Chapter 4. Operators

Section 4.1. Observable Properties Are Described by Operators

§ 1 *Introduction.* In this chapter I show that the expression for the average value of an observable A leads us to introduce a new object: the operator $\hat{A}$ representing the observable A. The pure states of the observable A and its spectrum can be calculated by solving the eigenvalue equation of $\hat{A}$.

Since operators are so central to quantum theory we need to study their properties. We define operations with operators (addition and multiplication) and functions of operators. Among these functions the Hermitian conjugate, the inverse, and the exponential of an operator play an important role. There are different kinds of operators, and in quantum mechanics Hermitian, anti-Hermitian, and unitary operators are most common and many general results of quantum theory are based on their properties.

§ 2 *The average value of an observable.* If we perform an experiment that puts a system in a state $|\psi\rangle$ and then we measure the value of an observable A, we can calculate the probability $P_\psi(a_n)$ that the result of the measurement is a_n by using

$$P_\psi(a_n) = |\langle a_n | \psi \rangle|^2 \tag{1}$$

Here $|a_n\rangle$ is a pure state of the observable A. A similar equation is valid for the probability $P_\psi(\alpha)\,\mathrm{d}\alpha$ that the measurement gives a value α in the continuous spectrum of A, located between α and $\alpha + \mathrm{d}\alpha$:

$$P_\psi(\alpha)\,\mathrm{d}\alpha = |\langle \alpha | \psi \rangle|^2\,\mathrm{d}\alpha \tag{2}$$

Often an experimentalist is not interested in studying the state $|\psi\rangle$ or the observable A in so much detail. He might be happy to know the average

value of the observable A, when the system is in a state $|\psi\rangle$. For example, we can expose a molecule to an ultra-short pulse of light to excite it to another electronic state. In this process we excite coherently many rotational states of the molecule. An experimentalist may be content to know only the average rotational energy of the excited molecule.

Probability theory has a simple definition for the average. If we measure a quantity X, which can take the values x_1, x_2, x_3, ... with the probabilities p_1, p_2, p_3, ..., then the average value $\langle X\rangle$ of X is defined by

$$\langle X\rangle \equiv \sum_{i=1}^{\infty} x_i p_i \tag{3}$$

If X takes continuous values $x \in D$ with the probability distribution $p(x)$ then the average value of X is

$$\langle X\rangle \equiv \int_{x\in D} x\, p(x)\, \mathrm{d}x \tag{4}$$

There is nothing unusual about these formulae: this is how you calculate the average grade of the students who took an examination, or the average family income in a city.

The same definition is used in quantum mechanics. This means that if a measurement of A can give one of the discrete values a_1, a_2, ... or one of the continuous values $\alpha \in D$, and the system is in state $|\psi\rangle$, the average value of A is

$$\langle A\rangle_\psi \equiv \sum_{n=1}^{\infty} P_\psi(a_n) a_n + \int_{\alpha\in D} \mathrm{d}\alpha\, P_\psi(\alpha)\alpha \tag{5}$$

Here $P_\psi(a_n)$ and $P_\psi(\alpha)\,\mathrm{d}\alpha$ are the probabilities defined by Eqs. 1 and 2. The notation $\langle A\rangle_\psi$ is often used in quantum mechanics for the average value of A when the system is in state $|\psi\rangle$. When it is clear which state the system is in, we use the notation $\langle A\rangle$.

§ 3 *The operator corresponding to an observable.* I want to rewrite Eq. 5 and I will use $|z|^2 = z^* z$, and $\langle x \,|\, y\rangle^* = \langle y \,|\, x\rangle$. The result is:

$$P_\psi(a_n) = |\langle a_n \,|\, \psi\rangle|^2 = \langle a_n \,|\, \psi\rangle^* \langle a_n \,|\, \psi\rangle = \langle \psi \,|\, a_n\rangle \langle a_n \,|\, \psi\rangle \tag{6}$$

Similarly,

$$P_\psi(\alpha) = \langle \psi \,|\, \alpha\rangle \, \langle \alpha \,|\, \psi\rangle \tag{7}$$

Using Eqs. 6 and 7 allows me to rewrite Eq. 5 as

$$\langle A\rangle_\psi = \sum_{n=1}^{\infty} \langle \psi \,|\, a_n\rangle \, a_n \, \langle a_n \,|\, \psi\rangle + \int_{\alpha\in D} \mathrm{d}\alpha \, \langle \psi \,|\, \alpha\rangle \, \alpha \, \langle \alpha \,|\, \psi\rangle \tag{8}$$

As was explained in Chapter 3, Dirac would write this expression as

$$\langle A\rangle_\psi = (\langle \psi \,|\,) \left(\sum_{n=1}^{\infty} |a_n\rangle a_n \langle a_n| + \int_{\alpha\in D} \mathrm{d}\alpha \, |\alpha\rangle \alpha \langle \alpha| \right) (\,|\,\psi\rangle) \tag{9}$$

and considered it to consist of the symbol

$$\hat{A} \equiv \sum_{n=1}^{\infty} |a_n\rangle \, a_n \, \langle a_n| + \int_{\alpha\in D} \mathrm{d}\alpha \, |\alpha\rangle \, \alpha \, \langle \alpha| \tag{10}$$

sandwiched between the bra $\langle\psi|$ and the ket $|\psi\rangle$:

$$\langle \hat{A}\rangle_\psi \equiv \langle \psi \,|\, \hat{A} \,|\, \psi\rangle \tag{11}$$

The symbol $\hat{A}$ is a new object for us. It acts on an arbitrary ket $|\psi\rangle$, to give another ket denoted by $\hat{A}\,|\,\psi\rangle$, according to the recipe:

$$\hat{A}|\psi\rangle = \sum_{n=1}^{\infty} |a_n\rangle \, a_n \, \langle a_n \,|\, \psi\rangle + \int_{\alpha\in D} \mathrm{d}\alpha \, |\alpha\rangle \, \alpha \, \langle \alpha \,|\, \psi\rangle \tag{12}$$

Here $\langle a_n \,|\, \psi\rangle$ and $\langle \alpha \,|\, \psi\rangle$ are complex numbers and a_n and α are real numbers (since they are possible results of a measurement of A). $|a_n\rangle \, a_n \, \langle a_n \,|\, \psi\rangle$ is a ket because multiplying the ket $|a_n\rangle$ by the number $a_n \langle a_n \,|\, \psi\rangle$ gives a ket.

The sum in Eq. 12 is a ket because a sum of kets is a ket. The integral in Eq. 12 also gives a ket, because an integral is a glorified sum. So, $\hat{A}|\psi\rangle$ is a ket.

We have good reason to use the notation $\hat{A}$ in Eq. 10: the right-hand side of that equation contains only quantities tied to the observable A; in particular, $\hat{A}$ does not depend on the state $|\psi\rangle$ of the system on which we perform the measurement.

Eq. 12 has all the "false generality" we encountered when we "derived" the completeness relation. We must keep in mind that the operator $\hat{A}$ defined by Eq. 12 *can only act on kets that belong to the same space as* $|a_n\rangle$ *and* $|\alpha\rangle$. It makes no sense to act with an operator defined by using the pure states of a harmonic oscillator on kets that describe the states of a hydrogen atom. As written, without carefully specifying the space in which $\hat{A}$ is defined, the formula appears to be much more general than it is.

The definition of $\hat{A}$ has another embarrassing shortcoming: it is valid only if we prove the convergence of the infinite sum and the existence of the integral. We leave such subtleties to mathematicians. Physical chemists are saved by the fact that many practical problems, concerning bound systems, are solved by assuming that we can neglect the integral and can use a finite number of terms in the sum. To test whether such a finite sum has enough terms to approximate the infinite sum, we redo the calculation by adding more terms to the finite sum, until the result of the numerical calculation no longer changes. A similar procedure works when the system is unbound (e.g. when two molecules collide, or when we study photodissociation or photoionization). The energy of such systems is continuous and one cannot neglect

the integral in the definition of the operator. However, in most practical applications one approximates the integral by a finite sum. Victory is declared when adding more terms to the sum does not change the magnitude of the observable being calculated. These methods do not guarantee convergence but they tend to work, in the sense that, when used carefully, they give results in agreement with the experiments.

§ 4 *An example: the energy operator.* Let us examine this definition for a particular case. If the observable is energy, and it has the spectrum E_1, E_2, ... and $e \in [0, \infty]$, we can associate with it the operator

$$\hat{H} = \sum_{n=1}^{\infty} |E_n\rangle \, E_n \, \langle E_n| + \int_0^{\infty} \mathrm{d}e \, |e\rangle \, e \, \langle e| \tag{13}$$

For example, the pure states of the hydrogen atom are $|n, \ell, m\rangle$ with $n = 1, 2, \ldots$, $\ell = 0, 1, \ldots, n-1$, and $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$. The energy of a bound state $|E_n\rangle$ is[1]

$$E_n = -\frac{\mu e^4}{2(4\pi\epsilon_0)^2\hbar^2} \, \frac{1}{n^2}, \quad n = 1, 2, \ldots$$

The hydrogen atom also has a continuous spectrum which is accessed experimentally when the atom absorbs a photon whose energy is higher than the binding energy of the electron (to the proton). After photon absorption the proton and the electron fly apart. The relative energy[2] of the dissociated

[1] μ is the reduced mass, e is the charge of the electron, and ϵ_0 is the permittivity of vacuum

[2] This is the energy of a system viewed by an observer that moves with the center of mass of the atom. Therefore, the formula does not contain the energy of the motion of the center of mass. The latter energy exists because the atom was moving before being ionized

electron-proton pair (i.e. the dissociated hydrogen atom) is

$$e_k = \frac{\hbar^2 k^2}{2\mu}, \quad k \in [0, \infty],$$

where $\hbar k$ is the relative momentum and μ is the reduced mass; the corresponding ket is denoted by $|k\rangle$.

According to the theory we have just developed, the operator corresponding to the energy of the hydrogen atom is

$$\begin{aligned} \hat{H} &= -\sum_{n=1}^{\infty} \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} |n, \ell, m\rangle \, \frac{\mu e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \, \frac{1}{n^2} \, \langle n, \ell, m| \\ &\quad + \int_{-\infty}^{+\infty} \mathrm{d}k_x \, \mathrm{d}k_y \, \mathrm{d}k_z \, |k_x, k_y, k_z\rangle \, \frac{\hbar^2 k^2}{2\mu} \langle k_x, k_y, k_z| \end{aligned} \tag{14}$$

The triple integral appears because the momentum is a vector with the components k_x, k_y and k_z. We use the notation $\hat{H}$ because the operator corresponding to the energy is called the Hamiltonian. Eq. 14 is a correct representation of the Hamiltonian of the hydrogen atom, even though it looks extremely different from the usual formula:

$$\hat{H} = -\frac{\hbar^2}{2\mu} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] - \frac{e^2}{4\pi\epsilon_0 r} \tag{15}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ is the distance between the electron and the proton and x, y and z are the coordinates of the electron in a coordinate system with the origin at the center of mass. We use Eq. 14 when we derive various properties of the Hamiltonian and Eq. 15 when we perform energy calculations.

Exercise 1 Write a formula similar to Eq. 14 for the operator corresponding to the angular momentum squared. The pure states of angular momentum squared are $|\ell, m\rangle$ with $\ell = 0, 1, 2, \ldots$ and $m = -\ell, -\ell + 1, \ldots, \ell$.

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§ 5 *The operators that represent observables are linear.* By definition, an operator $\hat{A}$ is linear when it satisfies the following conditions.

- If

$$|\eta\rangle = |\phi\rangle + |\psi\rangle \tag{16}$$

  where $|\phi\rangle$ and $|\psi\rangle$ are arbitrary kets, then

$$\hat{A}|\eta\rangle = \hat{A}|\phi\rangle + \hat{A}|\psi\rangle \tag{17}$$

- If

$$|\eta\rangle = \alpha|\psi\rangle \tag{18}$$

  where α is a complex number and $|\psi\rangle$ is an arbitrary ket, then

$$\hat{A}|\eta\rangle = \alpha\hat{A}|\psi\rangle \tag{19}$$

By 'arbitrary' in this context, I mean of course that the operations (e.g. application of $\hat{A}$) are meaningful. For example, if A is an observable pertaining to a harmonic oscillator then $|\psi\rangle$ should be a ket that represents properties of the *same* harmonic oscillator.

When $\hat{A}$ represents an observable, it is straightforward to verify that Eq. 17 is correct. If we ignore for a moment the second term in Eq. 10, then

$$\hat{A}|\eta\rangle = \sum_n |a_n\rangle\, a_n\, \langle a_n \,|\, \eta\rangle$$

One of the properties of the scalar product is that $\langle a_n \,|\, \eta\rangle \;= \langle a_n \,|\, \phi\rangle + \langle a_n \,|\, \psi\rangle$ when $|\eta\rangle$ is given by Eq. 16. Therefore

$$\hat{A}|\eta\rangle = \sum_n |a_n\rangle\, a_n\, \langle a_n \,|\, \phi\rangle + \sum_n |a_n\rangle\, a_n\, \langle a_n \,|\, \psi\rangle = \hat{A}|\phi\rangle + \hat{A}|\psi\rangle \tag{20}$$

The same property holds for the other part of Eq. 10, $\int \mathrm{d}\alpha\, |\alpha\rangle\, \alpha\, \langle\alpha|$, and therefore Eq. 17 is correct. Eq. 19 can be verified in a similar manner.

§ 6 *The eigenvalue problem.* One of the most important problems encountered in quantum mechanics is finding solutions to the equation

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle \tag{21}$$

where $\hat{O}$ is a known operator, $|\psi\rangle$ is an unknown ket, and λ is an unknown complex or real number. This is known as *the eigenvalue problem* for the operator $\hat{O}$. A ket $|\psi\rangle$ that satisfies Eq. 21 is called an *eigenket* or *eigenvector* or an *eigenstate* of $\hat{O}$. The number λ is called the *eigenvalue of* $\hat{O}$ *corresponding to eigenstate* $|\psi\rangle$. Eigenstates and eigenvalues come in pairs.

Most equations in physics have unique solutions once proper boundary or initial conditions are specified. The eigenvalue problem in quantum mechanics is an exception: it always has multiple solutions.

For linear operators, one source of multiplicity is trivial: if $|\psi\rangle$ is an eigenfunction of $\hat{O}$ for eigenvalue λ then $\alpha|\psi\rangle$ is also an eigenfunction of $\hat{O}$, for the same eigenvalue λ, for every number α. This fact is easily verified. Assume that $\hat{O}|\psi\rangle = \lambda|\psi\rangle$ and set $|\eta\rangle = \alpha|\psi\rangle$. Calculate

$$\hat{O}|\eta\rangle = \hat{O}(\alpha|\psi\rangle) = \alpha\hat{O}|\psi\rangle = \alpha\lambda|\psi\rangle = \lambda\alpha|\psi\rangle = \lambda|\eta\rangle$$

This calculation shows us that $|\eta\rangle$ is an eigenstate corresponding to eigenvalue λ.

So many solutions might have been an embarrassment of riches, but physics comes to the rescue. I will soon show that the eigenstates of interest to quantum mechanics must be normalized, namely they must satisfy

$$\langle\psi\,|\,\psi\rangle = 1$$

Suppose we have solved an eigenvalue problem and found an eigenstate $|\phi\rangle$ that is not normalized. What do we do about this? We remember that every multiple of $|\phi\rangle$ is also an eigenstate corresponding to the same eigenvalue. We write

$$|\chi\rangle = \alpha|\phi\rangle$$

and choose the number α to ensure that $|\chi\rangle$ is normalized:

$$1 = \langle\chi\,|\,\chi\rangle = \alpha^*\alpha\langle\phi\,|\,\phi\rangle$$

We see from this that

$$\alpha^*\alpha = \frac{1}{\langle\phi\,|\,\phi\rangle}$$

This relationship fixes the magnitude $|\alpha| = \sqrt{\alpha^*\alpha}$ of the complex number α but not its phase.[3] Therefore

$$\alpha = \frac{\mathrm{e}^{\mathrm{i}x}}{\sqrt{\langle\phi\,|\,\phi\rangle}},$$

where x is a real number, and the normalized eigenstate is

$$|\chi\rangle = \frac{\mathrm{e}^{\mathrm{i}x}|\phi\rangle}{\sqrt{\langle\phi\,|\,\phi\rangle}}$$

We are stuck with the unknown "phase factor" $\mathrm{e}^{\mathrm{i}x}$. It turns out that such phase factors cancel out when we use the state $|\chi\rangle$ to calculate measurable quantities.

It is straightforward to show that $|\chi\rangle$ is normalized:

$$\langle\chi\,|\,\chi\rangle = \frac{\mathrm{e}^{-\mathrm{i}x}}{\sqrt{\langle\phi\,|\,\phi\rangle}}\frac{\mathrm{e}^{-\mathrm{i}x}}{\sqrt{\langle\phi\,|\,\phi\rangle}}\langle\phi\,|\,\phi\rangle = 1$$

[3]Recall that a complex number α can be written as $|\alpha|\exp[\mathrm{i}x]$ where x is a real number called the phase of α. As usual, i is the square root of -1.

In summary, if we use an analytical or a numerical procedure for calculating eigenstates and obtain a ket $|\psi\rangle$ we convert it to a physically relevant eigenstate $|\eta\rangle$ by calculating

$$|\eta\rangle = \frac{|\psi\rangle}{\sqrt{\langle\psi\,|\,\psi\rangle}}$$

This is called *normalizing the eigenstate*.

There is another source of multiplicity of eigenstates, which is not as trivial as the one just discussed. The operators in quantum mechanics have more than one eigenstate and we should write Eq. 21 as

$$\hat{O}|\psi_i\rangle = \lambda_i|\psi_i\rangle \tag{22}$$

where i might take a finite number of values (e.g. for spin states) or an infinite but denumerable number of values (e.g. for harmonic-oscillator energy states), or belong to a continuous set (e.g. position or momentum states).

§ 7 *The pure states of an observable A are eigenstates of the operator $\hat{A}$ and the spectrum of A consists of all eigenvalues of $\hat{A}$.* The eigenvalue problem is important to quantum mechanics[4] because of the following statement.

Let $\hat{A}$ be the operator corresponding to an observable A. All pure states of the observable A are eigenstates of $\hat{A}$ and all allowed values of A (the spectrum of A) are eigenvalues of $\hat{A}$.

This means that the pure states $|a_n\rangle$ or $|\alpha\rangle$ of the observable A satisfy the eigenvalue equation

$$\hat{A}|a_n\rangle = a_n\,|a_n\rangle \tag{23}$$

[4]Eigenvalue problems are common to all branches of physics. All mathematics developed for solving problems in quantum mechanics can be used to solve problems in fluid mechanics, heat and mass transfer, acoustics or electrodynamics.

for states $|\,a_n\rangle$ corresponding to the discrete spectrum, and the equation

$$\hat{A}|\alpha\rangle = \alpha\,|\alpha\rangle \quad \alpha \in D \tag{24}$$

for the states $|\,\alpha\rangle$ corresponding to the continuous spectrum $\alpha \in D$.

I remind you that the pure states of any observable are orthonormal:

$$\langle a_n\,|\,a_m\rangle = \delta_{nm} \tag{25}$$

and

$$\langle a_n\,|\,\alpha\rangle = 0, \quad \alpha \in D \tag{26}$$

We can now prove the statement made above (in italics). Let us act with $\hat{A}$ (given by Eq. 10) on the pure state $|\,a_n\rangle$ and use the orthonormality of the pure states to simplify the result:

$$\begin{aligned} \hat{A}|a_n\rangle &= \sum_{m=1}^{\infty} |a_m\rangle\, a_m\, \langle a_m\,|\,a_n\rangle + \int_D \mathrm{d}\alpha|\alpha\rangle\, \alpha\, \langle\alpha\,|\,a_n\rangle \\ &= \sum_{m=1}^{\infty} |a_m\rangle\, a_m\, \delta_{mn} = a_n|a_n\rangle \end{aligned} \tag{27}$$

The integral disappears because of Eq. 26. Since the Kronecker delta is zero if $m \neq n$, and it is equal to 1 when $n = m$, the sum in the equation above is equal to $a_n\,|a_n\rangle$. This proves that Eq. 23 is correct. A similar argument shows that Eq. 24 is also correct.

Section 4.2. Various Kinds of Operators and Their Properties

§ 8 *Introduction.* We introduced above the concept of operator through Eq. 10, which was obtained by rewriting the equation for the average value of an observable. This is a very valuable result but, as a definition of an

operator, it is limited. We extend it to say that any operation that converts an element of a linear space into an element of the same linear space is an operator. A space of kets is a particular example of a linear space. For example, all the kets that are linear combinations of the pure states of a harmonic oscillator form one ket space. All the linear combinations of pure states of a hydrogen atom form another ket space. But these are not the only linear spaces of interest. The spaces L^2 and $\boldsymbol{\ell}^2$ are also important in quantum mechanics. Operators are defined on these linear spaces too.

Most of the operator properties derived here are valid for general operators defined to act on elements of a general linear space. They do not depend on the specific properties of the space.

It so happens that the operators of interest to quantum mechanics satisfy the following theorem: if the eigenvalues of an operator $\hat{B}$ are $b_n, n = 1, 2, \ldots$, and $\beta \in D$ and the corresponding eigenstates are $|b_n\rangle$ and $|\beta\rangle$ then the operator $\hat{O}$ satisfies

$$\hat{O} = \sum_{n=1}^{\infty} |\, b_n\rangle b_n \langle b_n\,| + \int_D \mathrm{d}\beta\, |\,\beta\rangle \beta \langle \beta\,| \tag{28}$$

We will use this property frequently when we prove various properties of operators. Mathematicians call Eq. 28 the *spectral resolution of the operator* $\hat{O}$.

Since operators are mathematical objects we need to define operations with them, such as addition and multiplication.

Not all operators are created equal, and Hermitian (or self-adjoint) and unitary operators, which will be defined shortly, play a special role in quantum mechanics. We define them and study their properties in what follows. Here is a preview.

As we have already discussed, the spectrum of an observable A consists of all the eigenvalues of the operator $\hat{A}$ representing that observable. Since the spectrum is the set of all values that A can take when it is measured, it must consist of real numbers. This condition is guaranteed only if the operator $\hat{A}$ is Hermitian.

Unitary operators convert a state of a system into a state that has the same measurable properties. Because of this, sometimes we can use unitary operators to rewrite a given set of states into an equivalent set whose physical content is easier to interpret. They are also sometimes used to convert an equation into a new equation that is simpler but gives the same physical results as the original (untransformed) equation.

To define Hermitian and unitary operators we need to define the adjoint of an operator and its inverse; these are functions of the original operator.

In this section we define these operators and derive their properties. You might find the material that follows tedious. You may be tempted to skip the proofs and accept obediently the results. This would be a mistake. The manipulations used in these proofs are so basic to quantum mechanics that you cannot master the subject unless you can use them with ease. For this you need the practice of going patiently and thoroughly through this chapter.

§ 9 *Operations with operators.* Let us start with some simple stuff. Operators are mathematical objects for which we can define addition and multiplication.

An operator $\hat{C}$ is the sum of the operators $\hat{A}$ and $\hat{B}$ if $\hat{C}$ operating on *any* ket $|\psi\rangle$ satisfies the equation

$$\hat{C}|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle \tag{29}$$

Since $\hat{A}|\psi\rangle$ is a ket and $\hat{B}|\psi\rangle$ is a ket, the sum $\hat{A}|\psi\rangle + \hat{B}|\psi\rangle$ is also a ket.

An operator $\hat{C}$ is the product $\hat{A}\hat{B}$ of the operators $\hat{A}$ and $\hat{B}$ if

$$\hat{C}|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle) \tag{30}$$

for *any* ket $|\psi\rangle$. The right-hand side of Eq. 30 indicates that first you act with $\hat{B}$ on $|\psi\rangle$ and obtain the ket $|\eta\rangle \equiv \hat{B}|\psi\rangle$, and then you act with $\hat{A}$ on $|\eta\rangle$.

Now that we have defined the product of two operators, we can define how to raise an operator to a power. $\hat{A}^2$ is

$$\hat{A}^2|\psi\rangle \equiv \hat{A}\hat{A}|\psi\rangle$$

and it is calculated as follows: act with $\hat{A}$ on $|\psi\rangle$ to obtain the ket $|\eta\rangle \equiv \hat{A}|\psi\rangle$ and then act with $\hat{A}$ on $|\eta\rangle$ to obtain $\hat{A}^2|\psi\rangle \equiv \hat{A}|\eta\rangle$. The meaning of $\hat{A}^n$, $n \geq 2$, should now be clear, and of course $\hat{A}^1 = \hat{A}$. By convention, $\hat{A}^0 \equiv \hat{I}$ is the unit operator (the "do nothing" operator), which is defined by $\hat{I}|\psi\rangle = |\psi\rangle$ for every ket $|\psi\rangle$.

The product of two operators *is not a commutative operation*:

$$\hat{A}\hat{B}|\psi\rangle \neq \hat{B}\hat{A}|\psi\rangle \text{ in general} \tag{31}$$

I am not saying that all operators must satisfy Eq. 31. Some operators do commute, that is, they satisfy $\hat{A}\hat{B}|\psi\rangle = \hat{B}\hat{A}|\psi\rangle$ for all $|\psi\rangle$.

The expression $\hat{A}\hat{B} - \hat{B}\hat{A}$ is called a *commutator* and is denoted by

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \tag{32}$$

When two operators commute, their commutator is identically zero.

§ 10 *Examples.* Quantum mechanics can be formulated in a variety of spaces (the space of abstract kets, or L^2, or $\boldsymbol{\ell}^2$, or C^N) and because of this I give examples of operators in each of these spaces.

In the space L^2 there are a variety of operators: differential, multiplicative, or integral. An example of differential operator is the derivative:

$$\hat{A}f(x) \equiv \frac{\mathrm{d}}{\mathrm{d}x}f(x) \tag{33}$$

The derivative is a legitimate operator if all elements of L^2 are differentiable. This is not the original definition of L^2, which only specified that a function belongs to L^2 if the integral

$$\int_{-\infty}^{\infty} \mathrm{d}x f(x)^* f(x) \tag{34}$$

is finite. If we want to work with differential operators we need to specify that they act on functions $f(x)$ that belong to a *subspace* of L^2 containing all functions $f(x)$ that satisfy Eq. 34 *and* are also differentiable.

An example of a multiplicative operator in L^2 is

$$\hat{B}f(x) \equiv V(x)f(x) \tag{35}$$

where $V(x)$ is some function such that $V(x)f(x)$ is an element of L^2 when $f(x)$ is.

An integral operator is, in general, of the form

$$\hat{C}f = \int_{-\infty}^{\infty} \mathrm{d}y\, K(x,y)f(y) \tag{36}$$

where "the kernel" $K(x,y)$ is such that the integral exist and the resulting function of x (namely $\hat{C}f$) is an element of L^2.

It is easy to show that the operators $\hat{A}$ and $\hat{B}$ defined above do not commute:

$$\begin{aligned} \hat{A}\hat{B}f(x) &= \hat{A}(V(x)f(x)) = \frac{\mathrm{d}}{\mathrm{d}x}(V(x)f(x)) \\ &= \frac{\mathrm{d}V(x)}{\mathrm{d}x}f(x) + V(x)\frac{\mathrm{d}f(x)}{\mathrm{d}x} \end{aligned} \tag{37}$$

and

$$\hat{B}\hat{A}f(x) = \hat{B}\left(\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right) = V(x)\frac{\mathrm{d}f(x)}{\mathrm{d}x} \tag{38}$$

We can write the commutator:

$$[\hat{A},\hat{B}]f(x) = (\hat{A}\hat{B} - \hat{B}\hat{A})f(x) = \hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x) = \frac{\mathrm{d}V(x)}{\mathrm{d}x}f(x) \tag{39}$$

Obviously $\hat{A}$ and $\hat{B}$ do not commute. The commutator is a new operator that multiplies the function $f(x)$ by $\mathrm{d}V/\,\mathrm{d}x$.

Linear operators in the space $\boldsymbol{\ell}^2$. The elements of $\boldsymbol{\ell}^2$ are sequences such as

$$|\,\eta\rangle \equiv \{\eta_1, \eta_2, \eta_3, \ldots\} \tag{40}$$

that satisfy the condition

$$\sum_{n=1}^{\infty} \eta_n^* \eta_n \leq M \tag{41}$$

where M is a finite, real number.

Consider now the operators $\hat{A}$ and $\hat{B}$ on $\boldsymbol{\ell}^2$ defined by

$$\hat{A}\{\eta_1, \eta_2, \ldots\} = \left\{\sum_{j=1}^{\infty} A_{1j}\eta_j,\ \sum_{j=1}^{\infty} A_{2j}\eta_j,\ \ldots\right\} \tag{42}$$

$$\hat{B}\{\eta_1, \eta_2, \ldots\} = \left\{\sum_{j=1}^{\infty} B_{1j}\eta_j,\ \sum_{j=1}^{\infty} B_{2j}\eta_j,\ \ldots\right\} \tag{43}$$

Here $|\eta\rangle = \{\eta_1, \eta_2, \ldots\}$ is an arbitrary element of $\boldsymbol{\ell}^2$ and the complex numbers A_{ij} and B_{ij} are given (they define the operators $\hat{A}$ and $\hat{B}$). It is easy to show that

$$\hat{B}\hat{A}|\eta\rangle = \left\{ \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} B_{1j}A_{ji}\eta_i,\ \sum_{i=1}^{\infty}\sum_{j=1}^{\infty} B_{2j}A_{ji}\eta_i,\ \ldots \right\} \tag{44}$$

If you are familiar with matrix algebra you can see that the multiplication of $\hat{B}$ with $\hat{A}$ follows the rule for matrix multiplication.

§ 11 *Functions of operators.* I remind you that we confined ourselves to operators that satisfy

$$\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n| + \int_{\alpha\in D} |\alpha\rangle\, \alpha\, \langle\alpha|\, \mathrm{d}\alpha \tag{45}$$

How can we define a function of this operator? Let me give an example to show why this is not a trivial matter. If the function is $f(x)$ and you want to define $f(\hat{A})$, you might think of replacing x with $\hat{A}$ and using the result as a definition of $f(\hat{A})$. Let's see how this works if $f(x) = \sqrt{x}\,\sin x$ and you assume $f(\hat{A}) \equiv \sqrt{\hat{A}}\,\sin\hat{A}$. This seems fine, but suppose the operator $\hat{A}$ is defined in L^2 and is $\frac{\partial}{\partial x}$: what is the meaning of $\sqrt{\frac{\partial}{\partial x}}$ or of $\sin\frac{\partial}{\partial x}$? If you try to give a workable (and useful) definition of this function you will convince yourself that this is not a trivial matter.

In Dirac's formulation, if $\hat{A}$ is given by Eq. 45 then $f(\hat{A})$ is defined as

$$f(\hat{A}) \equiv \sum_{n=1}^{\infty} |a_n\rangle\, f(a_n)\, \langle a_n| + \int_{\alpha\in D} |\alpha\rangle\, f(\alpha)\, \langle\alpha|\, \mathrm{d}\alpha \tag{46}$$

In the right-hand side, f acts on the numbers a_n and α so there is no ambiguity regarding the meaning of $f(a_n)$ and $f(\alpha)$. If you want to calculate $f(\hat{A})$, you solve the eigenvalue problem for $\hat{A}$ and use the result to write down the right-hand side of Eq. 46.

This definition may seem arbitrary but it has survived many tests and is very useful. It is also consistent with other definitions in use. One of the most popular applies if $f(x)$ can be represented by a convergent power-series

$$f(x) = f_0 + f_1 x + f_2 x^2 + \cdots \tag{47}$$

For such functions, $f(\hat{A})$ is defined by

$$f(\hat{A}) = f_0 + f_1 \hat{A} + f_2 \hat{A}^2 + \cdots \tag{48}$$

If we know $\hat{A}$ — and we are supposed to know it if we want to define the function $f(\hat{A})$ — we can evaluate the right-hand side of Eq. 48 because it involves only powers of $\hat{A}$.

When we write such infinite series, we must be concerned with convergence. If the power series in Eq. 47 is convergent, this does not mean that the power series in Eq. 48 is convergent. We have not even defined what we mean when we say that a power series of an operator is convergent. Mathematicians have answers to such questions but they are not practical for use in calculations. While using such an expansion in quantum mechanics, we have a recipe that allows us to declare that such an expansion is convergent. We approximate $f(\hat{A})$ with a finite sum $f(\hat{A}) \approx f_0 + f_1 \hat{A} + f_2 \hat{A}^2 + \cdots + f_N \hat{A}^N$. Then we use the result to calculate some observable. Any such calculation involves evaluating an expression of the form

$$\langle \psi \,|\, f(\hat{A}) \,|\, \psi \rangle = \sum_{n=0}^{N} f_n \langle \psi \,|\, \hat{A}^n \,|\, \psi \rangle \tag{49}$$

Now the sum involves only numbers. We can test that the sum converged by increasing N and showing that the result no longer changes. When this happens, we are satisfied with the approximation. This is not always a guarantee

that the series converges, but it works most of the time. In some calculations it happens that good results are obtained (i.e. agreement with experiment) if one uses a few terms in the series and the agreement deteriorates when the number of terms is increased. Series like that are called asymptotic and you will see examples of them when we discuss perturbation theory. A good physical chemist knows (and you will too, in time), from the physical properties of the system, when this is likely to happen.

It is very easy to show that the definition provided by Eq. 46 is consistent with Eq. 48 (but it is more general). Just replace $f(a_n)$ and $f(\alpha)$ in Eq. 45 with the expansion in Eq. 47.

The definition in Eq. 46 allows us to construct new and interesting operators. You will see that the operator $\exp\left[-\hat{H}/k_BT\right]$ is essential in statistical mechanics and the operator $\exp\left[-\mathrm{i}\hat{H}t/\hbar\right]$ gives the time evolution of the state of a system in quantum mechanics.

§ 12 *Adjoint, Hermitian, inverse, and unitary operators: definitions.* We defined the operator $\hat{A}$ through Eq. 45:

$$\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n| + \int_{\alpha\in D} |\alpha\rangle\, \alpha\, \langle\alpha|\, \mathrm{d}\alpha \tag{50}$$

Here $|a_n\rangle$ are the eigenstates of $\hat{A}$ and a_n are its discrete eigenvalues and the integral takes care of the contribution from the continuous spectrum. Starting from this expression we can define new operators, which are all functions of the operator $\hat{A}$.

1. The *adjoint* $\hat{A}^\dagger$ of $\hat{A}$ is

$$\hat{A}^\dagger \equiv \sum_{n=1}^{\infty} |a_n\rangle\, a_n^*\, \langle a_n| + \int_{\alpha\in D} |\alpha\rangle\, \alpha^*\, \langle\alpha|\, \mathrm{d}\alpha \tag{51}$$

Sometimes the adjoint of $\hat{A}$ is also called *the Hermitian conjugate* of $\hat{A}$.

2. An operator is *Hermitian* (or *self-adjoint*) if all its eigenvalues a_n and $\alpha \in D$ are real numbers. From Eqs. 50 and 51 it follows that $\hat{A}$ is Hermitian if and only if

$$\hat{A}^\dagger = \hat{A} \tag{52}$$

3. An operator is *unitary* if

$$|a_n| = 1 \text{ for all } n, \text{ and } |\alpha| = 1 \text{ for all } \alpha \in D \tag{53}$$

Here $|z|$ is the absolute value of the complex number z. You can verify that Eq. 53 is equivalent to requiring that

$$a_n = \mathrm{e}^{\mathrm{i}p_n} \text{ for } n \geq 1 \text{ and } \alpha = \mathrm{e}^{\mathrm{i}p(\alpha)} \text{ for } \alpha \in D \tag{54}$$

where p_n and $p(\alpha)$ are real numbers and $\mathrm{i} = \sqrt{-1}$.

4. The operator

$$\hat{A}^{-1} \equiv \sum_{n=1}^{\infty} |a_n\rangle \frac{1}{a_n} \langle a_n| + \int_{\alpha \in D} |\alpha\rangle \frac{1}{\alpha} \langle \alpha| \, \mathrm{d}\alpha \tag{55}$$

is called the *inverse* of $\hat{A}$. Note that if any one of the numbers a_n is zero, this expression makes no sense, and in that case we say that $\hat{A}$ *does not have an inverse* or that it is *singular*. If the integral in Eq. 55 is not well-defined, the operator does not have an inverse.

You will use these definitions, and the properties that follow from them, over, and over, and over. Other books use different, but equivalent, definitions. The ones used here lead most efficiently to useful results. The methods

used in other books (especially in mathematics books) are more rigorous but we do not need this additional rigor here.

§ 13 *Notation.* In what follows we derive some important properties that follow from the definitions given above. Before proceeding, let us establish some notation. If $|\eta\rangle \equiv \hat{A}|\psi\rangle$ then I either write

$$\langle\phi\,|\,\eta\rangle \equiv \langle\phi\,|\,\hat{A}\psi\rangle \tag{56}$$

or

$$\langle\phi\,|\,\eta\rangle \equiv \langle\phi\,|\,\hat{A}\,|\,\psi\rangle \tag{57}$$

Mathematicians tend to use Eq. 56 and physicists Eq. 57. I also use the notation

$$\langle\eta\,|\,\phi\rangle \equiv \langle\hat{A}\psi\,|\,\phi\rangle \tag{58}$$

§ 14 *Some properties of adjoint operators.*

Property 1. If $\hat{A}^\dagger$ is the adjoint of $\hat{A}$, then for any $|\phi\rangle$ and $|\psi\rangle$ we have

$$\langle\phi\,|\,\hat{A}\psi\rangle = \langle\hat{A}^\dagger\phi\,|\,\psi\rangle \tag{59}$$

and

$$\langle\hat{A}\phi\,|\,\psi\rangle = \langle\phi\,|\,\hat{A}^\dagger\psi\rangle \tag{60}$$

Here $\langle\hat{A}^\dagger\phi|$ and $\langle\hat{A}\phi|$ are the bras corresponding to the kets $\hat{A}^\dagger|\phi\rangle$ and $\hat{A}|\phi\rangle$, respectively. This relationship is useful if acting with $\hat{A}$ on $|\psi\rangle$ (in Eq. 59) is difficult but acting with $\hat{A}^\dagger$ on ϕ might be easy (maybe $\hat{A}^\dagger$ is a simpler operator than $\hat{A}$, or perhaps it is simpler to act on the ket $|\phi\rangle$ than on $|\psi\rangle$). Eq. 59 ensures that you get the same result for the scalar product in both procedures.

Eqs. 59 and 60 follow from the definition of the adjoint operator and the properties of the scalar product. To simplify our lives, I will discard the integral in the definition Eq. 50 of an operator. The integral is the limit of a sum, and therefore the method of proof for the sum works for the integral.

Now let us prove Eq. 59 by starting with $\langle \hat{A}^\dagger \phi \,|\, \psi \rangle$ and rewriting it, by using known relationships, to show that it is the same as $\langle \phi \,|\, \hat{A} \,|\, \psi \rangle$:

$$\begin{aligned}
\langle \hat{A}^\dagger \phi \,|\, \psi \rangle &= \langle \psi \,|\, \hat{A}^\dagger \phi \rangle^* && \text{(used } \langle x \,|\, y \rangle = \langle y \,|\, x \rangle^* \text{)} \\
&= (\textstyle\sum_{n=1}^{\infty} \langle \psi \,|\, a_n \rangle \, a_n^* \, \langle a_n \,|\, \phi \rangle)^* && \text{(used Eq. 51)} \\
&= \textstyle\sum_{n=1}^{\infty} \langle \psi \,|\, a_n \rangle^* \, a_n \, \langle a_n \,|\, \phi \rangle^* && \text{(used } (zw)^* = z^* w^* \text{)} \\
&= \textstyle\sum_{n=1}^{\infty} \langle \phi \,|\, a_n \rangle \, a_n \, \langle a_n \,|\, \psi \rangle && \text{(used } \langle x \,|\, y \rangle = \langle y \,|\, x \rangle^* \text{)} \\
&= \langle \phi \,|\, \hat{A} \psi \rangle && \text{(used Eq. 50)}
\end{aligned}$$

This proves Eq. 59. For Eq. 60, first note that, from the definition (Eq. 51), it follows that

$$(\hat{A}^\dagger)^\dagger = \hat{A} \tag{61}$$

Therefore

$$\begin{aligned}
\langle \phi \,|\, \hat{A}^\dagger \psi \rangle &= \langle (\hat{A}^\dagger)^\dagger \phi \,|\, \psi \rangle && \text{(used Eq. 59)} \\
&= \langle \hat{A} \phi \,|\, \psi \rangle && \text{(used Eq. 61)}
\end{aligned}$$

Many mathematicians prefer to use Eq. 59 as a definition of an adjoint operator, because it is more general than the one used here; it is valid for operators not covered by the definition Eq. 50 on which the material developed here is based.

Exercise 2 In the space L^2 the scalar product is defined by

$$\langle \phi \,|\, \psi \rangle \equiv \int_{-\infty}^{+\infty} \phi(x)^* \psi(x) \, \mathrm{d}x \tag{62}$$

and the space contains functions that satisfy

$$\int_{-\infty}^{+\infty} \psi(x)^* \psi(x)\,\mathrm{d}x < \infty \tag{63}$$

This condition ensures that all functions in L^2 are zero for infinite values (negative or positive) of x. Keeping these in mind find the Hermitian conjugate (the adjoint) of the operator $\frac{\mathrm{d}}{\mathrm{d}x}$. Also prove that the operator $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$ is equal to its own adjoint.

Property 2. If

$$\langle \hat{A}\psi \,|\, \phi \rangle = \langle \psi \,|\, \hat{B}\phi \rangle \tag{64}$$

for any $|\phi\rangle$ and $|\psi\rangle$, then $\hat{B}$ is the adjoint of $\hat{A}$ (meaning that $\hat{B} = \hat{A}^\dagger$).

Use $\langle x \,|\, y \rangle = \langle y \,|\, x \rangle^*$ to rewrite Eq. 64 as

$$\langle \phi \,|\, \hat{A}\psi \rangle^* = \langle \psi \,|\, \hat{B}\phi \rangle \tag{65}$$

Since this is valid for any kets $|\phi\rangle$ and $|\psi\rangle$, it is valid for the pure states $|a_n\rangle$ of A (eigenstates of $\hat{A}$). Therefore Eq. 65 gives (using Eq. 50 and orthonormality)

$$\langle a_n \,|\, \hat{B} \,|\, a_n \rangle = \langle a_n \,|\, \hat{A} \,|\, a_n \rangle^* = a_n^* \tag{66}$$

and, for $m \neq n$,

$$\langle a_n \,|\, \hat{B} \,|\, a_m \rangle = \langle a_n \,|\, \hat{A} \,|\, a_m \rangle^* = 0 \tag{67}$$

Since the set of pure states is complete, $\sum_n |a_n\rangle \langle a_n| = \hat{I}$, and we can write $\hat{B}$ as

$$\hat{B} = \hat{I}\hat{B}\hat{I} = \sum_n \sum_m |a_n\rangle \langle a_n \,|\, \hat{B} \,|\, a_m \rangle \langle a_m| = \sum_n |a_n\rangle\, a_n^* \,\langle a_n| \tag{68}$$

To obtain the last equality, I used Eqs. 66 and 67. If you check the definition of an adjoint operator, given in Eq. 51, you will see Eq. 68 shows that $\hat{B} = \hat{A}^\dagger$.

We will often have to deal with products of operators, such as $\hat{A}\hat{B}$. What is the adjoint of the product? That is, if we set $\hat{C} = \hat{A}\hat{B}$, what is $\hat{C}^\dagger$?

Property 3. $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$

From Property 1, we know that we can write

$$\langle\phi\,|\,\hat{C}\psi\rangle = \langle\hat{C}^\dagger\phi\,|\,\psi\rangle \tag{69}$$

for any operator $\hat{C}$. Let us replace $\hat{C}$ in the left-hand side of this equation with $\hat{C} = \hat{A}\hat{B}$ and use Property 1 twice:

$$\langle\phi\,|\,\hat{C}\psi\rangle = \langle\phi\,|\,\hat{A}(\hat{B}\psi)\rangle = \langle\hat{A}^\dagger\phi\,|\,\hat{B}\psi\rangle = \langle\hat{B}^\dagger\hat{A}^\dagger\phi\,|\,\psi\rangle \tag{70}$$

This is true for any kets $|\phi\rangle$ and $|\psi\rangle$. This means that (compare Eqs. 69 and 70) $\hat{C}^\dagger = \hat{B}^\dagger\hat{A}^\dagger$, which is what we set out to prove.

§ 15 *Properties of a self-adjoint (Hermitian) operator.*

Property 4. By definition *the eigenvalues of a Hermitian operator are real numbers*. I listed this as a property (even though in this presentation it is a definition) to make sure that you do not forget this statement. Since the eigenvalue of an operator representing an observable A are the values obtained when we measure A, they must be real. This is why any operator that represents an observable is Hermitian.

Property 5. $\hat{A}$ is Hermitian if and only if

$$\hat{A} = \hat{A}^\dagger \tag{71}$$

This is why in some texts Hermitian operators are called self-adjoint. Some texts use Eq. 71 as the definition of a Hermitian operator. Because of the if-and-only-if part of this statement our definition and the one using Eq. 71 are equivalent.

This property states that two operators (namely $\hat{A}$ and $\hat{A}^\dagger$) are equal. What does that mean? In these lecture notes this means that

$$\langle \psi \,|\, \hat{A} \,|\, \phi \rangle = \langle \psi \,|\, \hat{B} \,|\, \phi \rangle \tag{72}$$

for all kets $|\,\psi\rangle$ *and* $|\,\phi\rangle$ *in the space on which the operator is defined.* However, since all kets in the space are linear superpositions of the kets $\{|a_n\rangle\}_{n=1}^{\infty}$ (because this set provides a complete basis set) two operators are equal when $\langle a_n \,|\, \hat{A} \,|\, a_m \rangle = \langle a_n \,|\, \hat{B} \,|\, a_m \rangle$ *for all values* of m and n.

The proof of Eq. 71 is straightforward. By the definition of the adjoint of an operator (see Eq. 51), if $\hat{A}$ is defined by

$$\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle \, a_n \, \langle a_n| \tag{73}$$

then

$$\hat{A}^\dagger = \sum_{n=1}^{\infty} |a_n\rangle \, a_n^* \, \langle a_n| \tag{74}$$

Because $\hat{A}$ is Hermitian, the numbers a_n are real and this means that these two expressions (i.e. Eq. 73 and Eq. 74) are identical and $\hat{A} = \hat{A}^\dagger$, which is what we wanted to prove.

Conversely, if $\hat{A} = \hat{A}^\dagger$, then for any value of n,

$$\langle a_n \,|\, \hat{A}^\dagger \,|\, a_n \rangle = \langle a_n \,|\, \hat{A} \,|\, a_n \rangle \tag{75}$$

Using Eq. 74 and the fact that $\langle a_i \,|\, a_j \rangle = \delta_{ij}$, it is easy to see that $\langle a_n \,|\, \hat{A}^\dagger \,|\, a_n \rangle = a_n^*$. Similarly, using Eq. 73, $\langle a_n \,|\, \hat{A} \,|\, a_n \rangle = a_n$. Using these two results in

Eq. 75, tells us that $a_n^* = a_n$, which means that whenever $\hat{A} = \hat{A}^\dagger$, a_n must be a real number; $\hat{A} = \hat{A}^\dagger$ implies that $\hat{A}$ is Hermitian, which is what we stated.

Property 6. If $\hat{A}$ is self-adjoint, then $\langle \hat{A}\phi \,|\, \psi \rangle = \langle \phi \,|\, \hat{A}\psi \rangle$.

This much-used statement follows from Properties 1 and 5.

Exercise 3 Suppose that $\hat{A}$ and $\hat{B}$ are Hermitian. Prove the following.

(a) $(\hat{A}\hat{B})^\dagger = \hat{B}\hat{A}$.

(b) $\hat{A} + \hat{B}$ is Hermitian.

(c) $[\hat{A}, \hat{B}]^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} = -[\hat{A}, \hat{B}]$
where $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator of $\hat{A}$ with $\hat{B}$.

(d) $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ is Hermitian.

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§ 16 *Inverse operators.* If $\hat{A}$ is defined by

$$\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle \, a_n \, \langle a_n| \tag{76}$$

then its inverse is

$$\hat{A}^{-1} \equiv \sum_{n=1}^{\infty} |a_n\rangle \, \frac{1}{a_n} \, \langle a_n| \tag{77}$$

Note that we assume here that the operator $\hat{A}$ either does not have a continuous spectrum, or the phenomenon we examine is such that the continuous spectrum can be neglected. The continuous spectrum is important

in collision theory or in dealing with the fragmentation (photodissociation, photoionization, etc.), and it involves subtleties that are best dealt with when we examine those processes.

As noted earlier, if any a_n in the spectrum of $\hat{A}$ is equal to zero, then the operator $\hat{A}$ has no inverse (is singular). We know that each a_n is an eigenvalue of $\hat{A}$ and therefore we can state:

Property 7. If one of the eigenvalues of $\hat{A}$ is equal to zero, then $\hat{A}$ does not have an inverse. The reason for this is that if $a_3 = 0$ the term $1/a_3$ in the definition of $\hat{A}^{-1}$ becomes infinite.

Exercise 4 Suppose that in the example given above, I eliminate the ket $|a_3\rangle$ from the basis set (this defines a subspace of the original space). Will $\hat{A}$ defined in the subspace have an inverse? Explain your answer.

Property 8. If $\hat{A}$ and $\hat{B}$ satisfy

$$\hat{A}\hat{B} = \hat{B}\hat{A} = \hat{I} \tag{78}$$

and all the eigenvalues of $\hat{A}$ differ from zero, then $\hat{B} = \hat{A}^{-1}$.

Here $\hat{I}$ is the unit operator. Note that the equality in Eq. 78 means that $\langle\psi\,|\,\hat{A}\hat{B}\,|\,\phi\rangle = \langle\psi\,|\,\hat{B}\hat{A}\,|\,\phi\rangle = \langle\psi\,|\,\phi\rangle$ *for every* $|\psi\rangle$ and $|\phi\rangle$.

First, assume the Eq. 78 is valid and prove that $\hat{B}$ equals $\hat{A}^{-1}$. Write

$$\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n| \tag{79}$$

I have dropped the integral since that term can be dealt with in the same way as we handle the sum. From $\hat{B}\hat{A} = \hat{I}$, we have, for every n,

$$\langle a_n \,|\, \hat{B}\hat{A} \,|\, a_n \rangle = \langle a_n \,|\, \hat{I} \,|\, a_n \rangle = 1 \qquad (\text{used } \langle a_n \,|\, a_n \rangle = 1) \tag{80}$$

But also

$$\langle a_n \,|\, \hat{B}\hat{A} \,|\, a_n \rangle = a_n \langle a_n \,|\, \hat{B} \,|\, a_n \rangle \qquad (\text{used } \hat{A}|a_n\rangle = a_n|a_n\rangle) \tag{81}$$

Comparing these two values for $\langle a_n \,|\, \hat{B}\hat{A} \,|\, a_n \rangle$, we see that

$$\langle a_n \,|\, \hat{B} \,|\, a_n \rangle = 1/a_n \tag{82}$$

Starting again from $\hat{B}\hat{A} = \hat{I}$, we have

$$\langle a_n \,|\, \hat{B}\hat{A} \,|\, a_m \rangle = \langle a_n \,|\, \hat{I} \,|\, a_m \rangle = 0 \qquad (\text{used orthogonality}) \tag{83}$$

for every n and $m \neq n$. We conclude from Eqs. 82 and 82 that when all the eigenvalues of $\hat{A}$ differ from zero,

$$\langle a_n \,|\, \hat{B} \,|\, a_m \rangle = \delta_{nm}/a_m \tag{84}$$

Now, keep this in mind and write

$$\begin{aligned} \hat{B} &= \hat{I}\hat{B}\hat{I} = \sum_n \sum_m |a_n\rangle \langle a_n \,|\, \hat{B} \,|\, a_m \rangle \langle a_m| \\ &= \sum_n \sum_m |a_n\rangle \frac{\delta_{nm}}{a_m} \langle a_m| \qquad (\text{used Eq. 84}) \\ &= \sum_n |a_n\rangle \frac{1}{a_n} \langle a_n| (\text{used property of Kroneker delta}) \end{aligned} \tag{85}$$

Because of the definition of the inverse operator of $\hat{A}$, this expression proves that $\hat{B} = \hat{A}^{-1}$.

Inverse operators are formally used when we solve an equation of the form

$$\hat{A}|\psi\rangle = |\phi\rangle \tag{86}$$

where $|\psi\rangle$ is unknown and $\hat{A}$ and $|\phi\rangle$ are known. Acting with $\hat{A}^{-1}$ on Eq. 86 and using $\hat{A}^{-1}\hat{A} = \hat{I}$ and $\hat{I}|\psi\rangle = |\psi\rangle$ converts Eq. 86 to

$$|\psi\rangle = \hat{A}^{-1}|\phi\rangle \tag{87}$$

This seems to be a very efficient way of solving Eq. 86, but the trouble is that in many cases $\hat{A}^{-1}$ is hard to calculate. Nevertheless, the inverse of an operator is used often in quantum mechanics.

Exercise 5 Consider the following equation in L^2:

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = \phi(x)$$

You can formally write

$$\psi(x) = \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)^{-1}\phi(x)$$

Determine the explicit form of $\left(\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}\right)^{-1}$.

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§ 17 *Unitary operators.* I remind you that the operator $\hat{U}$ defined through

$$\hat{U} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n| \tag{88}$$

where $|a_n\rangle$ is an orthonormal set of kets, is called *unitary* if and only if

$$a_n^* a_n = 1, \quad n = 1, 2, \ldots \tag{89}$$

This is equivalent to requiring that

$$a_n = \mathrm{e}^{\mathrm{i}\phi_n}, \quad n = 1, 2, \ldots \tag{90}$$

where ϕ_n is a real number.

Property 9. The kets $|a_n\rangle$ that define an unitary operator (through Eq. 88) are the eigenkets of that operator and the numbers a_n are the corresponding eigenvalues. Therefore the eigenkets of a unitary operator are orthonormal and the absolute values of the eigenvalues are equal to 1 (see Eq. 89).

The proof of these statements is through a straightforward calculation: act with $\hat{U}$, given by Eq. 88, on the ket $|\,a_m\rangle$ and you will find that $\hat{U}\,|\,a_m\rangle = a_m\,|\,a_m\rangle$. This means that every $|\,a_m\rangle$ used in the definition Eq. 88 is an eigenket of $\hat{U}$.

Property 10. $\hat{U}$ is unitary if and only if it has an inverse and $\hat{U}^{-1} = \hat{U}^\dagger$.

The inverse of $\hat{U} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n|$ is $\hat{U}^{-1} = \sum_{n=1}^{\infty} |a_n\rangle\, \frac{1}{a_n}\, \langle a_n|$. If $\hat{U}$ is unitary, then $a_n = \exp[\mathrm{i}\phi_n]$ where ϕ_n is a real number. This means that

$$\frac{1}{a_n} = \exp[-\mathrm{i}\phi_n] = a_n^*$$

Therefore

$$\hat{U}^{-1} = \sum_{n=1}^{\infty} |a_n\rangle\, \frac{1}{a_n}\, \langle a_n| \sum_{n=1}^{\infty} |a_n\rangle\, a_n^*\, \langle a_n| = \hat{U}^\dagger$$

This proves the implication from left to right of Property 10.

Next, I assume that $\hat{U}^{-1} = \hat{U}^\dagger$ and prove that this forces $\hat{U}$ to be unitary. Using the definitions of $\hat{U}^{-1}$ and $\hat{U}^\dagger$, I can rewrite the equation $\hat{U}^{-1} = \hat{U}^\dagger$ as

$$\sum_{n=1}^{\infty} |a_n\rangle\, \frac{1}{a_n}\, \langle a_n| = \sum_{n=1}^{\infty} |a_n\rangle\, a_n^*\, \langle a_n| \tag{91}$$

Since $\langle a_m \,|\, a_n \rangle = \delta_{nm}$, Eq. 91 leads to (act with Eq. 91 on $|a_m\rangle$ and then act with $\langle a_m|$ on the result)

$$\frac{1}{a_m} = a_m^* \text{ for each } m \tag{92}$$

And this means that $a_m a_m^* = 1$ for each m and therefore $\hat{U}$ is unitary.

Property 11. If $\hat{A}$ is Hermitian then the operator $\hat{U} \equiv \exp[\,\mathrm{i}\,\lambda\,\hat{A}]$, where λ is a real number, is unitary. Also, if $\hat{U}$ is a unitary operator, then it can be written as $\hat{U} = \exp[\,\mathrm{i}\,\lambda\,\hat{B}]$ where $\hat{B}$ is Hermitian.

For $\hat{A} = \sum_{n=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n|$, the operator $\exp[\,\mathrm{i}\,\lambda\,\hat{A}]$ is defined by (we use the definition of a function of an operator)

$$\exp[\,\mathrm{i}\,\lambda\,\hat{A}] = \sum_{n=1}^{\infty} |a_n\rangle\, \mathrm{e}^{\,\mathrm{i}\,\lambda\, a_n}\, \langle a_n| \tag{93}$$

If $\hat{A}$ is Hermitian then a_n, $n = 1, 2, 3, \ldots$, are real numbers. By definition λ is a real number and so are all $\lambda\ a_n$, n= 1, 2, ... Therefore $(\mathrm{e}^{\,\mathrm{i}\,\lambda\, a_n})^* \mathrm{e}^{\,\mathrm{i}\,\lambda\, a_n} = \mathrm{e}^{-\,\mathrm{i}\,\lambda\, a_n} \mathrm{e}^{\,\mathrm{i}\,\lambda\, a_n} = 1$ for all n and $\exp[\,\mathrm{i}\,\lambda\,\hat{A}]$ is unitary. Thus for any given unitary operator $\hat{U}$ we can always construct a Hermitian operator $\hat{B}$ such that $\hat{U} = \exp[-\,\mathrm{i}\,\lambda\,\hat{B}]$.

Conversely, if an operator $\hat{U}$ is unitary then it must have the form

$$\hat{U} = \sum_{m=1}^{\infty} |u_m\rangle\, \mathrm{e}^{\mathrm{i}\phi_m}\, \langle u_m| \tag{94}$$

with ϕ_m real.

Consider now the operator $\hat{B}$ defined to have the spectrum ϕ_m, $m = 1, 2, \ldots$ and the pure states $|u_m\rangle$ $m = 1, 2, \ldots$, so that

$$\hat{B} = \sum_{m=1}^{\infty} |u_m\rangle\, \phi_m\, \langle u_m| \tag{95}$$

$\hat{B}$ is Hermitian because the ϕ_m are real numbers. A function $f(\hat{B})$ is defined by

$$f(\hat{B}) = \sum_{m=1}^{\infty} |u_m\rangle\, f(\phi_m)\, \langle u_m| \tag{96}$$

If f is the function $f(x) = \mathrm{e}^{\mathrm{i}\lambda x}$ then

$$f(\hat{B}) \equiv \mathrm{e}^{\mathrm{i}\lambda \hat{B}} = \sum_{m=1}^{\infty} |u_m\rangle\, \mathrm{e}^{\mathrm{i}\lambda \phi_m}\, \langle u_m| \tag{97}$$

which means that $\mathrm{e}^{\mathrm{i}\lambda \hat{B}}$ is unitary.

Property 12. If $\hat{A}$ is Hermitian and $\hat{U} \equiv \exp[\,\mathrm{i}\,\hat{A}]$ then $\hat{A}$ and $\hat{U}$ have the same eigenvectors (eigenkets): if $\hat{A}|a_n\rangle = a_n|a_n\rangle$ then $\hat{U}|a_n\rangle = u_n|a_n\rangle$ and vice versa. In addition, $u_n = \mathrm{e}^{\mathrm{i}a_n}$.

The proof of this is hidden in the proof of Property 9. You can prove it by direct calculation.

Exercise 6 Consider a function $f(x)$ of the real variable x for which the values $f(x)$ are complex ($\exp[\,\mathrm{i}\,x]$ is an example). Let $\hat{A}$ be a Hermitian operator with spectrum $\{a_n\}$ and eigenkets $\{|a_n\rangle\}$. Show that if

$$|f(a_n)| = 1 \quad \text{for all} \quad n \tag{98}$$

then $f(\hat{A})$ is unitary. Also show the converse: if $f(\hat{A})$ is unitary then Eq. 98 must hold.

Exercise 7 Show that if x varies along the real axis then $y \equiv (x - \mathrm{i})/(x + \mathrm{i})$ varies on the unit circle in the complex plane.

Exercise 8 Show that if $\hat{A}$ is Hermitian then

$$\hat{B} \equiv (\hat{A} - \mathrm{i}\hat{I})(\hat{A} + \mathrm{i}\hat{I})^{-1}$$

is unitary (show first that $\hat{A} + \mathrm{i}\hat{I}$ has an inverse). This is called a Cayley transform, and it is the basis of the Crank-Nicholson method for solving differential equations.

Property 13. $\hat{U}$ is unitary if and only if

$$\langle \hat{U}\phi \,|\, \hat{U}\psi \rangle = \langle \phi \,|\, \psi \rangle \text{ for any kets } |\phi\rangle, |\psi\rangle \tag{99}$$

We say that the *scalar product is invariant under a unitary transformation*.

It is easy to show that Eq. 99 holds for a unitary transformation:

$$\begin{aligned} \langle \hat{U}\phi \,|\, \hat{U}\psi \rangle &= \langle \phi \,|\, \hat{U}^\dagger \hat{U}\psi \rangle \quad \text{(used Property 1)} \\ &= \langle \phi \,|\, \hat{U}^{-1}\hat{U}\psi \rangle \quad \text{(used Property 4)} \\ &= \langle \phi \,|\, \psi \rangle \end{aligned}$$

Let us prove the converse: if Eq. 99 is valid then $\hat{U}$ is unitary. If $|u_n\rangle$ are the pure states of $\hat{U}$ then

$$\hat{U} = \sum_n |u_n\rangle \, u_n \, \langle u_n| \tag{100}$$

and

$$\hat{I} = \sum_n |u_n\rangle \, \langle u_n| \tag{101}$$

We start with Eq. 99:

$$\begin{aligned}
\langle\phi\,|\,\psi\rangle &= \langle\hat{U}\phi\,|\,\hat{U}\psi\rangle \\
&= \langle\phi\,|\,\hat{U}^\dagger\hat{U}\psi\rangle && \text{(used Property 1)} \\
&= \langle\phi\,|\,\textstyle\sum_m\sum_n |u_n\rangle\, u_n^*\,\langle u_n\,|\,u_m\rangle\, u_m\,\langle u_m\,|\,\psi\rangle && \text{(used Eq. 100)} \\
&= \langle\phi\,|\,\textstyle\sum_m\sum_n |u_n\rangle\, u_n^*\,\delta_{nm}\, u_m\,\langle u_m\,|\,\psi\rangle && \text{(used } \langle u_n\,|\,u_m\rangle = \delta_{nm}\text{)} \\
&= \langle\phi\,|\,\textstyle\sum_n |u_n\rangle\, u_n^*\, u_n\,\langle u_n\,|\,\psi\rangle
\end{aligned}$$

This is equal to $\langle\phi\,|\,\psi\rangle$ only if

$$\sum_n |u_n\rangle\, u_n^*\, u_n\,\langle u_n| = \hat{I}$$

Comparing this to Eq. 101 (completeness) implies that $u_n^*\, u_n = 1$ for all n, which means that $\hat{U}$ is unitary.

Property 14 Consider two sets of kets $\{|x_i\rangle\}_{i=1}^N$ and $\{|y_i\rangle\}_{i=1}^N$ in the same space, and $\{|y_i\rangle \equiv \hat{U}|x_i\rangle\}_{i=1}^N$, where $\hat{U}$ is an operator. If $\hat{U}$ is unitary and one of the sets is complete and orthonormal, then the other set is also complete and orthonormal. In addition, if both sets are complete and orthonormal then $\hat{U}$ is unitary.

This is a corollary of Property 13. Property 14 is extremely important in quantum mechanics. We will study its consequences in a future chapter.

Section 4.3 Summary of Definitions and Properties

The operators of interest to us are defined by

$$\hat{A} \equiv \sum_{n=1}^{\infty} |a_n\rangle\, a_n\,\langle a_n| \tag{102}$$

where a_n are numbers and $|a_n\rangle$ form a set of orthonormal kets. As a result, an operator defined in this way satisfies the eigenvalue equation

$$\hat{A}|a_n\rangle = a_n|a_n\rangle \tag{103}$$

Each operator can have an adjoint or an inverse. The definition of the adjoint $\hat{A}^\dagger$ of $\hat{A}$ is ($\hat{A}$ is defined by Eq. 102)

$$\hat{A}^\dagger \equiv \sum_{n=1}^{\infty} |a_n\rangle\, a_n^*\, \langle a_n| \tag{104}$$

The adjoint has the following properties.

1. $\langle \hat{A}\phi\,|\,\psi\rangle = \rangle\phi\,|\,\hat{A}^\dagger\psi\rangle$ for any $|\,\phi\rangle$ and $|\,\psi\rangle$.

2. $(\hat{A}^\dagger)^\dagger = \hat{A}$.

3. $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$.

The inverse $\hat{A}^{-1}$ of the operator $\hat{A}$ (defined by Eq. 102) is by definition

$$\hat{A}^{-1} \equiv \sum_{n=1}^{\infty} |\,a_n\rangle \frac{1}{a_n} \langle a_n\,| \tag{105}$$

If any one of the numbers a_n is equal to zero this expression makes no sense and we say that the operator $\hat{A}$ does not have an inverse. Since a_n is an eigenvalue of $\hat{A}$, it follows that operators that have an eigenvalue that is equal to zero do not have an inverse.

The inverse of an operator has the following properties.

1. $\hat{B}$ is the inverse of $\hat{A}$ if and only if $\hat{B}\hat{A} = \hat{A}\hat{B} = \hat{I}$.

2. If $\hat{C} \equiv \hat{A}\hat{B}$ then $\hat{C}^{-1} = \hat{B}^{-1}\hat{A}^{-1}$.

3. If $\hat{A}|x\rangle = |y\rangle$ then $|x\rangle = \hat{A}^{-1}|y\rangle + |z\rangle$ where $|z\rangle$ has the property $\hat{A}|z\rangle = 0$.

By definition an operator is Hermitian (or self-adjoint) if all a_n in Eq. 102 (which defines $\hat{A}$) are real numbers.

1. All operators that represent observables are Hermitian operators.

2. $\hat{A}$ is Hermitian if and only if $\hat{A} = \hat{A}^{\dagger}$.

3. $\hat{A}$ is Hermitian if and only if $\langle \hat{A}\psi \,|\, \phi\rangle = \langle \psi \,|\, \hat{A} \,|\, \phi\rangle$ for all $|\,\psi\rangle$ and $|\,\phi\rangle$. Here $\langle \hat{A}\psi\,|$ is the bra corresponding to $\hat{A}\,|\,\psi\rangle$.

Unitary operators are defined by

$$\hat{U} \equiv \sum_{n=1}^{\infty} |\,a_n\rangle a_n \langle a_n\,| \tag{106}$$

where $|\,a_n\rangle$ form an orthonormal set, and $a_n = exp[i\lambda]$ with λ a real number. Unitary operators have the following properties.

1. The eigenvectors of an unitary operator are orthonormal and the eigenvalues can be complex numbers but their absolute value must be equal to 1.

2. $\hat{U}$ is unitary if and only if $\hat{U}^{\dagger} = \hat{U}^{-1}$.

3. $\hat{U}$ is unitary if and only if $\langle \hat{U}\phi \,|\, \hat{U}\psi\rangle = \langle \phi \,|\, \psi\rangle$ for all $|\psi\rangle$ and $|\phi\rangle$ in the space.

4. If $\{|b_n\rangle\}_{n=1}^{\infty}$ is an orthonormal basis set and $\hat{U}$ is an operator then $\{\hat{U}|b_n\rangle\}_{n=1}^{\infty}$ is an orthonormal basis set if and only if $\hat{U}$ is unitary.

5. If $\hat{U} \equiv \exp[\mathrm{i}\lambda\hat{H}]$ then $\hat{U}$ is unitary if and only if $\hat{H}$ is Hermitian and λ is a real number.

6. For any unitary operator $\hat{U}$ there is a Hermitian operator $\hat{H}$ such that $\hat{U} = \exp[\mathrm{i}\hat{H}]$

Exercise 9 Suppose that $\{|a_n\rangle\}_{n=1}^{\infty}$ are pure states of an observable A. Show the following.

1. If $\hat{P} = |a_n\rangle\langle a_n|$ then $\hat{P}^2 = \hat{P}$.

2. If $\hat{P} = |a_n\rangle\langle a_n|$ and $\hat{Q} = |a_m\rangle\langle a_m|$, then $\hat{P}\hat{Q} = 0$ when $m \neq n$ and $[\hat{P}, \hat{Q}] = 0$.

3. If
$$\hat{A} = \sum_{i=1}^{\infty} |a_n\rangle\, a_n\, \langle a_n|$$
then
$$\hat{A}^m = \sum_{i=1}^{\infty} |a_n\rangle\, a_n^m\, \langle a_n|$$

Exercise 10 If $\{|a_n\rangle\}$, $n = 1, 2, \ldots$ and $\{|b_n\rangle\}$, $n = 1, 2, \ldots$ are pure states of two different observables A and B, and if $\hat{A}$ and $\hat{B}$ are the corresponding operators, find a condition that ensures that $[\hat{A}, \hat{B}] = 0$.

Exercise 11 Suppose that two operators $\hat{A}$ and $\hat{B}$ are defined by

$$\hat{A}f = \frac{\partial}{\partial x} f(x)$$

and

$$\hat{B}f = \int_{-\infty}^{+\infty} \mathrm{e}^{-(x-y)^2} f(x)\,\mathrm{d}x$$

Do these operators commute? Calculate the commutator.

Exercise 12 (technical). The trace of an operator $\hat{O}$ is defined by

$$Tr[\hat{O}] \equiv \sum_{n=1}^{\infty} \langle e_n \,|\, \hat{O} \,|\, e_n \rangle \tag{107}$$

where $\{\,|\,e_n\rangle\}_{n=1}^{\infty}$ is any complete, orthonormal basis set. Show that $\mathrm{Tr}[\hat{O}]$ is independent of the orthonormal basis set used in the definition.

Exercise 13 Show that $\mathrm{Tr}(\hat{X}\hat{Y}) = \mathrm{Tr}(\hat{Y}\hat{X})$ where $\hat{X}$ and $\hat{Y}$ are arbitrary operators. (Hint: use the definition of trace and a complete basis set.)

Exercise 14 (physics) Suppose that two Hermitian operators $\hat{A}$ and $\hat{B}$ anti-commute: $\hat{A}\hat{B} + \hat{B}\hat{A} = 0$. Do they have common eigenstates $|a_i, b_j\rangle$ (meaning that $\hat{A}|a_i, b_j\rangle = a_i|a_i, b_j\rangle$ and $\hat{B}|a_i, b_j\rangle = b_j|a_i, b_j\rangle$)?

Exercise 15 Is the operator $|e_n\rangle\langle e_n|$ Hermitian? How about $|e_n\rangle\langle e_m|$ and $|e_n\rangle\langle e_m| + |e_m\rangle\langle e_n|$?

Exercise 16 Calculate the Hermitian conjugate of $|e_n\rangle \langle e_m|$.

Exercise 17 Does the operator

$$\hat{H} \equiv |e_1\rangle \, a \, \langle e_1| + |e_2\rangle \, b \, \langle e_2 \, | \, + |e_1\rangle \, c \, \langle e_2|$$

where a, b, and c are real numbers, represent an observable?

Exercise 18 What is the inverse of the operator $\exp[\mathrm{i}\hat{A}]$, where $\hat{A}$ is an arbitrary operator? Is it possible that this operator does not have an inverse?

Exercise 19 An operator $\hat{H}$ is called *positive definite* if for any ket $|u\rangle$, we have $\langle u \, | \, \hat{H} \, | \, u\rangle \geq 0$. Show that the Hamiltonian of the harmonic oscillator is positive definite. Can you explain the reason why this is so?

Exercise 20 Show that if $\hat{A}$ and $\hat{B}$ are two operators and each has an inverse then $(\hat{A} \, \hat{B})^{-1} = \hat{B}^{-1} \hat{A}^{-1}$.

Exercise 21 Prove that

$$\hat{A} \, f(\hat{A}) = \sum_n |a_n\rangle \, a_n \, f(a_n) \, \langle a_n|$$

Exercise 22 Prove that

$$\phi[f(\hat{A})] = \sum_n |a_n\rangle \, \phi(f(a_n)) \, \langle a_n|$$

Exercise 23 When ϕ and f are ordinary functions of a complex variable and $\phi(f(x)) = x$, we call ϕ the inverse of f. Show that in this case $\phi[f(\hat{A})] = \hat{A}$.