4

Operators

4.1 Quantum mechanical operators

Dynamical variables used in classical mechanics are replaced by quantum-mechanical operators in quantum mechanics. Quantum mechanical operators can be used in either position space or momentum space. It was deduced in the last section that the dynamical variable *momentum* corresponds to the quantum mechanical operator $(\hbar / \mathrm{i})\,(\mathrm{d} / \mathrm{d}x)$ in position space, and the variable corresponds to the operator p in momentum space. All dynamical variables have quantum-mechanical operators in position and momentum space. Depending on the specific problem it may be more convenient to use either the position space or the momentum space representation to determine the expectation value of a variable. Table 4.1 summarizes the dynamical variables and their corresponding operators in position and momentum space.

DYNAMICAL VARIABLE		OPERATOR REPRESENTATION	
Variable		Position space	Momentum space
Position	x	x	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}$
Potential energy	$U(x)$	$U(x)$	$U\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}\right)$
	$f(x)$	$f(x)$	$\mathrm{f}\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}\right)$
Momentum	p_x	$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$	p_x
Kinetic energy	$\frac{p_x^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$\frac{p_x^2}{2m}$
	$f(p_x)$	$\mathrm{f}\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right)$	$f(p_x)$
Total energy	E_{total}	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}$	$-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}$
Total energy	E_{total}	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)$	$\frac{p_x^2}{2m}+U\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial p_x}\right)$

Table 4.1: Dynamical variables and corresponding quantum mechanical operators in their position space and momentum space representation. Depending on application it can be more convenient to use either position space or momentum space representation. The function $\mathrm{f}(x)$ denotes any mathematical function of x.

Two operator representations for the total energy are given in ***Table*** 4.1: The first one, $-(\hbar / \mathrm{i})(\partial / \partial t)$, follows from the 4th Postulate. The second one, $p_x^2 / (2\,m) + U(x)$, is the sum of kinetic and potential energy. The specific application determines which of the four operators is most convenient to calculate the total energy.

The total energy operator is an important operator. In analogy to the *hamiltonian function* in classical mechanics, the *hamiltonian operator* is used in quantum mechanics. The hamiltonian operator thus represents the total energy of the particle represented by the wave function $\psi(x)$

$$H\,\psi(x) \;=\; -\frac{\hbar^2}{2\,m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\psi(x) \;+\; U(x)\,\psi(x) \tag{4.1}$$

or equivalently,

$$H\,\Phi(p) \;=\; \frac{p^2}{2\,m}\,\Phi(p) \;+\; U\!\left(-\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}p}\right)\Phi(p)\;. \tag{4.2}$$

The hamiltonian operator is of great importance because many problems of quantum mechanics are solved by minimizing the total energy of a particle or a system of particles.

4.2 Eigenfunctions and eigenvalues

Any mathematical rule which changes one function into some other function is called an operation. Such an operation requires an *operator*, which provides the mathematical rule for the operation, and an operand which is the initial function that will be changed under the operation.

Quantum mechanical operators act on the wave function $\Psi(x, t)$. Thus, the wave function $\Psi(x, t)$ is the operand. Examples for operators are the differential operator $(\mathrm{d} / \mathrm{d}x)$ or the integral operator $\int \cdots \mathrm{d}x$. In the following sections we shall use the symbol ξ_{op} for an operator and the symbol $\mathrm{f}(x)$ for an operand.

The definition of the ***eigenfunction*** and the ***eigenvalue*** of an operator is as follows: If the effect of an operator ξ_{op} operating on a function $\mathrm{f}(x)$ is that the function $\mathrm{f}(x)$ is modified only by the multiplication with a scalar, then the function $\mathrm{f}(x)$ is called the *eigenfunction* of the operator ξ_{op}, that is

$$\xi_{op}\,\mathrm{f}(x) \;=\; \lambda_s\,\mathrm{f}(x) \tag{4.3}$$

where λ_s is a scalar (constant). λ_s is called the *eigenvalue* of the eigenfunction. For example, the eigenfunctions of the differential operator are exponential functions, because

$$\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{e}^{\lambda_s x} \;=\; \lambda_s\,\mathrm{e}^{\lambda_s x} \tag{4.4}$$

where λ_s is the eigenvalue of the exponential function and the differential operator.

4.3 Linear operators

Virtually all operators in quantum mechanics are *linear* operators. An operator is a linear operator if

$$\xi_{op}\, c\, \psi(x) \quad = \quad c\, \xi_{op}\, \psi(x) \tag{4.5}$$

where c is a constant. For example $\mathrm{d}/\mathrm{d}x$ is a linear operator, since the constant c can be exchanged with the operator $\mathrm{d}/\mathrm{d}x$. On the other hand, the logarithmic operator (log) is not a linear operator, as can be easily verified.

In classical mechanics, dynamical variables obey the ***commutation law***. For example, the product of the two variables *position* and *momentum* commutes, that is

$$x\, p \quad = \quad p\, x\ . \tag{4.6}$$

However, in quantum mechanics the two linear operators, which correspond to x and p, do not commute, as can be easily shown. One obtains

$$x\, p\, \psi(x) \quad = \quad x \left(\frac{\hbar}{\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}x} \right) \psi(x) \tag{4.7}$$

and alternatively

$$p\, x\, \psi(x) \quad = \quad \frac{\hbar}{\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}x}\, x\, \psi(x) \quad = \quad \frac{\hbar}{\mathrm{i}}\, \psi(x) \; + \; \frac{\hbar}{\mathrm{i}}\, x \frac{\mathrm{d}}{\mathrm{d}x}\, \psi(x)\ . \tag{4.8}$$

Linear operators do not commute, since the result of Eqs. (4.7) and (4.8) are different.

4.4 Hermitian operators

In addition to linearity, most of the operators in quantum mechanics possess a property which is known as hermiticity. Such operators are hermitian operators, which will be defined in this section. The expectation value of a dynamical variable is given by the 5th Postulate according to

$$\langle \xi \rangle \quad = \quad \int_{-\infty}^{\infty} \psi^*(x)\, \xi_{op}\, \psi(x)\, \mathrm{d}x\ . \tag{4.9}$$

The expectation value $\langle \xi \rangle$ is now assumed to be a physically observable quantity such as position or momentum. Thus, the dynamical variable ξ is real, and ξ is identical to its complex conjugate.

$$\xi \quad = \quad \xi^* \qquad \text{and} \qquad \langle \xi \rangle \quad = \quad \langle \xi^* \rangle\ . \tag{4.10}$$

It is important to note that $\xi_{op} \neq \xi_{op}{}^*$. To determine the complex conjugate form of Eq. (4.9) one has to replace each factor of the integrand with its complex conjugate.

$$\langle \xi^* \rangle \quad = \quad \int_{-\infty}^{\infty} \psi(x)\, \xi_{op}^*\, \psi^*(x)\, \mathrm{d}x\ . \tag{4.11}$$

With Eq. (4.10) one obtains

$$\int_{-\infty}^{\infty} \psi^*(x)\, \xi_{op}\, \psi(x)\, \mathrm{d}x \quad = \quad \int_{-\infty}^{\infty} \psi(x)\, \xi_{op}^*\, \psi^*(x)\, \mathrm{d}x\ . \tag{4.12}$$

Operators which satisfy Eq. (4.12) are called hermitian operators.

The definition of an hermitian operator is in fact more general than given above. In general, ***hermitian operators*** satisfy the condition

$$\int_{-\infty}^{\infty} \psi_1^*(x)\,\xi_{op}\;\psi_2(x)\,dx \quad = \quad \int_{-\infty}^{\infty} \psi_2(x)\,\xi_{op}^*\;\psi_1^*(x)\,dx \tag{4.13}$$

where $\psi_1(x)$ and $\psi_2(x)$ may be different functions. If $\psi_1(x)$ and $\psi_2(x)$ are identical, Eq. (4.13) simplifies into Eq. (4.12).

As an example, we consider the observable *variable momentum*. It is easily shown that the momentum operator is an hermitian operator. The momentum expectation value is given by

$$\langle p \rangle \quad = \quad \int_{-\infty}^{\infty} \psi^*(x)\;\frac{\hbar}{i}\frac{d}{dx}\;\psi(x)\,dx\ . \tag{4.14}$$

Integration by part (recall: $\int_a^b u'v\,dx = u\,v\big|_a^b - \int_a^b uv'\,dx$) and using $\psi(x \to \infty) = 0$ yields

$$\langle p \rangle \quad = \quad \int_{-\infty}^{\infty} \psi(x)\left(-\frac{\hbar}{i}\frac{d}{dx}\right)\psi^*(x)\,dx \tag{4.15}$$

which proves that p is an hermitian operator.

There are a number of consequences and implications resulting from the hermiticity of an operator. Two more properties of hermitian operators will explicitly mentioned. First, *eigenvalues of hermitian operators are real*. To prove this, suppose ξ_{op} is an hermitian operator with eigenfunction $\psi(x)$ and eigenvalue λ. Then

$$\int_{-\infty}^{\infty} \psi^*(x)\,\xi_{op}\;\psi(x)\,dx \quad = \quad \int_{-\infty}^{\infty} \psi^*(x)\,\lambda\,\psi(x)\,dx \tag{4.16}$$

$$= \quad \lambda\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx \tag{4.17}$$

and also due to hermiticity of the operator

$$\int_{-\infty}^{\infty} \psi(x)\,\xi_{op}^*\;\psi^*(x)\,dx \quad = \quad \int_{-\infty}^{\infty} \psi(x)\,\lambda^*\;\psi^*(x)\,dx \tag{4.18}$$

$$= \quad \lambda^*\int_{-\infty}^{\infty} \psi(x)\,\psi^*(x)\,dx \tag{4.19}$$

Since Eqs. (4.17) and (4.19) are identical, therefore $\lambda = \lambda^*$, which is only true if λ is real. Thus, eigenvalues of Hermitian operators are real.

Second, *eigenfunctions corresponding to two unequal eigenvalues of an hermitian operator are orthogonal to each other*. This is, if ξ_{op} is an hermitian operator and $\psi_1(x)$ and $\psi_2(x)$ are eigenfunctions of this operator and λ_1 and λ_2 are eigenvalues of this operator then

$$\int_{-\infty}^{\infty} \psi_1^*(x)\, \psi_2(x)\, \mathrm{d}x \quad = \quad 0 \ . \tag{4.20}$$

The two eigenfunctions $\psi_1(x)$ and $\psi_2(x)$ are ***orthogonal*** if they satisfy Eq. (4.20). The statement can be proven by using the hermiticity of the operator ξ_{op}. This yields

$$\int_{-\infty}^{\infty} \psi_1^*(x)\, \xi_{op}\, \psi_2(x)\, \mathrm{d}x \quad = \quad \int_{-\infty}^{\infty} \psi_2(x)\, \xi_{op}^*\, \psi_1^*(x)\, \mathrm{d}x \ . \tag{4.21}$$

Employing that λ_1 and λ_2 are the eigenvalues of $\psi_1(x)$ and $\psi_2(x)$ yields

$$\lambda_2 \int_{-\infty}^{\infty} \psi_1^*(x)\, \psi_2(x)\, \mathrm{d}x \quad = \quad \lambda_1 \int_{-\infty}^{\infty} \psi_1^*(x)\, \psi_2(x)\, \mathrm{d}x \ . \tag{4.22}$$

Since λ_1 and λ_2 may be unequal, Eq. (4.22) can only be true if $\psi_1(x)$ and $\psi_2(x)$ are orthogonal functions as defined in Eq. (4.20).

4.5 The Dirac bracket notation

A notation which offers the advantage of great convenience was introduced by Dirac (1926). As shown in the proceeding section, wave functions can be represented in position space and, with the identical physical content, in momentum space. Dirac's notation provides a notation which is *independent* of the representation, that is, a notation valid for the position-space and momentum-space representation.

Let $\Psi(x, t)$ be a wave function and let ξ_{op} be an operator; then the following integration is written with the Dirac bracket notation as

$$\left\langle \Psi \middle| \xi_{op} \middle| \Psi \right\rangle \quad = \quad \int_{-\infty}^{\infty} \Psi^*(x,t)\, \xi_{op}\, \Psi(x,t)\, \mathrm{d}x \tag{4.23}$$

and equivalently in momentum space

$$\left\langle \Psi \middle| \xi_{op} \middle| \Psi \right\rangle \quad = \quad \int_{-\infty}^{\infty} \Phi^*(p,t)\, \xi_{op}\, \Phi(p,t)\, \mathrm{d}p \ . \tag{4.24}$$

It is important to note the following two points. First, because Dirac's notation is valid for the position- and momentum-space representation, the dependences of the wave function on x, t, or p can be left out. Thus, only Ψ and not $\Psi(x, t)$ or $\Psi(p, t)$ may be used in the Dirac notation. However, if desirable, the explicit dependence of Ψ can be included, for example $\langle\psi(x) \mid \xi_{op} \mid \psi(x)\mid\rangle$. Second, the left-hand-side wave function in the bracket is by definition the complex conjugate of the right-hand-side wave function of the bracket. The integral notation still provides the explicit notation for the complex conjugate wave function, as shown by the asterisk (*).

If the operator equals the *unit-operator* $\xi_{op} = 1$, then

$$\left\langle \Psi \middle| \xi_{op} \middle| \Psi \right\rangle \quad = \quad \left\langle \Psi \middle| 1 \middle| \Psi \right\rangle \ . \tag{4.25}$$

For convenience the unit operator can be left out

$$\langle \Psi | 1 | \Psi \rangle \;=\; \langle \Psi | 1\, \Psi \rangle \;=\; \langle \Psi | \Psi \rangle \; . \tag{4.26}$$

The normalization condition, given in the 2nd Postulate can then be written as

$$\langle \Psi | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \Psi(x,t)\, \mathrm{d}x \;=\; 1 \; . \tag{4.27}$$

The Dirac notation can also be used to express expectation values. Writing the 5th Postulate in the Dirac's notation, one obtains the expectation value $\langle \xi \rangle$ of a dynamical variable ξ, which corresponds to the operator ξ_{op}, by

$$\langle \xi \rangle \;=\; \langle \Psi | \xi_{op} | \Psi \rangle \; . \tag{4.28}$$

Again, either position-space or momentum space representation of the wave function can be used.

In the Dirac notation, the operator acts on the function on the right hand side of the bracket. To visualize this fact one can write

$$\langle \Psi_1 | \xi_{op} | \Psi_2 \rangle \;=\; \langle \Psi_1 | \xi_{op}\, \Psi_2 \rangle \; . \tag{4.29}$$

If it is required that the operator acts on the first, complex conjugate function, the following notation is used

$$\langle \xi_{op}\, \Psi_1 | \Psi_2 \rangle \;=\; \int_{-\infty}^{\infty} \psi_2(x)\, \xi_{op}^*\, \psi_1^*(x)\, \mathrm{d}x \; . \tag{4.30}$$

Using this notation, the definition for hermiticity of operators reads

$$\langle \Psi_1 | \xi_{op}\, \Psi_2 \rangle \;=\; \langle \xi_{op}\, \Psi_1 | \Psi_2 \rangle \tag{4.31}$$

or equivalently

$$\langle \Psi_1 | \xi_{op} | \Psi_2 \rangle \;=\; \langle \Psi_2 | \xi_{op} | \Psi_1 \rangle^* \tag{4.32}$$

This equation is equivalent to the definition of hermitian operators in Eq. (4.13).

4.6 The Dirac delta function

A valuable function frequently used in quantum mechanics and other fields is the Dirac delta function. The delta function of the variable x is defined as

$$\delta(x - x_0) \;=\; \infty \qquad\qquad (x = x_0) \tag{4.33}$$

$$\delta(x - x_0) \;=\; 0 \qquad\qquad (x \neq x_0)\; . \tag{4.34}$$

The integral over the delta (δ) function remains finite and the integral has the unit value

$$\int_{-\infty}^{\infty} \delta(x - x_0)\, \mathrm{d}x \quad = \quad 1 \;. \tag{4.35}$$

The δ function can be understood as the limit of a gaussian distribution with an infinitesimally small standard deviation, that is

$$\delta(x - x_0) \quad = \quad \lim_{\sigma \to 0} \frac{1}{\sigma \sqrt{2\,\pi}} \; \exp\left[-\frac{1}{2} \left(\frac{x - x_0}{\sigma} \right)^2 \right] \;. \tag{4.36}$$

Gaussian functions with different standard deviations but the same area under the curve are shown in ***Fig***. 4.1.

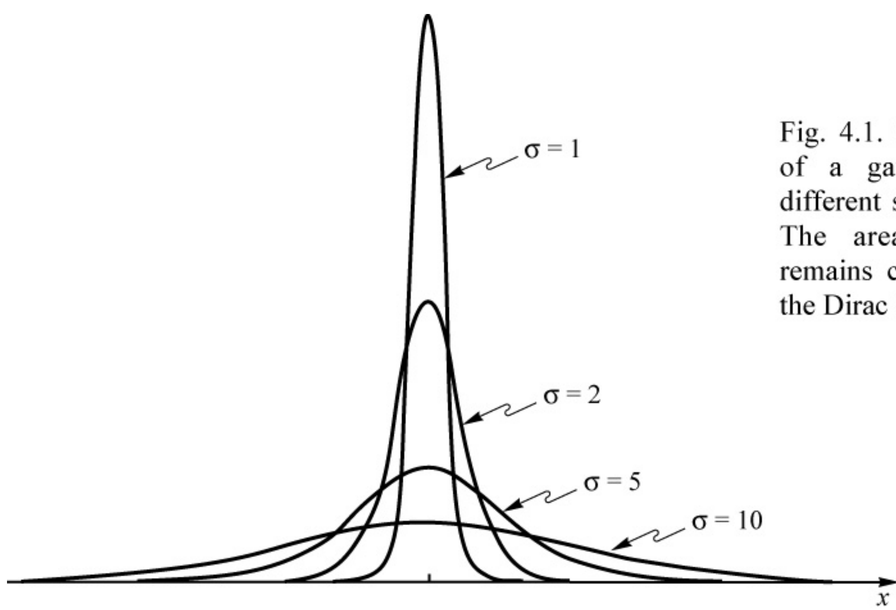

Fig. 4.1. Schematic illustration of a gaussian function for different standard deviations σ. The area under the curve remains constant. For σ → 0, the Dirac δ function is obtained.

The δ function can also be represented by its Fourier integral

$$\delta(x - x_0) \quad = \quad \frac{1}{2\,\pi} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(x - x_0)\,y} \, \mathrm{d}y \;\;. \tag{4.37}$$

The following equations summarize frequently used properties of the δ function

$$\delta(x) \quad = \quad \delta(-x) \tag{4.38}$$

$$\delta(\alpha\, x) \quad = \quad \frac{1}{\alpha}\, \delta(x) \tag{4.39}$$

$$\mathrm{f}(x)\, \delta(x - x_0) \quad = \quad \mathrm{f}(x_0)\, \delta(x - x_0) \tag{4.40}$$

$$\int_{-\infty}^{\infty} \mathrm{f}(x)\, \delta(x - x_0)\, \mathrm{d}x \quad = \quad \mathrm{f}(x_0) \tag{4.41}$$

$$\int_{-\infty}^{\infty} \mathrm{f}(x)\, \frac{\mathrm{d}}{\mathrm{d}x}\, \delta(x - x_0)\, \mathrm{d}x \quad = \quad -\frac{\mathrm{d}}{\mathrm{d}x}\, \mathrm{f}(x) \bigg|_{x=x_0} \tag{4.42}$$