10 Unitary transformations

10.1 Unitary operators

An operator $\hat{U}$ is said to be unitary if it is invertible and

$$\hat{U}^\dagger = \hat{U}^{-1}. \tag{10.1}$$

By definition of the inverse of an operator, $\hat{U}^{-1}\hat{U} = \hat{I} = \hat{U}\hat{U}^{-1}$ with $\hat{I}$ the identity operator. Therefore, if $\hat{U}$ is unitary,

$$\hat{U}^\dagger\hat{U} = \hat{I} = \hat{U}\hat{U}^\dagger. \tag{10.2}$$

- The eigenvalues of a unitary operator are real or complex numbers of modulus 1. (I.e., if $\hat{U}|\psi\rangle = \lambda|\psi\rangle$, it is always the case that $|\lambda| = 1$ when $\hat{U}$ is a unitary operator.)

  ☞ Proof: Suppose $\hat{U}|\psi\rangle = \lambda|\psi\rangle$ with $\langle\psi|\psi\rangle = 1$ (it is not restrictive to assume that $|\psi\rangle$ is normalized). As is explained in Section 4.3, it follows from this equation that $\langle\psi|\hat{U}^\dagger = \lambda^*\langle\psi|$, where $\hat{U}^\dagger$ is understood to act "on the left" on the bra vector $\langle\psi|$. Thus $\langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle = \lambda^*\lambda\langle\psi|\psi\rangle = |\lambda|^2$. However, we also have that $\langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle = \langle\psi|\psi\rangle = 1$. Thus $|\lambda| = 1$. □

- Eigenvectors of a unitary operator corresponding to different eigenvalues are always orthogonal. (I.e., if $\hat{U}$ is a unitary operator, $\hat{U}|\psi\rangle = \lambda|\psi\rangle$ and $\hat{U}|\phi\rangle = \mu|\phi\rangle$, it is always the case that $\langle\phi|\psi\rangle = 0$ if $\lambda \neq \mu$.)

  ☞ Proof: $\langle\phi|\hat{U}^\dagger = \mu^*\langle\phi|$ since $\hat{U}|\phi\rangle = \mu|\phi\rangle$, and therefore

  $$\langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle = \mu^*\lambda\langle\phi|\psi\rangle. \tag{10.3}$$

  However, we also have that

  $$\langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\phi|\hat{I}|\psi\rangle = \langle\phi|\psi\rangle. \tag{10.4}$$

  Subtracting Eq. (10.3) from Eq. (10.4) gives

  $$0 = (1 - \mu^*\lambda)\langle\phi|\psi\rangle. \tag{10.5}$$

  However $\mu \neq 0$ and $\mu^* = 1/\mu$ since $|\mu| = 1$, and thus

  $$0 = (1 - \lambda/\mu)\langle\phi|\psi\rangle = (\mu - \lambda)\langle\phi|\psi\rangle/\mu \tag{10.6}$$

  Hence $\langle\phi|\psi\rangle = 0$ if $\lambda \neq \mu$. □

- The most important property of unitary transformations is that they conserve the inner product: If $|\psi'\rangle = \hat{U}|\psi\rangle$, $|\phi'\rangle = \hat{U}|\phi\rangle$ and $\hat{U}$ is unitary,

$$\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle. \tag{10.7}$$

As a particular case of this relationship, $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle$ for any $|\psi\rangle$: unitary transformations conserve the norm.

☞ Proof: We use the relation, seen previously, that the bra vector conjugate to the ket vector $\hat{U}|\phi\rangle$ can be written as $\langle\phi|\hat{U}^\dagger$. Since $|\psi'\rangle = \hat{U}|\psi\rangle$ and $|\phi'\rangle = \hat{U}|\phi\rangle$, we see that $\langle\phi'|\psi'\rangle = \langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\phi|\hat{I}|\psi\rangle = \langle\phi|\psi\rangle$. □

☞ More generally, a unitary transformation is an inner product preserving one-to-one mapping from one Hilbert space to either the same Hilbert space or to another one. The word operator refers to mappings from one Hilbert space to the same one.

Representing ket vectors by column vectors is an example of a more general unitary transformations: Ket vectors and column vectors belong to different Hilbert spaces. However, given an orthonormal basis of ket vectors, there is a one-to-one correspondence between each ket vector and the column vector representing that ket vector in that basis. Furthermore, the inner product of any two ket vectors and the inner product of the two column vectors representing these ket vectors are always equal.

The Fourier transform is another example of a more general unitary transformation. Indeed, it can be shown that if $\phi_a(k)$ is the Fourier transform of $\psi_a(x)$ and $\phi_b(k)$ the Fourier transform of $\psi_b(x)$, then

$$\int_{-\infty}^{\infty} \psi_a^*(x)\psi_b(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \phi_a^*(k)\phi_b(k)\,\mathrm{d}k. \tag{10.8}$$

I.e., the inner product of $\psi_a(x)$ and $\psi_b(x)$ is equal to the inner product of their Fourier transforms.

10.2 Transformed operators

Suppose that the vector $|\psi\rangle$ is transformed into the vector $|\eta\rangle$ by a certain operator, $\hat{A}$:

$$|\eta\rangle = \hat{A}|\psi\rangle. \tag{10.9}$$

Suppose, further, that the vectors $|\psi\rangle$ and $|\eta\rangle$ are transformed into the vector $|\psi'\rangle$ and $|\eta'\rangle$ by a certain unitary operator, $\hat{U}$:

$$|\psi'\rangle = \hat{U}|\psi\rangle, \qquad |\eta'\rangle = \hat{U}|\eta\rangle. \tag{10.10}$$

Then we see that $|\eta'\rangle = \hat{U}\hat{A}|\psi\rangle = \hat{U}\hat{A}\hat{U}^\dagger|\psi'\rangle$, where in the last step we have used the facts that $|\psi\rangle = \hat{U}^{-1}|\psi'\rangle$ and that $\hat{U}^{-1} = \hat{U}^\dagger$. I.e.,

$$|\eta'\rangle = \hat{A}'|\psi'\rangle \tag{10.11}$$

with $\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$. Since this is the case for any $|\psi\rangle$ on which $\hat{A}$ acts, we can say that a unitary transformation which transforms ket vectors according to the equation

$$|\psi'\rangle = \hat{U}|\psi\rangle \tag{10.12}$$

transforms operators according to the equation

$$\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger. \tag{10.13}$$

The transformed operator $\hat{A}'$ has the same properties as $\hat{A}$ in the following sense:

1. If $\hat{A}$ is Hermitian, $\hat{A}'$ is also Hermitian. (The proof is left as an exercise.)
2. Sums and products of operators are transformed into sums and products of the transformed operators: e.g., if $\hat{A} = \alpha\hat{B} + \beta\hat{C}\hat{D}$ where α and β are two complex numbers, then $\hat{A}' = \alpha\hat{B}' + \beta\hat{C}'\hat{D}'$.

   ☞ Proof: We use the general relation between operators and their transformed, and also $\hat{U}\hat{U}^\dagger = \hat{I}$.

   $$\begin{aligned}\hat{A}' &= \hat{U}\hat{A}\hat{U}^\dagger \\ &= \hat{U}(\alpha\hat{B} + \beta\hat{C}\hat{D})\hat{U}^\dagger \\ &= \alpha\hat{U}\hat{B}\hat{U}^\dagger + \beta\hat{U}\hat{C}(\hat{U}^\dagger\hat{U})\hat{D}\hat{U}^\dagger \\ &= \alpha\hat{U}\hat{B}\hat{U}^\dagger + \beta(\hat{U}\hat{C}\hat{U}^\dagger)(\hat{U}\hat{D}\hat{U}^\dagger),\end{aligned}$$

   from which it follows that $\hat{A}' = \alpha\hat{B}' + \beta\hat{C}'\hat{D}'$. □

3. As a particular case of this relationship, if $[\hat{A}, \hat{B}] = \hat{C}$, then

$$[\hat{A}', \hat{B}'] = \hat{C}' = \hat{U}[\hat{A}, \hat{B}]\hat{U}^\dagger. \tag{10.14}$$

4. $\hat{A}$ and $\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$ have the same eigenvalues. (The proof is left as an exercise.)
5. $\langle\phi'|\hat{A}'|\psi'\rangle = \langle\phi|\hat{A}|\psi\rangle$ for any $|\phi\rangle$, $|\psi\rangle$. (The proof is also left as an exercise.)

Unitary transformations and matrix representation

We only consider representations of operators by finite matrices here, i.e., representations of operators acting in a finite-dimensional Hilbert space. As noted previously, the matrices and column vectors representing operators and vectors in a given basis depend on the basis used in the representation. Different choices of basis result in different matrices and column vectors. As we will now discuss, matrices and column vectors obtained in one basis are related to those obtained in another basis by a unitary transformation.

Consider an operator $\hat{A}$ acting in a Hilbert space of dimension N. Consider, also, two different orthonormal bases of this Hilbert space, namely a basis $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle\}$ and a basis $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_N\rangle\}$. That these two bases are orthonormal means that

$$\langle\phi_i|\phi_j\rangle = \langle\psi_i|\psi_j\rangle = \delta_{ij}, \tag{10.15}$$

and also that

$$\sum_{k=1}^{N} |\phi_k\rangle\langle\phi_k| = \sum_{k=1}^{N} |\psi_k\rangle\langle\psi_k| = \hat{I}, \tag{10.16}$$

where $\hat{I}$ is the identity operator. (This last equation is the completeness relation for these two bases, see Section 5.2.)

The operator $\hat{A}$ is represented by the matrix A of elements $A_{ij} = \langle\phi_i|\hat{A}|\phi_j\rangle$ when working in the $\{|\phi_n\rangle\}$ basis and by the matrix A' of elements $A'_{ij} = \langle\psi_i|\hat{A}|\psi_j\rangle$ when working in the $\{|\psi_n\rangle\}$ basis. These two matrices are usually different, although they represent the same operator. Likewise, a state vector $|\Psi\rangle$ is represented by the column vector c of elements $c_i = \langle\phi_i|\Psi\rangle$ when working in the $\{|\phi_n\rangle\}$ basis and by the column vector c' of elements $c'_i = \langle\psi_i|\Psi\rangle$ when working in the $\{|\psi_n\rangle\}$ basis. These two column vectors are usually different, although they represent the same state vector.

Now, given that the $\{|\phi_n\rangle\}$ basis is complete, it is always possible to write each of the $|\psi_j\rangle$ vectors as a linear combination of the $|\phi_i\rangle$ vectors. The coefficients of these linear combinations are complex numbers, which we will denote by M_{ij}. Specifically,

$$|\psi_j\rangle = \sum_{i=1}^{N} M_{ij}|\phi_i\rangle. \tag{10.17}$$

(Note the order of the indexes: the coefficient of $|\phi_i\rangle$ is denoted M_{ij}, not M_{ji}.) Since the $|\phi_i\rangle$ are orthonormal, $M_{ij} = \langle\phi_i|\psi_j\rangle$ (see Section 2.10). Moreover $M^*_{ij} = \langle\psi_j|\phi_i\rangle$ since $\langle\phi_i|\psi_j\rangle^* = \langle\psi_j|\phi_i\rangle$ (see Section 2.8).

These complex coefficients can be arranged in an $N \times N$ matrix M in the usual way:

$$\mathsf{M} = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1N} \\ M_{21} & M_{22} & \cdots & M_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ M_{N1} & M_{N2} & \cdots & M_{NN} \end{pmatrix}. \tag{10.18}$$

This matrix is unitary — i.e., $\mathsf{M}^\dagger\mathsf{M} = \mathsf{I}$, where I is the unit matrix.

☞ Proof: Let us work out the ij-element of the matrix $\mathsf{M}^\dagger\mathsf{M}$. Using Eq. (10.16),

$$\begin{aligned}\left(\mathsf{M}^\dagger\mathsf{M}\right)_{ij} &= \sum_{k=1}^{N} \left(\hat{M}^\dagger\right)_{ik}\left(\hat{M}\right)_{kj} \\ &= \sum_{k=1}^{N} M_{ki}^{*} M_{kj} \\ &= \sum_{k=1}^{N} \langle\psi_i|\phi_k\rangle\langle\phi_k|\psi_j\rangle \\ &= \langle\psi_i|\hat{I}|\psi_j\rangle = \langle\psi_i|\psi_j\rangle = \delta_{ij}.\end{aligned}$$

Since the elements of the unit matrix I are equal to δ_{ij} (the diagonal elements of I are all equal to 1 and all the other elements are equal to 0), we see that $\mathsf{M}^\dagger\mathsf{M} = \mathsf{I}$. Proving that $\mathsf{M}\mathsf{M}^\dagger = \mathsf{I}$ can be done similarly. □

We can thus pass from one basis to another by a unitary transformation. Transforming the basis from $\{|\phi\rangle_n\}$ to $\{|\psi\rangle_n\}$ as per the matrix M transforms both the column vectors representing quantum states and the matrices representing operators. This transformation is also unitary: If in the $\{|\phi\rangle_n\}$ basis the ket vector $|\psi\rangle$ is represented by the column vector c and the operator $\hat{A}$ is represented by the matrix A, and if the same ket vector and the same operator are represented by the column vector c' and the matrix $\hat{A}'$ in the $\{|\psi\rangle_n\}$ basis, then

$$\mathsf{c}' = \mathsf{M}^\dagger\mathsf{c} \quad \text{and} \quad \mathsf{A}' = \mathsf{M}^\dagger\mathsf{A}\mathsf{M}. \tag{10.19}$$

(The proof of these equations is left as an exercise. Note that the elements of the column vectors c transform according to $\mathsf{M}^\dagger$ whereas the basis vectors transform according to M.) These two equations can be brought to the same form as Eqs. (10.12) and (10.13) by rewriting them in terms of the adjoint of the basis change matrix: Setting $\mathsf{U} = \mathsf{M}^\dagger$,

$$\mathsf{c}' = \mathsf{U}\mathsf{c} \quad \text{and} \quad \mathsf{A}' = \mathsf{U}\mathsf{A}\mathsf{U}^\dagger. \tag{10.20}$$

However, note that these equations arise from a mere change of basis which has no impact on the ket vectors representing quantum states, whereas Eqs. (10.12) and (10.13) arise from a transformation of the ket vectors.

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