|\, a\rangle\}$ is its decomposition in an orthonormal basis $\{|v_i\rangle\}$, then

$$\sum_i |a_i|^2 = 1. \tag{A.8}$$

Exercise A.24. Suppose $\{|w_i\rangle\}$ is some basis in $\mathbb{V}$. It can be used to find an orthonormal basis $\{|v_i\rangle\}$ by applying the following equation in sequence to each basis element:

$$|v_{k+1}\rangle = \mathcal{N}\left[|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i|\, w_{k+1}\rangle\, |v_i\rangle\right], \tag{A.9}$$

where $\mathcal{N}$ is the normalization factor. This is called the *Gram-Schmidt procedure*.

Exercise A.25.* For a normalized vector $|\psi\rangle$ in an N-dimensional Hilbert space, and any natural number $m \le N$, show that it is possible to find a basis $\{|v_i\rangle\}$ such that $|\psi\rangle = 1/\sqrt{m}\sum_{i=1}^{m}|v_i\rangle$.

Exercise A.26.* Prove the *Cauchy-Schwarz inequality* for any two vectors $|a\rangle$ and $|b\rangle$:

$$|\langle a|\, b\rangle| \le \| \, |a\rangle \, \| \times \| \, |b\rangle \, \|. \tag{A.10}$$

Show that the inequality is saturated (i.e., becomes an equality) if and only if the vectors $|a\rangle$ and $|b\rangle$ are collinear (i.e., $|a\rangle = \lambda\,|b\rangle$).
Hint: Use the fact that $\| \, |a\rangle - \lambda\,|b\rangle \, \|^2 \ge 0$ for any complex number λ.

Exercise A.27. Prove the *triangle inequality* for any two vectors $|a\rangle$ and $|b\rangle$:

$$\|(|a\rangle + |b\rangle)\| \le \| \, |a\rangle \, \| + \| \, |b\rangle \, \|. \tag{A.11}$$

A.5 Adjoint Space

The scalar product $\langle a|\, b\rangle$ can be calculated as a matrix product (A.5) of a row and a column. While the column $\begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix}$ corresponds directly to the vector $|b\rangle$, the row $\begin{pmatrix} a_1^* & \dots & a_N^* \end{pmatrix}$ is obtained from the column corresponding to vector $|a\rangle$ by transposition and complex conjugation. Let us introduce a convention associating this row with the vector $\langle a|$, which we call the *adjoint* of $|a\rangle$.

Definition A.14. For the Hilbert space $\mathbb{V}$, we define the *adjoint space* $\mathbb{V}^\dagger$ (read "V-dagger"), which is in one-to-one correspondence with $\mathbb{V}$, in the following way: for each vector $|a\rangle \in \mathbb{V}$, there is one and only one *adjoint* vector $\langle a| \in \mathbb{V}^\dagger$ with the property

$$\text{Adjoint}(\lambda\,|a\rangle + \mu\,|b\rangle) = \lambda^*\,\langle a| + \mu^*\,\langle b|\,. \tag{A.12}$$

Exercise A.28. Show that $\mathbb{V}^\dagger$ is a linear space.

Exercise A.29. Show that if $\{|v_i\rangle\}$ is a basis in $\mathbb{V}$, $\{\langle v_i|\}$ is a basis in $\mathbb{V}^\dagger$, and if the vector $|a\rangle$ is decomposed into $\{|v_i\rangle\}$ as $|a\rangle = \sum a_i\,|v_i\rangle$, the decomposition of its adjoint is

$$\langle a| = \sum a_i^*\,\langle v_i|\,. \tag{A.13}$$

Exercise A.30. Find the matrix form of the vector adjoint to $|v_1\rangle + \mathrm{i}\,|v_2\rangle$ in the basis $\{\langle v_1|\,, \langle v_2|\}$.

"Direct" and adjoint vectors are sometimes called *ket* and *bra* vectors, respectively. The rationale behind this terminology, introduced by P. Dirac together with the symbols $\langle|$ and $|\rangle$, is that the bra-ket combination of the form $\langle a|\,b\rangle$, a "bracket", gives the inner product of the two vectors.

Note that $\mathbb{V}$ and $\mathbb{V}^\dagger$ are different linear spaces. We cannot add a bra-vector and a ket-vector.

A.6 Linear Operators

A.6.1 Operations with linear operators

Definition A.15. A *linear operator* $\hat{A}$ on a linear space $\mathbb{V}$ is a map[6] of linear space $\mathbb{V}$ onto itself such that, for any vectors $|a\rangle$, $|b\rangle$ and any scalar λ

$$\hat{A}(|a\rangle + |b\rangle) = \hat{A}\,|a\rangle + \hat{A}\,|b\rangle\,; \tag{A.14a}$$

$$\hat{A}(\lambda\,|a\rangle) = \lambda\hat{A}\,|a\rangle\,. \tag{A.14b}$$

Exercise A.31. Decide whether the following maps are linear operators[7]:

a) $\hat{A}\,|a\rangle \equiv 0$.
b) $\hat{A}\,|a\rangle = |a\rangle$.
c) $\mathbb{C}^2 \to \mathbb{C}^2 : \hat{A}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ -y \end{pmatrix}$.
d) $\mathbb{C}^2 \to \mathbb{C}^2 : \hat{A}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x+y \\ xy \end{pmatrix}$.
e) $\mathbb{C}^2 \to \mathbb{C}^2 : \hat{A}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x+1 \\ y+1 \end{pmatrix}$.
f) Rotation by angle ϕ in the linear space of two-dimensional geometric vectors (over $\mathbb{R}$).

Definition A.16. For any two operators $\hat{A}$ and $\hat{B}$, their sum $\hat{A}+\hat{B}$ is an operator that maps vectors according to

$$(\hat{A}+\hat{B})\,|a\rangle \equiv \hat{A}\,|a\rangle + \hat{B}\,|a\rangle\,. \tag{A.15}$$

For any operator $\hat{A}$ and any scalar λ, their product $\lambda\hat{A}$ is an operator that maps vectors according to

$$(\lambda\hat{A})\,|a\rangle \equiv \lambda(\hat{A}\,|a\rangle). \tag{A.16}$$

Exercise A.32. Show that the set of all linear operators over a Hilbert space of dimension N is itself a linear space, with the addition and multiplication by a scalar given by Eqs. (A.15) and (A.16), respectively.

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[6] A *map* is a function that establishes, for every element *keta* in $\mathbb{V}$, a unique "image" $\hat{A}\,|a\rangle$.

[7] $\mathbb{C}^2$ is the linear space of columns $\begin{pmatrix} x \\ y \end{pmatrix}$ consisting of two complex numbers.

a) Show that the operators $\hat{A}+\hat{B}$ and $\lambda\hat{A}$ are linear in the sense of Defn. A.15.
b) In the space of liner operators, what is the zero element and the opposite element $-\hat{A}$ for a given $\hat{A}$?
c)[§] Show that the space of linear operators complies with all the axioms introduced in Definition A.1.

Definition A.17. The operator $\hat{\mathbf{1}}$ that maps every vector in $\mathbb{V}$ onto itself is called the *identity operator*.

When writing products of a scalar with identity operators, we sometimes omit the symbol $\hat{\mathbf{1}}$, provided that the context allows no ambiguity. For example, instead of writing $\hat{A}-\lambda\hat{\mathbf{1}}$, we may simply write $\hat{A}-\lambda$.

Definition A.18. For operators $\hat{A}$ and $\hat{B}$, their *product* $\hat{A}\hat{B}$ is an operator that maps every vector $|a\rangle$ onto $\hat{A}\hat{B}|a\rangle \equiv \hat{A}(\hat{B}|a\rangle)$. That is, in order to find the action of the operator $\hat{A}\hat{B}$ on a vector, we must first apply $\hat{B}$ to that vector, and then apply $\hat{A}$ to the result.

Exercise A.33. Show that a product of two linear operators is a linear operator.

It does matter in which order the two operators are multiplied, i.e., generally $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. Operators for which $\hat{A}\hat{B}=\hat{B}\hat{A}$ are said to *commute*. Commutation relations between operators play an important role in quantum mechanics, and will be discussed in detail in Sec. A.9.

Exercise A.34. Show that the operators of counterclockwise rotation by angle $\pi/2$ and reflection about the horizontal axis in the linear space of two-dimensional geometric vectors do not commute.

Exercise A.35. Show that multiplication of operators has the property of associativity, i.e., for any three operators, one has

$$\hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}. \tag{A.17}$$

A.6.2 Matrices

It may appear that, in order to fully describe a linear operator, we must say what it does to every vector. However, this is not the case. In fact, it is enough to say how the operator maps the elements of some basis $\{|v_1\rangle,\ldots,|v_N\rangle\}$ in $\mathbb{V}$, i.e., it is enough to know the set $\{\hat{A}|v_1\rangle,\ldots,\hat{A}|v_N\rangle\}$. Then, for any other vector $|a\rangle$, which can be decomposed as

$$|a\rangle = a_1|v_1\rangle+\ldots+a_N|v_N\rangle,$$

we have, thanks to linearity,

$$\hat{A}|a\rangle = a_1\hat{A}|v_1\rangle+\ldots+a_N\hat{A}|v_N\rangle. \tag{A.18}$$

How many numerical parameters does one need to completely characterize a linear operator? Each image $\hat{A}\left|v_j\right\rangle$ of a basis element can be decomposed into the same basis:

$$\hat{A}\left|v_j\right\rangle = \sum_i A_{ij}\left|v_i\right\rangle. \tag{A.19}$$

For every j, the set of N parameters $A_{1j},\ldots,A_{Nj}$ fully describes $\hat{A}\left|v_j\right\rangle$. Accordingly, the set of N^2 parameters A_{ij}, with both i and j varying from 1 to N, contains full information about a linear operator.

Definition A.19. The *matrix of an operator* in the basis $\{|v_i\rangle\}$ is an $N\times N$ square table whose elements are given by Eq. (A.21). The first index of A_{ij} is the number of the row, the second is the number of the column.

Suppose, for example, that you are required to prove that two given operators are equal: $\hat{A}=\hat{B}$. You can do so by showing the identity for the matrices A_{ij} and B_{ij} of the operators in any basis. Because the matrix contains full information about an operator, this is sufficient. Of course, you should choose your basis judiciously, so that the matrices A_{ij} and B_{ij} are as easy as possible to calculate.

Exercise A.36. Find the matrix of $\hat{\mathbf{1}}$. Show that this matrix does not depend on the choice of basis.

Exercise A.37. Find the matrix representation of the vector $\hat{A}\left|v_j\right\rangle$ in the basis $\{|v_i\rangle\}$, where $\left|v_j\right\rangle$ is an element of this basis, j is given, and the matrix of $\hat{A}$ is known.

Exercise A.38. Show that, if $|a\rangle \simeq \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$ in some basis, then the vector $\hat{A}|a\rangle$ is given by the matrix product

$$\hat{A}|a\rangle \simeq \begin{pmatrix} A_{11} & \ldots & A_{1N} \\ \vdots & & \vdots \\ A_{N1} & \ldots & A_{NN} \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = \begin{pmatrix} \sum_j A_{1j}a_j \\ \vdots \\ \sum_j A_{Nj}a_j \end{pmatrix}. \tag{A.20}$$

Exercise A.39. Given the matrices A_{ij} and B_{ij} of the operators $\hat{A}$ and $\hat{B}$, find the matrices of the operators

a) $\hat{A}+\hat{B}$;
b) $\lambda\hat{A}$;
c) $\hat{A}\hat{B}$.

The last two exercises show that operations with operators and vectors are readily represented in terms of matrices and columns. However, there is an important caveat: matrices of vectors and operators depend on the basis chosen, in contrast to "physical" operators and vectors that are defined irrespectively of any specific basis.

This point should be taken into account when deciding whether to perform a calculation in the Dirac or matrix notation. If you choose the matrix notation to save ink, you should be careful to keep track of the basis you are working with, and write all the matrices in that same basis.

Exercise A.40. Show that the matrix elements of the operator $\hat{A}$ in an *orthonormal* basis $\{|v_i\rangle\}$ are given by

$$A_{ij} = \langle v_i| \left(\hat{A}\left|v_j\right\rangle\right) \equiv \langle v_i|\hat{A}\left|v_j\right\rangle. \tag{A.21}$$

Exercise A.41. Find the matrices of operators $\hat{R}_\phi$ and $\hat{R}_\theta$ that correspond to the rotation of the two-dimensional geometric space through angles ϕ and θ, respectively [Ex. A.31(f)]. Find the matrix of $\hat{R}_\phi \hat{R}_\theta$ using the result of Ex. A.39 and check that it is equivalent to a rotation through $(\phi + \theta)$.

Exercise A.42. Give an example of a basis and determine the dimension of the linear space of linear operators over a Hilbert space of dimension N (see Ex. A.32).

A.6.3 Outer products

Definition A.20. *Outer products* $|a\rangle\langle b|$ are understood as operators acting as follows:

$$(|a\rangle\langle b|)\,|c\rangle \equiv |a\rangle\,(\langle b|\,c\rangle) = (\langle b|\,c\rangle)\,|a\rangle\,. \tag{A.22}$$

(The second equality comes from the fact that $\langle b|\,c\rangle$ is a number and commutes with everything.)

Exercise A.43. Show that $|a\rangle\langle b|$ as defined above is a linear operator.

Exercise A.44. Show that $(\langle a|\,b\rangle)\,(\langle c|\,d\rangle) = \langle a|\,(|b\rangle\langle c|)\,|d\rangle$.

Exercise A.45. Show that the matrix of the operator $|a\rangle\langle b|$ is given by

$$|a\rangle\langle b| \simeq \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} \begin{pmatrix} b_1^* \dots b_N^* \end{pmatrix} = \begin{pmatrix} a_1 b_1^* & \dots & a_1 b_N^* \\ \vdots & & \vdots \\ a_N b_1^* & \dots & a_N b_N^* \end{pmatrix}. \tag{A.23}$$

This result explains the intuition behind the notion of the outer product. As discussed in the previous section, a ket-vector corresponds to a column and a bra-vector to a row. According to the rules of matrix multiplication, the product of the two is a square matrix, and the outer product is simply the operator corresponding to this matrix.

Exercise A.46. Let A_{ij} be the matrix of the operator $\hat{A}$ in an orthonormal basis $\{|v_i\rangle\}$. Show that

$$\hat{A} = \sum_{i,j} A_{ij}\,|v_i\rangle\left\langle v_j\right|. \tag{A.24}$$

Exercise A.47. Let $\hat{A}$ be an operator and $\{|v_i\rangle\}$ an orthonormal basis in the Hilbert space. It is known that $\hat{A}|v_1\rangle = |w_1\rangle, \ldots, \hat{A}|v_N\rangle = |w_N\rangle$, where $|w_1\rangle, \ldots, |w_N\rangle$ are some vectors (not necessarily orthonormal). Show that

$$\hat{A} = \sum_i |w_i\rangle\langle v_i|. \tag{A.25}$$

These exercises reveal the significance of outer products. First, they provide a way to convert the operator matrix into the Dirac notation as per Eq. (A.24). This result complements Eq. (A.21), which serves the reverse purpose, converting the operator from the Dirac form into the matrix notation. Second, Eq. (A.25) allows us to construct the expression for an operator based on our knowledge of how it maps elements of an arbitrary orthonormal basis. We find it to be of great practical utility when we try to associate an operator with a physical process.

Below are two practice exercises using these results, followed by one very important additional application of the outer product.

Exercise A.48. The matrix of the operator $\hat{A}$ in the basis $\{|v_1\rangle, |v_2\rangle\}$ is $\begin{pmatrix} 1 & -3\mathrm{i} \\ 3\mathrm{i} & 4 \end{pmatrix}$. Express this operator in the Dirac notation.

Exercise A.49. Let $\{|v_1\rangle, |v_2\rangle\}$ be an orthonormal basis in a two-dimensional Hilbert space. Suppose the operator $\hat{A}$ maps $|u_1\rangle = (|v_1\rangle + |v_2\rangle)/\sqrt{2}$ onto $|w_1\rangle = \sqrt{2}|v_1\rangle$ and $|u_2\rangle = (|v_1\rangle - |v_2\rangle)/\sqrt{2}$ onto $|w_2\rangle = \sqrt{2}(|v_1\rangle + 3\mathrm{i}|v_2\rangle)$. Find the matrix of $\hat{A}$ in the basis $\{|v_1\rangle, |v_2\rangle\}$.
Hint: Notice that $\{|u_1\rangle, |u_2\rangle\}$ is an orthonormal basis.

Exercise A.50. Show that for any orthonormal basis $\{|v_i\rangle\}$,

$$\sum_i |v_i\rangle\langle v_i| = \hat{\mathbf{1}}. \tag{A.26}$$

This result is known as *the resolution of the identity*. It is useful for the following application. Suppose the matrix of $\hat{A}$ is known in some orthonormal basis $\{|v_i\rangle\}$ and we wish to find its matrix in another orthonormal basis, $\{|w_i\rangle\}$. This can be done as follows:

$$\begin{aligned}
(\hat{A}_{ij})_{w\text{-basis}} &= \langle w_i|\hat{A}|w_j\rangle \\
&= \left\langle w_i\right|\hat{\mathbf{1}}\hat{A}\hat{\mathbf{1}}\left|w_j\right\rangle \\
&= \langle w_i|\left(\sum_k |v_k\rangle\langle v_k|\right)\hat{A}\left(\sum_m |v_m\rangle\langle v_m|\right)|w_j\rangle \\
&= \sum_k\sum_m \langle w_i|v_k\rangle\langle v_k|\hat{A}|v_m\rangle\langle v_m|w_j\rangle.
\end{aligned} \tag{A.27}$$

The central object in the last line is the matrix element of $\hat{A}$ in the "old" basis $\{|v_i\rangle\}$. Because we know the inner products between each pair of elements in the old and new bases, we can use the above expression to find each matrix element of $\hat{A}$ in the new basis. We shall use this trick throughout the course.

The calculation can be simplified if we interpret the last line of Eq. (A.27) as a product of three matrices. An example to that effect is given in the solution to the exercise below.

Exercise A.51. Find the matrix of the operator $\hat{A}$ from Ex. A.48 in the basis $\{|w_1\rangle, |w_2\rangle\}$ such that

$$|w_1\rangle = (|v_1\rangle + \mathrm{i}\,|v_2\rangle)/\sqrt{2}, \qquad (A.28)$$
$$|w_2\rangle = (|v_1\rangle - \mathrm{i}\,|v_2\rangle)/\sqrt{2}.$$

a) using the Dirac notation, starting with the result of Ex. A.48 and then expressing each bra and ket in the new basis;
b) according to Eq. (A.27).

Check that the results are the same.

A.7 Adjoint and self-adjoint operators

The action of an operator $\hat{A}$ on a ket-vector $|c\rangle$ corresponds to multiplying the square matrix of $\hat{A}$ by the column associated with $|c\rangle$. The result of this operation is another column, $\hat{A}\,|c\rangle$.

Let us by analogy consider an operation in which a row corresponding to a bra-vector $\langle b|$ is multiplied on the right by the square matrix of $\hat{A}$. The result of this operation will be another row corresponding to a bra-vector. We can associate such multiplication with the action of the operator $\hat{A}$ on $\langle b|$ *from the right*, denoted in the Dirac notation as $\langle b|\hat{A}$. The formal definition of this operation is as follows:

$$\langle b|\hat{A} \equiv \sum_{ij} b_i^* A_{ij} \langle v_j| , \qquad (A.29)$$

where A_{ij} and b_i are, respectively, the matrix elements of $\hat{A}$ and $|b\rangle$ in the orthonormal basis $\{|v_i\rangle\}$.

Exercise A.52. Derive the following properties of the operation defined by Eq. (A.29):

a) $\hat{A}$ acting from the right is a linear operator in the adjoint space;
b) $\langle a|\, b\rangle \langle c| = \langle a| (|b\rangle\langle c|)$;
c) for vectors $|a\rangle$ and $|c\rangle$,

$$\left(\langle a|\hat{A}\right) |c\rangle = \langle a| \left(\hat{A}\,|c\rangle\right); \qquad (A.30)$$

d) the vector $\langle a|\hat{A}$ as defined by Eq. (A.29) does not depend on the basis in which the matrix (A_{ij}) is calculated.

Let us now consider the following problem. Suppose we have an operator $\hat{A}$ that maps a ket-vector $|a\rangle$ onto ket-vector $|b\rangle$: $\hat{A}|a\rangle = |b\rangle$. What is the operator $\hat{A}^\dagger$ which, when acting from the right, maps *bra*-vector $\langle a|$ onto bra-vector $\langle b|$: $\langle a|\hat{A}^\dagger = \langle b|$? It turns out that this operator is not the same as $\hat{A}$, but is related relatively simply to it.

Definition A.21. An operator $\hat{A}^\dagger$ ("A-dagger") is called the *adjoint* (*Hermitian conjugate*) of $\hat{A}$ if for any vector $|a\rangle$,

$$\langle a|\hat{A}^\dagger = \text{Adjoint}\left(\hat{A}|a\rangle\right). \tag{A.31}$$

If $\hat{A} = \hat{A}^\dagger$, the operator is said to be *Hermitian* or *self-adjoint*.

Unlike bra- and ket-vectors, operators and their adjoints live in the same Hilbert space. More precisely, they live in both the bra- and ket- spaces: they act on bra-vectors from the right, and on ket-vectors from the left. Note that an operator cannot act on a bra-vector from the left or on a ket-vector from the right.

Exercise A.53. Show that the matrix of $\hat{A}^\dagger$ is related to the matrix of $\hat{A}$ through transposition and complex conjugation.

Exercise A.54. Show that, for any operator, $(\hat{A}^\dagger)^\dagger = \hat{A}$.

Exercise A.55. Show that the Pauli operators (1.7) are Hermitian.

Exercise A.56. By way of counterexample, show that two operators being Hermitian does not guarantee that their product is also Hermitian.

Exercise A.57. Show that

$$(|c\rangle\langle b|)^\dagger = |b\rangle\langle c|. \tag{A.32}$$

It may appear from this exercise that the adjoint of an operator is somehow related to its inverse: if the "direct" operator maps $|b\rangle$ onto $|c\rangle$, its adjoint does the opposite. This is not always the case: as we know from the Definition A.20 of the outer product, the operator $|c\rangle\langle b|$, when acting from the left, maps *everything* (not only $|c\rangle$) onto $|b\rangle$, while $|c\rangle\langle b|$ maps everything onto $|c\rangle$. However, there is an important class of operators, the so-called unitary operators, for which the inverse is the same as the adjoint. We discuss these operators in detail in Sec. A.10.

Exercise A.58. Show that

a)
$$(\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger; \tag{A.33}$$

b)
$$(\lambda\hat{A})^\dagger = \lambda^*\hat{A}^\dagger; \tag{A.34}$$

c)
$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger. \tag{A.35}$$

We can say that every object in linear algebra has an adjoint. For a number, its adjoint is its complex conjugate; for a ket-vector it is a bra-vector (and vice versa);

for an operator it is the adjoint operator. The matrices of an object and its adjoint are related by transposition and complex conjugation.

Suppose we are given a complex expression consisting of vectors and operators, and are required to find its adjoint. Summarizing Eqs. (A.12), (A.32) and (A.35), we arrive at the following algorithm:

a) invert the order of all products;
b) conjugate all numbers;
c) replace all kets by bras and vice versa;
d) replace all operators by their adjoints.

Here is an example.

$$\text{Adjoint}\left(\lambda\hat{A}\hat{B}\left|a\right\rangle\left\langle b\right|\hat{C}\right) = \lambda^*\hat{C}^\dagger\left|b\right\rangle\left\langle a\right|\hat{B}^\dagger\hat{A}^\dagger \tag{A.36}$$

This rule can be used to obtain the following relation.

Exercise A.59. Show that

$$\langle\phi|\hat{A}\,|\psi\rangle = \langle\psi|\hat{A}^\dagger\,|\phi\rangle^* . \tag{A.37}$$

A.8 Spectral decomposition

We will now prove an important theorem for Hermitian operators. I will be assuming you are familiar with the notions of determinant, eigenvalue, and eigenvector of a matrix and the methods for finding them. If this is not the case, please refer to any introductory linear algebra text.

Exercise A.60.* Prove the *spectral theorem*: for any Hermitian operator $\hat{V}$, there exists an orthonormal basis $\{|v_i\rangle\}$ (which we shall call the *eigenbasis*) such that

$$\hat{V} = \sum_i v_i\left|v_i\right\rangle\left\langle v_i\right|, \tag{A.38}$$

with all the v_i being real.

The representation of an operator in the form (A.38) is called the *spectral decomposition* or *diagonalization* of the operator. The basis $\{|v_i\rangle\}$ is called an *eigenbasis* of the operator.

Exercise A.61. Write the matrix of the operator (A.38) in its eigenbasis.

Exercise A.62. Show that the elements of the eigenbasis of $\hat{V}$ are the eigenvectors of $\hat{V}$ and the corresponding values v_i are its eigenvalues, i.e., for any i,

$$\hat{V}\left|v_i\right\rangle = v_i\left|v_i\right\rangle .$$

Exercise A.63.[*§] Show that a spectral decomposition (not necessarily with real eigenvalues) exists for any operator $\hat{V}$ such that $\hat{V}\hat{V}^\dagger = \hat{V}^\dagger\hat{V}$ (such operators are said to be *normal*).

Exercise A.64. Find the eigenvalues and eigenbasis of the operator associated with the rotation of the plane of two-dimensional geometric vectors through angle ϕ (see Ex. A.41), but over the field of *complex* numbers.

Exercise A.65.[§] In a three-dimensional Hilbert space, three operators have the following matrices in an orthonormal basis $\{|v_1\rangle, |v_2\rangle, |v_3\rangle\}$:

a) $\hat{L}_x \simeq \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$,

b) $\hat{L}_y \simeq \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}$;

c) $\hat{L}_z \simeq \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$.

Show that these operators are Hermitian. Find their eigenvalues and eigenvectors.

So we have found that every Hermitian operator has a spectral decomposition. But is the spectral decomposition of a given operator unique? The answer is affirmative as long as the operator has no *degenerate eigenvalues*, i.e., eigenvalues associated with two or more eigenvectors.

Exercise A.66. The Hermitian operator $\hat{V}$ diagonalizes in an orthonormal basis $\{|v_i\rangle\}$. Suppose there exists a vector $|\psi\rangle$ that is an eigenvector of $\hat{V}$ with eigenvalue v, but is not proportional to any $|v_i\rangle$. Show that this is possible only if v is a degenerate eigenvalue of $\hat{V}$ and $|\psi\rangle$ is a linear combination of elements of $\{|v_i\rangle\}$ corresponding to that eigenvalue.

Exercise A.67. Show that, for a Hermitian operator $\hat{V}$ whose eigenvalues are nondegenerate,

a) the eigenbasis is unique up to phase factors;
b) any set that contains all linearly independent normalized eigenvectors of $\hat{V}$ is identical to the eigenbasis of $\hat{V}$ up to phase factors.

The latter result is of primary importance, and we shall make abundant use of it throughout this course. It generalizes to Hilbert spaces of infinite dimension and even to those associated with continuous observables. Let us now look into the case of operators with degenerate eigenvalues.

Exercise A.68. Find the eigenvalues of the identity operator in the qubit Hilbert space and show that they are degenerate. Give two different examples of this operator's eigenbasis.

Exercise A.69. Show that eigenvectors of a Hermitian operator $\hat{V}$ that are associated with different eigenvalues are orthogonal. Do not assume non-degeneracy of the eigenvalues.

Exercise A.70. Suppose an eigenvalue v of an operator $\hat{V}$ is degenerate. Show that a set of corresponding eigenvectors forms a linear subspace (see Defn. A.8).

Exercise A.71.*

a) Show that if $\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{B}|\psi\rangle$ for all $|\psi\rangle$, then $\hat{A} = \hat{B}$.
b) Show that if $\langle\psi|\hat{A}|\psi\rangle$ is a real number for all $|\psi\rangle$, then $\hat{A}$ is Hermitian.

Definition A.22. A Hermitian operator $\hat{A}$ is said to be *positive (non-negative)* if $\langle\psi|\hat{A}|\psi\rangle > 0$ ($\langle\psi|\hat{A}|\psi\rangle \geq 0$) for any non-zero vector $|\psi\rangle$.

Exercise A.72. Show that a Hermitian operator $\hat{A}$ is positive (non-negative) if and only if all its eigenvalues are positive (non-negative).

Exercise A.73. Show that a sum $\hat{A}+\hat{B}$ of two positive (non-negative) operators is positive (non-negative).

A.9 Commutators

As already discussed, not all operators commute. The degree of non-commutativity turns out to play an important role in quantum mechanics and is quantified by the operator known as the commutator.

Definition A.23. For any two operators $\hat{A}$ and $\hat{B}$, their *commutator* and *anticommutator* are defined respectively by

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}; \quad \text{(A.39a)}$$
$$\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}. \quad \text{(A.39b)}$$

Exercise A.74. Show that:

a)
$$\hat{A}\hat{B} = \frac{1}{2}([\hat{A},\hat{B}] + \{\hat{A},\hat{B}\}); \quad \text{(A.40)}$$

b)
$$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]; \quad \text{(A.41)}$$

c)
$$[\hat{A},\hat{B}]^\dagger = [\hat{B}^\dagger,\hat{A}^\dagger]; \quad \text{(A.42)}$$

d)
$$[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}]; \quad \text{(A.43a)}$$
$$[\hat{A}+\hat{B},\hat{C}] = [\hat{A},\hat{C}] + [\hat{B},\hat{C}]; \quad \text{(A.43b)}$$

e)

$$[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C}+\hat{B}[\hat{A},\hat{C}]; \tag{A.44a}$$

$$[\hat{A}\hat{B},\hat{C}] = [\hat{A},\hat{C}]\hat{B}+\hat{A}[\hat{B},\hat{C}]; \tag{A.44b}$$

f)

$$\begin{aligned}[\hat{A}\hat{B},\hat{C}\hat{D}] &= \hat{C}\hat{A}[\hat{B},\hat{D}]+\hat{C}[\hat{A},\hat{D}]\hat{B}+\hat{A}[\hat{B},\hat{C}]\hat{D}+[\hat{A},\hat{C}]\hat{B}\hat{D} \\ &= \hat{A}\hat{C}[\hat{B},\hat{D}]+\hat{C}[\hat{A},\hat{D}]\hat{B}+\hat{A}[\hat{B},\hat{C}]\hat{D}+[\hat{A},\hat{C}]\hat{D}\hat{B}.\end{aligned} \tag{A.45}$$

When calculating commutators for complex expressions, it is advisable to use the relations derived in this exercise rather than the definition (A.39a) of the commutator. There are many examples to this effect throughout this book.

Exercise A.75. Express the commutators

a) $[\hat{A}\hat{B}\hat{C},\hat{D}]$;
b) $[\hat{A}^2+\hat{B}^2,\hat{A}+\mathrm{i}\hat{B}]$

in terms of the pairwise commutators of the individual operators $\hat{A},\hat{B},\hat{C},\hat{D}$.

Exercise A.76. For two operators $\hat{A}$ and $\hat{B}$, suppose that $[\hat{A},\hat{B}] = ic\hat{\mathbf{1}}$, where c is a complex number. Show that

$$[\hat{A},\hat{B}^n] = nc\hat{B}^{n-1}. \tag{A.46}$$

Exercise A.77. Show that, if $\hat{A}$ and $\hat{B}$ are Hermitian, so are

a) $i[\hat{A},\hat{B}]$;
b) $\{\hat{A},\hat{B}\}$.

Exercise A.78. Find the commutation relations of the Pauli operators (1.7).
Answer:

$$[\hat{\sigma}_m,\hat{\sigma}_j] = 2\mathrm{i}\varepsilon_{mjk}\sigma_k, \tag{A.47}$$

where ε is the Levi-Civita symbol given by

$$\varepsilon_{mjk} \equiv \begin{cases} +1 \text{ for } mjk = xyz,\ yzx \text{ or } zxy \\ -1 \text{ for } mjk = xzy,\ yxz \text{ or } zyx \\ \quad 0 \text{ otherwise.} \end{cases} \tag{A.48}$$

A.10 Unitary operators

Definition A.24. Linear operators that map all vectors of norm 1 onto vectors of norm 1 are said to be *unitary*.

Exercise A.79. Show that unitary operators preserve the norm of any vector, i.e., if $|a'\rangle = \hat{U}|a\rangle$, then $\langle a|\,a\rangle = \langle a'|\,a'\rangle$.

Exercise A.80. Show that an operator $\hat{U}$ is unitary if and only if it preserves the inner product of any two vectors, i.e., if $|a'\rangle = \hat{U}|a\rangle$ and $|b'\rangle = \hat{U}|b\rangle$, then $\langle a|\,b\rangle = \langle a'|\,b'\rangle$.

Exercise A.81. Show that:

a) a unitary operator maps any orthonormal basis $\{|w_i\rangle\}$ onto an orthonormal basis;
b) conversely, for any two orthonormal bases $\{|v_i\rangle\}, \{|w_i\rangle\}$, the operator $\hat{U} = \sum_i |v_i\rangle\langle w_i|$ is unitary (in other words, *any* operator that maps an orthonormal basis onto an orthonormal basis is unitary).

Exercise A.82. Show that an operator $\hat{U}$ is unitary if and only if $\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{1}$ (i.e., its adjoint is equal to its inverse).

Exercise A.83. Show the following:

a) Any unitary operator can be diagonalized and all its eigenvalues have absolute value 1, i.e., they can be written in the form $e^{i\theta}$, $\theta \in \mathbb{R}$.
Hint: use Ex. A.63.
b) A diagonalizable operator (i.e., an operator whose matrix becomes diagonal in some basis) with eigenvalues of absolute value 1 is unitary.

Exercise A.84. Show that the following operators are unitary:

a) the Pauli operators (1.7);
b) rotation through angle ϕ in the linear space of two-dimensional geometric vectors over $\mathbb{R}$.

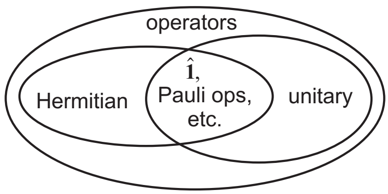

Fig. A.1 Relations among types of operators

The families of Hermitian and unitary operators overlap, but they are not identical (Fig. A.1). An operator that is both Hermitian and unitary must be self-inverse, as per Ex. A.82. Such operators are relatively rare.

A.11 Functions of operators

The concept of function of an operator has many applications in linear algebra and differential equations. It is also handy in quantum mechanics, as operator functions permit easy calculation of evolution operators.

Definition A.25. Consider a complex function $f(x)$ defined on $\mathbb{C}$. The *function of operator* $f(\hat{A})$ of a diagonalizable operator $\hat{A}$ is the following operator:

$$f(\hat{A}) = \sum_i f(a_i) \left| a_i \right\rangle \left\langle a_i \right|, \tag{A.49}$$

where $\{|a_i\rangle\}$ is an orthonormal basis in which $\hat{A}$ diagonalizes:

$$\hat{A} = \sum_i a_i \left| a_i \right\rangle \left\langle a_i \right|. \tag{A.50}$$

Exercise A.85. Show that, if the vector $|a\rangle$ is an eigenvector of a Hermitian operator $\hat{A}$ with eigenvalue a, then $f(\hat{A})\,|a\rangle = f(a)\,|a\rangle$.

Exercise A.86. Suppose that the operator $\hat{A}$ is Hermitian and the function $f(x)$, when applied to a real argument x, takes a real value. Show that $f(\hat{A})$ is a Hermitian operator, too.

Exercise A.87. Suppose that the operator $\hat{A}$ is Hermitian and function $f(x)$, when applied to any real argument x, takes a real non-negative value. Show that $f(\hat{A})$ is a non-negative operator (see Defn. A.22).

Exercise A.88. Find the matrices of $\sqrt{\hat{A}}$ and $\ln\hat{A}$ in the orthonormal basis in which

$$\hat{A} \simeq \begin{pmatrix} 1 & 3 \\ 3 & 1 \end{pmatrix}$$

Exercise A.89. Find the matrix of $e^{i\theta\hat{A}}$, where $\hat{A} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$.

Hint: One of the eigenvalues of $\hat{A}$ is 0, which means that the corresponding eigenvector does not appear in the spectral decomposition (A.50) of $\hat{A}$. However, the exponential of the corresponding eigenvalue is not zero, and the corresponding eigenvectors do show up in the operator function (A.49).

Exercise A.90. Show that, for any operator $\hat{A}$ and function f, $[\hat{A}, f(\hat{A})] = 0$.

Exercise A.91. Suppose $f(x)$ has a Taylor decomposition $f(x) = f_0 + f_1 x + f_2 x^2 + \ldots$. Show that $f(\hat{A}) = f_0 \hat{\mathbf{1}} + f_1 \hat{A} + f_2 \hat{A}^2 + \ldots$

Exercise A.92. Show that, if the operator $\hat{A}$ is Hermitian, the operator $e^{i\hat{A}}$ is unitary and $e^{i\hat{A}} = \left(e^{-i\hat{A}}\right)^{-1}$.

Exercise A.93.* Let $\vec{s} = (s_x, s_y, s_z)$ be a unit vector (i.e. a vector of length 1). Show that:

$$e^{i\theta\vec{s}\cdot\hat{\vec{\sigma}}} = \cos\theta\,\hat{\mathbf{1}} + i\sin\theta\,\vec{s}\cdot\hat{\vec{\sigma}}, \quad \text{(A.51)}$$

where $\hat{\vec{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$, $\vec{s}\cdot\hat{\vec{\sigma}} = s_x\hat{\sigma}_x + s_y\hat{\sigma}_y + s_z\hat{\sigma}_z$.
Hint: There is no need find the explicit solutions for the eigenvectors of the operator $\vec{s}\cdot\hat{\vec{\sigma}}$.

Exercise A.94.§ Find the matrices of the operators $e^{i\theta\hat{\sigma}_x}$, $e^{i\theta\hat{\sigma}_y}$, $e^{i\theta\hat{\sigma}_z}$ in the canonical basis.
Answer:

$$e^{i\theta\hat{\sigma}_x} = \begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix};$$
$$e^{i\theta\hat{\sigma}_y} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix};$$
$$e^{i\theta\hat{\sigma}_z} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}.$$

Definition A.26. Suppose the vector $|\psi(t)\rangle$ depends on a certain parameter t. The *derivative* of $|\psi(t)\rangle$ with respect to t is defined as the vector

$$\frac{d|\psi\rangle}{dt} = \lim_{\Delta t\to 0}\frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t}. \quad \text{(A.52)}$$

Similarly, the derivative of the operator $\hat{Y}(t)$ with respect to t is the operator

$$\frac{d\hat{Y}}{dt} = \lim_{\Delta t\to 0}\frac{\hat{Y}(t+\Delta t) - \hat{Y}(t)}{\Delta t}. \quad \text{(A.53)}$$

Exercise A.95. Suppose that the matrix form of the vector $|\psi(t)\rangle$ is

$$|\psi(t)\rangle = \begin{pmatrix} \psi_1(t) \\ \vdots \\ \psi_N(t) \end{pmatrix}$$

in some basis. Show that

$$\frac{d|\psi\rangle}{dt} = \begin{pmatrix} d\psi_1(t)/dt \\ \vdots \\ d\psi_N(t)/dt \end{pmatrix}.$$

Write an expression for the matrix form of an operator derivative.

Exercise A.96. Suppose the operator $\hat{A}$ is diagonalizable in an orthonormal basis and independent of t, where t is a real parameter. Show that $\frac{d}{dt}e^{i\hat{A}t} = i\hat{A}e^{i\hat{A}t} = ie^{i\hat{A}t}\hat{A}$.

Exercise A.97.* For two operators $\hat{A}$ and $\hat{B}$, suppose that $[\hat{A},\hat{B}] = ic\hat{\mathbf{1}}$, where c is a complex number. Prove the *Baker-Hausdorff-Campbell formula*[8]

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-ic/2} = e^{\hat{B}}e^{\hat{A}}e^{ic/2} \tag{A.54}$$

using the following steps.

a) Show that

$$[\hat{A}, e^{\hat{B}}] = ce^{\hat{B}}. \tag{A.55}$$

Hint: use the Taylor series expansion for the exponential and Eq. (A.46).

b) For an arbitrary number λ and operator $\hat{G}(\lambda) = e^{\lambda\hat{A}}e^{\lambda\hat{B}}$, show that

$$\frac{d\hat{G}(\lambda)}{d\lambda} = \hat{G}(\lambda)(\hat{A}+\hat{B}+\lambda c) \tag{A.56}$$

c) Solve the differential equation (A.56) to show that

$$\hat{G}(\lambda) = e^{\lambda\hat{A}+\lambda\hat{B}+\lambda^2 c/2}. \tag{A.57}$$

d) Prove the Baker-Hausdorff-Campbell formula using Eq. (A.57).

[8] This is a simplified form of the Baker-Hausdorff-Campbell formula. The full form of this formula is more complicated and holds for the case when $[\hat{A},\hat{B}]$ does not commute with $\hat{A}$ or $\hat{B}$.