Chapter 8. The Momentum Representation

§ 1 *Introduction.* In what follows we solve the eigenvalue equation for momentum and discuss the use of momentum representation for solving eigenvalue problems and its connection to the Fourier transform theory.

§ 2 *The momentum eigenfunctions in Schrödinger representation.* By definition, a system is in a pure momentum state $|p\rangle$ if a momentum measurement is certain to yield the value p. From general theory we know that $|p\rangle$ must be an eigenvector of the momentum operator $\hat{p}$:

$$\hat{p}|p\rangle = p|p\rangle \tag{1}$$

In the material presented so far we did not know how to solve this equation, because we did not know how to write down a "computable" expression for $\hat{p}$. By using what we learned in Chapter 7 we can convert Eq. 1 into a differential equation. The trick is to go to the coordinate representation, because in this representation we know the expression for the momentum operator. You do this by acting with $\langle x|$ on Eq. 1:

$$\langle x \,|\, \hat{p} \,|\, p\rangle = p\langle x \,|\, p\rangle \tag{2}$$

We have shown in the previous chapter that the left-hand side of Eq. 2 is

$$\langle x \,|\, \hat{p} \,|\, p\rangle = \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x}\langle x \,|\, p\rangle \tag{3}$$

Combining this with Eq. 2 gives

$$\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x}\langle x \,|\, p\rangle = p\langle x \,|\, p\rangle \tag{4}$$

By using Schrödinger notation

$$\langle x \,|\, p\rangle \equiv \psi_p(x), \tag{5}$$

we can write Eq. 4 as

$$\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x}\psi_p(x) = p\psi_p(x) \tag{6}$$

which is the form you are likely to have seen in your introductory course on quantum mechanics.

It is easy to verify that this equation is satisfied by

$$\langle x \,|\, p\rangle \equiv \psi_p(x) \equiv C \exp[\mathrm{i}\, p\, x/\hbar] \tag{7}$$

The constant C is determined from the normalization condition (momentum has a continuous spectrum):

$$\langle p \,|\, q\rangle = \delta(p - q) \tag{8}$$

where $|\,p\rangle$ and $|\,q\rangle$ are two pure momentum states.

For the evaluation of $\langle p\,|\,q\rangle$ we use our old friend:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\,|x\rangle\,\langle x| = \hat{I} \tag{9}$$

which allows us to write

$$\begin{aligned}
\langle p\,|\,q\rangle &= \textstyle\int_{-\infty}^{+\infty} \mathrm{d}x\,\langle p\,|\,x\rangle\,\langle x\,|\,q\rangle \\
&= \textstyle\int_{-\infty}^{+\infty} \mathrm{d}x\,(\langle x\,|\,p\rangle)^*\,\langle x\,|\,q\rangle && (\text{used } \langle a\,|\,b\rangle = \langle b\,|\,a\rangle^*) \\
&= C^*C \textstyle\int_{-\infty}^{+\infty} \mathrm{d}x\,\mathrm{e}^{-\mathrm{i}x\,p/\hbar}\,\mathrm{e}^{\mathrm{i}x\,q/\hbar} && (\text{used Eq. 7}) \\
&= \hbar C^*C \textstyle\int_{-\infty}^{+\infty} (\,\mathrm{d}x/\hbar)\,\mathrm{e}^{\mathrm{i}x(q-p)/\hbar} \\
&= \hbar C^*C \textstyle\int_{-\infty}^{+\infty} \mathrm{d}y\,\mathrm{e}^{\mathrm{i}y(q-p)} && (\text{change of variable } x/\hbar \to y)
\end{aligned} \tag{10}$$

I will now use the following formula for the δ function[1]:

$$\int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}y(q-p)}\,\mathrm{d}y = 2\pi\delta(p-q) \tag{11}$$

Using this equation we convert Eq. 10 to

$$\langle p\,|\,q\rangle = C^*C\hbar 2\pi\delta(p-q) \tag{12}$$

But this must be the same as Eq. 8, which can only be true if

$$2\pi\hbar C^*C = 1 \tag{13}$$

Therefore (dropping an irrelevant phase factor) I can take

$$C = \frac{1}{\sqrt{2\pi\hbar}} \tag{14}$$

[1]We have not mentioned this equation before and proving it would take us too far into the theory of Fourier transforms; just accept it and try to remember it because it is used often

Putting this into Eq. 7 gives

$$\langle x \,|\, p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ixp/\hbar} \tag{15}$$

This is not the only way to normalize the pure states of momentum.[2] The normalization $\langle q \,|\, p \rangle = \delta(q - p)$ is used frequently and it is necessary when you use a pure state $|p\rangle$ of momentum to calculate the probability $|\langle p \,|\, \psi \rangle|^2$ that a particle in state $|\psi\rangle$ has the momentum p.

§ 3 *Can we create a pure momentum state in the laboratory?* The short answer is no! There are two ways to understand this statement. One is to invoke the Heisenberg uncertainty principle. If momentum is exactly defined then we have complete uncertainty of position. This means that every position is just as probable as any other position. Since the particle is always located in some apparatus, not all positions are equally probable: we know for certain that the particle is not outside of our instrument. Therefore we must have some uncertainty in momentum unless we manage to create a particle alone in the universe.

One can arrive at the same conclusion by considering the fact that in a pure state of momentum, the momentum does not change. This means that to create such a state the particle must be in some space devoid of any forces. This in turn means a space devoid of any objects because collision with any object exerts a force on the particle.

[2] Sometimes one uses periodic boundary conditions and sometimes (in collision theory) one normalizes the momentum state to have a unit flux. We will discuss these alternatives when needed.

Any state that we can make in the laboratory is at best a coherent superposition $|\psi\rangle$ of pure states of momentum (or of the wave vector):

$$|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p\, A(p)\, |p\rangle \tag{16}$$

The function $A(p)$ will depend on the manner in which the state $|\psi\rangle$ is created by the experimenter. If more precise information is lacking, it is customary to assume that

$$A(k) = C \exp[-p^2/\beta^2] \tag{17}$$

where C and β are constants. C is obtained by normalizing ψ, and β describes the how uncertain our knowledge of momentum is (the probability that the wave vector is between p and $p+\,\mathrm{d}p$ is given by $\mid A(k) \mid^2 \mathrm{d}p$). We will discuss these "wave packets" in several chapters in what follows.

§ 4 *The use of the wave vector as a variable.* It is customary to define a new variable, the wave vector k, through

$$p = \hbar k \tag{18}$$

With this notation the eigenvalue equation for the momentum becomes

$$\frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x} \langle x \mid \hbar k \rangle = \hbar k \langle x \mid \hbar k \rangle \tag{19}$$

The $\hbar$ in $\langle x \mid \hbar k \rangle$ is superfluous and I will drop it and use the label $|k\rangle$ (instead of $\mid \hbar k \rangle$) to mean the pure state in which a measurement of the wave vector yields the value k. If a measurement of momentum is made on a system in state $|k\rangle$, the result will be $\hbar k$. Eq. 19 becomes

$$\frac{1}{\mathrm{i}} \frac{\partial}{\partial x} \langle x \mid k \rangle = k \langle x \mid k \rangle \tag{20}$$

This has the solution

$$\langle x \mid k \rangle = C e^{\mathrm{i}kx} \tag{21}$$

We normalize it so that

$$\langle k \mid k' \rangle = \delta(k - k') \tag{22}$$

Using this normalization condition, in the way we used the normalization of the states $|p\rangle$ in an earlier calculation, gives $C = 1/\sqrt{2\pi}$ and therefore

$$\langle x \mid k \rangle = \frac{1}{\sqrt{2\pi}} e^{\mathrm{i}kx} \tag{23}$$

If we compare this to

$$\langle x \mid p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\mathrm{i}kx} \tag{24}$$

we find that

$$|k\rangle = \frac{1}{\sqrt{\hbar}} |p\rangle \tag{25}$$

The kets $|k\rangle$ and $|p\rangle$ describe the same physical reality: a particle whose wave vector is k and whose momentum is $p = \hbar k$.

The factor $1/\sqrt{\hbar}$ in Eq. 25 appears because $|k\rangle$ and $|p\rangle$ have different units.

The simplest way of determining the unit of a ket is to use the completeness relation

$$\int |k\rangle \langle k| \; \mathrm{d}k = \int |p\rangle \langle p| \; \mathrm{d}p = \hat{I}$$

Both integrals are equal to $\hat{I}$ which is a dimensionless quantity. The units of $\mathrm{d}k$ are those of the wave vector (1/length). Therefore $|k\rangle \langle k|$ must have units of $1/k$, which means that $|k\rangle$ and $\langle k|$ each has the same units as $1/\sqrt{k}$. A similar argument leads us to conclude that the units of $|p\rangle$ and $\langle p|$ are $1/\sqrt{p}$. Now that you know this, you can show that $|k\rangle = (1/\sqrt{\hbar})|p\rangle$.

§ **5** *The momentum representation, the k-representation, and Fourier transforms.* The momentum and the wave vector are observables and therefore they satisfy the completeness relations

$$\int_{-\infty}^{+\infty} \mathrm{d}p \, |p\rangle \langle p| \tag{26}$$

and

$$\int_{-\infty}^{+\infty} \mathrm{d}k \, |k\rangle \langle k| \tag{27}$$

We can use either one of these relations to represent an arbitrary ket $|\psi\rangle$:

$$|\psi\rangle = \int_{-\infty}^{\infty} |p\rangle \langle p \,|\, \psi\rangle \, \mathrm{d}p \tag{28}$$

or

$$|\psi\rangle = \int_{-\infty}^{\infty} |k\rangle \langle k \,|\, \psi\rangle \, \mathrm{d}k \tag{29}$$

Eq. 28 gives $|\,\psi\rangle$ in the *momentum representation* and Eq. 29 gives $|\,\psi\rangle$ in the *k-representation*. Sometimes one says that $\langle p \,|\, \psi\rangle$ is $|\psi\rangle$ in the momentum representation and $\langle k \,|\, \psi\rangle$ is $|\psi\rangle$ in the k-representation.

In what follows I will show how we use the k-representation, because it is simpler and is used more widely. Whatever we do with the k-representation can be done with the momentum representation: the only difference is the presence of factors containing $\hbar$, which appear because momentum has different units from the wave vector.

The k-representation $\langle k \,|\, \psi\rangle$ of a ket $|\psi\rangle$ and the coordinate representation $\langle x \,|\, \psi\rangle$ (x is the coordinate) of the same ket are related by relationships called Fourier transforms. Let us "derive" these relationships by using the completeness relation for the wave vector to calculate $\langle x \,|\, \psi\rangle$:

$$\langle x \,|\, \psi\rangle = \int_{-\infty}^{\infty} \langle x|k\rangle \langle k \,|\, \psi\rangle \, \mathrm{d}k = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp[\mathrm{i}k\,x] \langle k \,|\, \psi\rangle \, \mathrm{d}k \tag{30}$$

I have used Eq. 23 for $\langle x \mid k \rangle$ to get the last equality. I will write this equation with the notation used frequently in mathematics:

$$\langle x \mid \psi \rangle \equiv \psi(x) \tag{31}$$

and

$$\langle k \mid \psi \rangle \equiv \bar{\psi}(x) \tag{32}$$

With this notation Eq. 30 can be rewritten as:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp[\mathrm{i}k\,x] \bar{\psi}(k)\,\mathrm{d}k \tag{33}$$

I will call the function $\bar{\psi}(k)$ *the Fourier transform of* $f(x)$. The operation that converts $\bar{\psi}(k)$ into $\psi(x)$ (namely the integral in Eq. 33) is called an *inverse Fourier transform.*

It is important to understand why I use the notation $\bar{\psi}(x)$ for $\langle k \mid \psi \rangle$ instead of $\psi(k)$ which would have seemed more natural within the Dirac formalism. The symbol $\psi(k)$ would imply that you evaluate it by replacing x in $\psi(x)$ with k. This is not correct: $\bar{\psi}$ *is a new function*, which has a different form than ψ, depending on a variable k that has different units than x. This is why we *must* use a different notation such as $\bar{\psi}(k)$. This is illustrated by the following example. Let us take $\bar{f}(k) \equiv \sqrt{2\pi}\frac{1}{1+k^2}$ and use Eq. 33 to calculate $f(x)$. `Mathematica` performs the integral (as long as x is a real number, which it is) and gives

$$f(x) = \mathrm{e}^{-|x|}$$

Obviously the function $f(x) = \exp[-|x|]$ is very different from the function $\bar{f}(k)$ and it would be a mistake to call the latter $f(k)$.

One interesting thing about Eq. 33 is that it can be "inverted": if you know $\psi(x)$, you can calculate $\bar{\psi}(x)$. To see how this is done let us use the coordinate representation to derive a formula for $\langle k \mid \psi \rangle \equiv \bar{\psi}(k)$:

$$\langle k \mid \psi \rangle = \int_{-\infty}^{\infty} \langle k|x \rangle \, \langle x \mid \psi \rangle \, \mathrm{d}x = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp[-\mathrm{i}k\,x] \langle x \mid \psi \rangle \, \mathrm{d}x \tag{34}$$

We can rewrite this with the notation Eq. 32 and Eq. 31 as

$$\bar{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp[-\mathrm{i}k\,x] \psi(x) \, \mathrm{d}x \tag{35}$$

The operation that converts $f(x)$ into $\bar{\psi}(k)$ is called a *Fourier transform*.

Unfortunately there is no dictator in mathematics, and the definition of the Fourier transform and its inverse vary from field to field and book to book. In particular, different people take different signs in the exponential and one man's Fourier transform may be one woman's inverse Fourier transform. There is no agreement whether one should use $\sqrt{2\pi}$ or 2π or 1 as factors in front of the integrals in the definitions. To make things worse there are unilateral or bilateral Fourier transforms, and sine and cosine Fourier transforms as well as sine, cosine, or exponential Fourier series. On top of all this all these operations have a discrete version (as in discrete Fourier transform). Whenever you read a book or an article, or use a computer program, make sure that you know what definition is being used. I use here the definition that is consistent with Dirac's notation. In these lectures when you go from coordinate representation to k-representation, you perform a Fourier transform; when you go from k-representation to coordinate representation, you perform an inverse Fourier transform.

At this point you have reason to think that this is a silly formal game: who needs to get back and forth between ψ and $\bar{\psi}$? You do. It turns out that if you Fourier-transform differential equations in ψ, you turn them into algebraic equations in $\bar{\psi}$. You solve these algebraic equations to get $\bar{\psi}$ and then you inverse Fourier transform it to get ψ. This solves your differential equation! It is almost this simple but not quite. Fourier transforms are routinely used to describe solids. It has been said that a solid state physicist is the Fourier transform of a solid state chemist; physicists tend to live in the k-representation, chemists in the coordinate representation. You'll have many opportunities to see Fourier transforms at work in the rest of the lectures. There is a chapter later dedicated to their properties.

This is fine, but why did I not stick to coordinate and momentum representation instead of changing the notation and telling you that you were doing Fourier transforms? The reason is that the theory of Fourier transforms is a venerable and well developed field of mathematics. If you know that the k-representation is related to the coordinate representation through Fourier transforms, you have access to a mathematical treasure: all the theorems concerning the properties of Fourier transforms and the software developed to calculate them numerically.

I comment again on the power of Dirac's notation. The essential equation of Fourier transform theory follows effortlessly from straightforward manipulations using this notation. Of course, as usual, some key points such as the nature of functions for which the integrals converge, are left to mathematicians.

§ 6 *The use of k-representation to solve eigenvalue problems.* I mentioned above that we can use momentum representation to solve problems in quantum mechanics. I will show below how this is done, by using the example of the energy eigenvalue

$$\hat{H}|\psi\rangle = E|\psi\rangle \tag{36}$$

of a one-dimensional system.

The idea is simple. Write $|\psi\rangle$ in the k-representation:

$$|\psi\rangle = \int_{-\infty}^{\infty} \mathrm{d}k\, |k\rangle\, \langle k \mid \psi\rangle \tag{37}$$

Determine the coefficients $\langle k \mid \psi\rangle$ by forcing $|\psi\rangle$ given by Eq. 37 to satisfy the eigenvalue equation Eq. 36. Manipulate the result to provide equations that can be solved to obtain the coefficients $\langle k \mid \psi\rangle$. Use the coefficients calculated in this way in Eq. 37 and you get $|\psi\rangle$.

Here is how we implement this idea. The Hamiltonian is

$$\hat{H} = \hat{K} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V} \tag{38}$$

where $\hat{K}$ is the kinetic energy and $\hat{V}$ is the potential energy. Because the kinetic energy is a function of the wave vector, I can write it as

$$\hat{K} = \int_{-\infty}^{\infty} \mathrm{d}k\, |k\rangle\, \frac{\hbar^2 k^2}{2m} \langle k\,| \tag{39}$$

I used the fact that the kinetic energy is $\frac{p^2}{2m}$ and $p = \hbar k$. Now let us use Eq. 39 in Eq. 38:

$$\int_{-\infty}^{\infty} \mathrm{d}k\, |k\rangle \frac{\hbar^2 k^2}{2m} \langle k \mid \psi\rangle + \hat{V}|\psi\rangle = E|\psi\rangle \tag{40}$$

Next, act on this equation with the bra $\langle q|$ that corresponds to a pure wave-vector state and use $\langle q \mid k\rangle = \delta(q-k)$ in the kinetic energy term. The result is (the δ-function allows us to perform the integral):

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}k\, \langle q \mid k\rangle \frac{\hbar^2 k^2}{2m} \langle q \mid \psi\rangle + \langle q \mid \hat{V} \mid \psi\rangle &= \frac{\hbar^2 q^2}{2m} \langle k \mid \psi\rangle + \langle q \mid \hat{V} \mid \psi\rangle \\ &= E\langle q \mid \psi\rangle \end{aligned} \tag{41}$$

Note an interesting thing: *because we used the k-representation (which is a "hidden" Fourier transform), the derivative in the kinetic energy has disappeared*. Unfortunately we are stuck with the term $\langle q \,|\, \hat{V} \,|\, \psi \rangle$ which depends on the ket ψ which we do not know. We want all unknown terms to be of the form $\langle \lambda \,|\, \psi \rangle$ where $\langle \lambda \,|$ is a bra corresponding to a pure state of the wave vector. We can achieve this by inserting the unit operator

$$\hat{I} = \int_{-\infty}^{\infty} \mathrm{d}\lambda \,|\, \lambda \rangle \langle \lambda \,|$$

between $\hat{V}$ and $|\, \psi \rangle$. The result is

$$\frac{\hbar^2 q^2}{2m} + \int_{-\infty}^{\infty} \mathrm{d}\lambda \langle q \,|\, \hat{V} \,|\, \lambda \rangle \langle \lambda \,|\, \psi \rangle = E \langle q \,|\, \psi \rangle \tag{42}$$

This is as far as we can go without performing numerical calculations. We converted the differential Schrödinger equation for $\langle x \,|\, \psi \rangle$ into an integral equation for the Fourier transform of the wave function. Often integral equations are easier to solve than the differential equations. If we solve for the functions $\langle q \,|\, \psi \rangle$ we obtain the Fourier transform of the wave function. Inverse Fourier transforming it gives us the wave function $\langle x \,|\, \psi \rangle$. This procedure may seem awkward to you since it is likely that you have not used integral equations frequently. However, you will find that this method is frequently used not only in quantum mechanics but in all fields of physics. We will study the Fourier transform and their use in detail in future chapters.

§ 7 *Three dimensions.* We go back now to one particle moving in three dimensions and calculate explicitly the eigenvalues of the momentum operator. The eigenvalue equation for momentum becomes

$$\hat{\vec{p}} | p_x, p_y, p_x \rangle = (\vec{e}_x \hat{p}_x + \vec{e}_y \hat{p}_y + \vec{e}_z \hat{p}_z) | p_x, p_y, p_x \rangle \tag{43}$$

Projecting on $\vec{e}_x$ (that is, taking the dot product of $\vec{e}_x$ with Eq. 43), we obtain

$$\hat{p}_x|p_x, p_y, p_x\rangle = p_x|p_x, p_y, p_x\rangle \tag{44}$$

Acting with $\langle x, y, z|$ on this from the left gives

$$\langle x, y, z\,|\,\hat{p}_x\,|\,p_x, p_y, p_x\rangle = p_x\langle x, y, z\,|\,p_x, p_y, p_x\rangle \tag{45}$$

Using Eq. 3 gives

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\langle x, y, z\,|\,p_x, p_y, p_x\rangle = p_x\langle x, y, z\,|\,p_x, p_y, p_x\rangle \tag{46}$$

Similarly,

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}\langle x, y, z\,|\,p_x, p_y, p_x\rangle = p_y\langle x, y, z\,|\,p_x, p_y, p_x\rangle \tag{47}$$

and

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}\langle x, y, z\,|\,p_x, p_y, p_x\rangle = p_z\langle x, y, z\,|\,p_x, p_y, p_x\rangle \tag{48}$$

We have three differential equations now. It is easy to verify that their solution is

$$\langle x, y, z\,|\,p_x, p_y, p_z\rangle = C\exp[-\frac{\mathrm{i}}{\hbar}(xp_x + yp_y + zp_z)] = C\exp\left[-\mathrm{i}\,\vec{r}\cdot\vec{p}/\hbar\right] \tag{49}$$

where $\vec{r} = \{x, y, z\}$ and $\vec{p} = \{p_x, p_y, p_z\}$.

The constant C is determined from the normalization condition. At this point we can repeat the calculation performed earlier for one dimension but I prefer to note that Eq. 49 can be written as a product of one-dimensional momentum wave functions:

$$\langle x, y, z\,|\,p_x, p_y, p_z\rangle = C\exp\left[\frac{\mathrm{i}xp_x}{\hbar}\right]\exp\left[\frac{\mathrm{i}yp_y}{\hbar}\right]\exp\left[\frac{\mathrm{i}zp_z}{\hbar}\right] \tag{50}$$

If each function in the right-hand side of Eq. 50 is normalized with the factor $(2\pi\hbar)^{-1/2}$, the normalized three-dimensional wave function needs to be

$$\langle x, y, z \mid p_x, p_y, p_z \rangle = (2\pi\hbar)^{-3/2} \exp\left[\frac{\mathrm{i}xp_x}{\hbar}\right] \exp\left[\frac{\mathrm{i}yp_y}{\hbar}\right] \exp\left[\frac{\mathrm{i}zp_z}{\hbar}\right] \tag{51}$$

§ **8** *Cartesian coordinates.* All this analysis was performed by using Cartesian coordinates. We often study systems where it is advantageous to use spherical or cylindrical coordinates. How do we "quantize" the momenta and what becomes of the coordinate representation when we use these other coordinate systems? Do we use $|r, \theta, \varphi\rangle$, and $\int \mathrm{d}r\, \mathrm{d}\theta\, \mathrm{d}\varphi\, |r, \theta, \varphi\rangle \langle r, \theta, \varphi|$, and $\hat{p}_r = \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial r}$, etc.? Certainly not!

Here is the simplest procedure. Always write the eigenvalue equations that are the starting point of your work *in Cartesian coordinates.* After that, convert to the coordinate system that you want to work with (spherical, cylindrical, etc.). This will keep you out of trouble. You'll see later a few examples of how this works.

§ **9** *We ignored the case when the particle is in an electromagnetic field.* In elementary mechanics, you learned that momentum is $\vec{p} = m\vec{v}$ where m is the mass and $\vec{v}$ is the velocity vector. This is true only in Cartesian coordinates, in the absence of an electromagnetic field. If an electromagnetic field is present, the momentum will acquire a new term: it will consist of a "mechanical momentum" and a contribution from the electromagnetic field. This is true in both classical and quantum mechanics. I will show you how this is done in a subsequent chapter.

§ **10** *Appendix: The derivative of Dirac delta* Our main task is done. We have learned how to turn abstract operators into differential operators which can be solved analytically or by using a computer. In what follows I will derive more equations pertaining to momentum in various representations. They come in handy sometimes.

We have determined that

$$\hat{p}|\psi\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, |x\rangle \, \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x} \langle x \,|\, \psi\rangle \tag{52}$$

This leads to

$$\langle \phi \,|\, \hat{p} \,|\, \psi\rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, \langle \phi \,|\, x\rangle \, \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x} \langle x \,|\, \psi\rangle \tag{53}$$

Formally this is equivalent to writing

$$\hat{p} = \int_{-\infty}^{+\infty} \mathrm{d}x\, |x\rangle \, \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x} \langle x| \tag{54}$$

It is not hard to show that

$$\hat{p}^n = \int_{-\infty}^{+\infty} \mathrm{d}x\, |x\rangle \left(\frac{\hbar}{\mathrm{i}}\right)^n \frac{\partial^n}{\partial x^n} \langle x| \tag{55}$$

We can start with Eq. 53 and replace ϕ with z and ψ with y. We obtain

$$\begin{aligned} \langle z \,|\, \hat{p} \,|\, y\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}x\, \langle z \,|\, x\rangle \, \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x} \langle x \,|\, y\rangle \\ &= \int_{-\infty}^{+\infty} \mathrm{d}x\, \delta(z - x) \, \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x} \delta(x - y) \\ &= \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial z} \delta(z - y) \end{aligned} \tag{56}$$

We have come across a novelty, the derivative of a δ-function. We need to examine this expression carefully to see what it means. We remember that δ-functions are meaningful only if used under an integral. So let us look at

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, f(x) \, \frac{\partial}{\partial x} \delta(x - y) \tag{57}$$

I perform an integration by parts to get

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathrm{d}x\, f(x)\, \frac{\partial}{\partial x}\delta(x-y) &= f(x)\,\delta(x-y)\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \mathrm{d}x\, \frac{\partial f(x)}{\partial x}\delta(x-y) \\ &= -\frac{\partial f(y)}{\partial y} \qquad (58)\end{aligned}$$

I used the fact that the δ-function is zero at $-\infty$ and $+\infty$. I could take this to be the definition of $\frac{\partial}{\partial x}\delta(x-y)$: whenever you encounter it under an integral over x, perform the integral by parts; or use Eq. 58.

Now let us see whether this is consistent with other formulae we have obtained. We have shown that

$$\langle \psi \,|\, \hat{p} \,|\, \phi \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, \langle \psi \,|\, x \rangle\, \frac{\hbar}{\mathrm{i}}\, \frac{\partial}{\partial x}\langle x \,|\, \phi \rangle \qquad (59)$$

We can also perform this calculation as follows:

$$\langle \psi \,|\, \hat{p} \,|\, \phi \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{d}y\, \langle \psi \,|\, x \rangle\, \langle x \,|\, \hat{p} \,|\, y \rangle\, \langle y \,|\, \phi \rangle \qquad (60)$$

Use Eq. 56 for $\langle x \,|\, \hat{p} \,|\, y \rangle$:

$$\langle \psi \,|\, \hat{p} \,|\, \phi \rangle = \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{d}y\, \langle \psi \,|\, x \rangle\, \frac{\hbar}{\mathrm{i}}\, \frac{\partial}{\partial x}\delta(x-y)\langle y \,|\, \phi \rangle \qquad (61)$$

When used in this equation, our definition of $\frac{\partial}{\partial x}\delta(x-y)$ (given by Eq. 58) must give Eq. 59.

Let us see if this is true. Start with Eq. 61 and integrate by parts:

$$\begin{aligned}\langle \psi \,|\, \hat{p} \,|\, \phi \rangle &= \frac{\hbar}{\mathrm{i}} \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{d}y\, \frac{\partial}{\partial x}\langle \psi \,|\, x \rangle \delta(x-y)\langle x \,|\, \phi \rangle \\ &= -\frac{\hbar}{\mathrm{i}} \int_{-\infty}^{+\infty} \mathrm{d}y\, \frac{\partial}{\partial y}\langle \psi \,|\, y \rangle\, \langle y \,|\, \phi \rangle\end{aligned}$$

Now integrate this by parts and use the fact that the system is bound and $\langle \psi \,|\, y \rangle \to 0$ as $y \to \infty$. You obtain

$$\langle \psi \,|\, \hat{p} \,|\, \phi \rangle = \int_{-\infty}^{+\infty} \mathrm{d}y\, \langle \psi \,|\, y \rangle\, \frac{\hbar}{\mathrm{i}}\, \frac{\partial}{\partial y}\langle y \,|\, \phi \rangle \qquad (62)$$

which is the same as Eq. 59. This shows that we can use the definition of $\frac{\partial}{\partial x}\delta(x-y)$ given above without running into trouble. You should avoid using $\langle x\,|\,\hat{p}\,|\,y\rangle = (\hbar/\mathrm{i})\frac{\partial}{\partial x}\delta(x-y)$ if you can. I gave it because you will encounter it in the literature.