APPENDIX B

A Few Words on Spaces, Vectors, and Functions

Vector Space

A vector space means a set V of elements $x, y, \ldots$ (i.e., $x, y, \ldots \in V$), that form an Abelian group, and can be "*added*" together[1] and "*multiplied*" by numbers α, β thus producing $z = \alpha x + \beta y$, $z \in V$. The multiplication (α, β are, in general, complex numbers) satisfies the usual rules:

$$
\begin{aligned}
&1 \cdot x = x \\
&\alpha(\beta x) = (\alpha\beta)x \\
&\alpha(x + y) = \alpha x + \alpha y \\
&(\alpha + \beta)x = \alpha x + \beta x
\end{aligned}
$$

Example 1. ***Integers***
The elements $x, y, \ldots$ are integers, "*addition*" means simply the usual addition of integers, the numbers $\alpha, \beta, \ldots$ are also integers, and "*multiplication*" means just the usual multiplication. Does the set of integers form a vector space? Let us see. The integers form a group (with addition as the operation in the group). Checking all the above axioms, one easily proves that they are satisfied by integers. Thus, the integers (with the operations defined above) form a vector space.

Example 2. ***Integers with real multipliers***
If, in the previous example, we admitted that α, β are real, then the multiplication of integers x, y by the real numbers would give the real numbers (not necessarily the integers). Therefore, in this case, $x, y, \ldots$ *do not* represent any vector space.

Example 3. ***Vectors***
Suppose that $x, y, \ldots$ are vectors, each represented by a N-element sequence of real numbers (they are called the vector components) $x = (a_1, a_2, \ldots a_N)$, $y = (b_1, b_2, \ldots b_N)$, etc. Their addition $(x + y)$ is an operation that produces the vector $z = (a_1 + b_1, a_2 + b_2, \ldots, a_N + b_N)$.

[1] See Appendix C available at booksite.elsevier.com/978-0-444-59436-5; to form a group, any pair of the elements can be "*added*" (operation in the group), the addition is associative, there exists a unit element, and to each element the inverse one exists.

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The vectors form an Abelian group because $x + y = y + x$, the unit ("*neutral*") element is $(0, 0, \ldots 0)$, the inverse element to $(a_1, a_2, \ldots a_N)$ is equal to $(-a_1, -a_2, \ldots -a_N)$. Thus, the vectors form a group. "*Multiplication*" of a vector by a real number α means $\alpha(a_1, a_2, \ldots a_N) = (\alpha a_1, \alpha a_2, \ldots \alpha a_N)$. Check that the above four axioms are satisfied. Conclusion: the vectors form a vector space.

Note that if only the positive vector components were allowed, then they would not form an Abelian group (no neutral element), and on top of that, their addition (which might mean a subtraction of components, because α, β could be negative) could produce vectors with non-positive components. Thus, the vectors with all positive components do not form a vector space.

Example 4. ***Functions***

This example is important in the scope of the book. This time, the vectors have real components.[2] Their "*addition*" means the addition of two functions $f(x) = f_1(x) + f_2(x)$. The "*multiplication*" means multiplication by a real number. The unit ("*neutral*") function means $f = 0$, the "*inverse*" function to f is $-f(x)$. Therefore, the functions form an Abelian group. A few seconds are needed to show that the above four axioms are satisfied. Such functions form a vector space.

Linear Independence A set of vectors is called a set of linearly independent vectors if no vector of the set can be expressed as a linear combination of the other vectors of the set. The number of the linear independent vectors in a vector space is called the dimension of the space.

Basis A set of n linearly independent vectors in the n -dimensional space.

Euclidean Space

A vector space (with real multiplying numbers α, β) represents an Euclidean space, if for any two vectors ϕ, ψ of the space we assign a real number called a *inner product* $\langle\phi|\psi\rangle$ with the following properties:

- $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle$
- $\langle\alpha\phi|\psi\rangle = \alpha\langle\phi|\psi\rangle$
- $\langle\phi_1 + \phi_2|\psi\rangle = \langle\phi_1|\psi\rangle + \langle\phi_2|\psi\rangle$
- $\langle\phi|\phi\rangle = 0$, only if $\phi = 0$

Inner Product and Distance The concept of the inner product is used to introduce the following:

- The *length of the vector* ϕ is defined as $\|\phi\| \equiv \sqrt{\langle\phi|\phi\rangle}$.
- The *distance between two vectors* ϕ and ψ is defined as a non-negative number $\|\phi - \psi\| = \sqrt{\langle\phi - \psi|\phi - \psi\rangle}$. The distance satisfies some conditions, which we treat as obvious from the everyday experience.

[2] Note a similarity of the present example with the previous one: a function $f(x)$ may be treated as a vector with the infinite number of the components. The components are listed in the sequence of increasing $x \in R$, the component $f(x)$ corresponding to x.

- The distance from Cracow to Cracow has to equal zero (just insert $\phi = \psi$).
- The distance from Cracow to Warsaw has to be the same as from Warsaw to Cracow (just exchange $\phi \leftrightarrow \psi$).
- The Cracow-Warsaw distance is shorter than or equal to the sum of two distances: Cracow-X and X-Warsaw for any town X (which is a little more difficult to show).

Schwartz Inequality For any two vectors belonging to the Euclidean space, the Schwartz inequality holds[3]:

$$|\langle\phi|\psi\rangle| \leq \|\phi\| \;\|\psi\|\,, \tag{B.1}$$

or, equivalently

$$|\langle\phi|\psi\rangle|^2 \leq \|\phi\|^2 \,\|\psi\|^2\,.$$

Orthogonal Basis All basis vectors ϕ_j, $j = 1, 2, \ldots N$ are orthogonal to each other: $\langle\phi_i|\phi_j\rangle = 0$ for $i \neq j$.

Orthonormal Basis An orthogonal basis set with all the basis vectors having length $\|\phi_i\| = 1$. Thus, for the orthonormal basis set we have $\langle\phi_i|\phi_j\rangle = \delta_{ij}$.

Example 5. ***Dot Product***

Let us take the vector space from Example 3 and let us introduce the dot product (representing the inner product) defined as

$$\langle\phi|\psi\rangle = \sum_{i=1}^{N} a_i b_i\,. \tag{B.2}$$

Let us check whether this definition satisfies the properties required for a inner product:

- $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle$, because the order of a and b in the sum is irrelevant.
- $\langle\alpha\phi|\psi\rangle = \alpha\,\langle\phi|\psi\rangle$, because the sum says that multiplication of each a_i by α is equivalent to multiplying by α, the inner product.
- $\langle\phi_1 + \phi_2|\psi\rangle = \langle\phi_1|\psi\rangle + \langle\phi_2|\psi\rangle$, because if the vector ϕ is decomposed into two vectors $\phi = \phi_1 + \phi_2$ in such a way that $a_i = a_{i1} + a_{i2}$ (with a_{i1}, a_{i2} being the components of ϕ_1, ϕ_2, respectively), then the summation of $\langle\phi_1|\psi\rangle + \langle\phi_2|\psi\rangle$gives $\langle\phi|\psi\rangle$.
- $\langle\phi|\phi\rangle = \sum_{i=1}^{N}\left(a_i\right)^2$, and this is equal to zero if and only if all the components $a_i = 0$. Therefore, the proposed formula operates as the inner product definition requires.

Unitary Space

If three changes are introduced in the definition of the Euclidean space, then we would obtain another space: the unitary space. These changes are as follows:

- The numbers $\alpha, \beta, \ldots$ are complex instead of real.

[3] The Schwartz inequality agrees with what everyone recalls about the dot product of two vectors: $\langle x|y\rangle = \|x\|\;\|y\|\cos\theta$, where θ is the angle between the two vectors. Taking the absolute value of both sides, we obtain $|\langle x|y\rangle| = \|x\|\;\|y\|\,|\cos\theta| \leq \|x\|\;\|y\|$.

- The inner product instead of $\langle \phi|\psi\rangle = \langle \psi|\phi\rangle$ has the property $\langle \phi|\psi\rangle = \langle \psi|\phi\rangle^*$.
- Instead of $\langle \alpha\phi|\psi\rangle = \alpha \langle \phi|\psi\rangle$, we have[4]: $\langle \alpha\phi|\psi\rangle = \alpha^* \langle \phi|\psi\rangle$.

After the new inner product definition is introduced, the related quantities, the length of a vector and the distance between the vectors, are defined in exactly the same way as in the Euclidean space. Also, the definitions of the orthogonality and the Schwartz inequality remain unchanged.

Hilbert Space

This is for us the most important unitary space–its elements are wave functions, which often will be denoted as $f, g, \ldots, \phi, \chi, \psi, \ldots$. etc. The wave functions with which we are dealing in quantum mechanics (according to John von Neumann) are the elements (i.e., vectors) of the Hilbert space. The inner product of two functions f and g means $\langle f|g\rangle \equiv \int f^* g d\tau$, where the integration is over the whole space of variables, on which both functions depend. The length of vector f is denoted by $||f|| = \sqrt{\langle f|f\rangle}$. Consequently, the orthogonality of two functions f and g means $\langle f|g\rangle = 0$ i.e., an integral $\int f^* g \, d\tau = 0$ over the whole range of the coordinates on which the function f depends. The Dirac notation, Fig. 1.6 and Eq. (1.9), is in fact the inner product of such functions in a unitary space.

David Hilbert (1862–1943), German mathematician and professor at the University of Göttingen. At the II Congress of Mathematicians in Paris, Hilbert formulated 23 goals of mathematics considered by him as very important. This had a great impact on mathematics and led to some unexpected results (e.g., the Gödel theorem). Hilbert's investigations in 1900–1910 on integral equations resulted in the concept of the Hilbert space. Hilbert worked also on the foundations of mathematics, on mathematical physics, number theory, variational calculus, etc. This hard-working and extremely prolific mathematician was deeply depressed by Hitler's seizing of power. He regularly came to his office, but did not write any single sheet of paper.

Let us imagine an infinite sequence of functions (i.e., vectors) $f_1, f_2, f_3, \ldots$ in a unitary space (Fig. B.1). The sequence will be called a *Cauchy sequence* if for a given $\varepsilon > 0$, a natural number N can be found, such that for $i > N$, we will have $\| f_{i+1} - f_i \| < \varepsilon$. In other words, in a Cauchy sequence, the distances between the consecutive vectors (functions) decrease, when we go to sufficiently large indices; i.e., the functions become more and more similar to each other. *If the converging Cauchy sequences have their limits (functions) that belong to the unitary space, then such a space is called the Hilbert space*

A basis in the Hilbert space is a set of the linearly independent functions (vectors) such that any function belonging to the space can be expressed as a linear combination of the basis set

[4] At the same time, $\langle x|\alpha y\rangle = \alpha \langle x|y\rangle$.

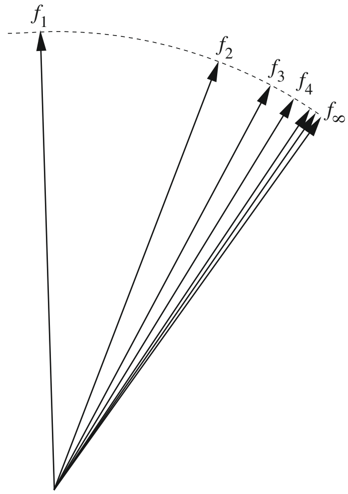

Fig. B.1. A pictorial representation of the Hilbert space. We have a vector space (each vector represents a wave function) and a series of unit vectors f_i, that differ less and less (Cauchy series). If any convergent Cauchy series has its limit belonging to the vector space, then the space represents the *Hilbert space*.

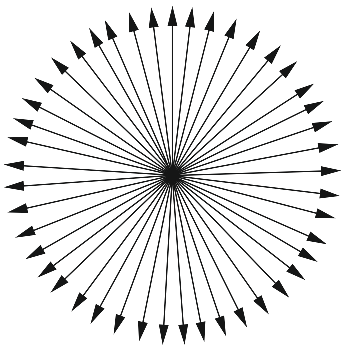

Fig. B.2. A pictorial representation of something that surely cannot be represented. Using poetic license, an orthonormal basis in the Hilbert space looks like a "*hedgehog*" of the unit vectors (their number equal to ∞), each pair of them orthogonal. This is in analogy to a 2-D or 3-D basis set, where the "*hedgehog*" has two or three orthogonal unit vectors.

functions. Because of the infinite number of dimensions, the number of the basis set functions is infinite. This is difficult to imagine. In analogy with a 3-D Euclidean space, we may imagine an orthonormal basis as the unit vectors protruding from the origin toward an infinite number of directions (like a "*hedgehog*"; Fig. B.2).

Each vector (function) can be represented as a linear combination of the "*hedgehog*" functions. It is seen, that we may rotate the "*hedgehog*" (i.e., the basis set)[5] and the completeness of the basis will be preserved; i.e., any vector of the Hilbert space can be represented as a linear combination of the new basis set vectors.

5 The new orthonormal basis set is obtained by a unitary transformation of the old one.

Linear Operator

Operator $\hat{A}$ transforms any vector ϕ from the operator's domain into vector ψ (both vectors ϕ, ψ belong to the unitary space): $\hat{A}(\phi) = \psi$, what is written as $\hat{A}\phi = \psi$. A *linear operator* satisfies $\hat{A}(c_1\phi_1 + c_2\phi_2) = c_1\hat{A}\phi_1 + c_2\hat{A}\phi_2$, where c_1 and c_2 stand for complex numbers.

We define the following:

- Sum of operators: $\hat{A} + \hat{B} = \hat{C}$ as $\hat{C}\phi = \hat{A}\phi + \hat{B}\phi$.
- Product of operators: $\hat{A}\hat{B} = \hat{C}$ as $\hat{C}\phi = \hat{A}(\hat{B}(\phi))$.

If for two operators we have $\hat{A}\hat{B} = \hat{B}\hat{A}$, then we say they *commute*, or their *commutator* $\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} = 0$. In general, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$; i.e., the operators do not commute.

- Inverse operator (if exists): $\hat{A}^{-1}(\hat{A}\phi) = \phi$.

Adjoint Operator

If for an operator $\hat{A}$ we can find a new operator $\hat{A}^\dagger$, such that for any two vectors ϕ and ψ of the unitary space[6], we have[7]

$$\left\langle \phi | \hat{A}\psi \right\rangle = \left\langle \hat{A}^\dagger \phi | \psi \right\rangle, \tag{B.3}$$

then we say that $\hat{A}^\dagger$ is the *adjoint* operator to $\hat{A}$.

Hermitian Operator

If $\hat{A}^\dagger = \hat{A}$, then the operator $\hat{A}$ will be called by us *self-adjoint* or *Hermitian* operator[8]:

$$\left\langle \phi | \hat{A}\psi \right\rangle = \left\langle \hat{A}\phi | \psi \right\rangle. \tag{B.4}$$

Unitary Operator

A unitary operator $\hat{U}$ transforms a vector ϕ into $\psi = \hat{U}\phi$, both belonging to the unitary space (the domain is the unitary space), and the *inner product is preserved*:

$$\left\langle \hat{U}\phi | \hat{U}\psi \right\rangle = \langle \phi | \psi \rangle .$$

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6 The formal definition is less restrictive, and the domains of the operators $\hat{A}^\dagger$ and $\hat{A}$ do not need to extend over the whole unitary space.

7 Sometimes in the Dirac notation, we make a useful modification: $\left\langle \phi | \hat{A}\psi \right\rangle \equiv \left\langle \phi | \hat{A} | \psi \right\rangle$.

8 The self-adjoint and Hermitian operators differ in mathematics (the matter of domains), but we will ignore this difference in this book.

This means that any unitary transformation preserves the angle between the vectors ϕ and ψ; i.e., the angle between ϕ and ψ is the same as the angle between $\hat{U}\phi$ and $\hat{U}\psi$. The transformation also preserves the length of the vector because $\left\langle \hat{U}\phi|\hat{U}\phi \right\rangle = \langle \phi|\phi \rangle$. This is why the operator $\hat{U}$ can be thought of as a *transformation related to a motion in the unitary space* (rotation, reflection, etc.). For a unitary operator, we have $\hat{U}^\dagger \hat{U} = 1$, because $\left\langle \hat{U}\phi|\hat{U}\psi \right\rangle = \left\langle \phi|\hat{U}^\dagger \hat{U}\psi \right\rangle = \langle \phi|\psi \rangle$.

Eigenvalue Equation

If for a particular vector ϕ, we have

$$\hat{A}\phi = a\phi, \tag{B.5}$$

where a is a complex number and $\phi \neq 0$, then ϕ is called an eigenvector[9] of the operator $\hat{A}$ corresponding to the eigenvalue a. The operator $\hat{A}$ may have an infinite number or a finite number (including number zero) of the eigenvalues, labeled by the subscript i:

$$\hat{A}\phi_i = a_i \phi_i.$$

Hermitian operators have the following important properties[10]:

> If $\hat{A}$ represents a Hermitian operator, its eigenvalues a_i are real numbers, and its eigenvectors ϕ_i that correspond to different eigenvalues are orthogonal.

9 In quantum mechanics, the eigenvector ϕ will correspond to a function (a vector in the Hilbert space) and therefore is called also the eigenfunction.

10 We have the eigenvalue problem $\hat{A}\phi = a\phi$. Finding the complex conjugate of both sides, we obtain $(\hat{A}\phi)^* = a^*\phi^*$. Multiplying the first equation by ϕ^* and integrating, and then using ϕ and doing the same with the second equation, we get $\left\langle \phi|\hat{A}\phi \right\rangle = a \langle \phi|\phi \rangle$ and $\left\langle \hat{A}\phi|\phi \right\rangle = a^* \langle \phi|\phi \rangle$. But $\hat{A}$ is Hermitian, and therefore the left sides of both equations are equal. Subtracting them, we have $(a - a^*) \langle \phi|\phi \rangle = 0$. Since $\langle \phi|\phi \rangle \neq 0$, because $\phi \neq 0$, then $a = a^*$. This is what we wanted to show.

The orthogonality of the eigenfunctions of a Hermitian operator (corresponding to different eigenvalues) may be proved as follows. We have $\hat{A}\phi_1 = a_1\phi_1$, $\hat{A}\phi_2 = a_2\phi_2$, with $a_1 \neq a_2$. Multiplying the first equation by ϕ_2^* and integrating, one obtains $\left\langle \phi_2|\hat{A}\phi_1 \right\rangle = a_1 \langle \phi_2|\phi_1 \rangle$. Then, let us make the complex conjugate of the second equation: $(\hat{A}\phi_2)^* = a_2\phi_2^*$, where we have used that $a_2 = a_2^*$ (this was proved above). Then, let us multiply it by ϕ_1 and integrate: $\left\langle \hat{A}\phi_2|\phi_1 \right\rangle = a_2 \langle \phi_2|\phi_1 \rangle$. Subtracting the two equations, we have $0 = (a_1 - a_2) \langle \phi_2|\phi_1 \rangle$, and taking into account that $a_1 - a_2 \neq 0$, this gives $\langle \phi_2|\phi_1 \rangle = 0$.

The number of the linear independent eigenvectors that correspond to a given eigenvalue a is called the degree of degeneracy of the eigenvalue. Such vectors form a basis of the *invariant space of the operator* $\hat{A}$; i.e., any linear combination of the vectors represents a vector that is also an eigenvector (with the same eigenvalue a). If the eigenvectors corresponded to different eigenvalues, then their linear combination *is not* an eigenvector of $\hat{A}$. Both things need a few seconds to appear.

One can show that the eigenvectors of a Hermitian operator form the complete basis set[11] in the Hilbert space; i.e., any function of class[12] Q can be expanded in a linear combination of the basis set.

Sometimes an eigenvector ϕ of the operator $\hat{A}$ (with the eigenvalue a) is subject to an operator $f(\hat{A})$, where f is an analytic function. Then[13]

$$f(\hat{A})\phi = f(a)\phi. \tag{B.6}$$

Commutation and Eigenvalues

At times, we will use a theorem that if two linear and Hermitian operators $\hat{A}$ and $\hat{B}$ commute, then they have a common set of the eigenfunctions, and *vice versa*.

We will prove this theorem in the case of no degeneracy (i.e., there is only one linearly independent vector). We have an eigenvalue equation $\hat{B}\psi_n = b_n\psi_n$. Applying to both sides of the operator $\hat{A}$ and using the commutation relation $\hat{A}\hat{B} = \hat{B}\hat{A}$, we get $\hat{B}\left(\hat{A}\psi_n\right) = b_n\left(\hat{A}\psi_n\right)$. This means that $\hat{A}\psi_n$ is an eigenvector of $\hat{B}$ corresponding to the eigenvalue b_n. But we know already such a vector–this is ψ_n. But this can happen only if the two vectors are proportional: $\hat{A}\psi_n = a_n\psi_n$, which means that ψ_n is an eigenvector of $\hat{A}$.

Now, let us look at the inverse theorem. We have two operators and any eigenvector of $\hat{A}$ is also an eigenvector of $\hat{B}$. We want to show that the two operators commute. Let us write the two eigenvalue equations: $\hat{A}\psi_n = a_n\psi_n$ and $\hat{B}\psi_n = b_n\psi_n$. Let us take a vector ϕ. Since the eigenvectors $\{\psi_n\}$ form the complete set, then

$$\phi = \Sigma_n c_n \psi_n.$$

[11] This basis set may be assumed to be orthonormal because the eigenfunctions are as follows:

- As square-integrable, they can be normalized.
- If they correspond to different eigenvalues, they are automatically orthogonal.
- If they correspond to the same eigenvalue, they can be orthogonalized (still remaining eigenfunctions) by a method described in Appendix J available at booksite.elsevier.com/978-0-444-59436-5.

[12] That is, continuous, single-valued and square integrable, see Fig. 2.6.

[13] The operator $f(\hat{A})$ is defined through the Taylor expansion of the function f: $f(\hat{A}) = c_0 + c_1\hat{A} + c_2\hat{A}^2 + \cdots$. If now the operator $f(\hat{A})$ acts on an eigenfunction of $\hat{A}$, then, because $\hat{A}^n x = a^n x$, we obtain the result.

Applying the commutator $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$, we have
$[\hat{A}, \hat{B}]\phi = \hat{A}\hat{B}\phi - \hat{B}\hat{A}\phi = \hat{A}\hat{B}\Sigma_n c_n \psi_n - \hat{B}\hat{A}\Sigma_n c_n \psi_n = \hat{A}\Sigma_n c_n \hat{B}\psi_n - \hat{B}\Sigma_n c_n \hat{A}\psi_n = \hat{A}\Sigma_n c_n b_n \psi_n - \hat{B}\Sigma_n c_n a_n \psi_n = \Sigma_n c_n b_n \hat{A}\psi_n - \Sigma_n c_n a_n \hat{B}\psi_n = \Sigma_n c_n b_n a_n \psi_n - \Sigma_n c_n a_n b_n \psi_n = 0$. This means that the two operators commute.