Chapter 12
Continuous Spectra

In this chapter we start by considering continuous spectra, which we have neglected thus far. Then we investigate the relationship between $\psi(x)$ and $|\psi\rangle$. With these results, the unification of the analytic and the algebraic approaches to quantum mechanics is completed.

So far, we have excluded *continuous spectra* from the discussion, e.g. by placing our quantum object between infinitely high potential walls,[1] thus discretizing the energy spectrum. The fact that we adopted this limitation had less to do with physical reasons, but rather almost exclusively with mathematical ones.[2] From a physical point of view, a continuous spectrum (e.g. the energy of a free quantum object) makes perfect sense. But we have the problem that the corresponding eigenfunctions are not square integrable, and therefore we cannot properly define a scalar product. This hurdle may be circumvented or alleviated, as we shall show in a moment, by the construction of *eigendifferentials* which leads to *improper vectors*. Finally, we examine the question of how a ket $|\Psi\rangle$ is related to the corresponding wavefunction $\Psi(\mathbf{r})$, or how we can transform abstract equations into 'concrete' equations, e.g. in the position or the momentum representation.

[1] Another possibility would be the introduction of periodic boundary conditions.

[2] Below the Planck scale ($\sim 10^{-35}$ m, $\sim 10^{-44}$ s), neither space nor time may exist, so that ultimately these variables would become 'grainy' or discrete. (On this scale, space is thought to be something like a foam bubbling with tiny black holes, continuously popping in and out of existence.) There are attempts to determine whether space is truly grainy, but results have so far been inconclusive. Experimentally, these orders of magnitude are still very far from being directly accessible (if they ever will be); the currently highest-energy accelerator, the LHC at CERN in Geneva, attains a spatial resolution of 'only' $\sim 10^{-19}$ m. Recently, however, indirect methods were proposed; see Jakob D. Bekenstein, 'Is a tabletop search for Planck scale signals feasible?', http://arxiv.org/abs/1211.3816 (2012); or Igor Pikovski et al., 'Probing Planck-scale physics with quantum optics', *Nature Physics* 8, 393–397 (2012). For a recent paper see e.g. V. Faraoni, 'Three new roads to the Planck scale', *American Journal of Physics* 85, 865 (2017); https://doi.org/10.1119/1.4994804

J. Pade, *Quantum Mechanics for Pedestrians 1*, Undergraduate Lecture Notes in Physics, https://doi.org/10.1007/978-3-030-00464-4_12

A remark on notation: discrete spectra are often written with Latin, continuous spectra with Greek letters (exceptions to this are position x and momentum k, as well as the energy E, which can have discrete and/or continuous values). For example, if the spectrum of the Hamiltonian is discrete or continuous, we write

$$H\,|\varphi_l\rangle = E_l\,|\varphi_l\rangle \;\text{ or }\quad H\,|\varphi_\lambda\rangle = E_\lambda\,|\varphi_\lambda\rangle, \tag{12.1}$$

or

$$H\,|E_l\rangle = E_l\,|E_l\rangle \;\text{ or }\quad H\,|E_\lambda\rangle = E_\lambda\,|E_\lambda\rangle. \tag{12.2}$$

In addition, a 'direct' terminology is common, in which a state of quantum number n or λ (the system 'has' the quantum number n or λ) is written as

$$\begin{aligned} &|n\rangle : \text{ discrete quantum number } n \\ &|\lambda\rangle : \text{ continuous quantum number } \lambda. \end{aligned} \tag{12.3}$$

12.1 Improper Vectors

Free motion (cf. Chap. 5) is a simple example of the continuous case. We have[3] $\varphi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, and with our notation

$$\int \varphi^*_{k'}(x)\,\varphi_k(x)\,\mathrm{d}x \equiv \langle\varphi_{k'}\,|\varphi_k\rangle \equiv \langle k'\,|k\rangle \tag{12.4}$$

for the scalar product, it follows that:

$$\langle k'\,|k\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ix(k-k')}\mathrm{d}x = \delta(k'-k). \tag{12.5}$$

The difficulty lies in the fact that the physical problem is not properly formulated: The Heisenberg uncertainty principle tells us that a state with a definite, sharp momentum has an infinite position uncertainty, as may indeed be read off directly from the function e^{ikx}. Mathematically, this is expressed by the fact that the integral in (12.5) is not defined 'properly'—the integral does not exist in the usual sense, but is a functional, namely the delta function $\delta(k'-k)$.[4] This means that the ket $|\varphi_k\rangle \equiv |k\rangle$ is well defined, but not the bra $\langle\varphi_k| \equiv \langle k|$. In other words, the state

[3] The factor $\frac{1}{\sqrt{2\pi}}$ is due to the normalization of the function, see below.

[4] It is clear that the delta function cannot be a function. That it is still denoted as one may be due to the often rather nonchalant or easygoing approach of physicists to mathematics. More is given on the delta function in Appendix H, Vol. 1.

$|\varphi_k\rangle$ is not normalizable. Such state vectors are commonly called *improper* states[5] (i.e. not square-integrable states), in contrast to the proper states, which are square integrable.[6]

We want to illustrate the problem by means of a simple example. The Hilbert space consists of all functions of x defined on the interval $-1 \leq x \leq 1$; the scalar product is given by $\int_{-1}^{1} u^*(x)v(x)\mathrm{d}x$. The problem is that the position operator x is indeed self-adjoint, but has no eigenvalues (so we cannot measure a local value). For if we want to solve the eigenvalue equation $xu_{x_0}(x) = x_0 u_{x_0}(x)$ for the eigenvalue x_0, we find $(x - x_0)\, u_{x_0}(x) = 0$, so that for $x \neq x_0$, the trivial solution $u_{x_0}(x) = 0$ is always obtained. The choice $u_{x_0}(x) = \delta\,(x - x_0)$ does not help, because the delta function is not square integrable and therefore not part of the Hilbert space. One can express this fact as mentioned above, by noting that such 'precise' measurements are not compatible with the uncertainty principle (and thus can be understood only in an idealized formulation).

We emphasize that for us, the problems with continuous spectra are based not primarily on mathematics (e.g. on the fact that such eigenfunctions depart from the mathematical structure of Hilbert space), but rather that *unphysical states* like the delta function states appear, which physically are not permissable in the context of quantum mechanics.[7] Since these unphysical states are not square integrable, the previously-developed probability concept of quantum mechanics cannot work with them (or at least not readily)—that is the essential difficulty.

The basic idea for getting the problem under control is to discretize[8] the continuous variable and then to let the gaps go to zero. We consider the following manipulations for general improper states $|\lambda\rangle$, which fulfill the equation (the 'substitute' of the ON relation for proper vectors)[9]:

$$\langle\lambda'\,|\lambda\rangle = \delta(\lambda' - \lambda). \tag{12.6}$$

As indicated in Fig. 12.1, we divide the continuum into fixed intervals of width $\Delta\lambda$ (the process is demonstrated here in one dimension; it works analogously in higher dimensions).[10] $|\lambda\rangle$ can be integrated within such an interval:

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[5] These states are also called *Dirac states*.

[6] The strict mathematical theory of continuous spectra is somewhat elaborate (keywords e.g. *rigged Hilbert space* or *Gel'fand triple*). We content ourselves here with a less rigorous and more heuristic approach.

[7] The electron is a point object, but not its wavefunction—that would be in contradiction to the uncertainty principle.

[8] Discretizations of continuous variables are used also in other areas, e.g. in lattice gauge theories or in the numerical treatment of differential equations. Moreover, a discrete space is taken as a basis for an alternative derivation/motivation of the SEq (hopping equation; see Appendix J, Vol. 1).

[9] Whoever wishes may keep in mind $\frac{1}{\sqrt{2\pi}} e^{i\lambda x}$ instead of $|\varphi_\lambda\rangle \equiv |\lambda\rangle$ — this is not quite correct, but may be helpful here and is preferable to the auxiliary notion of a column vector.

[10] Note that we cover the axis completely with non-overlapping intervals $\Delta\lambda$.

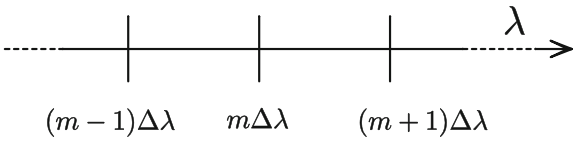

Fig. 12.1 Discretization of the continuous variable λ

$$|\lambda_m, \Delta\lambda\rangle := \frac{1}{\sqrt{\Delta\lambda}} \int_{\lambda_m}^{\lambda_m+\Delta\lambda} \left|\lambda'\right\rangle \mathrm{d}\lambda', \tag{12.7}$$

where λ_m is an integral multiple of the grid size $\Delta\lambda$: $\lambda_m = m\Delta\lambda$ with $m \in \mathbb{Z}$. The expression $|\lambda_m, \Delta\lambda\rangle$ is called an *eigendifferential*. Eigendifferentials, in contrast to continuous functions, are completely 'well-behaved'. In particular, the bras belonging to them exist, and they form an ON system:

$$\begin{aligned}
\langle\lambda_n, \Delta\lambda\,|\lambda_m, \Delta\lambda\rangle &= \frac{1}{\Delta\lambda} \int_{\lambda_n}^{\lambda_n+\Delta\lambda} \mathrm{d}\alpha\ \langle\alpha| \int_{\lambda_m}^{\lambda_m+\Delta\lambda} \mathrm{d}\beta\ |\beta\rangle \\
&= \frac{1}{\Delta\lambda} \int_{\lambda_n}^{\lambda_n+\Delta\lambda} \mathrm{d}\alpha \int_{\lambda_m}^{\lambda_m+\Delta\lambda} \mathrm{d}\beta\ \langle\alpha|\,\beta\rangle \\
&= \frac{1}{\Delta\lambda} \int_{\lambda_n}^{\lambda_n+\Delta\lambda} \mathrm{d}\alpha \int_{\lambda_m}^{\lambda_m+\Delta\lambda} \mathrm{d}\beta\ \delta(\alpha-\beta) \\
&= \frac{1}{\Delta\lambda} \int_{\lambda_m}^{\lambda_m+\Delta\lambda} \mathrm{d}\beta\ \delta_{\lambda_n\lambda_m} = \delta_{\lambda_n\lambda_m}.
\end{aligned} \tag{12.8}$$

Since we have covered the entire λ axis, the states $|\lambda_m, \Delta\lambda\rangle$ are complete and therefore form a CONS. Thus, the eigendifferentials constitute a basis, with which any ket $|\Psi\rangle$ can be represented as

$$|\Psi\rangle = \sum_{\lambda_m} |\lambda_m, \Delta\lambda\rangle\,\langle\lambda_m, \Delta\lambda\,|\Psi\rangle\,. \tag{12.9}$$

This is an approximation of the continuous system which gets better and better with increasingly finer subdivision of the intervals, i.e. with decreasing $\Delta\lambda$.[11] For sufficiently small $\Delta\lambda$, we can approximate the eigendifferential (12.7) using the mean value theorem for integration (see Appendix D, Vol. 1):

[11] A remark on the summation index: the range of values of λ runs through all integral multiples of the grid size $\Delta\lambda$.

$$|\lambda_m, \Delta\lambda\rangle \approx \frac{1}{\sqrt{\Delta\lambda}} \left|\lambda_\mu\right\rangle \Delta\lambda = \sqrt{\Delta\lambda}\, \left|\lambda_\mu\right\rangle; \quad m \le \mu \le m+1, \tag{12.10}$$

and it follows that

$$|\Psi\rangle \approx \sum_{\lambda_\mu} \left|\lambda_\mu\right\rangle \left\langle\lambda_\mu\right| \Psi\rangle\, \Delta\lambda. \tag{12.11}$$

We now go to the limiting case[12]:

$$|\Psi\rangle = \lim_{\Delta\lambda\to 0} \sum_{\lambda_\mu} \left|\lambda_\mu\right\rangle \left\langle\lambda_\mu\right| \Psi\rangle\, \Delta\lambda = \int |\lambda\rangle\, \langle\lambda\, |\Psi\rangle\, \mathrm{d}\lambda \tag{12.12}$$

or

$$\int |\lambda\rangle\, \langle\lambda|\, \mathrm{d}\lambda = 1, \tag{12.13}$$

so that we can also expand each state in a series of improper vectors. Although this process is mathematically not clearly defined, in view of the square integrability, we can permit it in the sense that (12.12) is an abbreviation for (12.9) (simply as an imagined limiting process).

The reason for this approach is that it is possibly much easier to work with improper vectors than with proper ones. It may well be very useful to describe a quantum object using plane waves[13] e^{ikx}, although they—being infinitely extended and everywhere equal in magnitude—certainly cannot represent real physical objects. The same is true for the delta function. One can imagine a wavefunction concentrated at a point and let it tend to a delta function in the mathematical limit—but it is impossible to realize such a state physically.

In short, delta functions and plane waves are, where appropriate, very practical tools for mathematical formulations, but one must not forget that a physical state is always represented only by a square-integrable wavefunction.

With this caveat, we also accept series expansions of improper vectors $|\varphi_\lambda\rangle \equiv |\lambda\rangle$. One speaks in this context of the *extended Hilbert space* (i.e. the set of proper and improper state vectors). Generally, the extended Hilbert space is also denoted by $\mathcal{H}$, i.e. by the same symbol as the proper Hilbert space. In summary, this means that we can work with improper vectors just as with proper ones, but we have to accept the occurrence of functionals such as the delta function. The orthonormality of proper and improper vectors is expressed by the equations

$$\langle\varphi_n\, |\varphi_{n'}\rangle = \delta_{nn'} \text{ and } \langle\varphi_{\lambda'}\, |\varphi_\lambda\rangle = \delta\left(\lambda - \lambda'\right) \tag{12.14}$$

[12] This is nothing more than the transition from a sum to an integral, well-known from school mathematics. One lets the length of the subdivisions tend to zero, so that the upper sum and lower sum approach and converge to the integral in the limit, i.e. for infinitesimal interval length. This process is reflected in the integral sign $\int$—it is simply a stylized 'S', for 'sum'.

[13] We repeat the remark that e^{ikx} is actually an *oscillation* in space. But one always refers in this context to a *wave*, because one keeps the time-dependent factor $e^{i\omega t}$ in mind, so to speak.

and their completeness by[14]:

$$\sum |\varphi_n\rangle \langle\varphi_n| = 1 \text{ and } \int |\varphi_\lambda\rangle \langle\varphi_\lambda| \, \mathrm{d}\lambda = 1. \tag{12.15}$$

The expansion theorem reads

$$|\Psi\rangle = \sum |\varphi_n\rangle \langle\varphi_n| \, \Psi\rangle \text{ and } |\Psi\rangle = \int |\varphi_\lambda\rangle \langle\varphi_\lambda \, |\Psi\rangle \, \mathrm{d}\lambda. \tag{12.16}$$

Thus, we can transfer our previous statements for the discrete case to the continuous case if we perform the following substitutions:

$$n \to \lambda; \sum \to \int \; ; \delta_{nn'} \to \delta(\lambda - \lambda'). \tag{12.17}$$

Indeed, we may make life even easier by introducing a new symbol,[15] namely $\sum\!\!\!\!\!\!\int$. The expansion theorem is then written as

$$|\Psi\rangle = \sum\!\!\!\!\!\!\int |\alpha_j\rangle\langle\alpha_j| \, \Psi\rangle \tag{12.18}$$

with

$$\sum\!\!\!\!\!\!\int |\alpha_j\rangle\langle\alpha_j| \, \Psi\rangle = \begin{cases} \sum\limits_j \\ \int \mathrm{d}j \\ \sum\limits_j + \int \mathrm{d}j \end{cases} \text{for} \begin{cases} \text{proper} \\ \text{improper} \\ \text{proper and improper} \end{cases} \text{states,} \tag{12.19}$$

and the completeness relation reads

$$\sum\!\!\!\!\!\!\int |\alpha_j\rangle\langle\alpha_j| \, \mathrm{d}j = 1. \tag{12.20}$$

Similarly, orthonormality can be expressed more compactly with the following new symbol (*extended* or *generalized Kronecker symbol*:)

$$\delta\,(i,\, j) = \begin{cases} \delta_{ij} & \text{for } i,\, j = \text{discrete} \\ \delta\,(i - j) & \text{for } i,\, j = \text{continuous,} \end{cases} \tag{12.21}$$

namely as

$$\langle\alpha_i \, |\alpha_j\rangle = \delta(i,\, j). \tag{12.22}$$

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[14] We recall that the increment of the sum is 1 (so we have $\Delta n = 1$). With this, one can emphasize the formal similarity between sums and integrals even more, e.g. in the form $\sum |\varphi_n\rangle \langle\varphi_n| \, \Delta n = 1$.

[15] There are other notations; e.g. Schwabl uses the symbol $\mathcal{S}$.

12.2 Position Representation and Momentum Representation

We will now address the question of how the ket $|\Psi\rangle$ is related to the wavefunction $\Psi(x)$.

First a preliminary remark: We have just considered why and how one can accept improper states in quantum mechanics. This allows the following formulation, using the example of position measurements considered above: Assume there is a quantum object at a point x in space,[16] i.e. with regard to its position, it is in the (abstract, improper) state $|x\rangle$. The measurement of its position can be symbolized by the position operator X, and we then have:

$$X|x\rangle = x|x\rangle . \tag{12.23}$$

In words: If we measure the state $|x\rangle$ (i.e. if we apply the position operator X to $|x\rangle$), then we find the number x as the measured value. $|x\rangle$ is an improper vector with

$$\langle x|x'\rangle = \delta(x - x') \quad \text{(ON)} \quad \text{and} \quad \int |x\rangle\langle x| \, dx = 1 \text{ (C)}. \tag{12.24}$$

After this remark, we go to a proper Hilbert space, i.e. a space spanned by a CONS of proper vectors $\varphi_n(x)$. A wavefunction $\Psi(x)$ can be expanded in terms of the CONS:

$$\Psi(x) = \sum\nolimits_n c_n \varphi_n(x) . \tag{12.25}$$

For the coefficients, we find:

$$c_n = \int \varphi_n^*(x)\, \Psi(x)\, dx. \tag{12.26}$$

Due to the orthonormality of $\{\varphi_n(x)\}$, we have

$$\int \Psi^*(x)\, \Psi(x)\, dx = \sum\nolimits_n c_n^* c_n. \tag{12.27}$$

We replace the coefficients by using (12.26), and obtain

$$\begin{aligned} \int \Psi^*(x)\, \Psi(x)\, dx &= \sum_n \int dx'\, \varphi_n(x') \Psi(x') \int dx\, \varphi_n^*(x)\, \Psi^*(x) \\ &= \int dx' \int dx \Psi(x') \Psi^*(x) \sum_n \varphi_n(x') \varphi_n^*(x). \end{aligned} \tag{12.28}$$

[16] It is clear that this is an idealized assumption which is not compatible with the uncertainty principle. But we can proceed on this assumption in terms of the above considerations concerning the eigendifferential.

Comparing the right- and left-hand sides, we see that the following equation must hold:

$$\sum\nolimits_n \varphi_n\left(x'\right)\varphi_n^*\left(x\right) = \delta\left(x' - x\right). \tag{12.29}$$

We note that the expression on the left-hand side is not a scalar product. Recalling our analogy ($\varphi \rightarrow$ column vector) introduced earlier, as well as ($\varphi^\dagger \rightarrow$ row vector), we can suppose that we have an expression of the form $\sum |\varphi_n\rangle \langle\varphi_n|$. In fact, we derived such an expression in the last chapter. Starting with $\langle\Psi|\ \Psi\rangle$ and carrying out exactly the same procedure (but only in the abstract space),[17] we obtained there the completeness relation in the form (see (12.15))

$$\sum\nolimits_n |\varphi_n\rangle \langle\varphi_n| = 1. \tag{12.30}$$

In other words, the (12.29) and (12.30) describe the same facts (completeness of the basis set), just with different notations. We see this more clearly if we transform (12.30) using (12.24):

$$\langle x|\left(\sum_n |\varphi_n\rangle \langle\varphi_n|\right)\left|x'\right\rangle = \sum_n \langle x|\ \varphi_n\rangle \langle\varphi_n\ \left|x'\right\rangle = \langle x|\ x'\rangle = \delta\left(x - x'\right). \tag{12.31}$$

The comparison of this equation with (12.29) suggests the following identification:

$$\varphi_n\left(x\right) = \langle x|\ \varphi_n\rangle \tag{12.32}$$

$\varphi_n\left(x\right)$ is called the *position representation* of the ket $|\varphi_n\rangle$. Formally, it is a scalar product of two abstract vectors, whose result is—as always—a scalar, and to which we can apply the (now) well-known rules of calculation. For example, we have

$$\langle\varphi_n|\ x\rangle = \langle x|\ \varphi_n\rangle^\dagger = \langle x|\ \varphi_n\rangle^* = \varphi_n^*\left(x\right). \tag{12.33}$$

So far so good. We now can 'play around' with this notation a bit. One question might be: If $\langle x|\ \varphi\rangle = \varphi\left(x\right)$ is the position representation of $|\varphi\rangle$, then what is the position representation of $\left|x'\right\rangle$? This state is characterized by the fact that a position measurement returns the result x'—the quantum object is at x', and only there can we

[17] We repeat this derivation briefly by writing the first line of (12.28) with bra-kets (remember: $\int f^* g \mathrm{d}x = \langle f\ |g\rangle$):

$$\int \Psi^*\left(x\right)\Psi\left(x\right)dx = \langle\Psi\ |\Psi\rangle = \sum_n \langle\varphi_n\ |\Psi\rangle \langle\Psi\ |\varphi_n\rangle$$

$$= \sum_n \langle\Psi\ |\varphi_n\rangle \langle\varphi_n\ |\Psi\rangle = \langle\Psi|\left(\sum_n |\varphi_n\rangle \langle\varphi_n|\right)|\Psi\rangle\,.$$

find it.[18] In fact, we have already answered the question with (12.24): The position representation of $\left|x'\right\rangle$ is $\langle x \left|x'\right\rangle = \delta\left(x - x'\right)$.

Another question: We have worked with states which are characterized not by a sharp position, but by a sharp momentum (or $k = p/\hbar$). In the abstract notation, this is the ket $|k\rangle$, whose position representation we already know—it is a plane wave[19] (the prefactor is due to the normalization):

$$\langle x|\ k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}. \tag{12.34}$$

By taking the adjoint, we obtain immediately the *momentum representation* of a state with a sharply-defined position:

$$\langle k|\ x\rangle = \frac{1}{\sqrt{2\pi}} e^{-ikx}, \tag{12.35}$$

and therefore

$$\langle k \left|k'\right\rangle = \delta\left(k - k'\right) \text{ (ON)} \quad \text{and} \int \mathrm{d}k\, |k\rangle\, \langle k| = 1 \text{ (C)}. \tag{12.36}$$

In short, the improper vectors $|k\rangle$ also form a CONS.

We can now write the ket $|\Psi\rangle$ in both the position and the momentum representations, namely as[20]

$$\begin{aligned} &\langle x\ |\Psi\rangle = \Psi(x)\text{: position representation} \\ &\langle k\ |\Psi\rangle = \hat{\Psi}(k)\text{: momentum representation.} \end{aligned} \tag{12.37}$$

How are these two representations related? We multiply by 1 and obtain

$$\begin{aligned} \langle x\ |\Psi\rangle &= \langle x| \int \mathrm{d}k\, |k\rangle\, \langle k\ |\Psi\rangle = \int \mathrm{d}k\, \langle x\ |k\rangle\, \langle k\ |\Psi\rangle \\ \langle k\ |\Psi\rangle &= \langle k| \int \mathrm{d}x\, |x\rangle\, \langle x\ |\Psi\rangle = \int \mathrm{d}x\, \langle k\ |x\rangle\, \langle x\ |\Psi\rangle\,, \end{aligned} \tag{12.38}$$

[18] We note again that this is an idealized formulation.

[19] Again, the above statement on oscillations and waves applies.

[20] Because these are two representations of the same ket $|\Psi\rangle$, sometimes the same symbol is used for both representations, i.e. $\Psi(x)$ and $\Psi(k)$, although these two functions are not the same (as mapping, that is, in the sense that one does not obtain $\Psi(k)$ by simply replacing x by k in $\Psi(x)$). What is precisely meant has to be inferred from the context. To avoid confusion, we use the notation $\hat{\Psi}(k)$.

or in the 'usual' notation:

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}k \; e^{ikx} \hat{\Psi}(k)$$
$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x \; e^{-ikx} \Psi(x). \tag{12.39}$$

We see that the position and momentum representations of a ket are *Fourier transforms* of each other.[21]

Finally the question arises as to how to derive equations and operators in the two representations. We consider an abstract eigenvalue equation of the form

$$A \left|\Psi\right\rangle = a \left|\Psi\right\rangle \tag{12.40}$$

and wish to write it in the position representation. For this purpose, we multiply first with a bra $\langle x|$:

$$\langle x| A \left|\Psi\right\rangle = a \langle x \left|\Psi\right\rangle \tag{12.41}$$

and then multiply the left-hand side by the identity:

$$\begin{gathered} \langle x| A \int \mathrm{d}x' \left|x'\right\rangle \left\langle x' \left|\Psi\right\rangle = a \langle x \left|\Psi\right\rangle \rightarrow \right. \\ \left. \int \mathrm{d}x' \langle x| A \left|x'\right\rangle \left\langle x' \left|\Psi\right\rangle = a \langle x \left|\Psi\right\rangle \right. . \end{gathered} \tag{12.42}$$

Now it depends on the matrix element $\langle x| A \left|x'\right\rangle$ how to continue. A significant simplification of the equation is obtained only if the following applies:

$$\langle x| A \left|x'\right\rangle = \delta(x - x') A(x). \tag{12.43}$$

In this case, one says that A is *diagonal* in the position representation, or that the operator A is a *local* operator.[22] With this understanding, (12.42) apparently may be written as

$$\int dx' \delta(x - x') A(x) \left\langle x' \left|\Psi\right\rangle = A(x) \langle x \left|\Psi\right\rangle = a \langle x \left|\Psi\right\rangle, \right. \tag{12.44}$$

or, in the familiar notation with a position variable,

$$A\Psi(x) = a\Psi(x), \tag{12.45}$$

[21] For an introduction to Fourier transforms, see Appendix H, Vol. 1.

[22] Quasi-local operators are defined via the derivative of the delta function:

$$\begin{aligned} A(x, y) &= a(x) \, \delta(x - y) \quad \text{local operator} \\ B(x, y) &= b(x) \, \delta'(x - y) \quad \text{quasi-local operator} \end{aligned}$$

where A now stands for the position representation of the operator. We point out again that the operators A in (12.40) and (12.45) are not identical. Though one usually writes the same symbol, they are quite different mathematical objects.

Finally, an example: We want to derive the position representation of the momentum operator p_{op} (which we know already, of course). For better readability, we indicate the operator for the moment by an index op.

We start with the abstract eigenvalue equation

$$p_{op} \, |k\rangle = \hbar k \, |k\rangle \, . \tag{12.46}$$

For the following considerations, we know nothing about the momentum operator apart from this eigenvalue equation. $|k\rangle$ is a state of well-defined momentum (note $p = \hbar k$), and $\hbar k$ is its eigenvalue or measured value. Multiplication with $\langle x|$ and insertion of the identity leads to:

$$\int \langle x| \, p_{op} \, |x'\rangle \langle x'| \, k\rangle \, \mathrm{d}x' = \hbar k \int \langle x| \, x'\rangle \langle x'| \, k\rangle \, \mathrm{d}x' = \hbar k \, \langle x| \, k\rangle = \frac{\hbar k}{\sqrt{2\pi}} e^{ikx}. \tag{12.47}$$

It follows that:

$$\int \langle x| \, p_{op} \, |x'\rangle e^{ikx'} \mathrm{d}x' = \hbar k \int \delta(x - x') e^{ikx'} \mathrm{d}x' = \frac{\hbar}{i} \int \delta(x - x') \frac{\partial}{\partial x'} e^{ikx'} \mathrm{d}x'. \tag{12.48}$$

Comparing the left- and right-hand sides yields

$$\langle x| \, p_{op} \, |x'\rangle = \delta(x - x') \frac{\hbar}{i} \frac{\partial}{\partial x}. \tag{12.49}$$

Thus, the momentum operator is diagonal in the position representation, and takes the well-known form—as was to be expected.

An example of a non-diagonal operator in the position representation (projection operator) can be found in the exercises. We have thus filled in a gap as promised in previous chapters.

12.3 Conclusions

We started in Chaps. 1 and 2 with two (at first sight completely different) descriptions of states, namely as position-dependent wavefunctions $\psi(\mathbf{r})$ (analytical approach, odd chapters) on the one hand, and as kets $|\varphi\rangle$ (algebraic approach, even chapters), with their representations as column vectors, on the other hand. After travelling long route, which encompassed necessarily a lot of other material (in large part, the path was also our destination),[23] we have combined the two approaches in this chapter

[23] "Caminante no hay camino, se hace camino al andar…" Antonio Machado, Spanish poet.

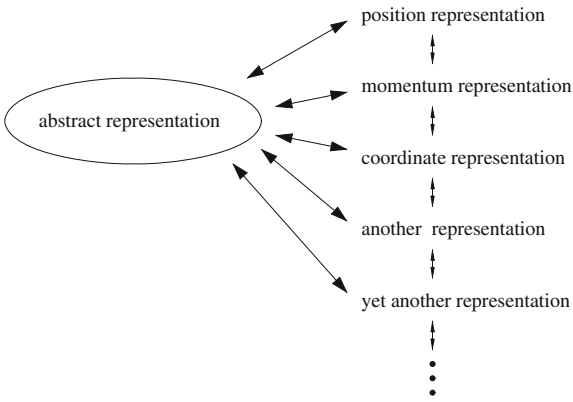

Fig. 12.2 The same physical situation permits various representations

and have seen that in the end, they are simply different formulations of the same facts; this also allows for other representations, cf. Fig. 12.2. We will take advantage of this circumstance in the following and will switch back and forth between the two formulations as proves be convenient for us—wave or matrix mechanics, or the abstract notation.

However, it is clear that wave mechanics cannot describe various properties, e.g. the spin (or, beyond the scope of this book, strangeness, charm, etc.). In other words, for any position-dependent wavefunction, there is a ket, but the converse is not true. But this is now no longer a problem, as we have extended wave mechanics to a general formalism in this chapter.

12.4 Exercises

1. Given an eigenstate $|k\rangle$ of the momentum operator; how is this state described in the position representation?
2. Show by using $\langle x|\ k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$ that the improper vectors $|k\rangle$ form a CONS.
3. Given an improper vector $|\varphi_\lambda\rangle$, what is the associated eigendifferential $\left|\varphi_{\lambda,\Delta\lambda}\right\rangle$?
4. Given the state $|k\rangle$ with the sharply-defined momentum k; we have $\langle x|\ k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$.
   (a) What is the (abstract) eigendifferential?
   (b) How is the eigendifferential expressed in the position representation?
   (c) Show that the eigendifferentials of (b) are orthonormal.
5. Given the SEq in the abstract formulation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi\rangle = H\,|\psi\rangle, \tag{12.50}$$

(a) Formulate this equation in the position representation and in the momentum representation.
(b) How can one calculate the matrix element $\langle k|\, H\, \left|k'\right\rangle$, if H is known in the position representation?

6. Given a CONS $\{|\varphi_n\rangle\}$; formulate the projection operator

$$P_1 = |\varphi_1\rangle\, \langle\varphi_1| \tag{12.51}$$

in the position representation.

7. A and B are self-adjoint operators with $[A, B] = i\hbar$, and $|a\rangle$ is an eigenvector of A with the eigenvalue a. Then we have

$$\langle a\, |[A, B]|\, a\rangle = \langle a\, |AB - BA|\, a\rangle = (a - a)\, \langle a\, |B|\, a\rangle = 0. \tag{12.52}$$

On the other hand, we also have:

$$\langle a\, |[A, B]|\, a\rangle = \langle a\, |i\hbar|\, a\rangle = i\hbar \neq 0. \tag{12.53}$$

Question: where is the flaw in this argument?