Lecture notes 10

10 More general formulation of quantum mechanics

In this course we have so far been using the **position representation** of quantum mechanics, and we have briefly touched upon the momentum representation. In these notes, we shall see that these formulations are special cases of a more general formulation.

This new formulation is important firstly because it offers a number of technical advantages, simplifying a number of calculations (once we get used to the new technique). The main advantage, however, is that the new formulation allows us to treat systems which cannot be described by wave mechanics, that is, with wave functions in x- or p-space. A central example is the description of spin degrees of freedom.

[You might want to supplement these notes with Hemmer's chapter 6, chapter 3 in Griffiths, and chapter 5 in B&J. Another reference is J.J. Sakurai, *Modern Quantum Mechanics*, chapter 1.]

10.1 Vectors in Hilbert space

10.1.a Central results in the position representation

Let us briefly review some central results in the theory presented so far:

The state of a particle at a given point in time can be described by a spatial wave function $\psi(x)$, if we consider a one-dimensional case. The value of ψ at the point x gives the probability amplitude of finding the particle in this position, in the sense that $|\psi(x)|^2$ gives the probability density. Thus, when we know the complete *function* $\psi(x)$, we know the amplitudes of finding the particle in all possible positions.

We are free to expand the wave function in terms of an arbitrary complete set of basis states. There are many such bases; we remember that for each observable there is a hermitian operator with a complete set of eigenfunctions. Examples are $\widehat{p}_x, \widehat{H}$ and $\widehat{x}$, with eigenvalue equations and eigenfunctions as follows:

$$\widehat{p}_x\psi_p(x) = p\psi_p(x) \quad ; \qquad \psi_p(x) = (2\pi\hbar)^{-1/2}e^{ipx/\hbar};$$

$$\widehat{H}\psi_n(x) = E_n\psi_n(x) \quad ; \qquad \psi_n(x) \text{ depends on the potential } V(x); \qquad \text{(T10.1)}$$

$$\widehat{x}\psi_{x'}(x) = x'\psi_{x'}(x) \quad ; \qquad \psi_{x'}(x) = \delta(x - x').$$

Here, we are assuming a discrete and non-degenerate energy spectrum $\{E_n\}$, so that we can use the orthonormality relation

$$\langle\, \psi_k, \psi_n \,\rangle \equiv \int \psi_k^*(x)\psi_n(x)dx = \delta_{kn}. \tag{T10.2}$$

All these sets of states are complete, in the sense that an arbitrary state $\psi(x)$ may be expanded in any of these sets. The expansion in terms of energy eigenfunctions then is a sum, while the expansions in momentum and position eigenfunctions become integrals, since the spectra $\{x'\}$ and $\{p\}$ are continuous:

$$\begin{aligned} \psi(x) &= \int dp\ \phi(p)\psi_p(x); \\ \psi(x) &= \sum_n c_n\psi_n(x); \\ \psi(x) &= \int dx'\ c(x')\psi_{x'}(x). \end{aligned} \tag{T10.3}$$

The expansion coefficients $\phi(p)$, c_n and $c(x')$ in these formulae characterize the state perfectly, like $\psi(x)$ itself, in the same way as the components of a vector in a given basis gives a perfect representation of the vector.

The expansion coefficients in (T10.3) are the projections of ψ onto the respective "basis vectors" ψ_p, ψ_n and $\psi_{x'}(x) = \delta(x - x')$:

$$\begin{aligned} \phi(p) &= (\psi_p, \psi) = \int \psi_p^*(x)\psi(x)dx; \\ c_n &= (\psi_n, \psi) = \int \psi_n^*(x)\psi(x)dx; \\ c(x') &= (\psi_{x'}, \psi) = \int \delta(x' - x)\psi(x)dx = \psi(x'). \end{aligned} \tag{T10.4}$$

Let us repeat the proof for the formula for c_n, by projecting $\psi(x) = \sum c_n\psi_n(x)$ on ψ_k. Interchanging the order of integration and summation, we find that

$$\langle\, \psi_k, \psi \,\rangle = \int \psi_k^*(x) \sum_n c_n\psi_n(x) = \sum_n c_n \int \psi_k^*(x)\psi_n(x)dx = \sum_n c_n\delta_{kn} = c_k, \quad \text{q.e.d.} \tag{T10.5}$$

A small exercise: Find the momentum wave function $\phi(p)$ by projecting ψ on ψ_p. Hint: Change the order of the integrations and use the delta-function "normalization"

$$\int \psi_{p'}^*(x)\psi_p(x)dx = \delta(p' - p).$$

In a similar manner you can derive the formula for $c(x')$ using the relation

$$\int \delta(x - x'')\delta(x - x')dx = \delta(x' - x'').$$

But it is even simpler to use the identity

$$\psi(x) = \int \psi(x')\delta(x - x')dx'.$$

We must also remember the physical interpretation of the expansion coefficients: $\psi(x')$ is (as already mentioned) the probability amplitude of finding the particle at the position x' (in the sense that $|\psi(x')|^2$ is the probability density in position space). In the same manner, $|\phi(p)|^2$ is the probability density in momentum space, and $|c_n|^2$ is the probability of measuring the energy E_n (and leaving the particle in the state ψ_n).

10.1.b State vectors in Hilbert space. Dirac notation

The most central aspect of the new formulation is that:

> With each wave function $\psi(x)$ we may associate an abstract vector which is called a **state vector**. For such vectors we shall use the symbol $|\ldots\rangle$, which was invented by Dirac. (T10.6)

For this so-called **ket** vector we may choose a suitable label to indicate which state we have in mind. As an example, we may denote the vector corresponding to the wave function $\psi(x)$ by $|\psi\rangle$. The vector corresponding to the energy eigenfunction $\psi_n(x)$ may be denoted by $|\psi_n\rangle$ (or $|n\rangle$ or $|E_n\rangle$). The vector corresponding to the position eigenfunction $\psi_{x'}(x) = \delta(x - x')$ may suitably be called $|x'\rangle$. The vector corresponding to the momentum eigenfunction $\psi_p(x) = (2\pi\hbar)^{-1/2} e^{ipx/\hbar}$ might be labeled $|p\rangle$ or $|\psi_p\rangle$, and so on. Thus (no matter which label we choose to use) we have a one-to-one correspondence between wave function and state vector:

$$\begin{aligned} \psi(x) &\iff |\psi\rangle, \\ \psi_n(x) &\iff |\psi_n\rangle = |n\rangle = |E_n\rangle, \\ \psi_{x'}(x) = \delta(x - x') &\iff |x'\rangle, \\ \psi_p(x) &\iff |p\rangle = |\psi_p\rangle, \end{aligned} \tag{T10.7}$$

and so on.

Here, we should not be confused by the fact that also wave functions are vectors (cf Lecture notes 2, or Griffiths); The ket vector $|\psi\rangle$ and the wave function $\psi(x)$ are *different objects*; they belong to two different vector spaces, with a one-to-one correspondence between the vectors in the two spaces. The space spanned by the ket vectors will from now on be denoted the Hilbert space $\mathcal{H}$, (even if also the wave functions $\psi(x)$ are vectors in a Hilbert space, mathematically speaking). [1]

An important property of Hilbert space (shared with *all* linear, complex vector spaces) is that an arbitrary linear combination of two vectors is also a vector in this space:

$$c_1|\psi_1\rangle + c_2|\psi_2\rangle = |\psi_3\rangle. \tag{T10.8}$$

[1] As you may recall from the discussion of the momentum eigenfunctions $\psi_p(x)$, these are not quadratically integrable. They therefore do not belong to the mathematical Hilbert space $\mathrm{L}_2(-\infty, \infty)$ of quadratically integrable functions, and neither do the position eigenfunctions $\psi_{x'}(x) = \delta(x - x')$. Correspondingly, the ket vectors $|\psi_p\rangle$ and $|x'\rangle$ do not really belong to the Hilbert space $\mathcal{H}$. However, these vectors function perfectly well as basis vectors for expansions of vectors in Hilbert space. Thus the sets $\{|\psi_p\rangle\}$ and $\{|x'\rangle\}$ are complete, together with the set $\{|\psi_n\rangle\}$. In quantum mechanics one therefore works with a kind of enlarged "Hilbert" space, where the vectors $|x'\rangle$ and $|\psi_p\rangle \equiv |p\rangle$ may largely be treated in the same way as the proper Hilbert-space vectors.

In particular $c|\psi\rangle$ gives a new vector $|\psi_1\rangle$:[2]

$$c|\psi\rangle = |\psi\rangle c = |\psi_1\rangle. \tag{T10.9}$$

Here, $|\psi\rangle$ corresponds to the wave function $\psi(x)$, and $|\psi_1\rangle$ corresponds to $c\psi(x) = \psi(x)c$. As you will remember, $\psi(x)$ and $c\psi(x)$ describe the same physical state. The same then holds for the ket-vectors $|\psi\rangle$ and $|\psi_1\rangle = c|\psi\rangle$.

10.1.c The dual Hilbert space. Scalar product

To get a new formulation that is equivalent with the old one, we must postulate the existence of a salar product (inner product) between ket vectors.

Before we define this product, it may be instructive to review how the scalar product is defined for ordinary complex vectors $\mathbf{A}$ and $\mathbf{B}$. In physics literature this product is usually defined as

$$\langle\, \mathbf{A}, \mathbf{B} \,\rangle = \mathbf{A}^* \cdot \mathbf{B} \equiv \sum_i A_i^* B_i. \tag{T10.10}$$

From this definition it follows that the (usually) complex scalar product satisfies the relation

$$\langle\, \mathbf{A}, \mathbf{B} \,\rangle = \langle\, \mathbf{B}, \mathbf{A} \,\rangle^* . \tag{T10.11}$$

Furthermore it is easy to see that, with c a complex number, the scalar product has the properties

$$\langle\, \mathbf{A}, c\mathbf{B} \,\rangle = c \,\langle\, \mathbf{A}, \mathbf{B} \,\rangle \qquad \text{and} \qquad \langle\, c\mathbf{A}, \mathbf{B} \,\rangle = c^* \,\langle\, \mathbf{A}, \mathbf{B} \,\rangle . \tag{T10.12}$$

We then say that the scalar product $\langle\, \mathbf{V}_1, \mathbf{V}_2 \,\rangle$ is **linear** with respect to vector no 2 ($\mathbf{V}_2$) and **anti-linear** with respect to vector no 1 ($\mathbf{V}_1$). Notice that the scalar product between functions has exactly the same properties:

$$\langle\, f, g \,\rangle = \int f^*\, g \, d\tau = \langle\, g, f \,\rangle^* ; \qquad \langle\, f, cg \,\rangle = c \,\langle\, f, g \,\rangle ; \qquad \langle\, cf, g \,\rangle = c^* \,\langle\, f, g \,\rangle . \tag{T10.13}$$

To obtain a convenient notation for the scalar product (inner product) $\langle\ |\psi_1\rangle\,, |\psi_2\rangle\ \rangle$ between two ket-vektorer in Hilbert space, Dirac introduced the so-called **dual** Hilbert space $\mathcal{H}^*$. We create this space by associating with every ket vector $|\psi\rangle$ in $\mathcal{H}$ a so-called **dual** vector $\langle\psi|$ in $\mathcal{H}^*$:

$$\langle\psi| \qquad \overset{\text{dual of}}{\longleftrightarrow} \qquad |\psi\rangle. \tag{T10.14}$$

Employing these new vectors $\langle\ldots|$, which Dirac called **bra** vectors, we can formulate rules of calculation and establish the Dirac notation, which are in fact easier to use than the wave-function formalism (and which may also be applied to problems for which there does not exist any wave functions, like e.g. for spin).

The main reason for introducing the bra vector is that it allows us to write the scalar product between $|\psi_1\rangle$ and $|\psi_2\rangle$ as a simple product of the *bra* vector $\langle\psi_1|$ and the ket vector $|\psi_2\rangle$:

$$\langle\ |\psi_1\rangle\,, |\psi_2\rangle\ \rangle = \langle\psi_1| \cdot |\psi_2\rangle \equiv \langle\psi_1|\psi_2\rangle. \tag{T10.15}$$

We can now understand why Dirac introduced the names **bra** and **ket**: The scalar product

$$\langle\psi_1| \cdot |\psi_2\rangle \equiv \langle\psi_1|\psi_2\rangle$$

[2] Some authors also use the notation $c|\psi\rangle = |\psi\rangle c = |c\psi\rangle$.

has the form $\langle$bra|ket$\rangle$, derived from the word $\langle$"**bracket**"$\rangle$. Notice that $\langle\psi_1|$ plays a role similar to $\mathbf{A}^*$ in the dot product $\langle\,\mathbf{A},\mathbf{B}\,\rangle = \mathbf{A}^*\cdot\mathbf{B}$, and to ψ_1^* in the scalar product $\langle\,\psi_1,\psi_2\,\rangle = \int\psi_1^*\psi_2 d\tau$. In (T10.15), we have an additional rule: In this inner product, the bra vector is always standing on the left and the ket vector is standing on the right.

The *physical interpretation* of $\langle\psi_1|\psi_2\rangle = \langle\,|\psi_1\rangle\,,|\psi_2\rangle\,\rangle$ — the projection of $|\psi_2\rangle$ on $|\psi_1\rangle$ — is exactly the same as for the corresponding wave functions: The projection is the probability amplitude that a measurement "finds" the system in the physical state corresponding to $|\psi_1\rangle$ (and to ψ_1) when the system is in the state corresponding to $|\psi_2\rangle$ (and to ψ_2) before the measurement. Thus

$$\boxed{\langle\psi_1|\cdot|\psi_2\rangle \equiv \langle\psi_1|\psi_2\rangle = \langle\,\psi_1,\psi_2\,\rangle \equiv \int\psi_1^*\psi_2 d\tau.} \tag{T10.16}$$

From the relation $\langle\,\psi_1,\psi_2\,\rangle = \langle\,\psi_2,\psi_1\,\rangle^*$ it then follows that

$$\langle\psi_2|\cdot|\psi_1\rangle = (\langle\psi_1|\cdot|\psi_2\rangle)^* = \quad \text{complex number},$$

or

$$\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle^*. \tag{T10.17}$$

We then see that

$$\underline{\langle\psi_1|\cdot c|\psi_2\rangle} = \langle\,\psi_1,c\psi_2\,\rangle = c\,\langle\,\psi_1,\psi_2\,\rangle = \underline{c\langle\psi_1|\cdot|\psi_2\rangle}. \tag{T10.18}$$

Thus the scalar product is linear in the ket vector (vector no 2). With $|\psi_1\rangle = c|\phi\rangle$ we see in the same manner that

$$\underline{\langle\psi_1|}\cdot|\psi_2\rangle = \langle\psi_2|\psi_1\rangle^* = (c\langle\psi_2|\phi\rangle)^* = \underline{c^*\langle\phi|}\cdot|\psi_2\rangle.$$

Thus the dual of $|\psi_1\rangle = c|\phi\rangle$ is $c^*\langle\phi|$:

$$c^*\langle\phi| \qquad \overset{\text{dual of}}{\longleftrightarrow} \qquad c|\phi\rangle, \tag{T10.19}$$

in analogy with $(c\mathbf{a})^* = c^*\mathbf{a}^*$. We shall use this relation frequently. Notice that this means that the scalar product is anti-linear with respect to vector no 1, just as $\langle\,f,g\,\rangle = \int f^*\,g\,d\tau$.

The relation between $|\psi\rangle$ and $\psi(x)$

While the wave function is now a well-known and hopefully dear friend, you are probably having difficulties in imagining what kind of object the abstract state vector $|\psi\rangle$ is. However, as you get more acquainted with the new formalism, you will learn to live with the abstractness, and you will probably end up appreciating the convenience of the new formalism, once you learn how to use it. We shall now attempt to present the central parts of these methods, not necessarily in the most systematic way.

Two important aspects have already been mentioned: The dual correspondence (T10.14) and (T10.19), together with the fact that the scalar product $\langle\psi_1|\psi_2\rangle$ is the same as between the corresponding wave functions. (See (T10.16)). Thus the **physical interpretation** of the new scalar product is the same as for the old one: For example, the scalar product $\langle\psi_n|\psi\rangle$ is the probability amplitude of finding the particle in the state described by the vector $|\psi_n\rangle$

(i.e., with the energy E_n) if it was in a state desrcibed by the vector $|\psi\rangle$ (corresponding to the wave function $\psi(x)$) before the measurement. In the same manner $\langle p|\psi\rangle$ is the amplitude of finding the particle described by the vector $|p\rangle$ (i.e., with momentum p).

Another example: We remember that the vector $|x'\rangle$ describes a state where the particle has the position x' (corresponding to the wave function $\psi_{x'}(x) = \delta(x - x')$). The scalar product $\langle x'|\psi\rangle$ therefore is the amplitude of finding the particle at x' when it is in the state $|\psi\rangle$. But this amplitude is precisely what the wave function $\psi(x')$ is. Thus the relation between the wave function $\psi(x)$ and the vector $|\psi\rangle$ is

$$\boxed{\langle x|\psi\rangle = \psi(x).} \tag{T10.20}$$

Notice also that

$$\langle \psi|x\rangle = \langle x|\psi\rangle^* = \psi^*(x). \tag{T10.21}$$

10.1.d Completeness

Thus the wave function $\psi(x) = \langle x|\psi\rangle$ is the "component of the Hilbert vector $|\psi\rangle$ in the $|x\rangle$-direction", or the projection of the vector $|\psi\rangle$ on the basis vector $|x\rangle$. In the same manner the scalar product $\langle \psi_n|\psi\rangle$ is the projection of $|\psi\rangle$ on another basis vector, $|\psi_n\rangle$. As the term "basis" indicates, these sets are **complete**, as are the corresponding sets of wave functions (cf (T10.1)). This means that an arbitrary vector $|\psi\rangle$ in Hilbert space may be expanded in terms of these basis sets, in analogy with the expansions (T10.3):

$$\begin{aligned} |\psi\rangle &= \int dp\ \phi(p)|p\rangle, \\ |\psi\rangle &= \sum_n c_n|\psi_n\rangle, \\ |\psi\rangle &= \int dx'\ c(x')|x'\rangle. \end{aligned} \tag{T10.22}$$

Here we must of course expect that the coefficients are the same as in (T10.4),

$$c_n = \langle\, \psi_n, \psi\, \rangle = \langle \psi_n|\psi\rangle, \quad \text{etc},$$

but let us check it, to get a little experience with the new formalism: By projecting the second of equations (T10.22) on $|\psi_k\rangle$ (that is, by multiplying from the elft by $\langle\psi_k|$), we find

$$\langle \psi_k|\psi\rangle = \sum_n c_n\langle \psi_k|\psi_n\rangle = \sum_n c_n\delta_{kn} = c_k, \quad \text{q.e.d..}$$

Here we have used (T10.16), which implies that the set $|\psi_k\rangle$ is orthonormal, just like the set $\psi_k(x)$:

$$\langle \psi_k|\psi_n\rangle = \langle\, \psi_k, \psi_n\, \rangle = \delta_{kn}. \tag{T10.23}$$

Inserting into (T10.22) now gives

$$|\psi\rangle = \sum_n \langle \psi_n|\psi\rangle\ |\psi_n\rangle. \tag{T10.24}$$

The corresponding expansions in terms of momentum and position vectors are

$$\begin{aligned} |\psi\rangle &= \int dp\, \langle p|\psi\rangle\, |p\rangle, \\ |\psi\rangle &= \int dx'\, \langle x'|\psi\rangle\, |x'\rangle. \end{aligned} \tag{T10.25}$$

This can be shown by projecting (T10.22) on $|x''\rangle$ and $|\psi_{p'}\rangle$, respectively. Both these are "continuum sets", with δ-function normalization, so that instead of (T10.23) we have [3]

$$\begin{aligned} \langle p'|p\rangle &= \langle\, p', p\,\rangle = \delta(p-p'), \\ \\ \langle x''|x'\rangle &= \langle\, \psi_{x''}, \psi_{x'}\,\rangle = \delta(x''-x'). \end{aligned} \tag{T10.26}$$

Hence

$$\langle x''|\psi\rangle = \int dx'\; c(x')\langle x''|x'\rangle = \int dx'\; c(x')\delta(x''-x') = c(x''),$$

so that

$$|\psi\rangle = \int dx'\; c(x')|x'\rangle = \int dx'\; \langle x'|\psi\rangle\, |x'\rangle = \int dx\; \langle x|\psi\rangle\, |x\rangle, \quad \text{q.e.d..}$$

In the same manner,

$$\langle p'|\psi\rangle = \int dp\; \phi(p)\langle p'|p\rangle = \int dp\; \phi(p)\delta(p-p') = \phi(p'), \quad \text{q.e.d..}$$

Notice that

$$\langle p|\psi\rangle = \phi(p) \tag{T10.27}$$

is the amplitude of finding the momentum p, that is, the momentum wave function.

Notice also that the formulae (T10.24) and (T10.25) are analogous to expansions of an ordinary vector in alternative basis sets $\hat{\mathbf{e}}_i$ and $\hat{\mathbf{e}}'_i$,

$$\mathbf{A} = \sum A_i \hat{\mathbf{e}}_i = \sum A'_i \hat{\mathbf{e}}'_i\;;$$

the components (A_i) depend on our choice of basis, while the vector $\mathbf{A}$ itself is basis-independent; it is an absolute geometric object. The same can be stated about the Hilbert vector $|\psi\rangle$.

The completeness relation

Equations (T10.24) and (T10.25) rely on the fact that the three basis sets are complete. A slight re-writing of (T10.24) gives [4]

$$\begin{aligned} |\psi\rangle &= \sum_n \langle\psi_n|\psi\rangle\, |\psi_n\rangle \\ &= \sum_n |\psi_n\rangle\langle\psi_n|\cdot|\psi\rangle \\ &= \left(\sum_n |\psi_n\rangle\langle\psi_n|\right)\cdot|\psi\rangle. \end{aligned} \tag{T10.28}$$

[3] Vectors with δ-function normalization (and the corresponding wave functions) strictly speaking do not belong to the respective Hilbert spaces, as already mentioned. In quantum mechanics we prefer to include these vectors into our formalism. This means that we are working with an "extended" Hilbert space, often simply called the Hilbert space.

[4] Notice that the scalar product $\langle\psi_n|\psi\rangle$ is a complex number, which may be moved wherever it suits us.

Since this holds for an arbitrary vector $|\psi\rangle$, it follows that

$$\boxed{\sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{1}. \qquad \text{(the completeness relation)}} \tag{T10.29}$$

This is the completeness relation in Dirac notation (for a discrete vector set). As we shall see below, both sides of this equation are **operators**. The quantity on the right-hand side is the **unit operator**; $\mathbb{1}|\psi\rangle = |\psi\rangle$.

In a similar manner we find for the two continuum sets:

$$|\psi\rangle = \int dx\, \langle x|\psi\rangle\, |x\rangle = \left(\int dx\, |x\rangle\langle x|\right)\cdot|\psi\rangle, \quad \text{etc.}$$

Thus the completeness relations for these sets are

$$\begin{aligned} \int dx\, |x\rangle\langle x| &= \mathbb{1}, \\ \int dp\, |p\rangle\langle p| &= \mathbb{1}. \qquad \text{(completeness)} \end{aligned} \tag{T10.30}$$

In what follows we shall see that these relations are easier to use than the corresponding relations for the wave functions (see e.g. B&J p 205):

$$\begin{aligned} \sum_n \psi_n(x)\psi_n^*(x') &= \delta(x-x'), \\ \int dp\, \psi_p(x)\psi_p^*(x') &= \delta(x-x'), \quad \text{etc.} \end{aligned} \tag{T10.31}$$

As an example we can re-write the square $\| \, |\psi\rangle \, \|^2 \equiv \langle\psi|\psi\rangle$ of the norm of $|\psi\rangle$ in several ways:

$$\begin{aligned} \langle\psi|\psi\rangle &= \langle\psi|\mathbb{1}|\psi\rangle = \langle\psi|\left(\int dx\, |x\rangle\langle x|\right)|\psi\rangle \\ &= \int dx\, \langle\psi|x\rangle\langle x|\psi\rangle = \int dx\, \psi^*(x)\psi(x) = \langle\, \psi, \psi\, \rangle\,, \\ \langle\psi|\psi\rangle &= \langle\psi|\left(\sum_n |\psi_n\rangle\langle\psi_n|\right)|\psi\rangle \\ &= \sum_n \langle\psi|\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n |\langle\psi_n|\psi\rangle|^2 \equiv \sum_n |c_n|^2, \\ \langle\psi|\psi\rangle &= \langle\psi|\left(\int dp\, |p\rangle\langle p|\right)|\psi\rangle \\ &= \int dp\, |\langle p|\psi\rangle|^2 \equiv \int dp\, |\phi(p)|^2. \end{aligned} \tag{T10.32}$$

These relations are generalized Parseval relations. Notice that the scalar product $\langle\psi|\psi\rangle$ is always a real non-negative number, so that we can define the norm of $|\psi\rangle$ as

$$\| \, |\psi\rangle \, \| = \langle\psi|\psi\rangle^{1/2} \geq 0. \tag{T10.33}$$

The technique applied above, of inserting the unit operators (T10.29) or (T10.31) (or a similar expression for another complete set) where it is suitable, is a trick that we shall use

frequently in what follows. Let us as an example use this trick to show the equivalence of (T10.29) and (T10.31): From the normalization condition (T10.26) we have:

$$\begin{aligned}\delta(x-x') &= \langle x|x'\rangle = \langle x|\mathbb{1}\,|x'\rangle \\ &= \langle x|\sum_n |\psi_n\rangle\langle\psi_n|x'\rangle \\ &= \sum_n \langle x|\psi_n\rangle\langle x'|\psi_n\rangle^* = \sum_n \psi_n(x)\psi_n^*(x'), \quad \text{q.e.d.}\end{aligned} \tag{T10.34}$$

10.2 Operators, eigenvectors, expectation values, etc

10.2.a General definition of operators

An operator applied to a function has the property

$$\text{operator} \cdot \text{function} = \text{new function.} \tag{T10.35}$$

The operators appearing in the new formulation have the same kind of property: When an operator $\widehat{A}$ acts on a Hilbert vector $|b\rangle$, the result is a new vector in Hilbert space, $|c\rangle = \widehat{A}|b\rangle$. In other words: Operators in Hilbert space map the space into itself. Notice that the operator is standing to the left of a ket vector.

Example: Projection operator

The expression $P_n \equiv |\psi_n\rangle\langle\psi_n|$ is an operator. Applied to an arbitrary vector $|\psi\rangle$ it gives

$$P_n|\psi\rangle \equiv (|\psi_n\rangle\langle\psi_n|)\,|\psi\rangle = \langle\psi_n|\psi\rangle\;|\psi_n\rangle \equiv c_n|\psi_n\rangle. \tag{T10.36}$$

Thus the operator $P_n \equiv |\psi_n\rangle\langle\psi_n|$ projects out the part of the vector $|\psi\rangle$ which points in the "$|\psi_n\rangle$ direction". It is therefore called a **projection operator**. Notice that

$$\sum_n P_n = \sum_n |\psi_n\rangle\langle\psi_n| = \mathbb{1}. \quad \text{(completeness relation)} \tag{T10.37}$$

Thus, as already mentioned, the expression on the left in the compleness relation is a sum of operators, adding up to the unit operator. Applying the trick of inserting this unit operator wherever it suits us, we must therefore always let the unit operator act from the left on a ket vector. It may also stand to the right of a bra vector. Some times we shall apply the unit operator to the right of an isolated $\langle$bra vector$|$; the resulting expression $\langle$bra vector$|\cdot\mathbb{1}$ may then be applied from the left on a $|$ket$\rangle$. (See section 10.3.b below.)

10.2.b Operators and eigenvectors

As you can see e.g. in section 6.4 in Hemmer' book, we may use the same postulates of quantum mechanics in the new formulation as in the old one, apart from the notation: Thus to each physical observable (e.g. x, p_x, E, etc) there corresponds a Hermitian operator. The problem with these Hilbert-space operators is that they are as abstract as the vectors — but again we shall see that we can live with the abstractness. For example, the only thing we

need to know about the operator $\widehat{p}_x$ is that it is *defineed* in such a way that it satisfies the **eigenvalue equation**

$$\widehat{p}_x|p\rangle = p|p\rangle. \tag{T10.38}$$

Similarly, the operator $\widehat{x}$ is defined by

$$\widehat{x}|x'\rangle = x'|x'\rangle. \tag{T10.39}$$

Thus the position vector $|x'\rangle$ is an eigenvector of the operator $\widehat{x}$ with the eigenvalue x'.

We shall see that (T10.38) and (T10.39) are sufficient to determine the action of the operators $\widehat{x}$ and $\widehat{p}_x$ on an arbitrary vector $|\psi\rangle$. Using the completeness relation for the set $\{|p\rangle\}$ of eigenvectors of $\widehat{p}_x$ we have

$$|\psi\rangle = \int dp\ |p\rangle\langle p|\psi\rangle. \tag{T10.40}$$

Using (T10.38) we then find that the operator acts as follows:

$$\begin{aligned} \widehat{p}_x|\psi\rangle &= \widehat{p}_x \int dp\ |p\rangle\langle p|\psi\rangle = \int dp\, \widehat{p}_x|p\rangle\langle p|\psi\rangle \\ &= \left(\int dp\ p|p\rangle\langle p|\right)\cdot|\psi\rangle. \end{aligned} \tag{T10.41}$$

Since this holds for all $|\psi\rangle$, we have a well-defined expression for the operator $\widehat{p}_x$:

$$\widehat{p}_x = \int dp\ |p\rangle p\langle p|. \tag{T10.42}$$

Here, the *number* p can be placed in any position in the integrand. This expression is the so-called **spectral representation** of the operator $\widehat{p}_x$; notice that the integral over p runs over the complete spectrum of the operator. Using the same method we find

$$\widehat{x} = \int dx'\ |x'\rangle x'\langle x'|. \tag{T10.43}$$

A similar procedure can obviously be carried through for all Hermitian operators (with complete sets of eigenvectors). An operator $\widehat{F}$ with a continuous spectrum $\{f\}$ and eigenvectors $|f\rangle$ can be expressed as

$$\widehat{F} = \int df\ |f\rangle f\langle f|. \tag{T10.44}$$

An operator $\widehat{A}$ with a discrete eigenvalue spectrum $\{a_n\}$ and eigenvectors $|a_n\rangle$ can be written as

$$\widehat{A} = \sum_n |a_n\rangle a_n\langle a_n|, \tag{T10.45}$$

and so on.

The same recipe can also be used to obtain an expression for an arbitrary power of a Hermitian operator. Applying $\widehat{p}_x$ once more in (T10.41) we find for example that

$$\widehat{p}_x^2 = \int dp\ |p\rangle p^2\langle p|,$$

and similarly for higher powers of $\widehat{p}_x$. This way we can also find an expression for an **operator-valued function** $\widehat{F}(\widehat{p}_x)$. Such operator functions are defined by a Taylor expansion of F in powers of the argument. Thus the operator $\widehat{F}(\widehat{p}_x)$ can be written as

$$\widehat{F}(\widehat{p}_x) = \int dp\ |p\rangle F(p)\langle p|, \tag{T10.46}$$

where $F(p)$ is the function F of the *variable* p. An example is the potential $V(x)$ for which the abstract potential *operator* is given by

$$\widehat{V}(\widehat{x}) = \int dx' \; |x'\rangle V(x') \langle x'|. \tag{T10.47}$$

10.2.c Adjoint

We have been discussing Hermitian operators, but without defining Hermiticity in Dirac notation. The new definition must of course be equivalent with the old one, that is, we must require that the operator is **self adjoint.** The "old" definition of the adjoint of the operator $\widehat{A}$ was

$$\int (\widehat{A}\psi_1)^* \psi_2 d\tau \equiv \int \psi_1^* \widehat{A}^\dagger \psi_2 d\tau, \tag{T10.48}$$

which may also be written as

$$\int \psi_1^* \widehat{A}^\dagger \psi_2 d\tau = \left(\int \psi_2^* \widehat{A} \psi_1 d\tau \right)^*,$$

or

$$(\psi_1, \widehat{A}^\dagger \psi_2) = (\psi_2, \widehat{A}\psi_1)^*.$$

The equivalent definition in Dirac notation is

$$\boxed{\langle a|\widehat{A}^\dagger|b\rangle = \langle b|\widehat{A}|a\rangle^*, \quad \text{(def. } \widehat{A}^\dagger\text{)}} \tag{T10.49}$$

where we have denoted the two arbitrary vectors by $|a\rangle$ and $|b\rangle$. Denoting the vector $\widehat{A}|a\rangle$ by $|c\rangle$, we have from (T10.49):

$$\underline{\langle a|\widehat{A}^\dagger}|b\rangle = \langle b|c\rangle^* = \underline{\langle c|}b\rangle.$$

Thus the dual of the vector $|c\rangle = \widehat{A}|a\rangle$ is $\langle a|\widehat{A}^\dagger$:

$$\boxed{\langle a|\widehat{A}^\dagger \quad \overset{\text{dual of}}{\longleftrightarrow} \quad \widehat{A}|a\rangle.} \tag{T10.50}$$

For a self adjoint (i.e. Hermitian) operator $\widehat{A} = \widehat{A}^\dagger$ we see that

$$\langle a|\widehat{A}|b\rangle = \langle b|\widehat{A}|a\rangle^*. \quad (\widehat{A} \text{ Hermitian}) \tag{T10.51}$$

Later we shall also see that the expectation values of Hermitian operators and their eigenvalues are real, as in the old formalism.

The equivalence between the old definition (T10.48) of the adjoint and the new one, (T10.49), implies that the rules of calculation for obtaining an adjoint (found in Lecture notes 2) apply equally well for Hilbert-space operators. Thus

$$\begin{aligned} (\widehat{A}\widehat{B})^\dagger &= \widehat{B}^\dagger \widehat{A}^\dagger \; ; \\ (\widehat{A}\widehat{B}\widehat{C})^\dagger &= \widehat{C}^\dagger \widehat{B}^\dagger \widehat{A}^\dagger \; , \;\; \text{etc;} \\ (c\widehat{F})^\dagger &= c^* \widehat{F}^\dagger \; , \;\; (c \text{ a complex number}). \end{aligned} \tag{T10.52}$$

We may also include the rule

$$(\widehat{A}^\dagger)^\dagger = \widehat{A}, \tag{T10.53}$$

which follows by applying (T10.51) twice:

$$\langle a|(\widehat{A}^\dagger)^\dagger|b\rangle = \langle b|\widehat{A}^\dagger|a\rangle^* = \langle a|\widehat{A}|b\rangle.$$

The bra vector $\langle a|$, which is dual to the ket vector $|a\rangle$, is often called **the adjoint** of $|a\rangle$ (and vice versa):

$$(|a\rangle)^\dagger = \langle a|\,, \qquad (\langle a|)^\dagger = |a\rangle. \tag{T10.54}$$

We may then obtain the adjoint of an arbitrary expression cantaining constants, operators and ket and bra vectors using the following substitutions:

$$\begin{aligned} c \quad &\longrightarrow \quad c^*\,; \qquad \text{(constant)} \\ \widehat{A} \quad &\longrightarrow \quad \widehat{A}^\dagger\,; \qquad \text{(operator)} \\ |\ \rangle \quad &\longrightarrow \quad \langle\ |\,; \qquad \text{(ket} \to \text{bra)} \\ \langle\ | \quad &\longrightarrow \quad |\ \rangle\,; \qquad \text{(bra} \to \text{ket)} \end{aligned} \tag{T10.55}$$

while the order of the terms is reversed. Note, however, that constants and scalar products like $\langle a|b\rangle$ and $\langle a|\widehat{A}|b\rangle$ can be moved around freely, because they are all complex numbers. Examples:

(i) The adjoint of the operator $c\langle u|\widehat{A}|v\rangle\,|\phi\rangle\langle\psi|$ is

$$|\psi\rangle\langle\phi|\,\langle v|\widehat{A}^\dagger|u\rangle c^* = c^*\langle v|\widehat{A}^\dagger|u\rangle\,|\psi\rangle\langle\phi|.$$

(ii) The adjoint of the ket vector $c|u\rangle\langle v|w\rangle$ is the bra vector

$$\langle w|v\rangle\,\langle u|c^* = c^*\langle w|v\rangle\,\langle u|.$$

10.2.d Expectation values

The expectation value of an observable F is in Dirac notation given by

$$\langle\, F\,\rangle_\psi = \langle\psi|\widehat{F}|\psi\rangle. \qquad \text{(expectation value)} \tag{T10.56}$$

Let us check that this definition is equivalent with the old one (cf Postulate C in Lecture notes 2): We take $\widehat{F} = \widehat{x}$ as an example and use the standard trick:

$$\begin{aligned} \langle\, x\,\rangle_\psi &= \langle\psi|\widehat{x}\cdot\mathbb{1}|\psi\rangle = \langle\psi|\widehat{x}\int dx'\,|x'\rangle\langle x'|\psi\rangle \\ &= \int dx'\,\langle\psi|x'\rangle x'\langle x'|\psi\rangle = \int dx'\,\psi^*(x')\,x'\,\psi(x'), \quad \text{q.e.d.} \end{aligned}$$

(You can derive the same result more directly by using (T10.43)).

Furthermore we have from (T10.27) and (T10.42):

$$\begin{aligned} \langle\,\widehat{p}_x\,\rangle_\psi &= \langle\psi|\widehat{p}_x|\psi\rangle = \int dp\,\langle\psi|p\rangle\,p\,\langle p|\psi\rangle \\ &= \int dp\,\phi^*(p)\,p\,\phi(p) = \int dp\,|\phi(p)|^2\,p, \end{aligned} \tag{T10.57}$$

where $\langle p|\psi\rangle = \phi(p)$ is the amplitude of finding the momentum p (i.e., the momentum wave function) and $|\phi(p)|^2$ is the probability density in momentum space.

More generally, we have for a (Hermitian) operator $\widehat{A}$ with eigenvalues a_n and eigenvectors $|a_n\rangle$ (cf (T10.45)):

$$\begin{aligned}\langle A\rangle_\psi &= \langle\psi|\widehat{A}|\psi\rangle \\ &= \langle\psi|\sum_n |a_n\rangle a_n\langle a_n|\psi\rangle \\ &= \sum_n \langle a_n|\psi\rangle^* a_n\langle a_n|\psi\rangle \\ &= \sum_n |\langle a_n|\psi\rangle|^2 a_n \equiv \sum_n P(a_n)a_n, \end{aligned} \tag{T10.58}$$

where $P(a_n) = |\langle a_n|\psi\rangle|^2$ is the probability of measuring a_n.

Notice that the Hermiticity of $\widehat{A}$ implies that $\langle A\rangle_\psi$ is real for all $|\psi\rangle$ (cf (T10.51)). In particular, if we set $|\psi\rangle = |a_n\rangle$, equation (T10.58) gives

$$\langle A\rangle_{|a_n\rangle} = a_n,$$

showing that all eigenvalues a_n are real, as we have seen before.

10.3 Equation of state. Position and momentum representations

10.3.a Equation of state

So far we have not discussed the time dependence of state vectors. A time-dependent wave function $\Psi(x,t)$ must correspond to a time-dependent Hilbert vector $|\Psi(t)\rangle$:

$$\Psi(x,t) = \langle x|\Psi(t)\rangle. \tag{T10.59}$$

We shall postulate that the quantum-mechanical equation of motion for $|\Psi(t)\rangle$, or the equation of state, generally has the same form as the Schrödinger equation,

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \widehat{H}|\Psi(t)\rangle, \tag{T10.60}$$

also for systems that *can not* be described by ordinary wave functions (cf spin degrees of freedom). We may call this equation a generalized Schrödinger equation. In this equation, $\widehat{H}$ is the Hamiltonian of the system, which determines how $|\Psi(t)\rangle$ develops as a function of time. Supposing that $\widehat{H}$ is Hermitian, we may say that $|\Psi(t)\rangle$ "rotates" in Hilbert space, since the norm is then conserved. This follows from (T10.60):

$$\begin{aligned}\frac{d}{dt}\langle\Psi(t)|\Psi(t)\rangle &= (\frac{d}{dt}\langle\Psi|)\cdot|\Psi\rangle + \langle\Psi|\cdot\frac{d}{dt}|\Psi\rangle \\ &= \frac{1}{-i\hbar}\langle\Psi|\widehat{H}^\dagger|\Psi\rangle + \langle\Psi|\frac{1}{i\hbar}\widehat{H}|\Psi\rangle \\ &= \frac{i}{\hbar}\langle\Psi|(\widehat{H}^\dagger - \widehat{H})|\Psi\rangle = 0, \quad \text{q.e.d.}, \end{aligned} \tag{T10.61}$$

since $\widehat{H}^\dagger = \widehat{H}$ when $\widehat{H}$ is Hermitian.

10.3.b Position and momentum representations

For systems which *can* be described by wave functions, equation (T10.60) must of course be equivalent to the Schrödinger equation, as is also indicated by the form of the proposed equation (T10.60). We shall see that the Schrödinger equation and the "old" formulation of quantum mechanics in position space, which we call the position representation, follows simply by projecting (T10.60) onto the $|x\rangle$ basis. In the same manner, the momentum representation will follow when we project (T10.60) on the momentum basis $|p\rangle$.

We start by establishing some simple formulae, which are very handy *tools* both here and in other connections:

$$\langle x'|\widehat{x} = x'\langle x'| \; ; \tag{T10.62}$$

$$\langle x'|\widehat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| \; ; \tag{T10.63}$$

$$\langle p|\widehat{p}_x = p\langle p| \; ; \tag{T10.64}$$

$$\langle p|\widehat{x} = -\frac{\hbar}{i}\frac{\partial}{\partial p}\langle p| \; . \tag{T10.65}$$

These formulae can be generalized, with the operators $\widehat{x}$ and $\widehat{p}_x$ replaced by powers of these operators, and hence also with operator-valued functions which can be expanded in powers:

$$\langle x'|\widehat{F}(\widehat{x},\widehat{p}_x) = \widehat{F}(x', \frac{\hbar}{i}\frac{\partial}{\partial x'})\langle x'| \; ; \tag{T10.66}$$

$$\langle p|F(\widehat{x},\widehat{p}_x) = \widehat{F}(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p)\langle p| \; . \tag{T10.67}$$

All these expressions become meaningful when they are applied from the left on a chosen ket vector.

Proof of the relations above:

Equations (T10.62) and (T10.64) follow by taking the adjoint of the eigenvector equations (T10.39) and (T10.38) (cf the rules (T10.55)). Formula (T10.63) is shown as follows: From the relation

$$\langle x'|p\rangle = \psi_p(x') = (2\pi\hbar)^{-1/2}\, e^{ipx'/\hbar} = \langle p|x'\rangle^* \tag{T10.68}$$

we have the identities

$$p\langle x'|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|p\rangle \qquad \text{and} \qquad x'\langle p|x'\rangle = -\frac{\hbar}{i}\frac{\partial}{\partial p}\langle p|x'\rangle. \tag{T10.69}$$

Using the standard trick with the completeness relation, we then have

$$\begin{aligned}
\langle x'|\widehat{p}_x \cdot \mathbb{1} &= \langle x'|\widehat{p}_x \int dp\, |p\rangle\langle p| \\
&= \langle x'| \int dp\, p|p\rangle\langle p| \\
&= \int dp\, \langle x'|p\rangle p\langle p| \\
&= \int dp\, \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|p\rangle\langle p| \\
&= \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| \int dp\, |p\rangle\langle p| = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| \cdot \mathbb{1}, \quad \text{q.e.d.}
\end{aligned} \tag{T10.70}$$

(Notice that the use of (T10.42) for the operator $\widehat{p}_x$ would save us from the first steps in this derivation). Equation (T10.65) is proved in the same manner.

The proof (T10.70) of equation (T10.63) can easily be generalized to arbitrary powers of $\widehat{p}_x$, so that a power $\widehat{p}_x^n$ to the right of $\langle x'|$ can be replaced by the corresponding power $(\frac{\hbar}{i}\frac{\partial}{\partial x'})^n$ to the left of $\langle x'|$. Similar statements are valid for all four of the relations (T10.62)–(T10.65). This also holds for sums of powers, that is, for Taylor expansions. This proves (T10.66) and (T10.67).

It is now a trivial matter to derive the Schrödinger equation from the generalized equation (T10.60). Projecting the latter on $|x'\rangle$ we find from (T10.66):

$$i\hbar \left.\frac{d}{dt}\right|_{x'} \langle x'|\Psi(t)\rangle = \langle x'|\widehat{H}(\widehat{x},\widehat{p}_x)|\Psi(t)\rangle = \widehat{H}(x', \frac{\hbar}{i}\frac{\partial}{\partial x'})\langle x'|\Psi(t)\rangle,$$

or

$$i\hbar\frac{\partial}{\partial t}\Psi(x',t) = \widehat{H}(x', \frac{\hbar}{i}\frac{\partial}{\partial x'})\Psi(x',t), \tag{T10.71}$$

which is the Schrödinger equation in the position representation.

It is now not really necessary to show that also the momentum representation follows from (T10.60), because we know that it follows from (T10.71) (which follows from (T10.60)). But let us do it anyway, to get some more practice: By projecting (T10.60) on $|p\rangle$ we have from (T10.67)

$$i\hbar \left.\frac{d}{dt}\right|_{p} \langle p|\Psi(t)\rangle = \langle p|\widehat{H}(\widehat{x},\widehat{p}_x)|\Psi(t)\rangle = \widehat{H}(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p)\langle p|\Psi(t)\rangle.$$

Here, $\langle p|\Psi(t)\rangle$ is the amplitude of finding the momentum p at the time t, which is of course identical to the momentum-space wave function $\Phi(p,t)$. Thus we have

$$i\hbar\frac{\partial}{\partial t}\Phi(p,t) = \widehat{H}(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p)\Phi(p,t), \tag{T10.72}$$

which is the Schrödinger equation in the momentum representation (cf Lecture notes 2).

The derivation of (T10.71) and (T10.72) show that $\widehat{x}$ and $\widehat{p}_x$ (and hence also $\widehat{H}$) in the position and momentum representations can be read straight out from the right-hand sides of equations (T10.62) – (T10.67). This is because if we let e.g. $\widehat{p}_x$ act on a vector $|\psi\rangle$, we get a new vector which we may call $|\tilde{\psi}\rangle$. This vector corresponds to the wave function

$$\begin{aligned} \tilde{\psi}(x') &= \langle x'|\tilde{\psi}\rangle = \langle x'|\widehat{p}_x|\psi\rangle \overset{\text{(T10.63)}}{=} \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|\psi\rangle \\ &= \frac{\hbar}{i}\frac{\partial}{\partial x'}\psi(x'). \end{aligned} \tag{T10.73}$$

This shows that the momentum operator in the position representation is $\frac{\hbar}{i}\frac{\partial}{\partial x'}$; which can be read out from the right-hand side of (T10.63).

As a small exercise, let us show that the Hilbert-space operators $\widehat{x}$ and $\widehat{p}_x$ satisfy the commutation relation

$$[\widehat{x},\widehat{p}_x] = i\hbar\mathbb{1}. \tag{T10.74}$$

There are several ways to show this. Here we do it by using the completeness relation together with (T10.62) and (T10.63):

$$\begin{aligned}
&\widehat{x}\widehat{p}_x - \widehat{p}_x\widehat{x} \\
&= \int dx' \, |x'\rangle\langle x'|(\widehat{x}\widehat{p}_x - \widehat{p}_x\widehat{x}) \\
&= \int dx' \, |x'\rangle(\langle x'|\widehat{x}\widehat{p}_x - \langle x'|\widehat{p}_x\widehat{x}) \\
&= \int dx' \, |x'\rangle \left(x'\langle x'|\widehat{p}_x - \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|\widehat{x} \right) \\
&= \int dx' \, |x'\rangle \left(x'\frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| - \frac{\hbar}{i}\frac{\partial}{\partial x'}x'\langle x'| \right) \\
&= \int dx' \, |x'\rangle \left(x'\frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| - \frac{\hbar}{i}\left(\frac{\partial x'}{\partial x'}\right)\langle x'| - x'\frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| \right) \\
&= \int dx' \, |x'\rangle \, i\hbar \, \langle x'| = i\hbar\mathbb{1}, \quad \text{q.e.d.}
\end{aligned}$$

Notice the order of the factors:

$$\langle x'|\widehat{x}\widehat{p}_x = x'\langle x'|\widehat{p}_x = x' \, \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'| \, ;$$

$$\langle x'|\widehat{p}_x\widehat{x} = \frac{\hbar}{i}\frac{\partial}{\partial x'}\langle x'|\widehat{x} = \frac{\hbar}{i}\frac{\partial}{\partial x'} \, x'\langle x'|.$$

10.4 Matrix mechanics

In the preceeding section we saw that the position and momentum representations follow when we project the equation of state (T10.60) on the $|x\rangle$- and $|p\rangle$-bases, respectively. These are two of many possible representations. In this section we shall see what kind of representation that results from the projection on a *discrete* basis.

10.4.a Matrix representations of vectors and operators

We consider a discrete set of basis vectors $|1\rangle, |2\rangle, \cdots,$ which are orthonormalized;

$$\langle k|n\rangle = \delta_{kn}. \tag{T10.75}$$

A vector

$$|a\rangle = \mathbb{1}|a\rangle = \sum_k |k\rangle\langle k|a\rangle = \sum_k \langle k|a\rangle|k\rangle$$

may then be represented by the components (or "coordinates") which we may call a_k;

$$\langle k|a\rangle \equiv a_k \;\; ; \qquad |a\rangle = \sum_k a_k|k\rangle. \tag{T10.76}$$

These components may conveniently be collected in a column matrix a. Similarly, the bra vector

$$\langle a| = \sum_k a_k^* \langle k|$$

may be represented by the row matrix

$$\mathrm{a}^\dagger = (a_1^*, a_2^*, \ldots).$$

We note that this row matrix is the adjoint (or Hermitian conjugate) of the column matrix a. [5] The scalar product may then be written as

$$\begin{aligned} \langle b|a\rangle &= \langle b|\mathbb{1}|a\rangle = \sum_k \langle b|k\rangle\langle k|a\rangle = \sum_k b_k^* a_k \\ &= (b_1^*, b_2^*, \ldots)\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \equiv \mathrm{b}^\dagger \mathrm{a}. \end{aligned} \tag{T10.77}$$

An operator $\widehat{A}$ is now represented by a matrix. This follows when we consider the components of the vector $|c\rangle = \widehat{A}|a\rangle$, which are

$$\langle k|c\rangle = \langle k|\widehat{A}|a\rangle = \sum_n \langle k|\widehat{A}|n\rangle\langle n|a\rangle,$$

that is,

$$c_k = \sum_n A_{kn} a_n,$$

or in matrix form:

$$\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & & \\ \vdots & & \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}. \tag{T10.78}$$

Similarly, employing two unit operators, we have

$$\begin{aligned} \langle b|\widehat{A}|a\rangle &= \sum_{k,n} \langle b|k\rangle\langle k|\widehat{A}|n\rangle\langle n|a\rangle \\ &= (b_1^*, b_2^*, \ldots)\begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & & \\ \vdots & & \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \\ &\equiv \mathrm{b}^\dagger \mathcal{A} \mathrm{a}. \end{aligned} \tag{T10.79}$$

A product of two operators is represented by the product of the two matrices:

$$(\widehat{A}\widehat{B})_{kn} = \langle k|\widehat{A}\widehat{B}|n\rangle = \sum_m \langle k|\widehat{A}|m\rangle\langle m|\widehat{B}|n\rangle = \sum_m A_{km} B_{mn},$$

that is,

$$(\mathcal{A}\mathcal{B}) = (\mathcal{A})(\mathcal{B}). \tag{T10.80}$$

For the adjoint of an operator $\widehat{A}$ we have from (T10.49)

$$(\widehat{A}^\dagger)_{kn} = \langle k|\widehat{A}^\dagger|n\rangle = \langle n|\widehat{A}|k\rangle^* = A_{nk}^*, \quad \text{or}$$

$$\mathcal{A}^\dagger = \tilde{\mathcal{A}}^*. \tag{T10.81}$$

Thus the operator $\widehat{A}^\dagger$ is represented by the adjoint (or Hermitian conjugate) of the matrix.

[5] Taking the adjoint, or Hermitian conjugate, of a matrix corresponds to taking the transpose conjugate; $M^\dagger \equiv \tilde{M}^*$.

10.4.b Change of basis ***[6]

The freedom in the choice of basis makes it interesting to see how a **change of basis** works. Suppose that we want to change from the original basis $|k\rangle$ (labeled by latin letters) to a new discrete set $|\alpha\rangle$ ($\alpha = 1, 2, \ldots$), labeled by greek letters (to distinguish between old and new components). The new basis vectors can be expressed in terms of the old ones:

$$|\alpha\rangle = \sum_k |k\rangle\langle k|\alpha\rangle \equiv \sum_k |k\rangle S_{k\alpha}. \tag{T10.82}$$

Here, $S_{k\alpha} \equiv \langle k|\alpha\rangle$ is the projection of the new vector number α on the old vector number k. Thus the numbers $S_{k\alpha}$ are the components of the new vectors in the old basis. These complex numbers may be collected in a matrix S. Thus we have

$$\begin{aligned} \langle k|\alpha\rangle &= S_{k\alpha}, \\ \langle \alpha|k\rangle &= \langle k|\alpha\rangle^* = S^*_{k\alpha} = (S^\dagger)_{\alpha k}. \end{aligned} \tag{T10.83}$$

If the new basis is to be orthonormal we must have

$$\delta_{\beta\alpha} \stackrel{!}{=} \langle \beta|\alpha\rangle = \sum_k \langle \beta|k\rangle\langle k|\alpha\rangle = \sum_k S^\dagger_{\beta k} S_{k\alpha} = (S^\dagger S)_{\beta\alpha}. \tag{T10.84}$$

In the same manner,

$$\delta_{kn} = \langle k|n\rangle = \sum_\alpha \langle k|\alpha\rangle\langle \alpha|n\rangle = \sum_\alpha S_{k\alpha} S^\dagger_{\alpha n} = (SS^\dagger)_{kn}.$$

When these relations are satisfied, the matrix S is said to be **unitary**:

$$S^\dagger S = SS^\dagger = \mathbb{1}; \quad S^\dagger = S^{-1}, \qquad \text{(unitarity)}. \tag{T10.85}$$

We may call S the transformation matrix, because it gives the connection between vector components in the old and new bases, and similarly for the operator matrices. Thus the new matrix elements of the operator $\widehat{A}$ are

$$\begin{aligned} A_{\beta\alpha} &\equiv \langle \beta|\widehat{A}|\alpha\rangle = \sum_{k,n} \langle \beta|k\rangle\langle k|A|n\rangle\langle n|\alpha\rangle \\ &= \sum_{k,n} S^\dagger_{\beta k} A_{kn} S_{n\alpha}, \end{aligned}$$

or on matrix form:

$$\mathcal{A}_{\text{new}} = S^\dagger \mathcal{A} S. \tag{T10.86}$$

Furthermore, the vector

$$|a\rangle = \sum_k |k\rangle\langle k|a\rangle$$

is in the new basis represented by the components

$$a_\alpha \equiv \langle \alpha|a\rangle = \sum_k \langle \alpha|k\rangle\langle k|a\rangle = \sum_k S^\dagger_{\alpha k} a_k,$$

[6] not compulsory

or on matrix form:

$$\mathrm{a}_{\mathrm{new}} = S^\dagger \mathrm{a}. \tag{T10.87}$$

For a bra vector we find similarly

$$\begin{aligned} b^*_\beta &= \langle b|\beta\rangle = \sum_n \langle b|n\rangle\langle n|\beta\rangle = \sum_n \langle n|b\rangle^*\langle n|\beta\rangle \\ &= \sum_n b^*_n S_{n\beta}, \end{aligned}$$

or on matrix form

$$\mathrm{b}^\dagger_{\mathrm{new}} = \mathrm{b}^\dagger S. \tag{T10.88}$$

Such a unitary transformation (change of basis) of course does not alter the *physics* of a given problem. For example, all scalar products are conserved under the transformation: By combining (T10.75) – (T10.78) we find that

$$\mathrm{b}^\dagger_{\mathrm{new}} \mathcal{A}_{\mathrm{new}} \mathrm{a}_{\mathrm{new}} = (\mathrm{b}^\dagger S)(S^\dagger \mathcal{A} S)(S^\dagger \mathrm{a}) = \mathrm{b}^\dagger \mathcal{A} \mathrm{a}.$$

This is how it should be, because the scalar product may also be written as $\langle b|\widehat{A}|a\rangle$, which is basis independent.

Diagonalization

Some times one wishes to find a new basis set $\{|\alpha\rangle\}$ which are eigenvectors of a given operator $\widehat{A}$,

$$\widehat{A}|\alpha\rangle = a_\alpha|\alpha\rangle, \tag{T10.89}$$

so that the matrix $\mathcal{A}_{\mathrm{nnew}}$ becomes diagonal:

$$A_{\beta\alpha} = \langle\beta|\widehat{A}|\alpha\rangle = a_\alpha \delta_{\beta\alpha}. \tag{T10.90}$$

Thus the task of finding the eigenvalues of the operator $\widehat{A}$ is equivalent to diagonalizing the $\mathcal{A}$-matrix. This diagonalization problem, i.e., to find the components $\langle k|\alpha\rangle$ (equal to $S_{k\alpha}$) of the vectors $|\alpha\rangle$, can in principle be solved starting with the non-diagonal matrix A_{kn} (in the old basis). This procedure is relevant when working with a finite-dimensional sub-space of the Hilbert space. From (T10.89) we then have:

$$\sum_{n=1}^{N} \langle k|\widehat{A}|n\rangle\langle n|\alpha\rangle = a_\alpha\langle k|\alpha\rangle, \quad \text{that is,}$$

$$\sum_n A_{kn} S_{n\alpha} = a_\alpha S_{k\alpha}\ ; \quad \alpha = 1, 2, \cdots, N;$$

or on matrix form:

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & & & \\ \vdots & & & \\ A_{N1} & \cdots & & A_{NN} \end{pmatrix} \begin{pmatrix} S_{1\alpha} \\ S_{2\alpha} \\ \vdots \\ S_{N\alpha} \end{pmatrix} = a_\alpha \begin{pmatrix} S_{1\alpha} \\ S_{2\alpha} \\ \vdots \\ S_{N\alpha} \end{pmatrix}. \tag{T10.91}$$

Column number α in the matrix S then is an eigenvector of the A_{kn} matrix. By solving this eigenvalue problem for the N eigenvalues a_α, one finds the N columns of the matrix S. Notice that the N eigenvalues are found by setting the **system determinant** equal to zero:

$$\det[\mathcal{A} - a_\alpha \cdot \mathbb{1}] = 0. \tag{T10.92}$$

Since the determinant is a polynomial in a_α of degree N, it follows that this so-called **characteristic equation** has N roots. These roots are the eigenvalues a_α; $\alpha = 1, 2, \cdots, N$. If one is interested only in the eigenvalues, it suffices to find these roots. If one also wishes to find the vectors $|\alpha\rangle$, then (T10.91) must be solved for the N eigenvalues a_α, so that the components $S_{n\alpha} = \langle n|\alpha\rangle$ of $|\alpha\rangle$ can be determined.

10.4.c Equation of state on matrix form

The projection of the equation of state (T10.60) on the $|k\rangle$ basis gives the equation

$$i\hbar\frac{d}{dt}\langle k|\Psi(t)\rangle = \langle k|\widehat{H}|\Psi(t)\rangle = \sum_n \langle k|\widehat{H}|n\rangle\langle n|\Psi(t)\rangle,$$

or

$$i\hbar\frac{d}{dt}\Psi_k(t) = \sum_n H_{kn}\Psi_n(t). \tag{T10.93}$$

The time-dependent "$|k\rangle$-components" $\Psi_k(t)$ of $|\Psi(t)\rangle$ thus are given by a coupled set of first-order differential equations in t. On matrix form:

$$i\hbar\frac{d}{dt}\begin{pmatrix}\Psi_1(t)\\ \Psi_2(t)\\ \vdots\end{pmatrix} = \begin{pmatrix}H_{11} & H_{12} & \cdots\\ H_{21} & & \\ \vdots & & \end{pmatrix}\begin{pmatrix}\Psi_1(t)\\ \Psi_2(t)\\ \vdots\end{pmatrix}. \tag{T10.94}$$

Note that if one diagonalizes this Hamiltonian matrix, then the diagonal elements (i.e., the eigenvalues of the $\mathcal{H}$ matrix) are the energies E_α of the stationary states of the system at hand. These energies are determined by equation (T10.92):

$$\det[\mathcal{H} - E_\alpha \cdot \mathbb{1}] = 0. \tag{T10.95}$$

Using the method described above, one can also find the corresponding eigenvectors $|\alpha\rangle$ of $\widehat{H}$, which correspond to the energy eigenstates of the system.

The matrix formulation of quantum mechanics is known as matrix mechanics, and is the formulation that was actually found first, by Werner Heisenberg in 1925, a few months before Schrødinger presented his wave mechanics.